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Formulation of the d-f interaction in ferromagnetic superconductors

H. Matsumoto, H. Umezawa, and J. P. Whitehead
Theoretical Physics Institute, Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2J1
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We present a formalism for the analysis of magnetic superconductors which includes, in a self-consistent manner, the pair-breaking effects, induced by the d-f interaction, arising from the scattering of the electrons by the localized-spin fluctuations and the polarization of the electrons by the localized spins. We take into account the shielding of the localized spins by the persistent current and the anisotropy of the localized-spin system. It will be shown how the effect of the spin fluctuations may be realized by means of a straightforward scaling law. The formalism provides an ideal basis for the analysis of the magnetic properties of reentrant materials such as $ErRh_4B_4$ in both bulk and thin films. In addition, a brief analysis of the Meissner state is presented.

I. INTRODUCTION

The recent discovery of the reentrant phenomena in $ErRh_4B_4$ (Ref. 1) and $HoMo_6S_8$ (Ref. 2) has stimulated a considerable amount of research concerning the interplay between magnetism and superconductivity. It is now well established that the coexistence of magnetism and superconductivity in the rare-earth ternary compounds such as RRh_4B_4 as well as RMo_6S_8 and RMo_6Se_8 is possible because of the relative weakness of the interaction between the d-band conduction electrons and the localized spins arising from the unfilled f-shell electrons of the rare-earth ions.

There are two predominant effects in these materials. The first concerns the electromagnetic interaction between the superconducting electrons and the rare-earth magnetic ions, in particular, the shielding of the localized magnetic moments by the persistent current. This effect, observed in the recent ultrasonic attenuation experiments,[3] is now generally believed to account for the modulated spin phase[4,5,6] observed in the narrow coexistence region above the reentrant temperature T_{c2}.[7–9]

The second effect concerns the pair-breaking effect arising from the scattering of the d electrons by the rare-earth spins through the d-f interaction. The terminology in the literature regarding the interaction between the localized electrons of the rare-earth ion and the conduction electrons in the rare-earth ternary superconductors is somewhat confusing. Many of the earlier papers in this field refer to this interaction as the s-f interaction in analogy with other rare-earth metals and compounds. There appears, however, to be an increasing tendency within the current literature to use the more accurate terminology and refer to it as the d-f interaction. It is the latter mode that we will employ here. While this effect is weak, it does give rise to an increase in the superconducting transition temperature with the substitution of the magnetic rare-earth ions by nonmagnetic ions[10] and may account for the deviation from the BCS result of the superconducting gap, obtained from tunneling measurements,[11] and the condensation energy, estimated from the magnetization curves.[12] Furthermore, calculations[13,14] indicate that the d-f interaction is important in order to account for the recent measurements of the magnetic properties of single-crystal $ErRh_4B_4$.[15,16]

Previous work[17] regarding the magnetic properties of the rare-earth ternary superconductors has emphasized the effect of the electromagnetic interaction by assuming that the effect of the d-f interaction (referred to as the s-f interaction in Ref. 17) could be absorbed in a *temperature-independent* renormalization of the physical parameters. While Ref. 17 shows that the electromagnetic interaction does have an important bearing on the magnetic properties of the rare-earth ternary superconductors and can in fact account reasonably well for the properties of the polycrystalline samples, it becomes immediately apparent, in light of the more recent single-crystal measurements,[15,16] that the incorporation of the d-f interaction solely through a temperature-independent renormalization of the parameter is inadequate. There therefore exists a need for a unified theory which includes both the electromagnetic interaction and the d-f interaction in a more detailed manner than that presented hitherto. In this paper we present such a formalism and examine the relative importance of various mechanisms in different physical conditions (such as the temperature dependence and field dependence) in order that their consequences may be discussed and compared. They will provide a basis for the interpretation and identification of possible mechanisms in the observed magnetic properties. The application of the present formalism to the analysis of the mixed state in $ErRh_4B_4$ (Ref. 18) will be presented in a subsequent paper. An extension of this work to consider the case of thin films is currently in progress.

The arrangement of this paper is as follows. In Sec. II we define the Hamiltonian and discuss the various contributions. In Sec. III we obtain the electron self-energy and present an expression for the superconducting gap in terms of the spin-splitting parameter μ and the effective coupling constant. We show how the gap may be obtained from the scaling of a two-parameter function. In Sec. IV we derive an expression for the free energy and define the field-dependent condensation energy. We show how the field-dependent condensation energy may also be obtained from the scaling of a two-parameter function. In Sec. V we discuss the Maxwell equations and present the scaling law for the London penetration depth. In Sec. VI we present the calculation of the magnetization and the susceptibility, including the shielding of the rare-earth magnetic moments by the persistent currents. The results of Sec. VII are then used to calculate the effective coupling constant and the scale factor for finite field and temperature. In Sec. VIII we present a summary of the important results, while devoting Sec. IX to some concluding remarks.

II. HAMILTONIAN

The dynamics of the system under consideration is assumed to be obtained from the following microscopic Hamiltonian density given by

$$\begin{aligned}\mathscr{H}(x)=&\psi^\dagger(x)\epsilon_0(-i[\vec{\nabla}-(ie/\hbar c)\vec{A}])\psi(x)-V\psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger(x)\psi_\downarrow(x)\psi_\uparrow(x)+\delta\epsilon_F\,\psi^\dagger(x)\psi(x)\\&-\tfrac{1}{2}\vec{M}(x)\cdot\gamma_0(-i\nabla)\vec{M}(x)-I\vec{M}(x)\cdot\psi^\dagger(x)\vec{\sigma}\psi(x)-\vec{M}(x)\cdot\vec{B}(x)\\&+\mu_B\psi^\dagger(x)\vec{\sigma}\psi(x)\cdot\vec{B}(x)+\frac{1}{8\pi}[\,|\vec{B}(x)|^2+|\vec{E}(x)|^2]\,. \qquad (2.1)\end{aligned}$$

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 $\vec{B}=\vec{\nabla}\times\vec{A}(x)$, and $M(x)$ 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.

III. SUPERCONDUCTING GAP

In this section we analyze the effect of the d-f interaction on the energy spectra of the superconducting electrons. There are 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 both of the above effects may 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 gap equation, 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 a temperature-dependent effective coupling constant as distinct from the temperature-independent effective coupling considered in Ref. 17.

In addition to considering the effects of the finite field this work includes a somewhat general treatment of the interactions present in the Hamiltonian; 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. (2.1) we obtain the following equation of motion for the electron fields $\psi_\uparrow$ and $\psi_\downarrow$:

$$\begin{aligned}i\partial_t\psi_\uparrow=&\,\epsilon_0(-i[\vec{\nabla}-(ie/\hbar c)\vec{A}])\psi_\uparrow-V\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow\\&-\delta\epsilon_F\,\psi_\uparrow+(I\vec{M}-\mu_B\vec{B})\cdot(\vec{\sigma}\psi)_\uparrow\,, \qquad (3.1)\end{aligned}$$

$$\begin{aligned}i\partial_t\psi_\downarrow=&\,\epsilon_0(-i[\vec{\nabla}-(ie/\hbar c)\vec{A}])\psi_\downarrow-V\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow\\&-\delta\epsilon_F\psi_\uparrow+(I\vec{M}-\mu_B\vec{B})\cdot(\vec{\sigma}\psi)_\downarrow\,. \qquad (3.2)\end{aligned}$$

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

$$V\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow=V\langle\psi_\downarrow\psi_\uparrow\rangle\psi_\downarrow^\dagger+V\langle\psi_\downarrow^\dagger\psi_\downarrow\rangle\psi_\uparrow \qquad (3.3)$$

and

$$V\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow=V\langle\psi_\uparrow\psi_\downarrow\rangle\psi_\uparrow^\dagger+V\langle\psi_\uparrow^\dagger\psi_\uparrow\rangle\psi_\downarrow\,. \qquad (3.4)$$

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

$$\phi=\begin{bmatrix}\psi\\ \psi_c\end{bmatrix} \qquad (3.5)$$

with

$$\psi_c=i\sigma_2[\psi^\dagger]^T\,, \qquad (3.6)$$

the equation of motion may be written as

$$[i\partial_t-\epsilon(-i\vec{\nabla})\tau_3+\Delta_0\tau_1-\mu\sigma_3]\phi =(I\vec{M}-\mu_B\vec{B})\cdot\vec{\sigma}\phi-\langle I\vec{M}-\mu_B\vec{B}\rangle\cdot\vec{\sigma}\phi \ , \quad (3.7)$$

where we have neglected the vector potential $\vec{A}$ and have assumed the applied field to point in the z direction, and where we have designated $\phi^\dagger\sigma_3\phi$ as the electron-spin density in the z direction. The parameters μ and Δ_0 in Eq. (3.7) are given by

$$\mu=\langle[I\vec{M}-\mu_B\vec{B}-(V/2)\vec{\sigma}]\rangle\cdot\vec{e}_3 \quad (3.8a)$$

and

$$\Delta_0=V\langle\psi_\downarrow(x)\psi_\uparrow(x)\rangle \ , \quad (3.8b)$$

respectively, where $\vec{e}_3$ denotes the unit vector in the z direction. The quantity Δ_0 may be thought of as the bare unrenormalized gap and μ is 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. (3.3) and (3.4).

The expression for μ may be written in terms of a renormalized d-f coupling constant $\tilde{I}$ and bare induction field $\vec{B}_0(x)$ created by vortices as

$$\mu=\tilde{I}\langle\vec{M}\rangle\cdot\vec{e}_3-\mu_B\vec{B}_0(x)\cdot\vec{e}_3 \ . \quad (3.9)$$

If calculated in the linear-response theory we obtain

$$\tilde{I}=\left[1-\frac{V}{2}\chi_\sigma\right]\left[I-4\pi\mu_B(1-I\mu_B\chi_\sigma)\times\frac{-\nabla^2}{-(1-4\pi\mu_B^2\chi_\sigma)\nabla^2+\lambda_L^{-2}C(-i\vec{\nabla})}\right] \quad (3.10a)$$

and

$$\vec{B}_0(x)=\frac{\lambda_L^{-2}C(-i\vec{\nabla})}{-(1-4\pi\mu_B^2\chi_\sigma)\nabla^2+\lambda_L^{-2}C(-i\vec{\nabla})}\vec{n}(x)\phi \ , \quad (3.10b)$$

where λ_L is the London penetration depth, $C(-i\vec{\nabla})$ is the nonlocal kernel appearing in the Meissner current, χ_σ is the susceptibility of the conduction electron, and $\vec{n}(x)\phi$ is the vortex density. The derivation of this result is presented in Appendix A.

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.[19] 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. (2.8) reduces to

$$\mu=I\langle\vec{M}\rangle\cdot\vec{e}_3 \quad (3.11)$$

or equivalently that

$$\tilde{I}=I \ . \quad (3.12)$$

The term on the right-hand side of Eq. (3.7) 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

$$\langle R[\phi(x)\phi^\dagger(y)]\rangle =\frac{i}{(2\pi)^4}\int d^4p\, e^{i[\vec{p}\cdot(\vec{x}-\vec{y})-p_0(t_x-t_y)]}S(p) \quad (3.13)$$

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

$$S^{-1}(p)=p_0-\epsilon(\vec{p})\tau_3+\Delta_0\tau_1+\mu\sigma_3-\Sigma(p) \ , \quad (3.14)$$

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

$$\Sigma(p)=\frac{\tilde{I}^2}{(2\pi)^3}\int d^3k\int dw\,dv\sum_i\rho_{ij}(w;k)\sigma_i\mathscr{S}(v;\vec{p}-\vec{k})\sigma_j\frac{e^{\beta(w+v)}}{(e^{\beta w}-1)(e^{\beta v}+1)}\frac{1}{(p_0-v-w+i\epsilon)} \ , \quad (3.15)$$

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

$$S(p)=\int d\alpha\,\mathscr{S}(v;\vec{p})\frac{1}{p_0-v+i\epsilon} \ , \quad (3.16)$$

so that

$$\mathscr{S}(p_0;\vec{p})=-\frac{1}{\pi}\mathrm{Im}S(p) \ , \quad (3.17)$$

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

$$\langle R[M_i(x)M_j(y)]\rangle=\frac{i}{(2\pi)^4}\int d^4k\, e^{i\vec{k}\cdot(\vec{x}-\vec{y})-ik_0(t_x-t_y)}\chi_{ij}(k) \quad (3.18)$$

and

$$\chi_{ij}(k)=\int dw\,\rho_{ij}(w;k)\frac{1}{k_0-w+i\epsilon}\;. \tag{3.19}$$

The derivation of Eq. (3.15) is tedious, but relatively straightforward, and is presented in Appendix B.

