Upper critical field and critical temperature for superconducting alloys described by the Anderson model*

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Extending some recent work by Shiba, we have used the Hartree-Fock approximation for the Anderson model of localized-impurity-electron states in a superconductor to obtain expressions for the critical temperature in zero magnetic field and for the upper critical field. The expression for the critical temperature reduces to Kaiser's result in the limit of no impurity magnetic moment, and Fulde and Maki's result in the magnetic limit. Between these two limits results are found which differ appreciably from those of either limit.

The d-electron (or f-electron) states localized on transition-metal (or rare-earth) impurities in simple metals are not orthogonal to the conductionelectron states of the host metal. This leads to a mixing, or hybridization, with conduction-electron states to form localized resonances.¹ Zuckermann² calculated the effect of a broad resonance (when the impurity has no magnetic moment) on the superconducting properties of these alloys. Takanaka and Takano, ³ and Ratto and Blandin⁴ extended Zuckermann's work to include the important effects of the Coulomb repulsion between localized electrons of opposite spin. Subsequently, Kiwi and Zuckermann,⁵ using the Hamiltonian of Ratto and Blandin, found that the energy gap decreased with concentration faster than the order parameter, suggesting the possibility of gapless superconductivity. However, Kaiser⁶ noted that the Ratto-Blandin Hamiltonian was time-reversal invariant in contrast to the case for a magnetic impurity. A general theorem⁷ stipulates that a time-reversal invariant Hamiltonian cannot give rise to gapless superconductivity.

Kaiser resolved this question by calculating the order parameter and energy gap for a superconductor containing localized nonmagnetic impurities in the Ratto-Blandin model. Using the fact that the resonance half-width is much greater than the range of energies about the Fermi surface which is important in superconductivity, he demonstrated that the energy gap vanishes if and only if the order parameter vanishes. Thus, there is no gapless behavior.

For the critical temperature in the absence of a magnetic field, Kaiser found

$$T_{c0} = 1.13 \Theta_c e^{-1/f (n_I)\lambda}$$

where Θ_c is a cutoff temperature (usually on the order of the Debye temperature) and $f(n_I)\lambda$ is an effective coupling constant, n_I being the impurity concentration (in atomic fraction). The quantity $f(n_I)$ is the ratio of the gap in the density of states

to the effective pairing potential Δ :

$$f(n_I) = \frac{\Delta_{r}}{\Delta} = \frac{1 - c(n_I)d}{1 + c(n_I)}$$
$$= \frac{1 - [n_I(2l+1)N_I(0)/N(0)][U_{eff}N_I(0)/\lambda]}{1 + n_I(2l+1)N_I(0)/N(0)},$$

where 2l + 1 is the orbital degeneracy factor for the impurity, $N_l(0)$ is the density of localized states admixed at the Fermi surface, and N(0) is the conduction-electron density of states at the Fermi surface. The effective on-site Coulomb repulsion is the Schrieffer-Mattis form⁸

$$U_{\text{off}} = \frac{U}{1 + (U/\pi E_d) \arctan(E_d/\Gamma)}$$

 E_d is the displacement of the center of the virtual levels from the Fermi surface, and Γ is the halfwidth of the virtual levels. U is the bare intraatomic Coulomb repulsion between localized electrons of opposite spin. The term $c(n_I)$ represents the fractional amount of localized states admixed at the Fermi level. The denominator of the expression for $f(n_I)$ represents what Kaiser referred to as a dilution effect. The density of conductionelectron states is diluted by the presence of these additonal virtual levels near the Fermi surface. The quantity d is the ratio of the "strength" of opposition to pairing to the "strength" of the pairing. This opposition arises due to the admixture of conduction-electron states into opposite-spin localized states which are separated in energy by $U\langle n_i \rangle \langle n_i \rangle$. This energy correlation between localized electrons of opposite spin induces, by admixture, a similar correlation between elements of a Cooper pair, having a negative effect on the stability of pairs. This is referred to as "pair weakening." The reflection of this weakening is in the term $c(n_i)d_i$. which is the fractional amount of admixture at the Fermi surface multiplied by the weakening due to admixture.

