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Theory of the upper critical field of a magnetic superconductor

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We have derived a general set of microscopic equations for the upper critical field of a magnetic superconductor which is valid for any concentration of normal impurity scattering and includes fully the dynamics of the phonons and of the spin fluctuations. As spin correlations can be long range, we avoid, in our derivation, the usual contact approximation and get an expression which behaves properly near the magnetic transition. Numerical estimates for various possible values of the magnetic parameters reveal that, for some regimes, the dynamics of the spin diffusions can be important. In addition it is found, from general symmetry considerations, that singlet-triplet amplitude mixing can occur in dirty superconductors with large band-splitting effects due to internal magnetization.

I. INTRODUCTION

The effect of single magnetic ions on superconducting properties has been extensively studied and is now reasonably well understood. This is not the case for stoichiometric concentrations of magnetic moments, possibly because the discovery of systems exhibiting reentrant behavior is much more recent. Still, considerable information has now been accumulated in $HoMo_6S_6$ and even more in $ErRh_4B_4$. In particular, the critical magnetic field of single-crystal tetragonal $ErRh_4B_4$ samples has been measured by, among others, Crabtree *et al.*,[1] supplementing previous polycrystalline studies by Behroozi *et al.*[2,3] In the single-crystal case the magnetic properties are found to be highly anisotropic. Because the Er magnetic moments are confined, by crystal-field effects,[4] to the basal plane, the tetragonal c axis shows weak paramagnetism (hard axis) with a resulting temperature dependence of the upper critical magnetic field which is very similar in shape to that of ordinary superconductors, even near the reentrant temperature T_{c2}. Along the easy axis, with field in the plane of the magnetic moments, the situation is radically altered by the strong paramagnetism, and $H_{c2}(T)$ becomes bell shaped with a maximum around 5.5 K.

Maekawa and Tachiki[5] have given an early theory of the upper critical magnetic field of reentrant superconductors. Their theory applies only to the dirty limit and employs the same BCS approximations as in the original work of Werthamer, Helfand, and Hohnberg[6] for ordinary superconductors. Furthermore, it is assumed that the magnetic frequencies involved are large compared with T_c (the "high-frequency" limit) which is equivalent to a BCS assumption for the phonon part. Such an assumption leads to greatly simplified formulas and the theory reduces to conventional form with an "effective pairing potential" that contains a correction for the magnetic interactions. In such a theory the magnetic interaction part always grows sufficiently fast, as the temperature is lowered, that it overwhelms the BCS attraction before the magnetic temperature T_M is reached. The high-frequency limit for the magnetic interactions is not made in the subsequent work of Machida and Younger.[7] Instead, these authors consider the opposite case, namely, the static limit. This leads to a theory of the same form as a conventional BCS microscopic theory of H_{c2} for a system with independent Abrikosov-Gorkov magnetic impurities, with the difference that the effective spin-flip scattering time is now temperature dependent. Quite different results from those of Maekawa and Tachiki are obtained in this limit. Furthermore, it has been emphasized by Lee[8] that the static limit of Machida and Younger suffers from an unphysical divergence of the magnetic interaction at the magnetic transition temperature which would always lead to the zero-order parameter as this temperature is reached. The divergence can be traced to the mode of integration used in the magnetic part of the electron self-energy and can be removed when the energy dependence in the magnetic susceptibility is properly accounted for.

Of course, other theoretical works have appeared dealing with the magnetic properties of ferromagnetic superconductors and the reader is referred to the review of Umezawa, Matsumoto, and Whitehead.[9] These authors adopt a somewhat different approach to the problem than that of Maekawa and Tachiki and of Machida and Younger and discuss extensions of these works. In particular, they consider in some detail a specific application of the theory to the H_{c2} data observed in single-crystal $ErRh_4B_4$ in which the electron band-splitting effect of the internal magnetic fields plays a prominent role (see also Sakai *et al.*[10]). While good agreement with experiment can be obtained in these theories with reasonable magnetic parameters, it should be noted that the proper dynamic nature of the spin fluctuations is not account for. Coffey, Levin, and Grest[11] have considered such effects in their work in the quasiparticle density of states of a reentrant superconductor and have stressed their importance. While the phonon part of the problem is handled in a BCS formalism, these authors treat fully, within an Eliashberg formalism, the dynamics of the spin fluctuations and no "high-" or "low-" frequency limit is taken. In addition, their hydrodynamic model for the dynamic spin susceptibility is properly constrained through a fit parameter to satisfy the susceptibility sum rule. As an example of the importance of such more sophisticated calculations, Coffey *et al.* conclude, among other things, that the high-frequency limit can greatly overestimate the effect of magnetism on the critical temperature and, by implication also, on other properties. A complementary work which deals only with the critical temperature but which uses an Eliashberg formalism in a form that follows the original work of Rainer[12] and also imposes the appropriate sum rule on the dynamic susceptibility, is that of Dupont *et al.*[13] These authors find that for a significant range of magnetic parameters, dynamic calculation gave results for the reentrant curve that are not very different from the static-limit results, concluding that a low-frequency approximation is better than a high-frequency approximation.

In this paper we develop a theory of the upper critical magnetic field of magnetic superconductors which follows closely the microscopic approach of Machida and Younger but which includes several generalizations and extensions as well as avoids many of their approximations. Rather than base our work on the BCS-type theory of H_{c2} given by Werthamer *et al.*,[6] we start from the theory given recently by Schossmann and Schachinger.[14] While this work considers only the electron-phonon interaction and no magnetic interaction, it derives equations for H_{c2} that fully account for strong-coupling effects. Here, an additional magnetic self-energy part involving the dynamic susceptibility is introduced and the generalized strong-coupling equations derived. They are not restricted to the dirty limit but apply to any impurity concentration. As in the previous work of Rainer *et al.*[15] we find that our generalized equations, couple, in principle, singlet to triplet states asymmetric in frequency and not in momentum.[16] Detailed numerical calculations of the importance of such effects are given including the importance of band splitting by the internal magnetic field, the dynamics of spin fluctuations and of the electron-phonon interaction itself, and the effect of finite concentrations of impurities.

This paper is structured into several parts. In Sec. II we describe our derivations of equations for the upper critical field H_{c2} which involve major extensions of the work of Helfand and Werthamer.[17] The original formalism is extended to include strong-coupling effects both for the phonon and for the spin fluctuations and also to treat accurately the long-range nature of the magnetic interaction. For the spin fluctuations themselves we use a hydrodynamic model along the lines described by Bennett and Martin[18] and Halperin and Hohenberg[19] but extended to include the effect of the magnetic field. The details are found in Sec. III. We restrict ourselves to weak magnetic fields in the sense that only linear effects are considered and therefore stay away from the saturation regime. In Sec. IV we present simplifications of our general formulas and give extensive numerical results, which can be divided into two broad categories. In the first set of results we ignore the effect of band splitting by the internal magnetic field and study the effect of spin fluctuation on H_{c2} comparing full dynamical results to static-limit results for a large range of magnetic parameters. We find that the importance of dynamics depends strongly on the size of the correlation length for the spin system. In the second set of results we consider only the band-splitting effects. It is shown that the matrix structure of the equations requires a mixing of some antiparallel spin states with parallel spin states, which has the effect of decreasing H_{c2} more than would be the case when such mixing is ignored. In addition, it is found that the mixing is increased when normal impurity scattering is taken into account.

II. FORMAL DEVELOPMENT

The Green's function of a superconductor is determined by the series

$$\hat{G}=\hat{G}_0+\hat{G}_0\sum_{n=1}^{\infty}(\hat{\Sigma}\hat{G}_0)^n , \tag{2.1}$$

where $\hat{G}$, $\hat{G}_0$, and $\hat{\Sigma}$ are 4×4 matrices in Nambu formalism and are, respectively, the interacting and noninteracting Green's function and the self-energy $\hat{\Sigma}$.

The self-energy consists of three parts. The first is due to the electron-phonon interaction

$$\hat{\Sigma}_{e\text{-ph}}(\mathbf{y},\mathbf{z},\omega_n)=-T\sum_m \tau_3\sigma_0\hat{G}(\mathbf{y},\mathbf{z},\omega_m) \times\tau_3\sigma_0 g^2 D(\mathbf{y}-\mathbf{z},\omega_n-\omega_m) , \tag{2.2}$$

with T the temperature, D the phonon Green's function, and g the electron-phonon coupling. In (2.2), ω_n is a Matsubara frequency. The localized spin part is

$$\hat{\Sigma}_s(\mathbf{y},\mathbf{z},\omega_n) =j_{fd}\{\tau\sigma\}^a\langle\mathbf{S}\rangle^a-T\sum_m\{\tau\sigma\}^a\hat{G}(\mathbf{y},\mathbf{z},\omega_m)\{\tau\sigma\}^b\chi^{ab} \times(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})j_{fd}^2 , \tag{2.3}$$

with χ the susceptibility, j_{fd} the magnetic electron exchange constant, and $\langle\mathbf{S}\rangle$ the average internal spin polarization. Finally, the non-spin-flip impurities give

$$\hat{\Sigma}_I(\mathbf{y},\mathbf{z},\omega_n)=-\frac{1}{2\pi\tau_{\text{imp}}}\tau_3\sigma_0\hat{G}(\mathbf{y}-\mathbf{z},\omega_n)\tau_3\sigma_0\delta(\mathbf{y}-\mathbf{z}) . \tag{2.4}$$

τ is the lifetime of electrons which results from the scattering potential:

$$\frac{1}{\tau_{\text{imp}}}=2\pi n_I N(0)\int\frac{d\Omega_{(k_{F'})}}{4\pi}\,|V(k_F,k_{F'})|^2 . \tag{2.5}$$

n_I is the concentration of impurities and $N(0)$ the density of states on the Fermi surface.