To evaluate (3.15) we assume that the spectral density $\rho_{ij}(k)$ may be written in the hydrodynamical form as

$$\rho_{ij}(w;\vec{k})=\frac{1}{\pi}\frac{w\Gamma}{w^2+\Gamma^2}\chi_{ij}(\vec{k}) \tag{3.20}$$

and expand the thermal weight in a low-frequency expansion:

$$\frac{e^{\beta(w+v)}+1}{(e^{\beta w}-1)(e^{\beta v}+1)}\simeq\frac{e^{\beta v}+1+\beta w e^{\beta v}+\cdots}{\beta w(1-\frac{1}{2}\beta w+\cdots)(e^{\beta v}+1)}=\left[\frac{1}{\beta w}+\frac{e^{\beta v}-1}{2(e^{\beta v}+1)}+O(w)\right]. \tag{3.21}$$

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

$$\Sigma(p)=\frac{\tilde{I}^2}{(2\pi)^3}\int d^3k\int dv\,\mathscr{S}(v;\vec{p}-\vec{k})\sum_i\chi_{ii}(\vec{k})\left[\beta^{-1}\frac{1}{p_0-v+i\Gamma}-\frac{e^{\beta v}-1}{2(e^{\beta v}+1)}\frac{i\Gamma}{p_0-v+i\Gamma}\right]. \tag{3.22}$$

There are two limiting cases where the gap equation assumes a rather familiar form. In the extreme elastic limit $\Gamma\to0$, the gap equation reduces to the result for the impurity case, while in the extreme inelastic limit $\Gamma\to\infty$ the gap equation reduces to

$$\Sigma(p)=-\frac{\tilde{I}^2}{(2\pi)^3}\int d^3k\int dv\,\mathscr{S}(v;\vec{p}-\vec{k})\sum_i\chi_{ii}(\vec{k})\frac{e^{\beta v}-1}{2(e^{\beta v}+1)}\;, \tag{3.23}$$

which was first considered in Ref. 20 and further analyzed in Ref. 21, and provides the starting point for our discussion.

From Eq. (3.7) and the approximations outlined in the preceding discussion, we obtain the following gap equation in the extreme inelastic limit:

$$\Delta(\vec{p})=\int\frac{d^3k}{(2\pi)^3}\left[V-\tilde{I}^2\sum_i\chi_{ii}(\vec{p}-\vec{k})\right]\frac{\Delta(\vec{k})}{2E(\vec{k})}\frac{1}{2}\left[\tanh\left[\frac{\beta(E(k)+\mu)}{2}\right]+\tanh\left[\frac{\beta(E(k)-\mu)}{2}\right]\right]. \tag{3.24}$$

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. (3.24) reduces to

$$1=g(T;H)N(0)\int_0^{\omega_D}d\epsilon\frac{1}{E}[1-f_F(E+\mu)-f_F(E-\mu)] \tag{3.25}$$

with

$$E=(\epsilon^2+\Delta^2)^{1/2}\;, \tag{3.26}$$

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

$$g(T;H)=\frac{1}{(4\pi)^2}\int_{|\vec{p}|=|\vec{k}|=k_F}d\Omega_p d\Omega_k\times\left[V-\tilde{I}^2\sum_i\chi_{ii}(\vec{p}-\vec{k})\right], \tag{3.27}$$

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

The equation

$$1=gN(0)\int_0^{\omega_D}d\epsilon\frac{1}{E}[1-f(E+\mu)-f(E-\mu)] \tag{3.28}$$

has been studied in detail by Sarma.[22] The resultant gap can be written in terms of a two-parameter function which we will denote by $\mathscr{D}(t;\tilde{\mu})$,

$$\frac{\Delta(T;\mu;gN)}{\Delta_0(gN)}=\mathscr{D}(t;\tilde{\mu})\;, \tag{3.29}$$

and which is given as the solution of

$$\ln\mathscr{D}(t;\tilde{\mu})=-\Phi_1\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\tilde{\mu});\frac{\pi e^{-\gamma}}{t}\tilde{\mu}\right] \tag{3.30}$$

with

$$\Phi_1(x;y)=\frac{x}{4}\mathrm{Re}\int_{-\infty}^{+\infty}dz\,\ln[z+(z^2-1)^{1/2}]\times\cosh^{-2}[\tfrac{1}{2}(xz+y)]\;. \tag{3.31}$$

The integrand is calculated along the contour shown in Fig. 1 with the branch line running between $z=\pm1$ and with

$$\lim_{v\to0}\ln[z+(z^2+1)^{1/2}]=\ln[u+(u^2-1)^{1/2}]\;\;\text{for } u>1\;, \tag{3.32}$$

where $z=u+iv$. $\Delta_0(gN(0);\omega_D)$ is given by

$$\Delta_0(gN(0);\omega_D)=2\omega_D\exp-\frac{1}{gN(0)}\;, \tag{3.33a}$$

$\tilde{\mu}$ is given by

$$\tilde{\mu}=\frac{\mu}{\Delta_0(gN(0);\omega_D)}\;, \tag{3.33b}$$

and t is the reduced temperature

$$t=T/T_c \; . \tag{3.33c}$$

Therefore, we then find that the solution to Eq. (3.25) may be obtained simply by scaling the solution (3.29), i.e.,

$$\frac{\Delta(T;\mu;g(T;H)N(0))}{\Delta_0(g(T_c;0))}=s(t;H)\mathscr{D}(t/s(t;H);\bar{\mu}/s(t;H)) \; , \tag{3.34}$$

where

$$s(t;H)=\exp\left[\frac{1}{g(T_c;0)N(0)}-\frac{1}{g(T;H)N(0)}\right] , \tag{3.35}$$

$$\bar{\mu}=\mu/\Delta_0(g(T_c)N(0);\omega_D) \; , \tag{3.36}$$

and we have normalized the gap by $\Delta_0(g(T_c;0)$. The calculation of the scale factor is presented in Sec. VII together with several examples of the resultant gap.

IV. FREE ENERGY

We now turn our attention to the calculation of the free energy. In evaluating the ground-state energy particular care has to be taken to ensure that certain contributions are not double counted. For example, the localized spins of the rare-earth atoms renormalize the superconducting electrons, in turn the superconducting electrons modify the behavior of the localized spins. While both effects must be included in the calculation of the ground-state energy, they both originate from the same term in the Hamiltonian. The approach used in this paper is to separate the Hamiltonian into electronic, magnetic, and electromagnetic terms,

$$\mathscr{H}(x)=\mathscr{H}_{\rm el}(x)+\mathscr{H}_M(x)+\mathscr{H}_{\rm EM}(x) \; , \tag{4.1}$$

where

$$\mathscr{H}_{\rm el}\equiv \psi^\dagger\epsilon_0(-i\vec{\nabla})\psi-V\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow -\tfrac{1}{2}(I\vec{\mathbf{M}}-g_J\mu_B\vec{\mathbf{B}})\cdot\psi^\dagger\vec{\sigma}\psi \; , \tag{4.2}$$

$$\mathscr{H}_M\equiv-\tfrac{1}{2}\vec{\mathbf{M}}\cdot\gamma_0(-i\vec{\nabla})\vec{\mathbf{M}}-\tfrac{1}{2}(I\psi^\dagger\vec{\sigma}\psi+\vec{\mathbf{B}})\cdot\vec{\mathbf{M}} \; , \tag{4.3}$$

and

$$\mathscr{H}_{\rm EM}\equiv\frac{1}{8\pi}(|\vec{\mathbf{E}}|^2+|\vec{\mathbf{B}}|^2)+\vec{\mathbf{j}}\cdot\left[\vec{\mathbf{A}}-\frac{\hbar c}{e}\vec{\nabla}f\right] -\tfrac{1}{2}(\vec{\mathbf{M}}-g_J\mu_B\psi^\dagger\vec{\sigma}\psi)\cdot\vec{\mathbf{B}} \; , \tag{4.4}$$

where we have divided the mutual interaction terms equally between the three contributions (e.g., $\frac{1}{2}\vec{\mathbf{M}}\cdot\psi^\dagger\vec{\sigma}\psi$ is included in $\mathscr{H}_{\rm el}$ and $\frac{1}{2}\vec{\mathbf{M}}\cdot\psi^\dagger\vec{\sigma}\psi$ is included in $\mathscr{H}_M$). Correspondingly, we define $U_{\rm el}$, U_M, and $U_{\rm EM}$ as

$$\frac{1}{V}\int d^3x\langle\mathscr{H}_{\rm el}\rangle\equiv U_{\rm el} \; , \tag{4.5}$$

$$\frac{1}{V}\int d^3x\langle\mathscr{H}_M\rangle=U_M \; , \tag{4.6}$$

and

$$\frac{1}{V}\int d^3x\langle\mathscr{H}_{\rm EM}\rangle=U_{\rm EM} \; . \tag{4.7}$$

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

The contribution to the internal energy from the electronic degrees of freedom, $U_{\rm el}$, may be calculated using the approximations introduced in the preceding section to give

$$U_{\rm el}=\int\frac{d^3k}{(2\pi)^3}\left[\epsilon-E+\frac{\Delta^2}{2E}[1-f_F(E-\mu)-f_F(E+\mu)]+(E-\mu)f_F(E-\mu)+(E+\mu)f_F(E+\mu) +\frac{\mu}{2}[f_F(E-\mu)-f_F(E+\mu)]\right] . \tag{4.8}$$

Since the derivation of the above result is somewhat tedious, the details of the calculation are presented in Appendix C. The entropy of the electronic states may be calculated to give

$$\beta^{-1}S_{\rm el}=\beta^{-1}\int\frac{d^3k}{(2\pi)^3}\{f(E+\mu)\ln f_F(E+\mu)+[1-f_F(E+\mu)]\ln[1-f_F(E+\mu)]\} +\beta^{-1}\int\frac{d^3k}{(2\pi)^3}\{f(E-\mu)\ln f_F(E-\mu)+[1-f_F(E-\mu)]\ln[1-f(E-\mu)]\} \; . \tag{4.9}$$

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

$$F_{\rm el}=U_{\rm el}-\beta^{-1}S_{\rm el} \; , \tag{4.10}$$

to be given by

$$F_{\rm el}^s=\int\frac{d^3k}{(2\pi)^3}\left[\epsilon-E+\frac{\Delta^2}{2E}[1-f(E-\mu)-f(E+\mu)]+\beta^{-1}\{\ln[1-f_F(E-\mu)]+\ln[1-f(E+\mu)]\} +\frac{\mu}{2}[f(E-\mu)-f(E+\mu)]\right] , \tag{4.11}$$

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

$$F_{\rm el}^N = \int \frac{d^3k}{(2\pi)^3} \left[\beta^{-1} \{ \ln[1 - f_F(\epsilon+\mu)] \} + \{ \ln[1 - f_F(\epsilon-\mu)] \} + \frac{\mu}{2} [f_F(\epsilon-\mu) - f_F(\epsilon+\mu)] \right] . \tag{4.12}$$