In the Ratto-Blandin Hamiltonian it is assumed

ab initio that the impurity is nonmagnetic. In the normal state, their Hamiltonian reduces to Hartree-Fock theory. When the impurity is allowed to have a moment, the Hamiltonian is no longer time-reversal invariant. One should expect the dilution effect to appear qualitatively the same as in the nonmagnetic case, since it depends only on the value of the density of up- and down- spinlocalized electrons at the Fermi level. The pair weakening should be modified, however, by the introduction of a pair-breaking interaction. Also, there should be another term arising from this pair breaking, the Abrikosov-Gorkov⁹ term. These are in fact our results. In addition, a unified theory of magnetic and nonmagnetic impurities in a superconductor should reproduce the Kaiser results in the limit of zero local moment, and the Abrikosov-Gorkov result in the magnetic limit $(U \gg \Gamma)$.

The purpose of this work is to obtain a useful expression for the critical temperature and upper critical field for localized impurities (magnetic or nonmagnetic) which are described by the Anderson model. Our expressions should reasonably interpolate between the well-known magnetic and nonmagnetic limit insofar as the Hartree-Fock approximation is valid.

Shiba¹⁰ has calculated the superconducting properties of alloys described by the Anderson model using the generalized Hartree-Fock approximation for the Hamiltonian and Nambu formalism. Our approach has been to obtain coupled linear Ginzburg-Landau equations microscopically, solving these at the phase boundary to find T_{c0} and H_{c2} . We find complete agreement between our expression for T_{c0} and that of Shiba, but we make further approximations which allow us to write a readily interpretable expression for the critical temperature.

In the interpolation regime between magnetic and nonmagnetic limits, we find (as did Shiba) results which may differ markedly from Abrikosov-Gorkov results for certain ranges of the parameters of our theory. We also find that Kaiser's results may be drastically modified by even a small amount of exchange scattering. By comparing our Anderson model results with those of the exchange model, we find a correspondence in the magnetic limit which is the same as the correspondence of Schrieffer and Wolff.¹¹ Outside of the magnetic limit, we find that we cannot unambiguously relate the Anderson model results to those of the exchange model. Our expressions for T_{c0} and H_{c2} may be readily interpreted as an amalgam of the Kaiser and the Abrikosov-Gorkov results.

Section I of the paper describes the Hamiltonian and the generalized Hartree-Fock approach as well as outlining the perturbation theoretic treatment employed. Feynman diagrams for the pair-correlation functions are evaluated, and a set of coupled linear Ginzburg-Landau equations is obtained. In Sec. II various approximations are made in order to develop these equations into a useful form. Section III deals with the establishment of a correspondence between the magnetic Anderson model results and the exchange model results. In Sec. IV graphs of the zero-field critical temperature as a function of concentration are obtained and discussed, with particular attention paid to the regime of small, but nonzero, exchange scattering, where effects due to the interdependence of pair-weakening and pair-breaking may be observed. In addition, graphs of the upper critical field as a function of reduced temperature for various concentrations and various amounts of exchange scattering are obtained and discussed.

I. CALCULATION OF GINZBURG-LANDAU EQUATION

We begin with the Hamiltonian

$$H = \int d\vec{\mathbf{r}} \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) \left(\frac{\left[(1/i) \vec{\nabla} - e \,\vec{\mathbf{A}}(\vec{\mathbf{r}}) \right]^{2}}{2m} - \mu \right) \psi_{\alpha}(\vec{\mathbf{r}}) + \sum_{i} \sum_{m} \epsilon_{i} \phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m\alpha}(\vec{\mathbf{R}}_{i}) \\ - \left| g \right| \int d\vec{\mathbf{r}} \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) \psi_{\beta}^{\dagger}(\vec{\mathbf{r}}) \psi_{\beta}(\vec{\mathbf{r}}) \psi_{\alpha}(\vec{\mathbf{r}}) + \frac{1}{2} U \sum_{i} \sum_{m,m'} \phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m\alpha}(\vec{\mathbf{R}}_{i}) \phi_{m'-\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m'-\alpha}(\vec{\mathbf{R}}_{i}) \\ + \frac{1}{2} (U - J) \sum_{i} \sum_{m\neq m'} \phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m\alpha}(\vec{\mathbf{R}}_{i}) \phi_{m'\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m'\alpha}(\vec{\mathbf{R}}_{i}) + \sum_{j} \int d\vec{\mathbf{r}} \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) W(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{j}) \psi_{\alpha}(\vec{\mathbf{r}}) \\ + \sum_{i,m} \int d\vec{\mathbf{r}} \left[V_{m}(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{i}) \phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \psi_{\alpha}(\vec{\mathbf{r}}) + V_{m}^{*}(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{i}) \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) \phi_{m\alpha}(\vec{\mathbf{R}}_{i}) \right] .$$
 (1.1)