τ_i and σ_i, $i=1,2,3$ are two sets of Pauli matrices and τ_0 as well as σ_0 are unit matrices. We define the "vector" matrix $\{\tau\sigma\}$,

$$\{\tau\sigma\}^a=(\tau_3\sigma_1,\tau_0\sigma_2,\tau_3\sigma_3) . \tag{2.6}$$

The electron-electron interaction mediated via phonons is assumed to be very short ranged and is therefore always approximated by a δ-function model

$$D(\omega_n-\omega_m,\mathbf{x}-\mathbf{x}')\approx D(\omega_n-\omega_m)\delta(\mathbf{x}-\mathbf{x}') \,. \tag{2.7}$$

In general, this is not the case for the spin part of the interaction which is described by $\chi^{ab}(\omega_n-\omega_m,\mathbf{x}-\mathbf{x}')$. In our homogeneous magnetic field parallel to the z axis this matrix has the form

$$\chi^{ab}=\begin{bmatrix}\chi^{11} & \chi^{12} & 0\\ \chi^{21} & \chi^{22} & 0\\ 0 & 0 & \chi^{33}\end{bmatrix} , \tag{2.8}$$

where $\chi^{21}=-\chi^{12}$ vanishes in the limit $H=0$.

For small stationary fields we adopt a hydrodynamic model for the spin diffusion which is described in more detail in Sec. III:

$$\chi^{11}(\mathbf{k},\omega_n)=\chi^{22}(\mathbf{k},\omega_n)=\chi^{33}(\mathbf{k},\omega_n)$$

$$=-\frac{\pi Dk^2\chi(k)}{\omega_n^2\tau_M+|\omega_n|+Dk^2} , \tag{2.9}$$

$$\chi^{12}(\mathbf{k},\omega_n)=-\chi^{21}(\mathbf{k},\omega_n)$$

$$=-B[\chi(\mathbf{k})-\chi(0)]\frac{\omega_n\tau_M+\mathrm{sgn}\omega_n}{\omega_n^2\tau_M+|\omega_n|+Dk^2} , \tag{2.10}$$

$$D=\frac{c}{\chi(\mathbf{q})} , \tag{2.11}$$

$$\chi(\mathbf{q})=\frac{1}{3}\frac{S(S+1)}{T-T_m+\xi_0^2q^2} . \tag{2.12}$$

$\chi(\mathbf{q})$ is the static susceptibility and ξ_0 a correlation length for the spin diffusion. The magnetic relaxation time τ and the constants c are not independent but have to be chosen to satisfy the sum rule

$$\int_{V_B}\frac{d^3q}{(2\pi)^3}\int_{-\infty}^{\infty}d\omega\frac{2\,\mathrm{tr}[\mathbf{B}(\mathbf{q},\omega)]}{1-e^{-\beta\omega}}=2\pi S(S+1)\int_{V_B}\frac{d^3\mathbf{q}}{(2\pi)^3} . \tag{2.13}$$

Here, V_B is the volume of the Brillouin zone and $\mathbf{B}$ is the spectral density for the spin fluctuations, namely,

$$\chi^{ab}(\omega_n,\mathbf{q})=\int dz\frac{B^{ab}(\mathbf{q},z)}{i\omega_n-z} , \tag{2.14}$$

which is also given in Sec. III.

For the upper critical magnetic field it is sufficient to neglect all off-diagonal terms in the perturbation series (1) which use higher than first order. In this case the diagonal part describes the normal state and is not affected by Cooper pair creation:

$$\hat{G}_n=\hat{G}_d=\begin{bmatrix}G_{\alpha\beta} & 0\\ 0 & G_{\alpha\beta}\end{bmatrix}=\hat{G}_0+\hat{G}_0\Sigma_d\hat{G}_n . \tag{2.15}$$

For the off-diagonal part, all the remaining terms can be combined to give

$$\hat{G}_{of}=\hat{G}_n\hat{\Sigma}_{of}\hat{G}_n . \tag{2.16}$$

As described by Helfand and Werthamer[17] the space dependence of the Green's function in a weak magnetic field results in the form

$$G_n(x,x',\tau,\tau')=G_n(x,x',\tau,\tau')\,|_{H=0}\exp\left[-i\frac{e}{c}\int_x^{x'}\mathbf{A}\cdot d\mathbf{s}\right] , \tag{2.17}$$

where $\mathbf{A}(x)$ is the vector potential. In the case of no magnetic field, Eq. (2.15) becomes translationally invariant and can be solved in momentum space with the ansatz

$$\begin{aligned}\hat{G}_n(\omega_n,k)&=[i\tilde{\omega}_n\tau_0\sigma_0-\epsilon\tau_3\sigma_0-b\tau_3\sigma_3]^{-1}\\ &=\frac{i}{2}\left[\frac{\tilde{\omega}_n-ib}{(\tilde{\omega}-ib)^2+\epsilon^2}+\frac{\tilde{\omega}_n+ib}{(\tilde{\omega}+ib)^2+\epsilon^2}\right]\tau_0\sigma_0+\frac{1}{2}\left[\frac{\epsilon}{(\tilde{\omega}_n-ib)^2+\epsilon^2}-\frac{\epsilon}{(\tilde{\omega}_n+ib)^2+\epsilon^2}\right]\tau_0\sigma_3\\ &\quad-\frac{1}{2}\left[\frac{\epsilon}{(\tilde{\omega}_n-ib)^2+\epsilon^2}+\frac{\epsilon}{(\tilde{\omega}_n+ib)^2+\epsilon^2}\right]\tau_3\sigma_0+\frac{i}{2}\left[\frac{\tilde{\omega}-ib}{(\tilde{\omega}_n-ib)^2+\epsilon^2}-\frac{\tilde{\omega}-ib}{(\tilde{\omega}_n+ib)^2+\epsilon^2}\right]\tau_3\sigma_3 .\end{aligned} \tag{2.18}$$

The state is assumed to be isotropic. It is also assumed that the self-energy does not vary very much in the region of the Fermi surface so that it can be evaluated right on the Fermi level, i.e., at k_F. The self-energy caused by spin diffusion can be written in the form

$$\Sigma_{SW,d}(\mathbf{k}_F,\omega_n)=-T\sum_m\int N(\epsilon')d\epsilon'\{\tau\sigma\}^aG_n(\epsilon',\omega_n)\{\tau\sigma\}^b\int\frac{d^2S'}{v_k'}j_{fd}^2\chi_{su}^{ab}(\mathbf{k}_F-\mathbf{k}',\omega_n-\omega_m) . \tag{2.19}$$

In (2.19), $N(\epsilon)$ is the density of states, dS' a constant energy surface average, and $v_{k'}$ the Fermi velocity. With the form of the spin fluctuations χ^{ab} given in (2.9) and (2.10), the integration over angle in (2.19) only gives functions which are symmetric with respect to ϵ' and so all parts of G_n antisymmetric in ϵ' can be neglected. Therefore only these parts of the Green's function (2.18) which are proportional to $\tau_0\sigma_0$ and $\tau_3\sigma_3$ give contributions to the integral in (2.19). These two parts can be expressed by the real and imaginary parts of the newly defined function

$$\lambda_{SW}^{ab}(\omega_n,\omega_m)=-\int\frac{d^3k'}{(2\pi)^3}\frac{(\tilde{\omega}_m+ib)\mathrm{sgn}\omega_m}{\pi[(\tilde{\omega}_m+ib)^2+\epsilon^2(k')]}j_{fd}^2\chi^{ab}(\omega_n-\omega_m,\mathbf{k}_F-\mathbf{k}') . \tag{2.20}$$

As already mentioned, the interaction length of the phonons is so small that its momentum dependence can be neglected. This part can be treated in the usual way by using the function

$$\lambda_{e\text{-ph}}(\omega_n-\omega_m)=\frac{1}{N(0)}\int_0^\infty d\Omega\frac{2\Omega}{\Omega^2+(\omega_n-\omega_m)^2}\alpha^2F(\Omega)\ , \tag{2.21}$$

where the Eliashberg function

$$\alpha^2F(\Omega)=\frac{\int(d^2S/v_F)\int(d^2S'/v_F)\,|g(\mathbf{k},\mathbf{k}')|^2B(\Omega,\mathbf{k}_F-\mathbf{k}_{F'})}{\int(d^2S/v_{F'})} \tag{2.22}$$

has been introduced.