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

$$\begin{aligned} \frac{H_c^2(T;H)}{8\pi} &\equiv F_{\rm el}^N(T;H) - F_{\rm el}^s(T;H) \\ &= -2N(0) \int_0^{\omega_D} d\epsilon \left[\epsilon - E - \frac{\Delta^2}{2E} - \frac{E^2+\epsilon^2}{2E} [f_F(E-\mu) + f_F(E+\mu)] + 2\epsilon f_F(\epsilon) + \frac{\mu}{2} [f_F(E-\mu) - f_F(E+\mu)] \right] \\ &= 2N(0) \left[\tfrac{1}{4}\Delta^2 - \frac{\pi^2}{6}\beta^{-2} + \int_0^\infty d\epsilon \frac{E^2+\epsilon^2}{2E} [f_F(E-\mu) + f_F(E+\mu)] - \frac{\mu}{2} \int_0^\infty d\epsilon [f_F(E-\mu) - f_F(E+\mu)] \right] . \end{aligned} \tag{4.13}$$

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

As in the discussion of the preceding section, the effect of the temperature- and field-dependent effective coupling constant may be realized through the scaling of a two-parameter function

$$\frac{H_c(T;H)}{H_{c0}} = s(t;H) \mathscr{H}(t/s(t;H);\bar{\mu}/s(t;H)) , \tag{4.14}$$

where

$$\begin{aligned} \mathscr{H}^2(t;\bar{\mu}) = \mathscr{D}^2(t;\bar{\mu}) - \frac{2\pi^2}{3} \Bigg[& \frac{t^2}{\pi e^{-\gamma}} - \frac{3\mathscr{D}^2(t;\bar{\mu})}{\pi^2} \Phi_3 \left[\frac{\pi e^{-\gamma}}{t} \mathscr{D}(t;\bar{\mu}); \frac{\pi e^{-\gamma}}{t} \bar{\mu} \right] \\ & - \frac{3\bar{\mu}\mathscr{D}(t;\bar{\mu})}{\pi^2} \Phi_4 \left[\frac{\pi e^{-\gamma}}{t} \mathscr{D}(t;\bar{\mu}); \frac{\pi e^{-\gamma}}{t} \bar{\mu} \right] \Bigg] . \end{aligned} \tag{4.15}$$

Here the functions $\mathscr{D}(t;\bar{\mu})$ and $s(t;H)$ are those defined in the preceding section [Eqs. (3.30) and (3.36)]. The functions $\Phi_3(x;y)$ and $\Phi_4(x;y)$ are given by

$$\Phi_3(x;y) = \frac{x}{4} {\rm Re} \int_{-\infty}^{+\infty} dz\, z(z^2-1)^{1/2} \times \cosh^{-2}[\tfrac{1}{2}(xz+y)] \tag{4.16}$$

and

$$\Phi_4(x;y) = \frac{x}{4} {\rm Re} \int_{-\infty}^{+\infty} dz (z^2-1)^{1/2} \times \cosh^{-2}[\tfrac{1}{2}(xz+y)] , \tag{4.17}$$

while the normalization factor H_{c0} is given by

$$H_{c0} = [4\pi N(0) \Delta_0^2(g(T_c;0))]^{1/2} , \tag{4.18}$$

where Δ_0 is given by Eq. (3.33) 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

$$\begin{aligned} U_M = &-\tfrac{1}{2} \langle \vec{\rm M} \rangle \gamma_0(-i\nabla) \cdot \langle \vec{\rm M} \rangle \\ &- \tfrac{1}{2} (I \langle \psi^\dagger \vec{\sigma} \psi \rangle - \langle \vec{\rm B} \rangle) \cdot \langle \vec{\rm M} \rangle , \end{aligned} \tag{4.19}$$

while the entropy may be calculated to give

$$\beta^{-1} S_M = -\beta^{-1} N \ln Z_J(g_J J \mu_B \,|\, \vec{\rm H}_{\rm MF} \,|\,) - \vec{\rm H}_{\rm MF} \cdot \langle \vec{\rm M} \rangle , \tag{4.20}$$

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

$$Z_J(x) = \sinh \left[\frac{1}{2J} x \right] \Big/ \sinh \left[\frac{1}{2J+1} x \right] ,$$

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

$$\vec{\rm H}_{\rm MF} = \gamma_0(-i\nabla) \langle \vec{\rm M} \rangle + \langle \vec{\rm B} \rangle + I \langle \psi^\dagger \sigma \psi \rangle . \tag{4.21}$$

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

$$\begin{aligned} F_M &\equiv U_M - \beta^{-1} S_M \\ &= \tfrac{1}{2} \langle \vec{\rm M} \rangle \cdot \vec{\rm H}_{\rm MF} - \beta^{-1} N \ln Z_J(g_J J \mu_B B \,|\, \vec{\rm H}_{\rm MF} \,|\,) . \end{aligned} \tag{4.22}$$

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

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

$$U_{\rm EM}=\frac{1}{8\pi}(\,|\langle\vec{\rm E}\rangle|^2+|\langle\vec{\rm B}\rangle|^2)-\tfrac{1}{2}\langle\vec{\rm j}\rangle\cdot\left[\langle\vec{\rm A}\rangle-\frac{\hbar c}{e}\vec{\nabla}f\right]$$

$$-\tfrac{1}{2}(\langle M\rangle-g\mu_B\langle\psi^\dagger\vec{\sigma}\psi\rangle)\cdot\langle\vec{\rm B}\rangle\ , \qquad (4.23)$$

which, after some manipulation involving the Maxwell equations, may be written as[23]

$$U_{\rm EM}=\frac{1}{8\pi}\int_V d^3x\langle\vec{\rm H}\rangle\cdot\frac{\hbar c}{e}\vec{\nabla}\times\vec{\nabla}f \qquad (4.24)$$

$$=\frac{1}{V}\frac{1}{8\pi}\int_V d^3x\langle\vec{\rm H}\rangle\cdot\vec{\rm n}\phi \qquad (4.25)$$

in the case of the superconducting state, where $\vec{\rm n}$ denotes the vortex density, $\phi=hc/2e$, and $\vec{\rm H}$ is the internal magnetic field defined by $\vec{\rm H}=\vec{\rm B}-4\pi(\vec{\rm M}-\mu_B\psi^\dagger\vec{\sigma}\psi)$. 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

$$U_{\rm EM}=\frac{1}{V}\int_V d^3x\langle\vec{\rm H}\rangle\cdot\langle\vec{\rm B}\rangle\ . \qquad (4.26)$$

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

$$F_s=-\frac{H_c^2}{8\pi}+\frac{1}{8\pi}\langle\vec{\rm H}\rangle\cdot\vec{\rm n}\phi+\tfrac{1}{2}\langle\vec{\rm H}_{\rm MF}\rangle\cdot\langle\vec{\rm M}\rangle$$

$$-\beta^{-1}N\ln(g_J J\mu_B B\,|\vec{\rm H}_{\rm MF}|)+E_{\rm core}\ . \qquad (4.27)$$

The last term in Eq. (4.27), $E_{\rm core}$, corresponds to the effect of the vortices on the energy spectra of the superconducting electrons. It is calculated in the manner outlined in Ref. 23. It should be noted that the above expression has an identical form to that presented in Ref. 17, 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.

V. MAXWELL EQUATIONS

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

$$\vec{\nabla}\times\langle\vec{\rm B}\rangle=\frac{4\pi}{e}\langle\vec{\rm j}\rangle+4\pi\vec{\nabla}\times(\langle\vec{\rm M}\rangle-\mu_B\langle\psi^\dagger\vec{\sigma}\psi\rangle)\ . \qquad (5.1)$$

In the superconducting state the current $\vec{\rm j}$ is related to the vector potential $\vec{\rm A}$ through the expression

$$\frac{4\pi}{e}\langle\vec{\rm j}\rangle=-\lambda_L^{-2}C(-i\vec{\nabla})\left[\langle\vec{\rm A}\rangle-\frac{\hbar c}{e}\vec{\nabla}f\right]\ , \qquad (5.2)$$

where $C(\vec{\rm k})$ is the nonlocal kernel of the Meissner current, λ_L is the London penetration depth, and $f(x)$ is the phase of the order parameter. The combination $\vec{\rm A}_f=\vec{\rm A}-(\hbar c/e)\vec{\nabla}f$ appears as a requirement of the gauge invariance.

Using the approximations presented in Sec. III, we obtain the following expression for the London penetration depth λ_L:

$$\frac{\lambda_L^{-2}(T;H)}{\lambda_{L0}^{-2}}=\left[1+\int_0^\infty d\epsilon\left[\frac{\partial f(E+\mu)}{\partial E}+\frac{\partial f(E-\mu)}{\partial E}\right]\right]\ , \qquad (5.3)$$

where the normalization factor λ_{L0} is defined as

$$\lambda_{L0}^{-2}=\frac{8\pi e^2 v_f^2 N(0)}{3\hbar^2 c}\ . \qquad (5.4)$$

Similar to the calculations presented in the preceding two sections, the effect of the temperature-dependent coupling may be realized through the scaling of a two-parameter function. Specifically, we have

$$\frac{\lambda_L^{-2}(T;H)}{\lambda_{L0}^{-2}}=\mathscr{L}^{-2}(t/s(t;H);\bar{\mu}/s(t;H))\ , \qquad (5.5)$$

where

$$\mathscr{L}^{-2}(t;\bar{\mu})=1-\Phi_2\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\bar{\mu});\frac{\pi e^{-\gamma}}{t}\bar{\mu}\right] \qquad (5.6)$$

with

$$\Phi_2(x;y)=\frac{x}{4}{\rm Re}\int_{-\infty}^{+\infty}dz\frac{z}{(z^2-1)^{1/2}}\cosh^{-2}[\tfrac{1}{2}(xz+y)]\ . \qquad (5.7)$$

Here the integrand in Φ_2 is defined in a manner analogous to Φ_1.

The calculation of the nonlocal kernel $C(\vec{\rm k})$ is rather involved when the polarization effect is included. Since the polarization appears explicitly only through the Fermi distributions, at $T=0$ K, the d-f interaction manifests itself solely through the modification of the gap and the coupling constant. Thus the result at $T=0$ K may be obtained by simply scaling the results for the nonmagnetic case.