Here ϵ_i is the distance of the unperturbed localized levels from the Fermi surface. The localized electrons (assumed orbitally degenerate) have z component of angular momentum m, and spin α (we sum over repeated Greek indices). The effective Bardeen-Cooper-Schrieffer (BCS) interaction is |g|. The local atomic Coulomb repulsion between opposite-spin electrons is U, while J is the intra-atomic exchange energy. Ordinary impurity-potential scattering is represented by $\sum_j W(\vec{\mathbf{r}} - \vec{\mathbf{R}}_j)$, and $V_m(\vec{\mathbf{r}} - \vec{\mathbf{R}}_i)$ is the transfer integral between a conduction electron at $\vec{\mathbf{r}}$ and a localized electron of angular momentum z component m

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at the impurity site R_i .

Following Ratto and Blandin,⁴ we make a generalized Hartree-Fock approximation to obtain

$$H_{\text{eff}} = H_0 + H_1 + H_2 , \qquad (1.2)$$

$$H_0 = \int d\vec{\mathbf{r}} \,\psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) \left(\frac{\left[(1/i) \,\vec{\nabla} - e \,\vec{\mathbf{A}}(\vec{\mathbf{r}}) \right]^2}{2m} - \mu \right) \psi_{\alpha}(\vec{\mathbf{r}}) + \sum_i E_{I\alpha} \,\phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_i) \phi_{m\alpha}(\vec{\mathbf{R}}_i) , \qquad (1.3)$$

$$H_{1} = -\frac{1}{2} \sum_{m,m'} \sum_{i} \left[\Delta_{i}^{*}(\vec{\mathbf{R}}_{i})_{\alpha\beta}^{mm'} \phi_{m'\beta}(\vec{\mathbf{R}}_{i}) \phi_{m\alpha}(\vec{\mathbf{R}}_{i}) + \phi_{m\alpha}^{\dagger}(\vec{\mathbf{R}}_{i}) \phi_{m'\beta}^{\dagger}(\vec{\mathbf{R}}_{i}) \Delta_{l}(\vec{\mathbf{R}}_{i})_{\beta\alpha}^{m'm} \right] - \frac{1}{2U} \sum_{i} \sum_{m,m'} \Delta_{i}^{*}(\vec{\mathbf{R}}_{i})_{\alpha\beta}^{mm'} \Delta_{l}(\vec{\mathbf{R}}_{i})_{\beta\alpha}^{m'm}$$

$$-\frac{1}{2}\int d\vec{r} \left[\Delta^{*}(\vec{r})_{\alpha\beta}\psi_{\beta}(\vec{r})\psi_{\alpha}(\vec{r})+\psi_{\alpha}^{\dagger}(\vec{r})\psi_{\beta}^{\dagger}(\vec{r})\Delta(\vec{r})_{\beta\alpha}\right]+\frac{1}{2|g|}\int d\vec{r}\,\Delta^{*}(\vec{r})_{\alpha\beta}\,\Delta(\vec{r})_{\beta\alpha}\,,\tag{1.4}$$

$$H_{2} = \sum_{j} \int d\vec{\mathbf{r}} \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) W(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{j}) \psi_{\alpha}(\vec{\mathbf{r}}) + \sum_{i,m} \int d\vec{\mathbf{r}} \left[V_{m}(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{i}) \phi_{m\,\omega}^{\dagger}(\vec{\mathbf{R}}_{i}) \psi_{\alpha}(\vec{\mathbf{r}}) + V_{m}^{*}(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{i}) \psi_{\alpha}^{\dagger}(\vec{\mathbf{r}}) \phi_{m\,\alpha}(\vec{\mathbf{R}}_{i}) \right].$$
(1.5)