Finally, the impurity part of the self-energy can be treated in a similar way. By inserting the self-energy into the inverted form of Eq. (2.15) and by comparing the coefficients of $\tau_0\sigma_0$ and $\tau_3\sigma_3$, the following two equations result:

$$\tilde{\omega}_n=\omega_n+\pi T\sum_m\{\lambda_{e\text{-ph}}(\omega_n-\omega_m)+\mathrm{Re}\,tr[\boldsymbol{\lambda}_{SW}(\omega_n,\omega_m)]+2\,\mathrm{Im}\lambda_{SW}^{12}(\omega_n,\omega_m)\}\mathrm{sgn}\omega_m+\frac{1}{\tau_{\mathrm{imp}}}\mathrm{sgn}\omega_n\ , \tag{2.23}$$

$$b=-\pi T\sum_m\{\mathrm{Im}[\lambda^{11}(\omega_n,\omega_m)+\lambda^{22}(\omega_n,\omega_m)-\lambda^{33}(\omega_n,\omega_m)]-2\,\mathrm{Re}[\lambda^{12}(\omega_n,\omega_m)]\}\mathrm{sgn}\omega_m-j_{df}\langle\mathbf{S}\rangle_3\ . \tag{2.24}$$

In order to simplify all further calculations, we choose, for the off-diagonal matrix, the ansatz

$$\hat{G}_{of}(\mathbf{x},\mathbf{x}',\omega_n)=F_S(\mathbf{x},\mathbf{x}',\omega_n)\tau_2\sigma_2-iF_t(\mathbf{x},\mathbf{x}',\omega_n)\tau_1\sigma_1\ , \tag{2.25}$$

with F_s and F_t real functions. The triplet amplitude F_t is not new and can already be found in the work of Rainer *t al.*[15] It differs from the triplet pairing discussed by Fenton and Psaltakis.[16] Their work deals with a triplet pair amplitude asymmetric in momentum space, while ours is asymmetric in frequency as in the case of Rainer *et al.*[15]

The matrix of the normal-state Green's function (2.18) is of a form that only the diagonal elements are nonzero and therefore it is easy to calculate explicitly each part of the matrix $\hat{G}_{\mathrm{eff}}$. The equation for G_{14} is

$$\begin{aligned}F_S(\mathbf{x},\mathbf{x}',\omega_n)&+iF_t(\mathbf{x},\mathbf{x}',\omega_n)\\&=\int d^3y\int d^3z\,G_{11}(\mathbf{x},\mathbf{y},\omega_n)\Bigg[T\sum_m\{[F_S(\mathbf{y},\mathbf{z},\omega_m)+iF_t(\mathbf{y},\mathbf{z},\omega_m)][g^2D_{e\text{-ph}}(\omega_n-\omega_m)\delta(\mathbf{y}-\mathbf{z})-j_{fd}^2\chi^{33}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\\&\qquad-[F_S(\mathbf{y},\mathbf{z},\omega_m)-iF_t(\mathbf{y},\mathbf{z},\omega_m)]j_{fd}^2\\&\qquad\times[\chi^{11}(\omega_n-\omega_m,\mathbf{y},\mathbf{z})+\chi^{22}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})+2i\chi^{12}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\}\\&\qquad+\frac{1}{2\pi\tau_{\mathrm{imp}}}[F_S(\mathbf{y},\mathbf{z},\omega_n)+iF_t(\mathbf{y},\mathbf{z},\omega_n)]\Bigg]G_{44}(\mathbf{z},\mathbf{x}',\omega_n)\ ,\end{aligned} \tag{2.26}$$

and for G_{23} is

$$\begin{aligned}F_S(\mathbf{x},\mathbf{x}',\omega_n)&-iF_t(\mathbf{x},\mathbf{x}',\omega_n)\\&=\int d^3y\int d^3z\,G_{22}(\mathbf{x},\mathbf{y},\omega_n)\\&\quad\times\Bigg[T\sum_m[F_S(\mathbf{y},\mathbf{z},\omega_m)-iF_t(\mathbf{y},\mathbf{z},\omega_m)][g^2D_{e\text{-ph}}(\omega_n-\omega_m)\delta(\mathbf{y}-\mathbf{z})-j_{fd}^2\chi^{33}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\\&\quad-[F_S(\mathbf{y},\mathbf{z},\omega_n)+iF_t(\mathbf{y},\mathbf{z},\omega_m)]j_{fd}^2[\chi^{11}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})+\chi^{22}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})-2i\chi^{12}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\\&\quad+\frac{1}{2\pi\tau_{\mathrm{imp}}}[F_S(\mathbf{y},\mathbf{z},\omega_n)-iF_t(\mathbf{y},\mathbf{z},\omega_n)]\Bigg]G_{33}(\mathbf{z},\mathbf{x}',\omega_n)\ .\end{aligned} \tag{2.27}$$

The equations for G_{32} and G_{41} are only the complex conjugate forms of G_{23} and G_{14}.

It is not possible to apply the method of Helfand and Werthamer[17] in a straightforward way to the spin fluctuations χ^{ab} because they are not necessarily short ranged enough to be approximated by a δ-function model. This is in contrast to the short-range-phonon exchange case for which the eigenstate of the Cooper pairs with the lowest eigenvalue has the form

$$F(\mathbf{x},\mathbf{x},\omega_n)=e^{-\alpha|\mathbf{x}_L|^2}f(\omega_n)\ , \tag{2.28}$$

where $\alpha=eH/m$ and $\mathbf{x}_L$ means the component orthogonal to the magnetic field. This is a Gaussian function which becomes a constant in the limit of $H=0$ and it tells us the behavior of the two-point function $\mathbf{F}(\mathbf{x},\mathbf{x}',\omega_n)$ in the limit $\mathbf{x}\rightarrow\mathbf{x}'$. In this case, the behavior of this function for $\mathbf{x}\neq\mathbf{x}'$ is not important for estimating H_{c2}. However, we know that for $H=0$, $F(\mathbf{k},\omega_n)$ is of the form

$$F(\mathbf{k},\omega_n)=\frac{\Delta}{\omega_n^2+\epsilon^2+\Delta^2}\ , \tag{2.29}$$

which is very easy to transform into an $\mathbf{x}$-space representation. Neglecting all Δ terms of higher than first order, $F(\mathbf{x},\mathbf{x}',\omega_n)$ is proportional to

$$F(\mathbf{x},\mathbf{x}',\omega_n)\sim\frac{k_F^2}{v_F}\Delta\exp\left[-\frac{|\omega_n|}{v_F}|\mathbf{x}-\mathbf{x}'|\right]\times\frac{\sin(k_F|\mathbf{x}-\mathbf{x}'|)}{k_F|\mathbf{x}-\mathbf{x}'|}\ . \tag{2.30}$$

This is a fast oscillating function and these oscillations can be of importance when spin diffusion is included in the theory, as shown by other authors.

In order to construct a method of solving Eqs. (2.21) and (2.22), we assume that the electron-electron interactions are only important for determining the first oscillating behavior of the Green's function with respect to variations $\Delta\mathbf{x}=\mathbf{x}-\mathbf{x}'$ and this should not be changed significantly by a weak magnetic field. The magnetic field itself only determines the shape of the function $F(\mathbf{x},\mathbf{x}',\omega_n)$ on a scale very large compared to k_F^{-1}. We assume therefore that these two influences can be accounted for approximately by the product ansatz

$$F_{S,t}(\mathbf{x},\mathbf{x}',\omega_n)\approx\phi(\mathbf{x})F_{S,t}(\mathbf{x}-\mathbf{x}',\omega_n)\ , \tag{2.31}$$

where $\phi(x)$ describes the slow varying behavior in a magnetic field and rewrite (2.21) and (2.22) in such a way that the influence of the magnetic field is completely separated in these equations from the influence of the Lagrange electron-electron interaction. Equation (2.21) reduces to

$$\begin{aligned}\phi(\mathbf{x})[F_S(\mathbf{x}-\mathbf{x}',\omega_n)+iF_t(\mathbf{x}-\mathbf{x}',\omega_n)]&=\int d^3y'\,G_{11}(\mathbf{x},\mathbf{y}',\omega_n)\phi(\mathbf{y}',\omega_n)G_{44}(\mathbf{y}',\mathbf{x},\omega_n)\\&\quad\times\frac{1}{N}\int d^3y\int d^3z\,G_{11}(\mathbf{x}-\mathbf{y},\omega_n)|_{H=0}\\&\quad\times\left[T\sum_m\{[F_S(\mathbf{y}-\mathbf{z},\omega_m)+iF_t(\mathbf{y}-\mathbf{z},\omega_m)][g^2D_{e\text{-ph}}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})-j_{fd}^2\chi^{33}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\right.\\&\quad\quad-[F_S(\mathbf{y}-\mathbf{z},\omega_m)-iF_t(\mathbf{y}-\mathbf{z},\omega_m)]j_{pd}^2\\&\quad\quad\times[\chi^{11}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})+\chi^{22}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})-2i\chi^{12}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\}\\&\quad\left.+\frac{1}{2\pi\tau_{\text{imp}}}[F_S(\mathbf{y}-\mathbf{z},\omega_n)+iF_t(\mathbf{y}-\mathbf{z},\omega_n)]\right]G_{44}(\mathbf{x}-\mathbf{y},\omega_n)|_{H=0}\ ,\end{aligned} \tag{2.32}$$