At finite temperature complications arise since the thermal distributions are now modified by the spin splitting due to the effective field μ. However, since we expect the effect of the d-f interaction to be more pronounced at lower temperatures, it is reasonable to suppose that such complications may be avoided by simply extending the scaling arguments at zero temperature to finite temperature. In essence one is assuming that the correlation length is related to the inverse of the superconducting gap, which is at least qualitatively correct. Therefore, based on the results of Ref. 24, we can write

$$C(\vec{\rm k})=\exp-\nu[\,|\vec{\rm k}|\,\xi(T;H)]^\eta\ , \qquad (5.8)$$

where

$$\nu=-0.4527g(T;H)N(0)+0.559\ , \qquad (5.9)$$

$$\eta=-0.7857g(T;H)N(0)+2.207\ , \qquad (5.10)$$

and

$$\xi(T;H)\simeq\frac{v_F}{\pi\Delta(T;H)}\ . \qquad (5.11)$$

VI. MAGNETIZATION AND THE MAGNETIC SUSCEPTIBILITIES

In order to complete the analysis of the preceding sections we require 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

$$\langle \vec{M} \rangle = g_J \mu_B J N B_J(\beta g_J \mu_B \, | \vec{H}_{MF} |) \, , \tag{6.1}$$

where J is the spin of the localized spin, g_J is the Landé g factor, N is the density of magnetic ions, B_J is the Brillouin function, and $\vec{H}_{MF}$ is given by

$$\vec{H}_{MF} = \langle \vec{B} \rangle + \gamma_0(-i\nabla)\langle \vec{M} \rangle + I \langle \psi^\dagger \vec{\sigma} \psi \rangle \, . \tag{6.2}$$

The thermal average of the electron-spin density may be obtained even in the case of finite polarization as

$$\langle \psi^\dagger(x) \vec{\sigma} \psi(x) \rangle = \int d^4y \, \chi_\sigma(x-y)[I\langle \vec{M}(y) \rangle - \mu_B \langle \vec{B}(y) \rangle] \, , \tag{6.3}$$

where $\chi_\sigma(x-y)$ is a 3×3 matrix obtained from the electron-spin correlation function (see Appendix A):

$$\chi_\sigma(x-y)_{ij} = \frac{i}{2} \left\{ \left\langle R\left[\sum_k \sigma_k(x)\sigma_k(y) \right] \right\rangle \delta_{ij} - \langle R[\sigma_j(x)\sigma_i(y)] \rangle \right\} \, , \tag{6.4}$$

where $R[\;]$ denotes the retarded product. Since the quantities $\langle \vec{M} \rangle$ and $\langle \vec{B} \rangle$ are independent of time, then Eq. (6.3) reduces to

$$\langle \psi^\dagger \vec{\sigma} \psi \rangle = \chi_\sigma(I\langle \vec{M} \rangle - \mu_B \langle \vec{B} \rangle) \, , \tag{6.5}$$

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. (6.2), may then be written as

$$\vec{H}_{MF} = (1 - I\chi_\sigma \mu_B)\langle \vec{B} \rangle + [\gamma_0(-i\nabla) + I^2\chi_\sigma]\langle \vec{M} \rangle \, . \tag{6.6}$$

Since $\langle B \rangle$, $\langle H \rangle$, $\langle M \rangle$, and $\langle \psi^\dagger \vec{\sigma} \psi \rangle$ are related through

$$\langle \vec{B} \rangle = \langle \vec{H} \rangle + 4\pi(\langle \vec{M} \rangle - \mu_B \langle \psi^\dagger \vec{\sigma} \psi \rangle) \, , \tag{6.7}$$

the expression for the mean field may be written in terms of $\vec{H}$ and $\vec{M}$ as

$$\vec{H}_{MF} = \frac{1-\mu_B I \chi_\sigma}{1-4\pi\mu_B^2\chi_\sigma}\langle \vec{H} \rangle + \left[\gamma_0 + I^2\chi_\sigma + \frac{4\pi(1-\mu_B I\chi_\sigma)^2}{1-4\pi\mu_B^2\chi_\sigma} \right] \langle \vec{M} \rangle \, . \tag{6.8}$$

If we neglect the paramagnetic interaction, then the above expression simplfiies to give

$$\vec{H}_{MF} = \langle \vec{H} \rangle + (\gamma_0 + I^2\chi_\sigma + 4\pi)\langle \vec{M} \rangle \, . \tag{6.9}$$

In the case of $ErRh_4B_4$ we assume (6.9) together with (6.1) determines 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

$$\chi_\sigma^s \simeq \chi_\sigma^N \simeq \chi_\sigma^N |_{\mu=0} \, . \tag{6.10}$$

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 $\delta h_{ext}(x)$ that acts on the localized spins. This will produce a change in the fields $\langle \vec{B} \rangle$, $\langle \vec{M} \rangle$, and $\langle \psi^\dagger \vec{\sigma} \psi \rangle$, 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:

$$[-\nabla^2 + \lambda_L^{-2}C(-i\vec{\nabla})]\delta\vec{b} = -4\pi\nabla^2[T](\delta\vec{m} - \mu_B\delta\vec{\sigma}) \, , \tag{6.11}$$

$$\delta\vec{m}_3 = \frac{C}{T}\alpha_J(\delta\vec{h}_{MF}\cdot\vec{e}_3) \, , \tag{6.12}$$

$$\delta\vec{m} \times \vec{H}_{MF} = \langle \vec{M} \rangle \times \delta\vec{h}_{MF} \, , \tag{6.13}$$

and

$$\delta\vec{\sigma} = \chi_\sigma(I\,\delta\vec{m} - \mu_B\,\delta\vec{b}) \, , \tag{6.14}$$

where C denotes the Curie constant, $\delta\vec{h}_{MF}$ denotes the change in the mean field induced by the external field $\delta\vec{h}_{ext}(x)$ and is given by

$$\delta\,\vec{h}_{MF} = \delta\vec{b} + \gamma_0(-i\nabla)\delta\vec{m} + I\,\delta\vec{\sigma} + \delta\vec{h}_{ext} \, , \tag{6.15}$$

and where α_J is given by

$$\alpha_J = \frac{3J}{J+1}B_J'\left[\frac{g_J\mu_B J}{k_B T} \, | \vec{H}_{MF} | \right] \, . \tag{6.16}$$

From (6.11) and (6.14), $\delta\vec{b}$ and $\delta\vec{\sigma}$ may be eliminated from (6.15) to give

$$\delta\,\vec{h}_{MF} = \tilde{\gamma}(-i\vec{\nabla})\delta\vec{m} + \delta\vec{h}_{ext} \, , \tag{6.17}$$

with $\tilde{\gamma}$ given by

$$\tilde{\gamma}(\vec{k}) = \gamma(\vec{k}) - 4\pi\frac{(1-\mu_B I\chi_\sigma)^2}{(1-\mu_B^2 4\pi\chi_\sigma)} \times \frac{C(\vec{k})}{(1-4\pi\mu_B^2\chi_\sigma)\lambda_L^2 \, | \vec{k} |^2 + C(\vec{k})}[T] \tag{6.18}$$

and $\gamma(\vec{k})$ given by

$$\gamma(\vec{k}) = \gamma_0(\vec{k}) + I^2\chi_\sigma + 4\pi\frac{(1-\mu_B I\chi_\sigma)^2}{1-4\pi\mu_B^2\chi_\sigma}[T] \, . \tag{6.19}$$

Equation (6.17) together with (6.12) and (6.13) yields

$$\delta\vec{m} = \chi(-i\vec{\nabla})\delta\vec{h}_{ext} \tag{6.20}$$

with

$$\chi^{-1}(\vec{k}) = \begin{bmatrix} \frac{H_{MF}}{\langle M \rangle} & 0 & 0 \\ 0 & \frac{H_{MF}}{\langle M \rangle} & 0 \\ 0 & 0 & \frac{T}{\alpha JC} \end{bmatrix} - \tilde{\gamma}(\vec{k}) , \tag{6.21}$$

which may be inverted to give

$$\chi_{33}(\vec{k}) = \frac{C\alpha_J}{T - \alpha_J C \gamma_{33}(\vec{k})} \tag{6.22}$$

and

$$\chi_{ii}(\vec{k}) = \frac{1}{H_{MF}/\langle M \rangle - \gamma_{ii}(\vec{k})} \quad \text{for } i = 1,2 , \tag{6.23}$$

neglecting the effect of the transverse operator $[T]$ in (6.18) and (6.19). Parametrizing $\gamma_{ii}(\vec{k})$ as

$$\gamma_{ii}(\vec{k}) = \frac{T_m^{(i)}}{C} - \frac{D}{C} |\vec{k}|^2 , \tag{6.24}$$

we obtain

$$\chi_{33}(\vec{k}) = C \Bigg/ \left[\frac{T}{\alpha_J} - T_m^{(3)} + D|\vec{k}|^2 + 4\pi C \frac{1-\mu_B I \chi_\sigma}{1 - 4\pi\mu_B^2 \chi_\sigma} \frac{C(\vec{k})}{(1-4\pi\mu_B^2\chi_\sigma)|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] \tag{6.25}$$

and

$$\chi_{ii}(\vec{k}) = C \Bigg/ \left[\frac{1-\mu_B I \chi_\sigma}{1-4\pi\mu_B^2\chi_\sigma} \frac{C\langle H_3 \rangle}{\langle M_3 \rangle} + (T_m^{(3)} - T_m^{(i)}) + D|\vec{k}|^2 + 4\pi C \frac{1-\mu_B I \chi_\sigma}{1-4\pi\mu_B^2\chi_\sigma} \frac{C(\vec{k})}{(1-4\pi\mu_B^2\chi_\sigma)|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] \quad \text{for } i = 1,2 . \tag{6.26}$$

When we neglect the paramagnetic contribution the analysis simplifies somewhat and we obtain

$$\chi_{33}(\vec{k}) = C \Bigg/ \left[\frac{T}{\alpha_J} - T_m^{(3)} + D|\vec{k}|^2 - 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] \tag{6.27}$$

and

$$\chi_{ii}(\vec{k}) = C \Bigg/ \left[\frac{C\langle H_3 \rangle}{\langle M_3 \rangle} + (T_m^{(3)} - T_m^{(i)}) + D|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] \quad \text{for } i = 1,2 , \tag{6.28}$$

respectively.

Equations (6.25) and (6.26) together with the limiting cases (6.27) and (6.28) illustrate how the effect of the finite field modifies the calculation of the spin susceptibility. The expression given by Eqs. (6.27) and (6.28) represents the generalization of the result of Ref. 25 to consider finite field. The last term in the denominator represents the effect of the shielding of the localized magnetic moments by the persistent current. As was shown in Ref. 25, in the zero-field limit, the susceptibility given by Eqs. (6.27) and (6.28) 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. (6.24) to include the effect of the anistropy in the momentum dependence. We therefore replace Eq. (6.24) with

$$\gamma_{ii}(\vec{k}) = \frac{T_m^{(i)}}{C} - \frac{D}{C}[1 + \tfrac{3}{2}\alpha(1-\cos^2\theta)]|\vec{k}|^2 , \tag{6.29}$$

where θ denotes the angle between the vector $\vec{Q}$ and the momentum $\vec{k}$. Equations (6.27) and (6.28) then become

$$\chi_{33}(\vec{k}) = C \Bigg/ \left[\frac{T}{\alpha_J} - T_m^{(3)} + D[1 + \tfrac{3}{2}\alpha(1-\cos^2\theta)]|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] , \tag{6.30}$$

$$\chi_{ii}(\vec{k}) = C \Bigg/ \left[\frac{C\langle H_3 \rangle}{\langle M_3 \rangle} + (T_m^{(3)} - T_m^{(i)}) + D[1 + \tfrac{3}{2}\alpha(1-\cos^2\theta)]|\vec{k}|^2 + 4\pi C \frac{C(\vec{k})}{|\vec{k}|^2\lambda_L^2 + C(\vec{k})} \right] , \tag{6.31}$$

respectively.