Here we have defined the parameters

$$\Delta_{I}(\vec{\mathbf{R}}_{i})_{\alpha\beta}^{mm'} \equiv -U\langle \phi_{m\alpha}(\vec{\mathbf{R}}_{i})\phi_{m'\beta}(\vec{\mathbf{R}}_{i}) \rangle_{\text{off}} = -U \frac{\text{Tr}[e^{-\beta H \text{off}}\phi_{m\alpha}(\vec{\mathbf{R}}_{i})\phi_{m'\beta}(\vec{\mathbf{R}}_{i})]}{\text{Tr}[e^{-\beta H \text{off}}]}, \qquad (1.6)$$

$$\Delta(\vec{\mathbf{r}})_{\alpha\beta} = -\left|g\right| \left\langle \psi_{\alpha}(\vec{\mathbf{r}})\psi_{\beta}(\vec{\mathbf{r}}) \right\rangle_{\text{eff}} = -\left|g\right| \frac{\operatorname{Tr}\left[e^{-\beta H_{\text{eff}}}\psi_{\alpha}(\vec{\mathbf{r}})\psi_{\beta}(\vec{\mathbf{r}})\right]}{\operatorname{Tr}\left[e^{-\beta H_{\text{eff}}}\right]} \quad .$$

$$(1.7)$$

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Following Shiba, we have set

$$E_{l\alpha} \equiv E_l + v\alpha , \qquad (1.8)$$
$$E_l \equiv \epsilon_l + \frac{1}{2} [(2l+1)U + 2l(U-J)] [\langle n, \rangle + \langle n, \rangle] , \qquad (1.9)$$

$$v = -\frac{1}{2} [(2l+1)U - 2l(U-J)] [\langle n, \rangle - \langle n, \rangle] . \qquad (1.10)$$

The term $\langle n_{\alpha} \rangle$ is the thermal average of the number of localized electrons of spin α . Since the orbital degeneracy of the localized electrons is not broken

$$\Delta_{l}(\vec{\mathbf{R}}_{i})_{\alpha\beta}^{mm'} = \Delta_{l}(\vec{\mathbf{R}}_{i})_{\alpha\beta} \,\delta_{m,m'} \,. \tag{1.11}$$

To account for the degenerate localized states we use the approximation

$$e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_{i}} V_{m}(\vec{\mathbf{k}}) = \int d\vec{\mathbf{r}} e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_{i}} e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} V_{m}(\vec{\mathbf{r}})$$
$$= (4\pi)^{1/2} Y_{im}(\hat{n}_{k}) e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_{i}} , \qquad (1.12)$$

where V is a constant and $Y_{lm}(\hat{n}_k)$ is a spherical harmonic [using the approximation that the angular dependence of $V_m(\hat{\mathbf{r}})$ is of the form $Y_{lm}(\theta, \psi)$ for suitably chosen localized orbitals].

We will determine H_{c2} and T_{c0} by calculating

$$\left\langle \psi_{i}^{\dagger}(\vec{\mathbf{r}})\psi_{i}^{\dagger}(\vec{\mathbf{r}})\right\rangle_{\text{eff}},$$

$$\sum_{i,m} \left\langle \delta(\vec{\mathbf{r}}-\vec{\mathbf{R}}_{i})\phi_{m,i}^{\dagger}(\vec{\mathbf{r}})\phi_{m,i}^{\dagger}(\vec{\mathbf{r}}) \frac{\Delta_{i}(\vec{\mathbf{r}})_{i,i}}{\Delta(\vec{\mathbf{r}})_{i,i}}\right\rangle_{\text{eff}},$$

$$(1.13)$$

using standard temperature-diagram techniques. We expand these averages to lowest nonvanishing order in the non-particle-conserving portion of H_{eff} , obtaining