and (2.22) becomes

$$\begin{aligned}\phi(\mathbf{x})[F_S(\mathbf{x}-\mathbf{x}',\omega_n)-iF_t(\mathbf{x}-\mathbf{x}',\omega_n)]&=\int d^3y'\,G_{22}(\mathbf{x},\mathbf{y}',\omega_n)\phi(\mathbf{y}',\omega_n)G_{33}(\mathbf{y}',\mathbf{x},\omega_n)\\&\quad\times\frac{1}{N}\int d^3y\int d^3z\,G_{22}(\mathbf{x}-\mathbf{y},\omega_n)|_{H=0}\\&\quad\times\left[T\sum_m\{[F_S(\mathbf{y}-\mathbf{z},\omega_n)-iF_t(\mathbf{y}-\mathbf{z},\omega_m)][g^2D_{e\text{-ph}}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})-j_{fd}^2\chi^{33}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\right.\\&\quad\quad-[F_S(\mathbf{y}-\mathbf{z},\omega_m)+iF_t(\mathbf{y}-\mathbf{z},\omega_m)]j_{fd}^2\\&\quad\quad\times[\chi^{11}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})+\chi^{22}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})-2i\chi^{12}(\omega_n-\omega_m,\mathbf{y}-\mathbf{z})]\}\\&\quad\left.+\frac{1}{2\pi\tau_{\text{imp}}}[F_S(\mathbf{y}-\mathbf{z},\omega_n)-iF_t(\mathbf{y}-\mathbf{z},\omega_n)]\right]G_{33}(\mathbf{x}-\mathbf{y},\omega_n)|_{H=0}\ .\end{aligned} \tag{2.33}$$

The normalization factor $1/N$ is necessary to provide the proper limits for $H=0$. The advantage of this step is that the $F(\mathbf{x}-\mathbf{x}')$ part has become translationally invariant and can easily be transformed into momentum space. The integration acting on $\phi(\mathbf{x})$ is the same as in the theory of Werthamer, Helfand, and Hohnberg and it can be replaced by the eigenstate with the lowest eigenvalue:

$$\int d^3y\, G_{11}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})G_{44}(\mathbf{y},\mathbf{x})=-\alpha(\omega_n)\phi(\mathbf{x}) , \tag{2.34}$$

$$\int d^3y\, G_{22}(\mathbf{x},\mathbf{y})\phi(\mathbf{y})G_{33}(\mathbf{y},\mathbf{x})=-\alpha^*(\omega_n)\phi(\mathbf{x}) , \tag{2.35}$$

$$\alpha(\omega_n)=2\pi N(0)\frac{1}{\sqrt{x}}\int_0^\infty dq\, e^{-q^2}\tan^{-1}\left[\frac{x^{1/2}q}{(\tilde{\omega}_n+ib)\mathrm{sgn}\omega_n}\right] , \tag{2.36}$$

$$x=eB_{c2}v_F^2 . \tag{2.37}$$

It remains to discuss the equations for F_S and F_t. Equation (2.27) is now

$$\begin{aligned}F_S(\mathbf{k},\omega_n)+iF_t(\mathbf{k},\omega_n)=&-\frac{\alpha(\omega_n)}{N}[G_{11}(\mathbf{k},\omega_n)G_{44}(\mathbf{k},\omega_n)]\,|_{H=0}\\ &*\int\frac{d^3k'}{(2\pi)^3}\left[\sum_m\{[F_S(\mathbf{k}',\omega_m)+iF_t(\mathbf{k}',\omega_m)][g^2(\mathbf{k},\mathbf{k}')D_{e\text{-ph}}(\omega_n-\omega_m)-j_{fd}^2\chi^{33}(\omega_n-\omega_m,\mathbf{k}-\mathbf{k}')]\right.\\ &\qquad-[F_S(\mathbf{k}',\omega_m)-iF_t(\mathbf{k}',\omega_m)]j_{fd}^2\\ &\qquad\times[\chi^{11}(\omega_n-\omega_m,\mathbf{k}-\mathbf{k}')+\chi^{22}(\omega_n-\omega_m,\mathbf{k}-\mathbf{k}')+2i\chi^{12}(\omega_n-\omega_m,\mathbf{k}-\mathbf{k}')]\}\\ &\left.\qquad+\frac{1}{2\pi\tau_{\mathrm{imp}}}[F_S(\mathbf{k}',\omega_n)+iF_t(\mathbf{k}',\omega_n)]\right] .\end{aligned} \tag{2.38}$$

It is easy to see that with the form (2.15) the condition

$$G_{11}(\mathbf{k},\omega_n)G_{44}(\mathbf{k},\omega_n)\,|_{H=0}=G_{22}^*(\mathbf{k},\omega_n)G_{33}^*(\mathbf{k},\omega_n)\,|_{H=0} \tag{2.39}$$

is satisfied. Therefore, Eq. (2.33) transforms in the same way as (2.32) and the complex conjugate form of (2.38) results. This proves that the ansatz (2.25) is correct and that further considerations can be restricted to (2.38).

F_S and F_t can now be regarded as off-diagonal parts of the Green's function without magnetic field. For a linearized theory we make an ansatz for the Green's function of the form

$$G(k,\omega_n)=[G_n^{-1}(k,\omega_n)-\Delta_S(\omega_n)\tau_2\tau_2+i\Delta_t(\omega_n)\tau_1\sigma_1]^{-1} . \tag{2.40}$$

According to the Dyson equation the gap functions $\Delta_{s,t}$ are proportional to the self-energy. For these we always take averages over the momentum right on the Fermi surface and this is the reason why the gaps are not functions of the momentum. With the form (2.18) for G_n and by explicit insertion in (2.38) the ansatz is

$$\begin{aligned}F_S(\mathbf{k},\omega_n)&+iF_t(\mathbf{k},\omega_n)\\ &=[\Delta_S(\omega_n)+i\Delta_t(\omega_n)]G_{11}(\mathbf{k},\omega_n)G_{44}(\mathbf{k},\omega_n) .\end{aligned} \tag{2.41}$$

If (2.41) is inserted in (2.38) the integration over momentum is of a form expressible by (2.20) and (2.21)

$$\begin{aligned}\Delta_S(\omega_n)+i\Delta_t(\omega_n)=\frac{\alpha(\omega_n)}{N}\Bigg[T\sum_m\Bigg\{&\frac{\Delta_S(\omega_m)+i\Delta_t(\omega_m)}{(\tilde{\omega}_m+ib)\mathrm{sgn}\omega_n}[\lambda_{e\text{-ph}}(\omega_n-\omega_m)-\lambda_{SW}^{33}(\omega_n,\omega_m)]\\ &+\frac{\Delta_S(\omega_m)-i\Delta_t(\omega_m)}{(\tilde{\omega}_m-ib)\mathrm{sgn}\omega_m}[\lambda_{SW}^{*11}(\omega_n,\omega_m)+\lambda_{SW}^{*22}(\omega_n,\omega_m)-2i\lambda_{SW}^{*12}(\omega_n,\omega_m)]\Bigg\}\\ &+\frac{1}{2\pi\tau_{\mathrm{imp}}}\frac{\Delta_S(\omega_n)+i\Delta_t(\omega_n)}{(\tilde{\omega}_n+ib)\mathrm{sgn}\omega_n}\Bigg] .\end{aligned} \tag{2.42}$$

For (2.42) one has to take care that $F_S(\mathbf{k},\omega_n)-iF_t(\mathbf{k},\omega_n)$ is replaced by the complex conjugate form of (2.41). Finally, we have to choose the right factor N, which is done by postulating the limit

$$\lim_{H\to 0}\frac{\alpha(\omega_n)}{N}=1 , \tag{2.43}$$

which means

$$N=\frac{\pi N(0)}{(\tilde{\omega}_n+ib)\mathrm{sgn}\omega_n} . \quad (2.44)$$

With (2.43) inserted in (2.42), one recovers the correct T_c equation, which is in agreement with other authors.[8,13] For convenience we make the replacement

$$\Delta_S(\omega_n)+i\Delta_t(\omega_n)=\frac{\alpha(\omega_n)}{N(0)}(\tilde{\omega}_n+ib)\mathrm{sgn}\omega_n[\bar{\Delta}_S(\omega_n)+i\bar{\Delta}_t(\omega_n)] \quad (2.45)$$

and analogous for its complex conjugate. The equation becomes

$$\begin{aligned}\bar{\Delta}_S(\omega_n)+i\bar{\Delta}_t(\omega_n)=\pi T\sum_m \Bigg\{ &\frac{\alpha(\omega_m)}{N(0)}[\bar{\Delta}_S(\omega_m)+i\bar{\Delta}_t(\omega_m)][\lambda_{e\text{-ph}}(\omega_n-\omega_m)-\lambda^{33}(\omega_n,\omega_m)-\mu^*]\\ &-\frac{\alpha^*(\omega_m)}{N(0)}[\bar{\Delta}_S(\omega_m)-i\bar{\Delta}_t(\omega_m)][\lambda_{SW}^{*11}(\omega_n,\omega_m)+\lambda_{SW}^{*22}(\omega_n,\omega_m)-2i\lambda_{SW}^{*12}(\omega_n,\omega_m)]\Bigg\}\\ &+\frac{1}{2\pi\tau_{\mathrm{imp}}}\frac{\alpha(\omega_n)}{N(0)}[\bar{\Delta}_S(\omega_n)+i\bar{\Delta}_t(\omega_n)] . \end{aligned} \quad (2.46)$$

In (2.46) the additional factor of μ^* has been introduced to describe the Coulomb pseudopotential. This result gives, together with (2.23) and (2.24), and a closed set of equations.