VII. EFFECTIVE COUPLING CONSTANT

With the finite-field susceptibilities given by Eqs. (6.31) and (6.32), we can calculate the coupling constant $g(T;h)$ using Eq. (3.27) in the London limit [i.e., $C(k)=1$] as

$$g(T;h)=\frac{1}{4k_F^2}\int_0^{4k_F^2}dl^2\int_0^1 d\cos\theta\left\{V-\tilde{I}^2\left[C\Big/\left[\frac{T}{\alpha_J}-T_m^{(3)}+D[1+\alpha\tfrac{3}{2}(1-\cos^2\theta)]l^2+\frac{4\pi C}{l^2\lambda_L^2+1}\right]\right]\right.$$
$$-\sum_{i=1}^{2}\tilde{I}^2\left[C\Big/\left[\frac{C\langle H_3\rangle}{\langle M_3\rangle}+(T_m^{(3)}-T_m^{(i)})\right.\right.$$
$$\left.\left.\left.+\;D[1+\tfrac{3}{2}\alpha(1-\cos^2\theta)]l^2+\frac{4\pi C}{l^2\lambda_L^2+1}\right]\right]\right\}. \tag{7.1}$$

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 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.,

$$\tfrac{3}{2}\alpha(1-\cos^2\theta)\simeq\alpha\;, \tag{7.2}$$

and thus Eq. (7.1) reduces to give

$$g(T;h)=\frac{1}{4k_F^2}\int_0^{4k_F^2}dl^2\left\{V-\tilde{I}^2\left[C\Big/\left[\frac{T}{\alpha_J}-T_m^{(3)}+D(1+\alpha)l^2+\frac{4\pi C}{l^2\lambda_L^2+1}\right]\right]\right.$$
$$\left.-\sum_i\tilde{I}^2\left[C\Big/\left[\frac{C\langle H_3\rangle}{\langle M_3\rangle}+T_m^{(3)}-T_m^{(i)}+D(1+\alpha)l^2+\frac{4\pi C}{l^2\lambda_L^2+1}\right]\right]\right\}. \tag{7.3}$$

This may be integrated to give an analytical expression for the effective coupling constant at finite field as

$$g(T;H)=V-\tilde{I}^2\left[G_3[\epsilon_{\parallel}^{(3)}(t;H)]+\sum_{i=1,2}G_i[\epsilon_{\perp}^{(i)}(t;H)]\right], \tag{7.4}$$

where

$$G_{(i)}(\epsilon)=\frac{C^{(i)}}{8\pi d_f^{(i)}(1+\alpha)}\left[\ln\left[\frac{d_f^{(i)2}(1+\alpha)+d_f^{(i)}[\epsilon+d^{(i)}(1+\alpha)]+d^{(i)}(\epsilon+C^{(i)})}{d^{(i)}(\epsilon+C^{(i)})}\right]+[d^{(i)}(1+\alpha)-\epsilon]I^{(i)}(\epsilon)\right],$$

with

$$I^{(i)}(\epsilon)=\frac{1}{[\Omega_{(i)}(\epsilon)]^{1/2}}\ln\left[\frac{2d_f^{(i)}(1+\alpha)+[d^{(i)}(1+\alpha)+\epsilon]-[\Omega_{(i)}(\epsilon)]^{1/2}}{2d_f^{(i)}(1+\alpha)+[d^{(i)}(1+\alpha)+\epsilon]+[\Omega_{(i)}(\epsilon)]^{1/2}}\right.$$
$$\left.\times\frac{d^{(i)}(1+\alpha)+\epsilon+[\Omega_{(i)}(\epsilon)]^{1/2}}{d^{(i)}(1+\alpha)+\epsilon-[\Omega_{(i)}(\epsilon)]^{1/2}}\right]\quad\text{for }\Omega_{(i)}(\epsilon)>0 \tag{7.6}$$

and

$$I^{(i)}(\epsilon)=\frac{1}{[-\Omega_{(i)}(\epsilon)]^{1/2}}\left[\tan^{-1}\frac{2d_F^{(i)}(1+\alpha)+d^{(i)}(1+\alpha)+\epsilon}{[-\Omega_{(i)}(\epsilon)]^{1/2}}-\tan^{-1}\frac{\epsilon+d^{(i)}(1+\alpha)}{[-\Omega_{(i)}(\epsilon)]^{1/2}}\right]\quad\text{for }\Omega_{(i)}(\epsilon)<0\;, \tag{7.7}$$

with

$$\Omega_{(i)}(\epsilon)=\{\epsilon+d^{(i)}(1+\alpha)+2[d^{(i)}(1+\alpha)C^{(i)}]^{1/2}\}\{\epsilon-d^{(i)}(1+\alpha)+[d^{(i)}(1+\alpha)C^{(i)}]^{1/2}\}\;. \tag{7.8}$$

The parameters $d^{(i)}$, $d_F^{(i)}$, and $C^{(i)}$ are defined as

$$C^{(i)}=\frac{4\pi C}{T_m^{(i)}},\quad d^{(i)}=\frac{D}{T_m^{(i)}\lambda_L^2},\quad d_F^{(i)}=\frac{4Dk_F^2}{T_m^{(i)}}\;,$$

and $\epsilon_{\perp}^{(i)}(t;H)$ and $\epsilon_{\parallel}^{(3)}(t;H)$ are given by

$$\epsilon_{\parallel}^{(3)}(t;H)=\frac{t}{t_m^{(3)}\alpha_J}-1 \tag{7.9}$$

and

$$\epsilon_{\perp}^{(i)}(t;H)=\frac{C}{T_m^{(i)}}\frac{H}{\langle M_3\rangle}-1+T_m^{(3)}-T_m^{(i)} . \tag{7.10}$$

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 (7.4) then becomes

$$g(T;H)=g(1;0)\left[1-\frac{\tilde{I}^2}{g(1)}\{G_{(3)}[\epsilon_{\parallel}^{(3)}(t;H)]-G_{(3)}[\epsilon_{\parallel}^{(3)}(1;H=0)]\}\right.$$
$$\left.-\sum_{i=1,2}\frac{\tilde{I}^2}{g(1)}\{G_{(i)}[\epsilon_{\perp}^{(i)}(t;H)]-G_{(i)}[\epsilon_{\perp}^{(i)}(1;H=0)]\}\right] . \tag{7.11}$$

We note that

$$\epsilon_{\parallel}^{(i)}(t;0)=\epsilon_{\perp}^{(i)}(t;0)\equiv\epsilon^{(i)}(t)=\left[\frac{t}{t_m^{(i)}}-1\right] . \tag{7.12}$$

The renormalized coupling constant $g(1;0)$ is given by

$$g(1;0)=V-\tilde{I}^2\sum_i G_{(i)}[\epsilon^{(i)}(1)] , \tag{7.13}$$

where

$$G_{(i)}[\epsilon^{(i)}(1)]=\frac{C}{4\pi d_F}\ln\left[\frac{\epsilon^{(i)}(1)+d_F^{(i)}(1+\alpha)}{\epsilon^{(i)}(1)}\right] . \tag{7.14}$$

Here we used the fact that $\lambda_L\to\infty$ at $T=T_c$.

With the effective coupling constant given by (7.7), the scale factor $s(t;H)$ may be computed from Eq. (3.35) and the superconducting quantities may be calculated from the scaling laws which will be summarized in the next section.

VIII. SUMMARY AND RESULTS

In the preceding sections we have shown how the effect of the magnetic ions on the superconducting properties such as Δ, λ_L, and H_c may be calculated. In particular, it was shown how the effect of the spin fluctuations may be realized through a simple rescaling of certain two-parameter functions involving the temperature and the effective field of the electrons, namely μ. In this section we wish to summarize the relevant formula and present some numerical results to illustrate the various effects arising from the d-f interaction.

In Sec. III the superconducting gap $\Delta(T;H)$ was found to be given by

$$\frac{\Delta(T;H)}{\Delta_0}=s(t;H)\mathscr{D}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{8.1}$$

In Sec. IV the field-dependent condensation energy was found to be

$$\frac{H_c(T;H)}{H_{c0}}=s(t;H)\mathscr{H}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{8.2}$$

In Sec. V the London penetration depth λ_L was found to be

$$\frac{\lambda_L(T;H)}{\lambda_{L0}}=\mathscr{L}(t/s(t;H);\bar{\mu}/s(t;H)) . \tag{8.3}$$

The normalization parameters Δ_0, H_{c0}, and λ_{L0} are given by

$$\Delta_0=2\omega_D\exp\frac{-1}{g(T_c;0)N(0)} , \tag{8.4}$$

$$H_{c0}^2=4\pi\Delta_0^2N(0) , \tag{8.5}$$

and

$$\lambda_{L0}^{-2}=\frac{8\pi}{3C^2}e^2v_F^2N(0) . \tag{8.6}$$

We wish to emphasize that the above normalization constants do not correspond to the observable gap and critical field at $T=0$ K. They are instead related simply to the quantities for nonmagnetic superconductors with a similar structure.

The spin-splitting parameter $\bar{\mu}$ is also a function of t and H and is given by

$$\bar{\mu}(t;H)=\frac{\tilde{I}\langle M_3(t;H)\rangle}{\Delta_0} , \tag{8.7}$$

where $\langle M_3(t;H)\rangle$ is determined in Sec. VI.

The two-parameter functions $\mathscr{D}(t;\mu)$, $\mathscr{H}(t;\mu)$, and $\mathscr{L}(t;\mu)$ are given by

$$\ln\mathscr{D}(t;\bar{\mu})=-\Phi_1\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\bar{\mu});\frac{\pi e^{-\gamma}}{t}\bar{\mu}\right] , \tag{8.8}$$

$$\mathscr{H}^2(t;\bar{\mu})=\mathscr{D}^2(t;\bar{\mu})-\frac{2\pi^2}{3}\left[\frac{t^2}{\pi e^{-\gamma}}-\frac{3\mathscr{D}^2(t;\bar{\mu})}{\pi^2}\Phi_3\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\bar{\mu});\frac{\pi e^{-\gamma}}{t}\bar{\mu}\right]\right.$$
$$\left.-\frac{3\bar{\mu}\mathscr{D}(t;\bar{\mu})}{\pi^2}\Phi_4\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\bar{\mu});\frac{\pi e^{-\gamma}}{t}\bar{\mu}\right]\right] , \tag{8.9}$$

and

$$\mathscr{L}^{-2}(t;\bar{\mu})=1-\Phi_2\left[\frac{\pi e^{-\gamma}}{t}\mathscr{D}(t;\bar{\mu});\frac{\pi e^{-\gamma}}{t}\bar{\mu}\right], \quad (8.10)$$

where the functions (Φ_i) may be written as

$$\Phi_i(x;y)=\frac{x}{4}\mathrm{Re}\int_{-\infty}^{+\infty}dz\,T_i(z)\cosh^{-2}\tfrac{1}{2}(xz+y)\,. \quad (8.11)$$

The functions $[T_i(z)]$ are complex functions and all are defined on the Riemann sheet with the branch line running between $z=\pm 1$ shown in Fig. 1 with

$$\lim_{\mathrm{Im}z\to 0}T_i(z)=T_i(\mathrm{Re}z)\ \ \text{for}\ \mathrm{Re}z>1\,, \quad (8.12)$$

where

$$T_1(z)=\ln[z+(z^2-1)^{1/2}]\,, \quad (8.13)$$

$$T_2(z)=\frac{z}{(z^2-1)^{1/2}}\,, \quad (8.14)$$

$$T_3(z)=z(z^2-1)^{1/2}\,, \quad (8.15)$$

$$T_4(z)=(z^2-1)^{1/2}\,. \quad (8.16)$$

The scale factor $s(t;H)$ is given by

$$s(t;H)=\exp\left[\frac{1}{g(1;0)N(0)}-\frac{1}{g(t;H)N(0)}\right], \quad (8.17)$$

where $g(t;H)$ is the effective coupling constant evaluated in Sec. VII.

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 $\mathscr{D}$, $\mathscr{H}$, and $\mathscr{L}$ 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. The temperature dependence of the gap, the condensation energy, and the London penetration depth in the case of zero field are shown in Figs. 2, 3, and 4, respectively, for the parameters shown in Table I which are felt to be appropriate to the case of $ErRh_4B_4$, together with the results of the BCS theory. (A detailed discussion of the particular choice of the parameters will be given together with a detailed analysis of the magnetic properties of the mixed state in $ErRh_4B_4$ in a forthcoming paper.) These results clearly show the effect of the suppression of the superconducting quantities at low temperature 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[26] and thin-film[27] 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 magnetizaton curves of single-crystal $ErRh_4B_4$ (Ref. 28) 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 Fig. 3 if we choose a value of $H_{c0}\simeq 1.4$ kG, a value consistent with similar measurements on $LuRh_4B_4$ obtained from specific-heat measurements which give $H_{c0}\simeq 1.85$ kG.[29] Accurate determination of the condensation energy for various temperatures would be extremely useful in that it

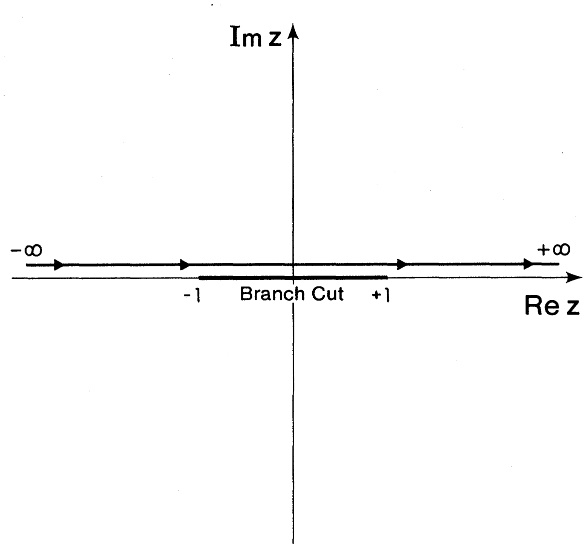

FIG. 1. Contour for the complex integrals contained in the expressions for $\{\phi_i(x;y)\}$, $i=1,4$.