$$\lim_{u^{+} \to u} \langle \psi_{i}^{\dagger}(\vec{\mathbf{r}}, u)\psi_{i}^{\dagger}(\vec{\mathbf{r}}, u^{+})\rangle_{eff} \approx \lim_{u^{+} \to u} \frac{\operatorname{Tr}\left\{e^{-\beta (H_{0} + H_{2})} \int_{0}^{\beta} du_{1} T[H_{1}(u_{1})\psi_{i}^{\dagger}(\vec{\mathbf{r}}, u)\psi_{i}^{\dagger}(\vec{\mathbf{r}}, u^{+})]\right\}}{\operatorname{Tr}\left[e^{-\beta (H_{0} + H_{2})}\right]} , \qquad (1.14)$$
$$\lim \sum_{u^{+} \to u} \sum_{u^{+} \to u^{+}} \frac{\Delta_{I}(\vec{\mathbf{r}})}{\Delta_{I}(\vec{\mathbf{r}})} \phi_{m,i}^{\dagger}(\vec{\mathbf{r}}, u)\phi_{m,i}^{\dagger}(\vec{\mathbf{r}}, u^{+})\rangle$$

$$\approx \lim_{u^{*} \to u} \frac{\operatorname{Tr}\left\{e^{-\beta (H_{0}^{*}H_{2})} \int_{0}^{\beta} du_{1} T[H_{1}(u_{1}) \sum_{i,m} \delta(\vec{\mathbf{r}} - \vec{\mathbf{R}}_{i}) [\Delta_{I}(\vec{\mathbf{r}})/\Delta(\vec{\mathbf{r}})] \phi_{m}^{\dagger}(\vec{\mathbf{r}}, u) \phi_{m}^{\dagger}(\vec{\mathbf{r}}, u^{*})]\right\}}{\operatorname{Tr}\left\{e^{-\beta (H_{0}^{*}H_{2})}\right\}}$$
(1.15)

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Working by analogy with Kaiser's approach, we define the ratio

 $d(\mathbf{\vec{r}}) \equiv -\Delta_I(\mathbf{\vec{r}}) / \Delta(\mathbf{\vec{r}}) , \qquad (1.16)$

assuming that the limit

 $\lim_{\Delta \to 0} d(\mathbf{r})$

exists. Because we will configuration-average all quantities, we make the ansatz that d is independent of \vec{r} .

The remaining thermal averages are then calculated by making a perturbation expansion in H_2 .

Employing the phase-integral approximation to account for the effects of the magnetic field, configuration averaging and using the dirty limit near

(A A)

 $H = H_{c2}$, we obtain two coupled differential equations which can be solved at H_{c2}^{12} :

$$\frac{1}{|g|} \Delta^*(\vec{\mathbf{r}}) = \lim_{r_2 \to r} K_s(\vec{\Pi}^\dagger(\vec{\mathbf{r}}_2)^2) \Delta^*(\vec{\mathbf{r}}_2) , \qquad (1.17)$$

$$n_{I}(2l+1)(d^{2}/U)\Delta^{*}(\vec{\mathbf{r}}) = \lim_{r_{2} \neq r} K_{I}(\vec{\Pi}^{\dagger}(\vec{\mathbf{r}}_{2})^{2})\Delta^{*}(\vec{\mathbf{r}}_{2}) .$$
(1.18)

The kernels K_s and K_t are given by the diagrams in Fig. 1:

$$K_{s}(\vec{\Pi}^{\dagger}(\vec{\mathbf{r}}_{2})^{2}) = \frac{1}{2} k_{B} T \sum_{n} \sum_{k} \sum_{\alpha} \langle G_{\alpha}(\vec{\mathbf{k}} + \vec{\mathbf{q}}, i\omega_{n}) \rangle \\ \times G_{-\alpha}(-\vec{\mathbf{k}}, -i\omega_{n}) \Lambda_{s}(\vec{\mathbf{q}}, i\omega_{n}, -i\omega_{n})_{\alpha-\alpha} \rangle \Big|_{q^{2} = \vec{\Pi}^{\dagger}(\vec{\mathbf{r}}_{2})^{2}} , \qquad (1.19)$$

$$K_{I}(\vec{\Pi}^{\dagger}(\vec{\mathbf{r}}_{2})^{2}) = -n_{I}(2l+1)\frac{1}{2}k_{B}T \sum_{\alpha} \sum_{n} \left\langle dC_{\alpha}\left(i\omega_{n}\right) C_{-\alpha}(-i\omega_{n})\Lambda_{I}(\vec{\mathbf{q}},i\omega_{n},-i\omega_{n})_{\alpha-\alpha} \right\rangle \Big|_{q^{2}=\vec{\Pi}^{\dagger}(\vec{\mathbf{r}}_{2})^{2}} .$$

$$(1.20)$$

Each Λ_s vertex function carries implicitly a restriction of the summation over the integers *n* of the Matsubara frequencies. The notation \sum_n' with the prime indicates that the range of the integral representation of the sum is $|\omega| < \omega_D$, where ω_D is the Debye frequency.