III. SPIN DIFFUSION IN A HOMOGENEOUS MAGNETIC FIELD

We need the spin-diffusion propagator of a ferromagnet when a homogeneous magnetic field is applied. This propagator has already been investigated by several other authors[18,19] in the zero-magnetic-field limit and we extend their results using a hydrodynamic model.

The change in the local spin by the diffusion process is described by

$$\frac{\partial S_{\mathrm{diff}}}{\partial t}=D\nabla^2 S^i , \quad (3.1)$$

where D is the diffusion coefficient. The influence of magnetic fields on the motion of spins is easily derived from the quantum-mechanical single-spin equation

$$\frac{1}{i}\frac{\partial S^i}{\partial t}=[\hat{H},S^i] , \quad (3.2)$$

$$\hat{H}=-\mu_B S^i[B_0^i+B^i(\sigma)] . \quad (3.3)$$

B_0^i is the constant homogeneous field and $B^i(\sigma)$ an additional perturbation from which the susceptibility will be derived. The S^i are operators which obey the usual commutation laws of angular momentum. Equations (3.2) and (3.3) together result in the equation of motion

$$\frac{\partial S^i}{\partial t}=\mu_B\epsilon_{ijk}S^j[B_0^k+B^k(t)] . \quad (3.4)$$

The spin operators are composed of two parts

$$S^i(t)=\langle S^i\rangle+\delta S^i(t) , \quad (3.5)$$

$$\langle S^i\rangle=\chi(0)B^i , \quad (3.6)$$

where S^i describes the average polarization of the spins in the homogeneous magnetic field. We regard $\delta S^i(t)$ and $H^i(t)$ to be weak perturbations and find the linearized equation

$$\left.\left[\frac{\partial S^i}{\partial t}\right]\right|_{H_0}=\mu_B\epsilon_{ijk}[\delta S^i(t)B_0^k+\langle S^j\rangle B^k(t)] , \quad (3.7)$$

which describes the additional influence of a homogeneous magnetic field. Finally, we get the change of the spin in an alternating magnetic field by

$$\left.\left[\frac{\partial S^i}{\partial t}\right]\right|_{SUS}=\chi\frac{\partial B^i}{\partial t} . \quad (3.8)$$

The complete change with time of the spin is given by the sum of all these influences (3.1), (3.7), and (3.8),

$$\frac{\partial S^i}{\partial t}=D\nabla^2 S^i+\mu_B\epsilon_{ijk}[S^jB_0^k+\langle S^j\rangle B^k(t)]+\chi\frac{\partial B^i(k)}{\partial t} . \quad (3.9)$$

In momentum and frequency representation this is

$$\begin{aligned}[(i\omega+Dq^2)\delta_{i,k}+\mu_B\epsilon_{ijk}B_0^j]S^k(\omega,\mathbf{q})\\ =\mu_B\epsilon_{ijk}\langle S^j\rangle B^k(\omega,\mathbf{q})+\omega\chi(q)B^i(\omega,\mathbf{q}) . \end{aligned} \quad (3.10)$$

The matrix acting on $S^k(\omega,\mathbf{q})$ can be inverted and multiplying (3.10) with

$$(i\omega+Dq^2)\delta_{ij}+\mu_B\epsilon_{ijk}B_0^k-\frac{\mu_B^2}{i\omega+Dq^2}B_0^iB_0^j , \quad (3.11)$$

we get the form

$$S^i(\omega,\mathbf{q})=\chi^{ij}(\omega,\mathbf{q})B^j(\omega,\mathbf{q}) , \quad (3.12)$$

where the dynamic susceptibility is

$$\chi^{ij}(\omega,\mathbf{q})=\frac{[(i\omega+Dq^2)\chi(0)-\chi(\mathbf{q})]\mu_B B_0\epsilon_{ijk}+[(i\omega+Dq^2)\chi(\mathbf{q})+\mu_B^2\chi(0)B_0^2]\delta_{ij}-\mu_B^2\chi(0)B_0^iB_0^j}{(i\omega+Dq^2)^2-\mu_B^2\,|\,\mathbf{B}_0\,|^2} . \tag{3.13}$$

In a constant field parallel to the z axis the nonvanishing terms are

$$\chi^{11}(\omega,\mathbf{q})=\chi^{22}(\omega,\mathbf{q})=\frac{(i\omega Dq^2)\chi(\mathbf{q})+\mu_B^2\chi(0)\,|\,\mathbf{B}_0\,|^2}{(i\omega+Dq^2)^2-\mu_B^2\,|\,\mathbf{B}_0\,|^2} , \tag{3.14a}$$

$$\chi^{33}(\omega,\mathbf{q})=\frac{(i\omega+Dq^2)\chi(q)}{(i\omega+Dq^2)-\mu_B^2\,|\,\mathbf{B}_0\,|^2} , \tag{3.14b}$$

$$\chi^{12}(\omega,\mathbf{q})=-\chi^{21}(\omega,\mathbf{q})$$

$$=-\frac{(i\omega+Dq^2)\chi(0)-\chi(\mathbf{q})}{(i\omega+Dq^2)^2-\mu_B^2\,|\,\mathbf{B}_0\,|^2}\mu_B\,|\,\mathbf{B}_0\,| \tag{3.14c}$$

We assume $\mathbf{B}_0$ to be weak enough that as a first approximation all terms of higher than first order in $|\,\mathbf{B}_0\,|$ can be neglected.

The spectral density is found by taking the imaginary part of χ^{11} and the real part of χ^{12},

$$B^{11}(\omega,\mathbf{q})=B^{22}(\omega,\mathbf{q})$$

$$=B^{33}(\omega,q)=\frac{1}{\pi}\,\frac{\omega Dq^2\chi(q)}{\omega^2+(Dq^2-\omega\tau_m)^2} , \tag{3.15a}$$

$$B^{12}(\omega,\mathbf{q})=-\frac{i}{\pi}\,\frac{Dq^2[\chi(\mathbf{q})-\chi(0)]\,|\,\mathbf{B}_0\,|}{\omega^2+(Dq^2-\omega^2\tau_m)^2} , \tag{3.15b}$$

where we introduced the additional parameters τ_m which provide a cutoff at high frequencies and which are interpreted as magnetic relaxation time. With these spectral densities the forms (2.7) and (2.8) for the spin-diffusion propagator in temperature representation follow.

IV. NUMERICAL RESULTS

In Eq. (2.46) the real and imaginary part of the gap are mixed because the eigenvalues $\alpha(\omega_n)$ and the spin fluctuation λ_{SW}^{ab} are complex functions. The imaginary part of the gap $\Delta_t(\omega_n)$ has the matrix structure $\tau_2\sigma_2$ and therefore transforms like a spin $S=1$ state under rotations in space described by

$$U=\exp\left[\frac{i}{2}\boldsymbol{\phi}\{\tau\sigma\}\right] , \tag{4.1}$$

$$\hat{G}\to\hat{G}=U^{-1}\hat{G}U . \tag{4.2}$$

This means that the Pauli exclusion principle is not satisfied by the parallel pairing of electrons nor by a symmetric space configuration which is the same for the real and imaginary parts of the gap. However, it can be shown that the following relations hold:

$$\alpha(\omega_n)=\alpha^*(-\omega_n) , \tag{4.3}$$

$$\lambda_{SW}^{ab}(\omega_n,\omega_m)=\lambda_{SW}^{ab*}(-\omega_n,-\omega_m)\ \text{ for } a=b , \tag{4.4}$$

$$\lambda_{SW}^{12}(\omega_n,\omega_m)=-\lambda_{SW}^{12}(-\omega_n,\omega_m) . \tag{4.5}$$

We see that it is sufficient to choose the ansatz

$$\Delta_S(\omega_n)=\Delta_S(-\omega_n) , \tag{4.6}$$

$$\Delta_t(\omega_n)=-\Delta_t(-\omega_n) . \tag{4.7}$$

The antisymmetry of the imaginary part (4.7) can be interpreted as antisymmetry in time on the real axis and in this way takes care of the Pauli principle.

From the form of the eigenvalue (2.36) we see that the band-splitting term b plays the same role as Pauli paramagnetism. The polarization term proportional to $\langle\mathbf{S}\rangle$ which itself is strongly temperature dependent can make a large contribution to b and can by itself cause a significant depression of B_{c2} as discussed by Umezawa *et al.*[9] This means there are two effects which can cause the reentrant behavior, namely, band splitting and spin fluctuations. We will regard each case separately, that is, we will consider only the effect of spin fluctuations and then only band splitting.