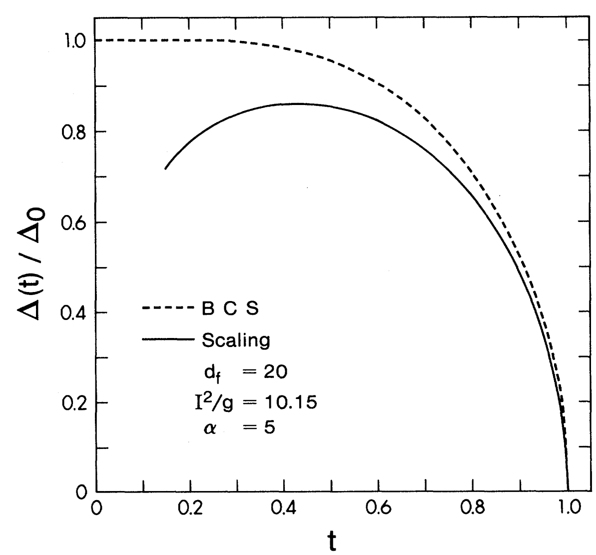

FIG. 2. Temperature dependence of the superconducting gap including the effect of the spin fluctuations (solid curve) and the BCS result for comparison (dashed curve). The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, and $I^2/g=10.15$.

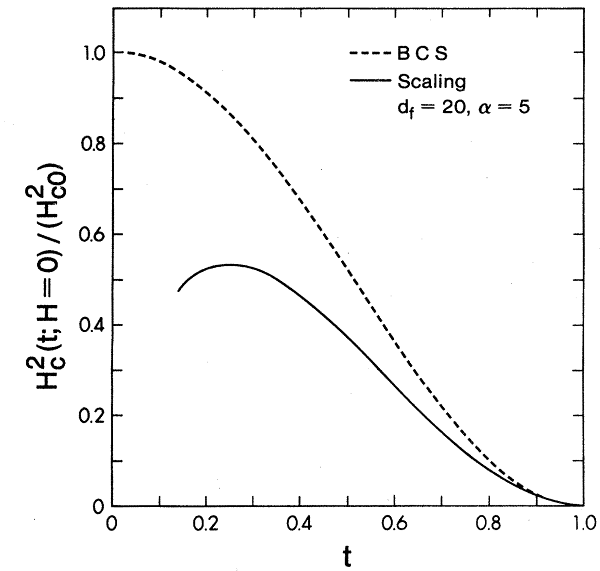

FIG. 3. Temperature dependence of the condensation energy including the effect of the spin fluctuations (solid curve) and the BCS result (dashed curve) for comparison. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, and $I^2/g=10.15$.

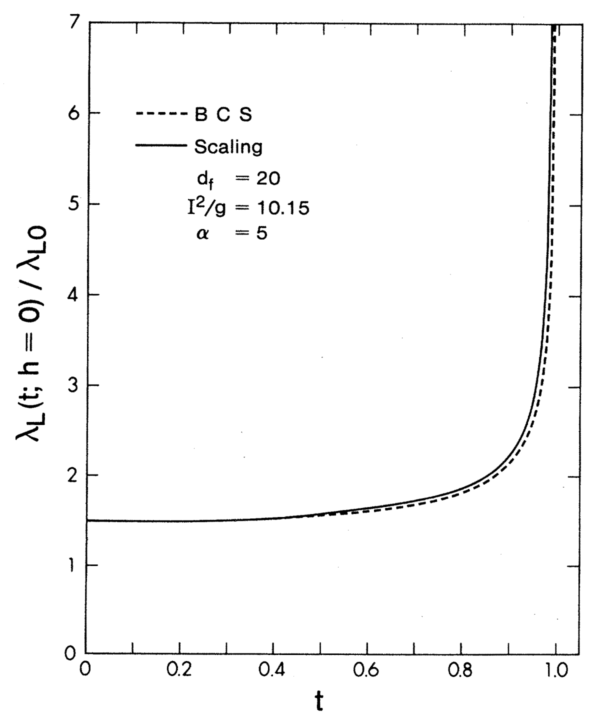

FIG. 4. Temperature dependence of the London penetration depth including the effect of the spin fluctuations (solid curve) and the BCS result (dashed curve) for comparison. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, and $I^2/g=10.15$.

TABLE I. Parameters which are appropriate to the case of $ErRh_4B_4$.

$t_m^a \equiv \frac{T_m^a}{T_c} = 0.115$	$g(T_c)N(0) = 0.3$
$t_m^c \equiv \frac{T_m^c}{T_c} = -2.300$	$d \equiv \frac{D}{T_m \lambda_L^2} = 0.452\times 10^{-2}$
$t_p \equiv \frac{T_p}{T_c} = 0.092$	$J = 7.5$
$C \equiv \frac{4C}{T_m^a} = 2.312$	

The parameters d_f, U, and I are defined as

$$d_f \equiv \frac{4Dk_F^2}{T_m^a}$$

$$U \equiv \frac{M}{\phi/\lambda_{L0}^2}$$

$$\tilde{I} \equiv \frac{IM}{\Delta_0} = \left[\frac{8\pi^5}{3} g(T_c)N(0)\frac{I^2}{g(T_c)}\right]^{1/2} \frac{U}{k_B}$$

would provide information regarding the strength and the role of the spin fluctuations in modifying the superconducting state as we approach the coexistence 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 $2\Delta_{max}/k_B T_c$ have 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[11] for both polycrystalline and single-crystal $ErRh_4B_4$. The results show that the value of the superconducting gap inferred from the dI/dV-versus-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 $2\Delta_{max}/k_B T_c$ appears to be in the region 3.8 to 4.2, in contrast to the results presented here.

The London penetration depth shown in Fig. 3 does not show such a dramatic change. While it is the case that the London penetration depth may be obtained from surface-independence measurements, the exact nature of the relationship is complicated by the possible appearance of surface magnetization states.[30] Further analytical work in this direction is in progress.

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:

(1) It will suppress the spin fluctuation, leading to an increase in the effective coupling constant $g(T;H)$ and therefore enhancing the superconductivity.

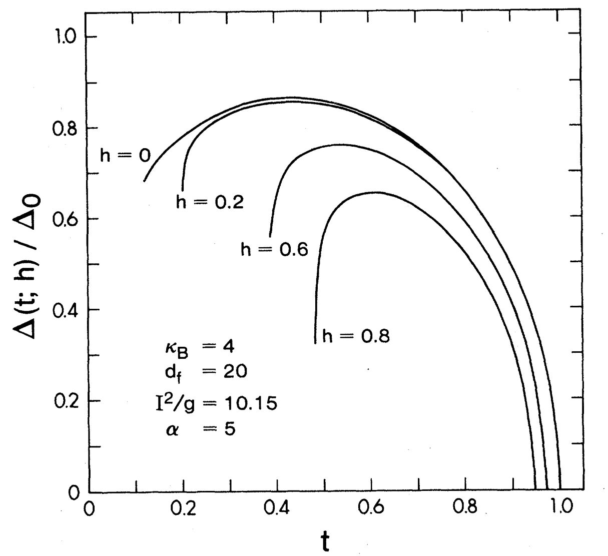

FIG. 5. Temperature dependence of the gap for various values of the reduced internal field $h(\equiv H/\phi\lambda_{L0}^{-2})$. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

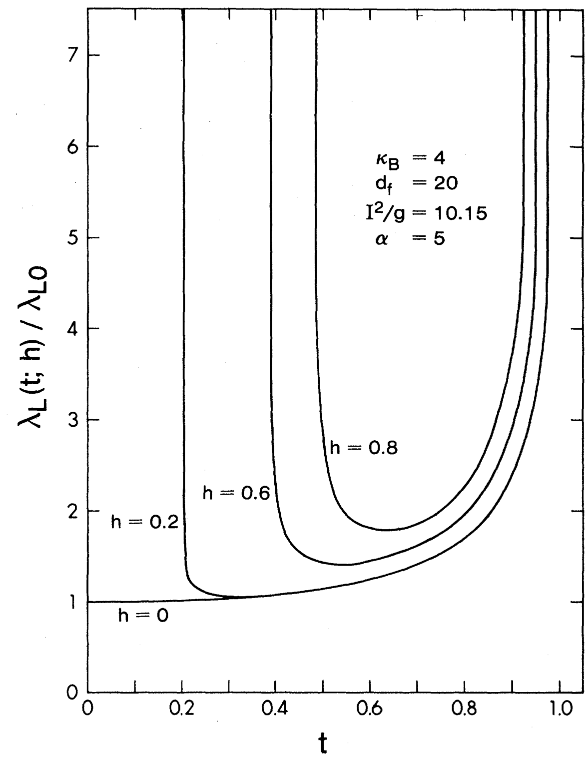

FIG. 7. Temperature dependence of the London penetration depth for various values of the reduced internal field $h(=H/\phi\lambda_{L0}^{-2})$. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

(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 Figs. 5, 6, and 7 we present graphs showing the temperature dependence of the gap, the field-dependent condensation energy, and the London penentration depth under the presence of an internal field. In Figs. 8, 9, and 10 we present the field dependences of the gap, the condensation energy, and the London penetration depth, respectively, for various temperatures. 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 tempera-

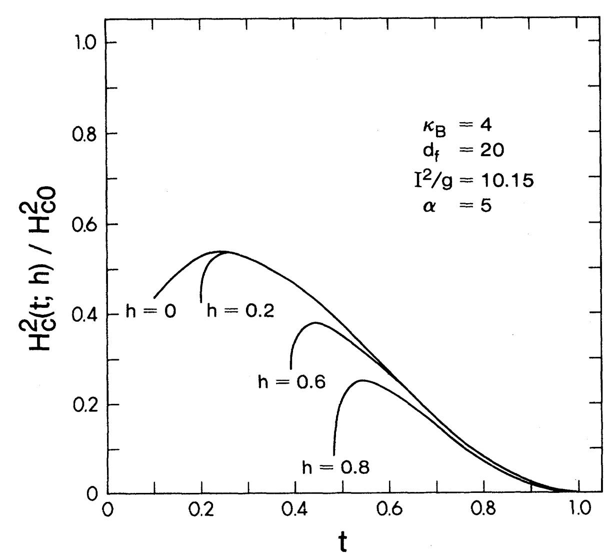

FIG. 6. Temperature dependence of the field-dependent condensation energy for various values of the reduced internal field $h(\equiv H/\phi\lambda_{L0}^{-2})$. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