The dressed conduction-electron Green's function is

$$G_{\alpha}(\vec{k}, i\omega_n) = \frac{1}{i\tilde{\omega}_{n\alpha} - \epsilon(\vec{k}) - \phi_{\alpha}(\tilde{\omega}_n)} , \qquad (1.21)$$

and the dressed localized electron Green's function is

$$C_{\alpha}(i\omega_{n}) = 1/(i\tilde{\omega}_{n} - E_{l\alpha}) , \qquad (1.22)$$

where

$$\hat{\omega}_{n} = \omega_{n} + \Gamma \omega_{n} / |\omega_{n}| , \qquad (1.24)$$

$$\phi_{\alpha}(\hat{\omega}_{n}) = -n_{I}(2l+1) \langle |V|^{2} E_{I\alpha}/(\hat{\omega}_{n}^{2} + E_{I\alpha}^{2}) \rangle , \qquad (1.25)$$

$$\Gamma = \pi N(0) \left| V \right|^2 \,. \tag{1.26}$$

The term in Eq. (1.23) multiplying ω_n is the fractional admixture of conduction electrons of spin α into the localized states. The next two terms are the electron lifetime due to potential scattering, $1/\tau_1$, and that due to scattering of electrons of spin α by the localized impurity, respectively. Γ is the half-width of the resonance while $\phi_{\alpha}(\hat{\omega}_n)$ is the energy contribution due to the polarization of conduction electrons by the internal-exchange field. The angular bracketing represents an average over impurity spin orientation (see Appendix A).

The vertex functions are given by the diagrams in Fig. 1:

$$\Lambda_{s}(\vec{q}, i\omega_{n}, -i\omega_{n})_{\pm} = \frac{1 - n_{I}(2l+1) \langle |V|^{2} / [(\hat{\omega}_{n} \pm iv)^{2} + E_{i}^{2}] \rangle d}{1 - \{1/\tau_{1} + 2n_{I}(2l+1) \langle |V|^{2} \Gamma / [(\hat{\omega}_{n} \pm iv)^{2} + E_{i}^{2}] \rangle \} \{(1/|\overline{\omega}_{n\pm}|) [1 - \frac{1}{3}(v_{F}q/\overline{\omega}_{n\pm})^{2}] \}} , \quad (1.27)$$

$$\Lambda_{l}(\mathbf{\bar{q}}, i\omega_{n}, -i\omega_{n})_{\pm} = -d + 2\Gamma(1/\left|\overline{\omega}_{n\pm}\right|) \left[1 - \frac{1}{3}(v_{F}q/\overline{\omega}_{n\pm})^{2}\right] \Lambda_{s}(\mathbf{\bar{q}}, i\omega_{n}, -i\omega_{n})_{\pm} , \qquad (1.28)$$

where

$$\left|\overline{\omega}_{n\pm}\right| \equiv \left|\widetilde{\omega}_{n+}\right| + \left|\widetilde{\omega}_{n+}\right| \pm i I(\widetilde{\omega}_n) , \quad I(\widetilde{\omega}_n) \equiv \phi_{+}(\widetilde{\omega}_n) - \phi_{+}(\widetilde{\omega}_n) , \quad \hat{\omega}_{n\pm} \equiv \hat{\omega}_{n\pm} i v .$$

The calculation of these vertex functions is considered in Appendix B.