In the case where the polarization term is neglected, a term $\mathrm{Re}\lambda^{12}(\omega_n,\omega_m)$ remains in Eq. (2.24). Since λ^{12} is to first order linearly dependent on the magnetic field, its influence on B_{c2} is of second order and thus can be neglected. With $b=0$, all the functions λ_{SW}^{ab} defined by (2.20) become real. This will result in considerable simplifications.

The equation for the real part is

$$\Delta_S(\omega_n)=\pi T\sum_m \alpha(\omega_m)\{\lambda_{e\text{-ph}}(\omega_n-\omega_m)-\mathrm{tr}[\lambda_{SW}(\omega_n,\omega_m)]-\mu\}\times\Delta_S(\omega_m)+\frac{1}{\tau_{\mathrm{imp}}}\alpha(\omega_n)\Delta_S(\omega_n) , \tag{4.8}$$

which gives, together with

$$\tilde{\omega}_n=\omega_n+\pi T\sum_m\{\lambda_{e\text{-ph}}(\omega_n-\omega_m)+\mathrm{tr}[\lambda_{SW}(\omega_n,\omega_m)]\}\times\mathrm{sgn}\omega_m+\frac{1}{\tau_{\mathrm{imp}}}\mathrm{sgn}\omega_n , \tag{4.9}$$

a closed set of Eliashberg equations. The spin-fluctuation part is given by

$$\lambda_{SW}^{ab}(\omega_n,\omega_m)=j_{fd}^2\int\frac{d^3k}{(2\pi)^3}\,\frac{|\,\omega_m\,|}{(\tilde{\omega}_m^2+\epsilon^2)\pi}\times\frac{Dk^2\chi^{ab}(\mathbf{k}_F-\mathbf{k})}{(\omega_n-\omega_m)^2\tau_M+|\,\omega_n-\omega_m\,|+Dk^2} . \tag{4.10}$$

It is possible but a rather lengthy task to integrate (4.10) analytically. Details are given in the Appendix. In the static limit $\omega_n-\omega_m=0$ the result is fairly simple:

$$\lambda^{11}_{SW}(\omega_n,\omega_m)=\frac{S(S+1)}{12\xi_0^2 q_F^2} j_{fd}^2 N(0) \ln \left[\frac{(4k_F^2/T_m)\xi_0^2+(T-T_m/T_m)}{[(\xi_0^2 k_F/T_m)^{1/2}\,|\tilde{\omega}_n|\,/2\epsilon_F+(T-T_m/T_m)^{1/2}]^2} \right] , \tag{4.11}$$

which is in agreement with the result of Lee[8] and is always the dominant part of the interaction even when dynamics is included. In this last instance it is necessary to employ the full equation (A4). We note that this expression was derived for the momentum-dependent static susceptibility given in Eq. (2.12) and the dynamic extension including the magnetic relaxation time τ_M [Eqs. (2.9)–(2.11)] without the need for approximation.

In Figs. 1 and 2 we show two sets of $B_{c2}(T)$ diagrams as a function of temperature for two values of the magnetic correlation length ξ_0 which enters Eq. (2.12) for the static-limit magnetic susceptibility. In Fig. 1, which we discuss first, $\xi_0^2 k_F^2/T_m=0.3$ (a rather small value). The top curve is included for comparison and applies to the case when spin fluctuations are completely omitted. In this case, as in all the others, the electron-phonon spectral density $\alpha^2F(\Omega)$ of Eq. (2.22) is taken to be that of Nb metal with a mass enhancement factor λ set equal to 1. The Coulomb pseudopotential μ^* is chosen to get a critical temperature T_{c0} of 1.0 meV. The set of lower curves is labeled by the value of the effective strength between the superconducting electrons and the spins, namely, $N(0)j_{df}^2$. We see that, with increasing values of this parameter, the resulting $B_{c2}(T)$ curves start to deviate from our reference curve in two distinctive ways. First, the spin fluctuations reduce the upper critical temperature T_{c1}. For $N(0)j_{df}^2=0.056$ meV, T_{c1} is already less than half its initial value $T_c=1.0$ meV. Further important modifications occur resulting from the introduction of spin fluctuations at low temperatures near the magnetic critical temperature T_m which was set equal to 0.1 meV. Even for the case $N(0)j_{fd}^2=0.012$ meV, which is the smallest value for this parameter that is shown in Fig. 1, superconductivity is destroyed on reaching T_M. This is due to the effect that at the temperature T_m the spin fluctuation is determined only by the value $\ln(\epsilon_F/\tilde{\omega})$ and the chemical potential was chosen to be rather large with $\epsilon_F=5$ eV. For larger values of the electron-magnetic coupling, the reentrant temperature T_{c2} can be significantly larger than T_m. This feature is due to the large increase in the magnetic susceptibility[2,12] that occurs as T approaches T_m. We note that, for small $N(0)j_{fd}^2$, the maximum in $B_{c2}(T)$ is found to be closer to T_m so that an important resemblance to the usual curve $B_{cs}^0(T)$ remains. At high values of $N(0)d_{fd}^2$ this resemblance is lost entirely. In closing the discussion of this figure, we note that all results described so far were calculated using the full dynamical theory $\lambda^{ab}_{SW}(\omega_n,\omega_m)$ but also coincide with the static-limit results, Eq. (4.12). This is not the case for Fig. 2 where $\xi_0^2k_F^2/T_m=3.0$. In this case, the resulting $B_{c2}(T)$ curves are quite different from the curves previously described. For the same value of $N(0)d_{fd}^2$, the superconducting transition temperature T_{c1} is smaller when ξ_0 is small. Also, the curves remain closer to the $B_{c20}(T)$ curve and the drop near the magnetic transition temperature T_m is less significant. In fact, for the upper curves, T_{c1} falls below T_m. For each value of $N(0)j_{fd}^2$, labeling the curves in Fig. 2 we find three distinct cases. The solid curves

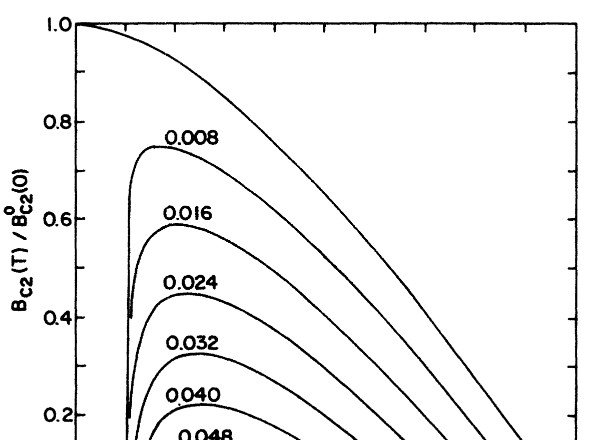

FIG. 1. Suppression of $B_{c2}(T)$ by spin fluctuations with increasing $j_{fd}^2N(0)$ given in meV. The magnetic correlation length is $\xi_0^2k_F^2/T_m=0.3$ and other parameters are $S=1.5$. T_c without spin fluctuations is taken to be 1.0 meV (11.5 K) and the magnetic transition set at $T_m=0.1$ meV. The difference between a fully dynamic calculation of spin fluctuations and a static approximation is too small to show up.

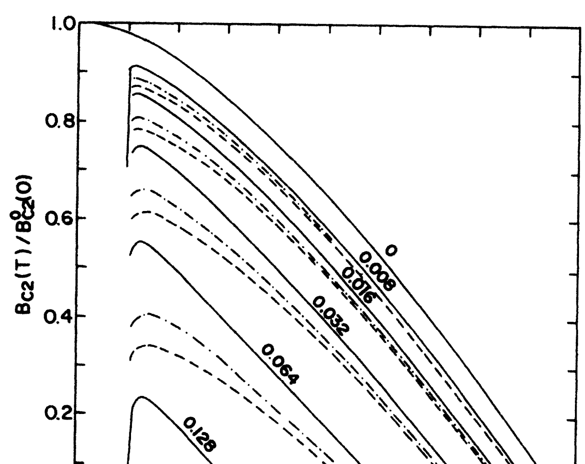

FIG. 2. Same as Fig. 1 but the magnetic correlation length is taken as $\xi_0^2k_F^2/T_m=3.0$. The dashed curve (— — —) is for $\tau_m=0.1$ meV^{-1} and the dashed-dotted curve (—·—·—·) for $\tau_m=0.01$ meV^{-1}, where the spin diffusion is calculated with full dynamic. (τ_M is the magnetic relaxation time.) The solid line describes the static limit.

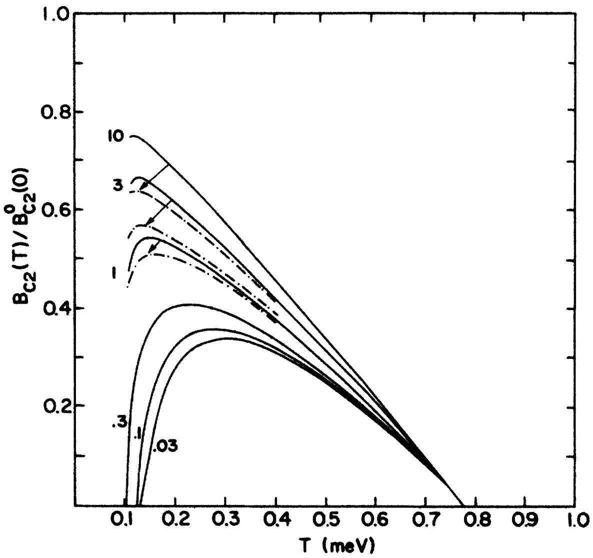

FIG. 3. $B_{c2}(T)$ for different values of the magnetic coherence length $\xi_0^2 k_F^2/T_m$ given by the numbers above the curves. In all cases $S=1.5$, the magnetic temperature is 0.1 meV, and the superconducting temperature without spin fluctuations is set at $T_{c0}=1.0$ meV. The solid lines (——) are the result of a static approximation for the spin fluctuation, while the dashed-dotted curves (—·—·—·) were obtained using the full dynamic with $\tau_m=0.1$ meV^{-1}.