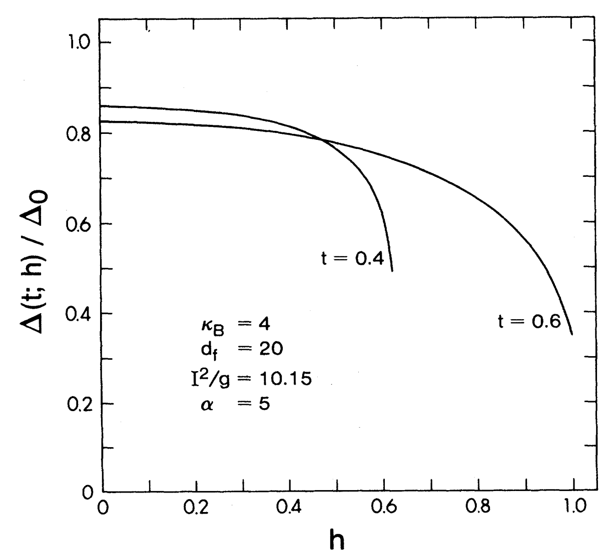

FIG. 8. Field dependence of the superconducting gap for various values of the reduced temperature. The parameters used are those given in Table II together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

TABLE II. Field dependence of the condensation energy. Calculated values of the condensation energy $H_c^2(t;h)/H_{c0}^2$ for various values of $h(=H/\phi\lambda_L^2)$ and $t(=T/T_c)$. The parameters used are those given in Table I together with $d_f=20$, $\alpha=5$, and $k_B=4$.

h	$t=0.2$	$t=0.4$	$t=0.6$
0.00	0.523 616	0.466 289	0.269 145
0.01	0.523 638	0.466 290	0.269 145
0.02	0.523 702	0.466 295	0.269 147
0.03	0.523 805	0.466 303	0.269 149
0.04	0.523 940	0.466 313	0.269 152
0.05	0.524 097	0.466 327	0.269 155
0.06	0.524 261	0.466 342	0.269 160
0.07	0.524 410	0.466 359	0.269 165
0.08	0.524 512	0.466 377	0.269 170
0.09	0.524 519	0.466 395	0.269 176
0.10	0.524 365	0.466 414	0.269 182

ture is lowered further. This arises from the increase in the spin-splitting parameter μ due to the increased ordering of the magnetic ions. A closer examination of the numerical results, however, reveals that as H is increased for a given temperature, H_c^2 is seen first to rise due to the increase in the effective coupling $g(T;H)$ before decreasing rapidly at higher values of the field. While the actual increase is very small for the present choice of parameters (see Table II) and is not discernible on the graphs presented in Fig. 9 which shows the field dependence of $H_c^2(T;H)$ for various temperatures, such an increase at low-field values may be important when one considers the nature of the transition around the lower critical field H_{c1} in a type-II superconductor.

While the direct observation of the effect of the internal field on the superconducting properties is extremely difficult, the effect on the magnetic and thermodynamic quantities will be quite marked. A detailed study of the magnetic properties of $ErRh_4B_4$ using this formalism has been completed and a report on the results is currently in preparation and will include a detailed comparison with the recent experimental measurements of single-crystal $ErRh_4B_4$.[15,16] Also, since the polarization effect is quite drastic when the internal field reaches a certain critical value, the magnetic properties of thin films may be affected considerably. Such an analysis is in progress.

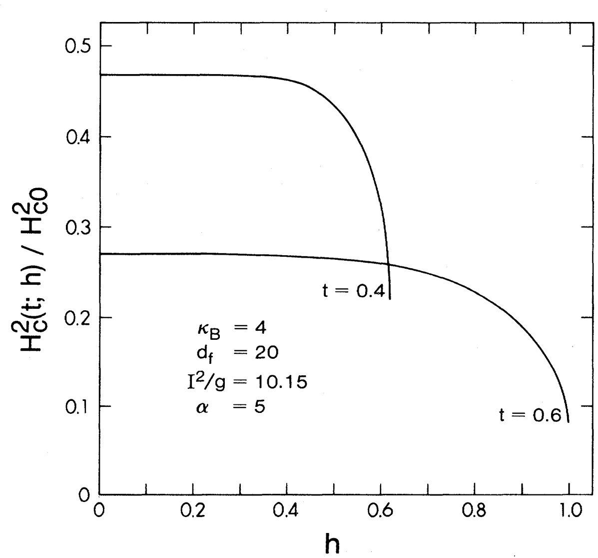

FIG. 9. Field dependence of the field-dependent condensation energy for various values of the reduced temperature. The parameters used are those given in Table II together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

IX. CONCLUSIONS

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, summarized in Sec. VIII, 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 properties 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

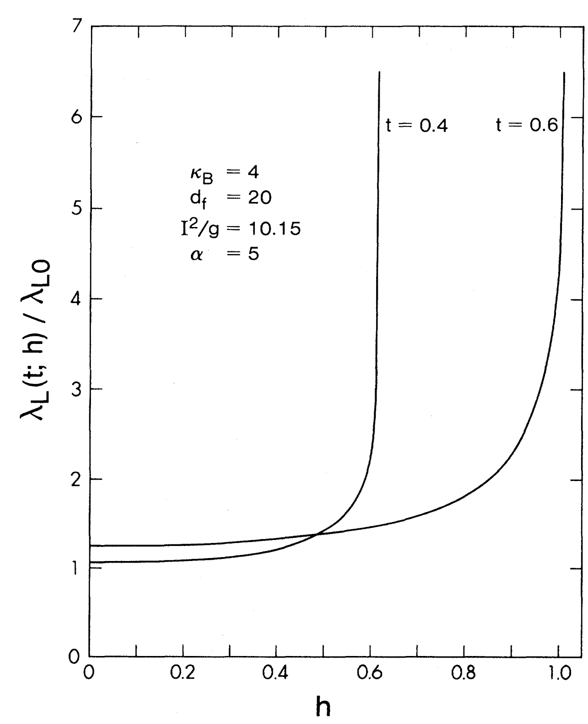

FIG. 10. Field dependence of the London penetration depth for various values of the reduced temperature. The parameters used are those given in Table II together with $d_f=20$, $\alpha=5$, $I^2/g=10.15$, and $k_B=4$.

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.

Second, it is both interesting and somewhat surprising that the resultant expression for the free energy given in Eq. (4.27) has the same form as that presented in Ref. 17, 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 paper can be used to extend work presented in Ref. 17 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 $H_c^2(H;T)/8\pi$ for increasing H, for low values of the field proceeded by the rapid decrease for high values of H, shown in Fig. 9. This suggests that the response of the localized-spin fluctuations to an applied field will be of importance in determining the behavior 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 in the analysis of magnetic superconductors. The results obtained show several interesting features and allow for the extension of previous work on the mixed state to include the effect of the d-f and the paramagnetic interactions. The application of the present formalism to a specific material (such as $ErRh_4B_4$) will be presented elsewhere.

ACKNOWLEDGMENTS

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APPENDIX A: RENORMALIZED COUPLING $\tilde{I}$

In this appendix we show how the expression for the renormalized coupling constant $\tilde{I}$ given in Eq. (3.10) may be calculated. We begin with the equation of motion for the $S_i(t)$ defined as

$$S_i(t)=\int d^3x\,\phi^\dagger\sigma_i\phi\ , \tag{A1}$$

which is given as

$$\partial_t S_i(t)=-\epsilon_{ijk}\int d^3x[IM_j(x)-\mu_B B_j(x)]\sigma_k(x)\ . \tag{A2}$$

Thus we have

$$\partial_t\langle R[\sigma_i(x)S_j(t)]\rangle=\delta(t-t_x)\langle[S_j(t),\sigma_i(x)]\rangle-\epsilon_{jlk}\left\langle R\left[\sigma_i(x)\int d^3y[IM_l(y)-\mu_B B_l(y)]\sigma_k(y)\right]\right\rangle\ . \tag{A3}$$

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

$$\langle\sigma_i(x)\rangle=\frac{1}{2i}(\delta_{jl}\delta_{ik}-\delta_{jk}\delta_{il})\int d^4y\,\langle R\{\sigma_j(x)\sigma_k(y)[IM_l(y)-\mu_B B_l(y)]\}\rangle\ . \tag{A4}$$

Calculating this in the mean-field approximation yields the result of Eqs. (6.3) and (6.4):

$$\langle\sigma_i(x)\rangle=\int d^4y\,\chi_\sigma^{ij}(x-y)[I\langle M_j(y)\rangle-\mu_B B_j(y)]\ , \tag{A5}$$

where χ_σ is a 3×3 matrix;

$$\chi_\sigma^{ij}(x-y)=\frac{i}{2}\left[\delta_{ij}\sum_k\langle R[\sigma_k(x)\sigma_k(y)]\rangle-\langle R[\sigma_j(x)\sigma_i(y)]\rangle\right]\ . \tag{A6}$$

Thus the expression for μ may be written as

$$\mu=I\langle M_3\rangle-\mu_B\langle B\rangle-\frac{V}{2}\langle\sigma_3\rangle=\left[1-\frac{V}{2}\chi_\sigma^{33}(i\partial)\right](I\langle M_3\rangle-\mu_B\langle B_j\rangle)\ . \tag{A7}$$

Now from the Maxwell equation of (5.1) and (5.2) we have

$$[\nabla^2-\lambda_L^{-2}C(-i\vec{\nabla})]B(x)=\lambda_L^{-2}C(-i\vec{\nabla})n(x)\phi+4\pi\nabla^2(\langle M\rangle-\mu_B\langle\sigma\rangle)$$
$$=-\lambda_L^{-2}C(-i\vec{\nabla})n(x)\phi+4\pi\nabla^2(1-\mu_B I\chi_\sigma^{33})\langle M\rangle+\mu_B^2\chi_\sigma^{33}4\pi\nabla^2\langle B(x)\rangle \ . \quad \text{(A8)}$$

Here all fields lie along the z axis and $n(x)\phi=(\hbar c/e)[\vec{\nabla}\times\vec{\nabla}f(x)]\cdot\vec{e}_3$. Thus we obtain

$$B(x)=\left[(1-4\pi\mu_B^2\chi_\sigma^{33})\nabla^2-\frac{1}{\lambda_L^2}C(-i\vec{\nabla})\right]^{-1}\left[-\frac{1}{\lambda_L^2}C(-i\vec{\nabla})n(x)\phi+4\pi\nabla^2(1-\mu_B I\chi_\sigma^{33})\langle M\rangle\right] , \quad \text{(A9)}$$

and hence that

$$\mu=-\mu_B\left[1-\frac{V}{2}\chi_\sigma^{33}\right][-(1-4\pi\mu_B^2\chi_\sigma^{33})\nabla^2+\lambda_L^{-2}C(-i\vec{\nabla})]^{-1}\lambda_L^{-2}C(-i\vec{\nabla})n(x)\phi$$
$$+\left[1-\frac{V}{2}\chi_\sigma^{33}\right]\{I-4\pi\mu_B(1-I\mu_B\chi_\sigma^{33})(-\nabla^2)[-(1-4\pi\mu_B^2\chi_\sigma^{33})\nabla^2+\lambda_L^{-2}C(-i\vec{\nabla})]^{-1}\}\langle M\rangle \ . \quad \text{(A10)}$$

APPENDIX B: ELECTRON SELF-ENERGY

In order to discuss the calculation of the electron propagator at finite temperature, we use the formalism of thermofield dynamics (TFD). The TFD formalism is dealt with extensively in the literature[31–36] and its relation to other techniques such as the Matsubara method[35] and the C^* algebra approach is now well understood.[36] Briefly, TFD introduces temperature by doubling the number of degrees of freedom; for example, the electron field $\psi(x)$ is now generalized to a doublet field $\psi^\alpha(x)$ ($\alpha=1,2$) which satisfies the usual canonical anticommutation relations and which satisfies Eq. (3.7), namely,

$$[i\partial_t-\epsilon(i\vec{\nabla})\tau_3+\Delta_0\tau_1+\mu\sigma_3]\phi^\alpha$$
$$=I(\vec{\mathrm{M}}^\alpha-\langle\vec{\mathrm{M}}\rangle)\cdot\vec{\sigma}\phi^\alpha-\mu_B(\vec{\mathrm{B}}^\alpha-\langle\vec{\mathrm{B}}\rangle)\cdot\vec{\sigma}\phi^\alpha \ . \quad \text{(B1)}$$