At the phase boundary, H_{c2} and T_{c0} are given by the coupled equations

$$K_s(q^2) = 1/|g|$$
, (1.29)

$$K_{I}(q^{2}) = -[n_{I}(2l+1)/U]d^{2}, \qquad (1.30)$$

for $q^2 = 2eH_{c2}$ and $q^2 = 0$, respectively. The second equation provides an expression for d, which is contained in the first equation:

$$\overline{K}_{s}(q^{2}) = \pi N(0) k_{B} T \sum_{n}' \sum_{\pm} \frac{\left[1 - \langle n_{I}(2l+1) | V |^{2} / (\hat{\omega}_{n\pm}^{2} + E_{I}^{2}) \rangle d \right]}{B(q^{2}, |\overline{\omega}_{n\pm}|)^{-1} - \left[1 / \tau_{1} + \langle 2n_{I}(2l+1) | V |^{2} / (\hat{\omega}_{n\pm}^{2} + E_{I}^{2}) \Gamma \rangle \right]},$$
(1.31)

$$\overline{K}_{d}(q^{2}) = \frac{1}{2} d^{2} n_{I}(2l+1) \sum_{n=\infty} \sum_{\pm} \left(\frac{1}{\hat{\omega}_{n\pm}^{2} + E_{I}^{2}} \right) - d\pi N(0) k_{B} T \sum_{n} \sum_{\pm} \frac{\langle n_{I}(2l+1) | V|^{2} / (\hat{\omega}_{n\pm}^{2} + E_{I}^{2}) \rangle \left[1 - \langle n_{I}(2l+1) | V|^{2} / (\hat{\omega}_{n\pm}^{2} + E_{I}^{2}) \rangle d \right]}{B(q^{2}, |\overline{\omega}_{n\pm}|)^{-1} - \left[1 / \tau_{1} + \langle 2n_{I}(2l+1) | V|^{2} / (\hat{\omega}_{n\pm}^{2} + E_{I}^{2}) \Gamma \rangle \right]},$$
(1.32)

where

$$B(q^{2}, \left|\overline{\omega}_{n\pm}\right|)^{-1} = \frac{\left|\overline{\omega}_{n\pm}\right|}{1 - \frac{1}{3}(v_{F}q)^{2}/\left|\overline{\omega}_{n\pm}\right|^{2}} \quad .$$
(1.33)

For $\Gamma \gg 2\pi k_B T$

$$\frac{1}{2}k_{B}T\sum_{n=-\infty}^{\infty}\sum_{\pm}\left(\frac{1}{\hat{\omega}_{n\pm}^{2}+E_{I}^{2}}\right)\approx\frac{1}{2\pi}\int_{0}^{\infty}d\omega\left(\frac{1}{(\omega+\Gamma+i\nu)^{2}+E_{I}^{2}}+\frac{1}{(\omega+\Gamma-i\nu)^{2}+E_{I}^{2}}\right)$$
$$=\frac{1}{\pi}\left(\frac{1}{E_{I_{1}}+E_{I_{1}}}\right)\left[\arctan\left(\frac{E_{I_{1}}}{\Gamma}\right)+\arctan\left(\frac{E_{I_{1}}}{\Gamma}\right)\right].$$
(1.34)

Define U_{eff} so that

$$\frac{1}{U_{eff}} - \frac{1}{U} = \frac{1}{\pi} \left(\frac{1}{E_{I} + E_{I}} \right) \left[\arctan\left(\frac{E_{I}}{\Gamma} \right) + \arctan\left(\frac{E_{I}}{\Gamma} \right) \right] .$$
(1.35)

 $U_{\rm eff}$ is the effective Coulomb repulsion experienced by localized electrons of opposite spin. Consider

$$\left\langle \frac{n_{I}(2l+1)|V|^{2}}{\hat{\omega}_{n\pm}^{2}+E_{I}^{2}} \right\rangle = \left\langle n_{I}(2l+1)|V|^{2} \frac{\hat{\omega}_{n}^{2}+E_{I}^{2}+v^{2}-2v^{2}\mp 2i\hat{\omega}_{n}v}{(\hat{\omega}_{n}^{2}+E_{I},E_{I})^{2}+4\hat{\omega}_{n}^{2}v^{2}} \right\rangle \quad .$$
(1.36)

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We rewrite this as

$$\left\langle c(\hat{\omega}_n) - \frac{1}{2\tau_s(\hat{\omega}_n)\Gamma} \mp i \frac{1}{2\tau_s(\hat{\omega}_n)\Gamma} \frac{\hat{\omega}_n}{v} \right\rangle.$$
 (1.37)