(——) describe the static limit, i.e., the spin fluctuations are treated in the approximation $\omega_n-\omega_m=0$ with $\lambda_{SW}^{ab}(\omega_n,\omega_m)$ reducing to formula (4.11). The other two curves employ the full dynamic expression for $\lambda_{SW}^{ab}(\omega_n,\omega_m)$ given by Eq. (A6). In this case, it is necessary to specify the value of the magnetic relaxation time τ_m which plays the role of a cutoff. There is little knowledge about this parameter and we consider two values, namely, $\tau_m=0.1$ meV^{-1} (dashed curve) (— — —) and 0.01 meV^{-1} (dashed-dotted curve) (—·—·—·). Another parameter that enters the dynamic calculations for spin fluctuations is the constant c which relates the spin-diffusion parameter D in Eq. (2.11) to the inverse of the static susceptibility. This constant is, however, not arbitrary once τ_m is chosen and is to be determined from the sum rule (2.13). The importance of satisfying this sum rule has been stressed by Dupont *et al.*[13] It is also present in the work of Coffey *et al.*,[11] which we have followed closely except for the important fact that we chose τ_M and varied c.

On comparing static and dynamic results in Fig. 2 it becomes obvious that, in all cases, the dynamic corrections are significant and the differences in the results become very pronounced for large values of $N(0)j_{fd}^2$. This effect is further emphasized in Fig. 3 where the magnetic coherence length ξ_0 is varied and dynamic (—·—·—·) and static (——) results are compared. All curves are for $\tau_m=0.1$ meV^1. The coupling strength $N(0)j_{fd}^2$ is not fixed in these graphs but rather has been adjusted to get the same superconducting temperature $T_{c1}=9$ K (0.78 meV). It is clear that for small values of ξ_0 the static limit is sufficient but this does not follow when ξ_0 is large, in which case quantitative results can only be obtained with full inclusions of the dynamics. We now want to discuss the effects of band splitting on $B_{c2}(T)$ curves.

If the term χ^{12} in the spin fluctuations is not negligible, its main contribution will result, according to Eqs. (2.46) and (2.24), in an effective band splitting. The same effect will also result from the polarization term $\langle S\rangle$. In our second case, we regard next a superconductor without spin fluctuations but with this polarization term included. Equation (2.46) reduces then to the coupled set

$$\Delta_S(\omega_n)=\frac{\pi T}{N(0)}\sum_{m=0}^{\infty}[\mathrm{Re}\alpha(\omega_m)\Delta_S(\omega_m)-\mathrm{Im}\alpha(\omega_m)\Delta_t(\omega_m)]\times[\lambda_{e\text{-ph}}(n-m)+\lambda_{e\text{-ph}}(n+m+1)-2\mu^*]+\frac{1}{2\tau_{\mathrm{imp}}}\frac{1}{N(0)}[\mathrm{Re}\alpha(\omega_n)\Delta_S(\omega_n)-\mathrm{Im}\alpha(\omega_t)\Delta_t(\omega_n)]\ , \tag{4.12}$$

$$\Delta_t(\omega_n)=\frac{\pi T}{N(0)}\sum_{m=0}^{\infty}[\mathrm{Re}\alpha(\omega_m)\Delta_t(\omega_m)+\mathrm{Im}\alpha(\omega_n)\Delta_S(\omega_m)]\times[\lambda_{e\text{-ph}}(n-m)-\lambda_{e\text{-ph}}(n+m+1)]+\frac{1}{2\tau_{\mathrm{imp}}}\frac{1}{N(0)}[\mathrm{Re}\alpha(\omega_n)\Delta_t(\omega_n)+\mathrm{Im}\alpha(\omega_n)\Delta_s(\omega_n)]\ . \tag{4.13}$$

The sum over the negative Matsubara frequencies has been converted to one over the positive ones using only the symmetries (4.37)–(4.7). We see that for the imaginary part the phonon interactions largely cancel and the Coulomb repulsion μ^* has dropped out; however, a strong mixing with the real part can be caused by the impurities. Similar equations have already been used by Schossmann and Schachinger[14] to explain the $B_{c2}(T)$ of V_3Si as due to Pauli paramagnetic limiting. For the polarization it is sufficient to assume the simplest possible model for the susceptibility that is valid in this region, namely,

$$b=j_{fd}\langle \mathbf{S}\rangle_3=-j_{fd}\frac{S(S+1)}{3k_B(T-T_m)}\mu_B B\ , \tag{4.14}$$

and to introduce the polarization parameter

$$p=j_{fd}\frac{S(S+1)}{3k_B T_m}\frac{1}{\pi}\ . \tag{4.15}$$

In Fig. 4 we show reentrant $B_{c2}(T)$ curves resulting from band splitting for different values of the parameter p. In each case the reentrant temperature T_{c2} is 0.1 meV, corresponding to a divergence in b due to the assumed form of the model susceptibility in (4.14). Also the superconducting transition temperature T_{c1} is fixed at 1 meV. The electron-phonon spectral density is as always that of

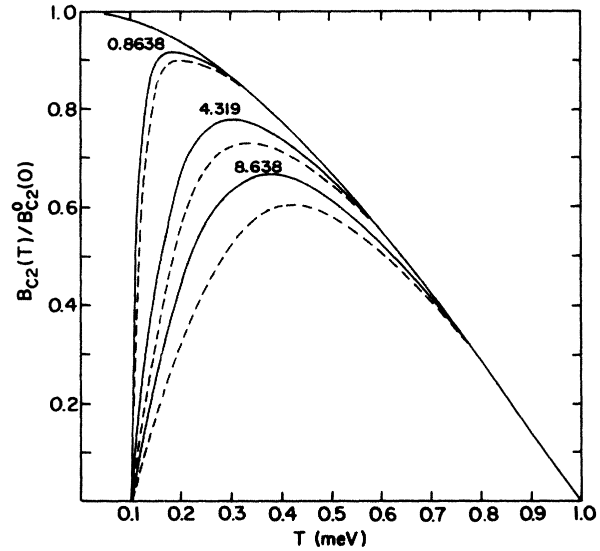

FIG. 4. Suppression of $B_{c2}(T)$ due to band splitting, ignoring spin-fluctuation effects. The waves are labeled by the value of the parameter p which is explained in the text. The solid line (——) represents results in which the mixing with parallel spin Cooper pairs is ignored, while the dashed curves (— — —) fully include this mixing. For all curves the normal impurity scattering density is fixed at $1/\tau_{\text{imp}}=1.0$ meV. The Fermi velocity v_F is chosen to give a $B^0_{c2}(0)$ of 2 T.

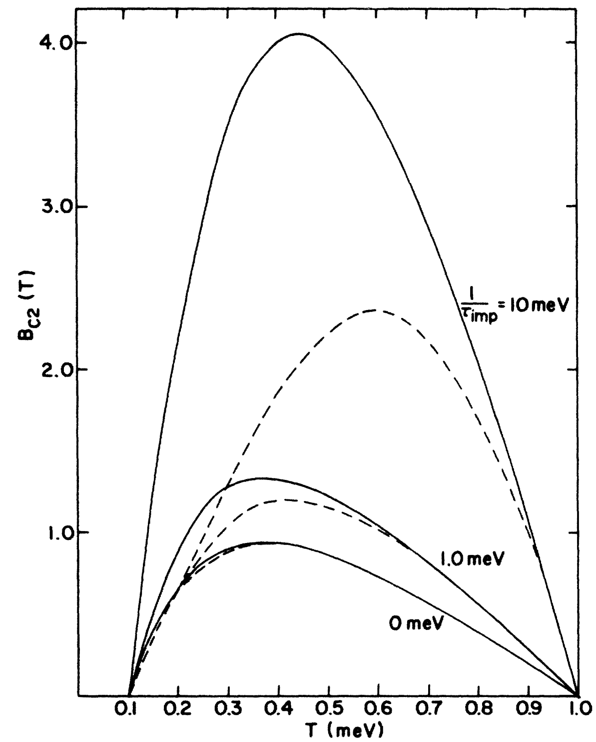

FIG. 5. $B_{c2}(T)$ for different impurity concentrations and with pure band splitting ($p=8.638$). Dashed and solid lines are the same as in Fig. 4.