The relation between thermal doublet is constructed in such a way that the thermal expectation value of a particular operator A may be relaized within a canonical field theory as the vacuum expectation value of $A^{\alpha=1}$, specifically

$$\langle A\rangle\equiv\langle\beta|A^{\alpha=1}|\beta\rangle , \quad \text{(B2)}$$

where $\langle\beta|$ denotes the "thermal vacuum." In particular, the thermal expectation of the *time-ordered* product $T[\phi(x)\phi^\dagger(y)]$ may be obtained from the TFD Green's function as

$$\langle T[\phi(x)\phi^\dagger(y)]\rangle=\langle\beta|T[\phi^\alpha(x)\phi^\beta(y)^\dagger]|\beta\rangle,\ \ \alpha=\beta=1 \ . \quad \text{(B3)}$$

From Eq. (B1) and neglecting the B field contribution, we obtain

$$\left[\frac{i\partial}{\partial t}-\epsilon(-i\vec{\nabla})\tau_3+\Delta_0\tau_1+\mu\sigma_3\right]\langle\beta|T[\phi^\alpha(x)\phi^\beta(y)^\dagger]|\beta\rangle=i\delta^{\alpha\beta}\delta(x-y)+I\sigma_i\langle\beta|T\{[M_i^\alpha(x)-\langle M_i(x)\rangle]\phi^\alpha(x)\phi^\beta(y)^\dagger\}|\beta\rangle \ . \quad \text{(B4)}$$

In the lowest order of perturbation we have

$$\langle\beta|T\{[M_i(x)-\langle M_i(x)\rangle]\phi^\alpha(x)[\phi^\beta(y)]^\dagger\}|\beta\rangle$$
$$\simeq-iI\int d^4z\langle\beta|T\left[\sum_a\vec{\mathrm{M}}^a(z)[\psi^a(z)]^\dagger\vec{\sigma}\psi(z)^a[M_i(x)-\langle M_i(x)\rangle]\phi^\alpha(x)[\phi^\beta(y)]^\dagger\right]|\beta\rangle \ .$$
$$\simeq-iI\int d^4z\sum_a\langle\beta|T\{[M_i(x)-\langle M_i(x)\rangle][M_j(z)-\langle M_j(z)\rangle]\}|\beta\rangle$$
$$\times\langle\beta|T\{\phi^\alpha(x)[\phi^\beta(z)]^\dagger\}|\beta\rangle\sigma_i\langle\beta|T\{\phi^\alpha(z)[\phi^\beta(y)]^\dagger\}|\beta\rangle , \quad \text{(B5)}$$

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

$$\langle\beta|T\{\phi^\alpha(x)[\phi^\beta(y)]^\dagger\}|\beta\rangle$$
$$=\frac{i}{(2\pi)^4}\int d^4p\,e^{-ip(x-y)}S^{\alpha\beta}(p) \quad \text{(B6)}$$

and

$$\langle\beta|T\{[M_i(x)-\langle M_i(x)\rangle][M_j(y)-\langle M_j(y)\rangle]\}|\beta\rangle$$
$$=\frac{i}{(2\pi)^4}\int d^4k\,e^{-ik(x-y)}\chi_{ij}^{\alpha\beta}(k) , \quad \text{(B7)}$$

with $p\cdot x=\vec{\mathrm{p}}\cdot\vec{\mathrm{x}}-p_0t_x$, then Eq. (B4) together with Eq. (B5) yields

$$S^{-1}(p)^{\alpha\beta}=[p_0-\epsilon(\vec{p})\tau_3+\Delta_0\tau_1]S_{\alpha\beta}-\frac{iI^2}{(2\pi)^4}\int d^4k\sum_i\chi_{ij}^{\alpha\beta}(k)\sigma_i S^{\alpha\beta}(p-k)\sigma_j\ . \tag{B8}$$

The propagators $\chi_{ij}^{\alpha\beta}(k)$ and $S^{\alpha\beta}(k)$ may be written in the spectral representation as[33]

$$\chi_{ij}^{\alpha\beta}(k)=\int dw\,\rho_{ij}(w;\vec{k})[U_B(w)\tau(k_0-w+i\delta\tau)^{-1}\times U_B(w)]^{\alpha\beta} \tag{B9}$$

and

$$S^{\alpha\beta}(p)=\int dv\,\mathscr{S}(v;\vec{p})[U_F(v)(p_0-w+i\delta\tau)^{-1}U_F(v)]^{\alpha\beta}\ , \tag{B10}$$

where

$$U_B(w)=\begin{bmatrix}\cosh\theta(w) & \sinh\theta(w)\\ \sinh\theta(w) & \cosh\theta(w)\end{bmatrix} \tag{B11}$$

with

$$\sinh^2\theta(w)=\frac{1}{e^{\beta w}-1} \tag{B12}$$

and

$$U_F(v)=\begin{bmatrix}\cos\zeta(v) & \sin\zeta(v)\\ -\sin\zeta(v) & \cos\zeta(v)\end{bmatrix} \tag{B13}$$

with

$$\sin^2\zeta(v)=\frac{1}{e^{\beta v}+1}\ , \tag{B14}$$

while τ is a matrix operating on the thermal doublet

$$\tau=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\ . \tag{B15}$$

Using the integration formulas given in Ref. 34 we obtain

$$\Sigma^{\alpha\beta}(p)\equiv\frac{iI^2}{(2\pi)^4}\int d^4k\,\chi_{ij}^{\alpha\beta}(k)\sigma_i S^{\alpha\beta}(p-k)\sigma_j=\int d\kappa\,\rho(\kappa;\vec{p})[U_F(\kappa)(p_0-\kappa+i\delta\tau)^{-1}U_F(\kappa)]^{\alpha\beta} \tag{B16}$$

with

$$\rho(\kappa;\vec{p})=\frac{I^2}{(2\pi)^3}\int d^3k\int dw\,dv\,\rho_{ij}(w;\vec{k})\sigma_i\mathscr{S}(v;\vec{p}-\vec{k})\sigma_j\delta(\kappa-w-v)\frac{e^{\beta\kappa}+1}{(e^{\beta w}-1)(e^{\beta w}+1)}\ . \tag{B17}$$

If we now define the matrices $S(p)$ and $\Sigma(p)$ as

$$S(p)^{\alpha\beta}=[U_F(p_0)S(p)U_F^{\dagger}(p_0)]_{\alpha\beta} \tag{B18}$$

and

$$\Sigma(p)^{\alpha\beta}=[U_F(p_0)\Sigma(p)U_F^{\dagger}(p_0)]_{\alpha\beta}\ , \tag{B19}$$

then we can easily show that $S(p)$ and $\Sigma(p)$ 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.

Thus we obtain the result of Eqs. (3.14) and (3.15):

$$S^{-1}(p)=p_0-\epsilon(\vec{p})\tau_3+\Delta_0\tau_1+\mu\sigma_3-\Sigma(p) \tag{B20}$$

with

$$\Sigma(p)=\frac{I^2}{(2\pi)^3}\int d^3k\int dw\int dv\,\rho_{ij}(w;\vec{k})\sigma_i\mathscr{S}(v;\vec{p}-\vec{k})\sigma_j\frac{e^{\beta(v+w)}+1}{(e^{\beta w}-1)(e^{\beta v}+1)}\frac{1}{p_0-w-v+i\epsilon}\ . \tag{B21}$$

APPENDIX C: CONDENSATION ENERGY

The electronic contribution to the Hamiltonian was defined in Eq. (4.2) as

$$\mathscr{H}_{\rm el}=\psi^{\dagger}\epsilon(-i\vec{\nabla})\psi-V\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}\psi_{\downarrow}\psi_{\uparrow}-\tfrac{1}{2}\{I\vec{M}-g_J\mu_B\vec{B}\}\cdot\psi^{\dagger}\vec{\sigma}\psi\ . \tag{C1}$$

We define F_ϕ as

$$[i\partial_t-\epsilon(-i\vec{\nabla})\tau_3+\Delta\tau_1+\mu\sigma_3]\phi=F_\phi\ , \tag{C2}$$

where F_ϕ is given as

$$-F_\phi=\begin{bmatrix}V\psi_{\downarrow}^{\dagger}\psi_{\downarrow}\psi_{\uparrow}+(IM_3-g_J\mu_BB_3-\mu)\psi_{\uparrow}+2(IM_--g\mu_BB_-)\psi_{\downarrow}-\Delta\psi_{\downarrow}^{\dagger}\\ V\psi_{\uparrow}^{\dagger}\psi_{\uparrow}\psi_{\downarrow}-(IM_3-g_J\mu_BB_3-\mu)\psi_{\downarrow}+2(IM_+-g\mu_BB_+)\psi_{\uparrow}+\Delta\psi_{\uparrow}^{\dagger}\\ -V\psi_{\downarrow}^{\dagger}\psi_{\uparrow}^{\dagger}\psi_{\uparrow}+(IM_3-g_J\mu_BB_3-\mu)\psi_{\downarrow}^{\dagger}-2(IM_--g\mu_BB_-)\psi_{\uparrow}^{\dagger}-\Delta\psi_{\uparrow}\\ V\psi_{\uparrow}^{\dagger}\psi_{\downarrow}^{\dagger}\psi_{\downarrow}+(IM_3-g_J\mu_BB_3-\mu)\psi_{\uparrow}^{\dagger}+2(IM_+-g\mu_BB_+)\psi_{\downarrow}^{\dagger}-\Delta\psi_{\downarrow}\end{bmatrix}\ . \tag{C3}$$

With F_ϕ thus defined we may write the expression in (C1) as

$$\int d^3x\, \mathscr{H}_{\rm el} = V \int \frac{d^3k}{(2\pi)^3}(\epsilon+\mu) + \int d^3x\, \phi^\dagger[\epsilon(-i\nabla)\tau_3 - \Delta\tau_1 - \mu\sigma_3]\phi + \frac{\mu}{2}\int d^3x\, \phi^\dagger\sigma_3\phi + \frac{\Delta}{2}\int d^3x\, \phi^\dagger\tau_1\phi + \tfrac{1}{4}\int d^3x(\phi_1^\dagger F_{\phi_1} + \phi_2 F_{\phi_2}^\dagger - \phi_3 F_{\phi_3}^\dagger - \phi_4 F_{\phi_4}^\dagger) . \tag{C4}$$

Taking the thermal expectation value, we obtain

$$\frac{1}{V} d^3x \langle \mathscr{H}_{\rm el}\rangle = \int \frac{d^3k}{(2\pi)^3}(\epsilon+\mu) - \frac{i}{(2\pi)^4}\oint_+ d^4k\, {\rm Tr}\{S(k)[\epsilon(\vec{k}) - \Delta\tau_1 - \mu\sigma_3]\} + \tfrac{1}{2}\int d^3k\, {\rm Tr}[(\mu\sigma_3 + \Delta\tau_1)S(k)] + \frac{1}{2V}\int d^3x\, {\rm Re}\langle \phi F_\phi\rangle . \tag{C5}$$

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 B, then this term will not contribute since the self-energy and the counter terms Δ and μ will exactly cancel. The resultant expression for the self-energy is

$$\frac{1}{V}\int d^3x \langle \mathscr{H}_{\rm el}\rangle = \int \frac{d^3k}{(2\pi)^3}\Big\{ (\epsilon - E) + \frac{\Delta^2}{2E}[1 - f_F(E-\mu) - f_F(E+\mu)] + (E-\mu) f(E-\mu) - (E+\mu) f_F(E+\mu) + \frac{\mu}{2}[f_F(E-\mu) - f_F(E+\mu)]\Big\} , \tag{C6}$$

which is the result given in Eq. (4.8).

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