Nb with the mass enhancement factor set equal to 1 ($\lambda=1$) and the Coulomb pseudopotential is adjusted to get the assumed T_{c1}. The impurity scattering time is set $1/\tau_{\text{imp}}=1.0$ meV and the Fermi velocity chosen to give $B_{c2}(0)=1.0T$ and we plot $B_{c2}(T)/B_{c2}(0)$ versus T. The solid lines are results from Eqs. (4.12) and (4.13) in which the triplet part is ignored while the dashed curves include this part. It is obvious that the mixing of the triplet part of the amplitudes in (4.12) and (4.13) can be significant and depresses $B_{c2}(T)$ below the value calculated without such effects. This is emphasized further in Fig. 5. In this figure we use the same parameters as employed in Fig. 4 except that the polarization parameter $p=8.638$ is used for all curves and the impurity content ($1/\tau_{\text{imp}}$) changes from 0 to 1.0 and finally to 10.0 meV. We see clearly that for large impurity content the $B_{c2}(T)$ curves with triplet mixing are completely different from those without such a mixing.

In connection with the band-splitting effects introduced in Figs. 4 and 5 we should mention several additional points. First, such effects have been discussed in the literature and the reader is referred to the review of Umezawa *et al.*[9] for details. They can explain the very large anisotropy observed in single-crystal $ErRh_4B_4$ between easy and hard axis since along the easy axis the spin polarization will be large, while it will be small along the hard axis. This is in striking contrast to the effe ts of spin fluctuation which cannot explain the occurrence of large anisotropies because it is now the trace of the susceptibility ($\text{tr}\{\chi_{SW}\}$) that enters the equations so that the resulting $B_{c2}(T)$ remains isotropic in this theory.

Furthermore, triplet mixing decreases $B_{c2}(T)$. This result can be understood in a simple limit as due to an effective reduction in the pairing potential and impurity scattering in the single channel through the inclusion of triplet pairing. To see this we ignore the small electron-phonon term in Eq. (4.13) and get the immediate solution for Δ_t in terms of Δ_S:

$$\Delta_t(\omega_n)=\frac{(1/2\tau_{\text{imp}})[1/N(0)]\text{Im}\alpha(\omega_n)}{1-(1/2\tau_{\text{imp}})[1/N(0)]\text{Re}\alpha(\omega_n)}\Delta_S(\omega_n)\ . \tag{4.16}$$

Substitution of (4.16) into (4.12) gives

$$\Delta_S(\omega_n)=\frac{\pi T}{N(0)}\sum_{m=0}^{\infty}\text{Re}\alpha(\omega_m)\left[1-\frac{(1/2\tau_{\text{imp}})[1/N(0)][\text{Im}\alpha(\omega_m)]^2}{\{1-(1/2\tau_{\text{imp}})[1/N(0)]\text{Re}\alpha(\omega_n)\}\text{Re}\alpha(\omega_n)}\right]$$
$$\times[\lambda_{e\text{-ph}}(n-m)+\lambda_{e\text{-ph}}(n+m+1)-2\mu^*]$$
$$+\frac{\text{Re}\alpha(\omega_n)}{2\tau_{\text{imp}}N(0)}\left[\frac{(1/2\tau_{\text{imp}})[1/N(0)][\text{Im}(\omega_n)]^2}{\{1-(1/2\tau_{\text{imp}})[1/N(0)]\text{Re}\alpha(\omega_n)\}\text{Re}\alpha(\omega_n)}\right]\Delta_S(\omega_n)\ . \tag{4.17}$$

This last equation has the same form as (4.12) with Δ_t set equal to zero but with the effective coupling and impurity content reduced by the factor

$$1-\frac{(1/2\tau_{\rm imp})[1/N(0)][{\rm Im}\alpha(\omega_n)]^2}{\{1-(1/2\tau_{\rm imp})[1/N(0)]{\rm Re}\alpha(\omega_n)\}{\rm Re}\alpha(\omega_n)}\ ,$$

which is clearly less than 1 for the case of $\tau_{\rm imp}$ large since the denominator in the second term is near 1.

V. CONCLUSION

We have presented a microscopic theory for the upper critical magnetic field $B_{c2}(T)$ of a ferromagnetic superconductor in the paramagnetic region. A fundamental set of Eliashberg-type equations is derived which fully includes the dynamics, as well as the band-splitting effect caused by the polarization of the spin system. In our derivations, which are valid for any amount of normal impurities, the long-range nature of the spin correlations in space are accounted for by making a new ansatz for the pair amplitude in a magnetic field which does not assume a contact interaction. This is necessary in order to avoid an unphysical singularity which would otherwise be introduced near the magnetic temperature due to the divergence in the static magnetic susceptibility at that temperature. In our formulation it is found, from general symmetry considerations, that the singlet and triplet amplitudes are naturally mixed, a result already present in the work of Rainer *et al.*[15] Detailed numerical evaluations of the full set of equations show that without approximation the effect of spin fluctuations in the $B_{c2}(T)$ curves can be very significant for a certain range of values of the assumed magnetic parameters. Furthermore, when the magnetic coherence length (ξ_0) is large, the dynamics of the spin fluctuation cannot be ignored in quantitative calculations. These effects are, however, less significant when ξ_0 is small. As for the effects of band splitting, we find, as in previous works reviewed by Umezawa *et al.*,[9] that they can be very large and can explain the observed large anisotropies in single crystals. Furthermore, we find that the B_{c2} curves are sensitive to the amount of normal impurities present and that they can be greatly affected by triplet mixing for some ranges of values of the relevant parameters.

APPENDIX

In Sec. II we have defined the spin-diffusion part of the interaction

$$\lambda_{SW}^{ab}(\omega_n,\omega_m)=-\int\frac{d^3k'}{(2\pi)^3}\,\frac{(\tilde{\omega}_m+ib){\rm sgn}\omega_m}{\pi[(\tilde{\omega}_m+ib)^2+\epsilon^2(k')]}\times j_{fd}^2\chi^{ab}(\omega_n-\omega_m,\mathbf{k}_F-\mathbf{k}')\ . \qquad (A1)$$

By assuming a spherical Fermi surface the only remaining angular dependence is in χ^{ab} and the integration over angles can be performed as a first step. For χ^{11} this is

$$\int d^2S(k')\chi^{11}(\omega_n-\omega_m,\mathbf{k}_F-\mathbf{k}')=-\frac{k'\pi S(S+1)}{6k_F\xi_0^2}\ln\left[\frac{\Omega-t^2+\left[\dfrac{\xi_0^2}{T_m}(k_F+k')^2+t\right]^2}{\Omega-t^2+\left[\dfrac{\xi_0^2}{T_m}(k_F-k')^2+t\right]^2}\right]-\frac{k'\pi S(S+1)}{6k_F\xi_0^2}\,\frac{t}{(\Omega-t^2)^{1/2}}$$
$$*\ln\left[\frac{\left[\dfrac{\xi_0^2}{T_m}(k+k_F)^2+t+(t^2-\Omega)^{1/2}\right]\left[\dfrac{\xi_0^2}{T_m}(k-k_F)^2+t-(t^2-\Omega)^{1/2}\right]}{\left[\dfrac{\xi_0^2}{T_m}(k+k_F)^2+t-(t^2-\Omega)^{1/2}\right]\left[\dfrac{\xi_0^2}{T_m}(k-k_F)^2+t+(t^2-\Omega)^{1/2}\right]}\right]\ , \qquad (A2)$$

where

$$\Omega=\frac{\xi_0^2S(S+1)}{3T_m^2C}[(\omega_n-\omega_n)^2\tau_n+|\omega_n-\omega_m|]\ , \qquad (A3)$$

$$t=\frac{T-T_m}{2T_m}\ . \qquad (A4)$$

For the integral over the energy the dynamics of electrons is approximated over the Fermi surface by

$$k\approx k_F+\frac{\epsilon}{v_F} \qquad (A5)$$

and we get a rather lengthy expression for λ^{11} after considerable algebra:

$$\lambda_{SW}^{11}(\omega_n,\omega_m)=\frac{j_{fd}^2N(0)S(S+1)}{24\xi_0^2q_F^2}\left\{\ln\left[\frac{(4x_0+t)^2-t^2+\Omega}{\{w^2+(2\omega)^{1/2}[t+(\Omega)^{1/2}]^{1/2}+(\Omega)^{1/2}\}^2}\right]\right.$$
$$+\frac{t}{(t^2-\Omega)^{1/2}}\left[\ln\left[\frac{4x_0+t+(t^2-\Omega)^{1/2}}{4x_0+t-(t^2-\Omega)^{1/2}}\right]\right.$$
$$\left.\left.-2\ln\left[\frac{w+[t+(t^2-\Omega)^{1/2}]^{1/2}}{w+[t-(t^2-\Omega)^{1/2}]^{1/2}}\right]\right]\right\}, \quad \text{(A6)}$$

where we defined

$$x_0=\frac{\xi_0^2k_F^2}{T_m} \quad \text{(A7)}$$

and

$$w=\left[\frac{\xi_0^2k_F^2}{T_m}\right]^{1/2}\frac{(\tilde{\omega}_m+ib)\mathrm{sgn}\omega_m}{2\epsilon_F}\,. \quad \text{(A8)}$$

For the case that $\sqrt{\Omega}>t$ the logarithm can be analytically continued to inverse tangent function.

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