For v = 0 (nonmagnetic limit) this is just $c(\hat{\omega}_n)$. Using

$$E_{1}^{2} + E_{1}^{2} = 2E_{1}, E_{1} + 4v^{2} = 2E_{1}^{2} + 2v^{2} , \qquad (1.38)$$

$$\frac{1}{2} \left\langle n_{I}(2l+1) \left| V \right|^{2} \left(\frac{1}{\hat{\omega}_{n}^{2} + E_{I}^{2}} + \frac{1}{\hat{\omega}_{n}^{2} + E_{I}^{2}} \right) \right\rangle = c(\hat{\omega}_{n}) .$$
(1.39)

Thus

$$\left|\overline{\omega}_{n\pm}\right| = \left[1 + c(\widehat{\omega}_n)\right] 2 \left|\omega_n\right| + 1/\tau_1 + 2c(\widehat{\omega}_n)\Gamma \pm i\langle I(\widehat{\omega}_n)\rangle$$
(1.40)
and

we find that

$$\frac{1}{B(q^{2}, |\overline{\omega}_{n\pm}|)^{-1} - [1/\tau_{1} + \langle n_{I}(2l+1)|V|^{2}/(\widehat{\omega}_{n\pm}^{2} + E_{I}^{2})2\Gamma\rangle]} = \left[1 - \frac{1}{3}\left(\frac{v_{F}q}{|\overline{\omega}_{n\pm}|}\right)^{2}\right] \left[2[1 + c(\widehat{\omega}_{n})|\omega_{n}| + \tau_{s}(\widehat{\omega}_{n})^{-1} \pm i\left\langle I(\widehat{\omega}_{n}) + \frac{\widehat{\omega}_{n}}{\tau_{s}(\widehat{\omega}_{n})v}\right\rangle + \left(\frac{1}{\tau_{1}} + 2c(\widehat{\omega}_{n})\Gamma - \tau_{s}(\widehat{\omega}_{n})^{-1} \pm i\left\langle\frac{\widehat{\omega}_{n}}{\tau_{s}(\widehat{\omega}_{n})v}\right\rangle\right)\frac{(v_{F}q)^{2}}{3|\overline{\omega}_{n\pm}|^{2}}\right]^{-1}. (1.41)$$

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Using (1.36), (1.37), and (1.40) we define

$$P(\hat{\omega}_n) \equiv I(\hat{\omega}_n) + \frac{\hat{\omega}_n}{\tau_s(\hat{\omega}_n)v} = 2n_I(2l+1) |V|^2 \frac{(\Gamma^2 + E_I^2 - v^2 - \omega_n^2)v}{(\hat{\omega}_n^2 + E_I)^2 + 4\hat{\omega}_n^2 v^2}.$$
 (1.42)

 $\langle P(\hat{\omega}_n) \rangle$ is the total polarization of conduction electrons by the internal exchange field. For randomly oriented spins this average is zero.

In the dirty limit

$$\frac{1}{3} \frac{1/\tau_1 + [2c(\hat{\omega}_n)\Gamma - \tau_s(\hat{\omega}_n)^{-1} \mp i \langle \hat{\omega}_n / \tau_s(\hat{\omega}_n)v \rangle] (v_F q)^2}{\{2[1 + c(\hat{\omega}_n)] | \omega_n | + 1/\tau_1 + 2c(\hat{\omega}_n)\Gamma \pm i \langle I(\hat{\omega}_n) \rangle\}^2}$$

10

$$-\left(\frac{1}{1/\tau_1 + 2c(\hat{\omega}_n)\Gamma \pm i\langle I(\hat{\omega}_n)\rangle} - \frac{\tau_s(\hat{\omega}_n)^{-1} \pm i\langle P(\hat{\omega}_n)\rangle}{[1/\tau_1 + 2c(\hat{\omega}_n)\Gamma \pm i\langle I(\hat{\omega}_n)\rangle]^2}\right) \frac{(v_F q)^2}{3} \quad . \tag{1.43}$$

Assuming that

$$\tau_{s}(\hat{\omega}_{n})^{-1}, \quad \langle P(\hat{\omega}_{n}) \rangle, \quad \langle I(\hat{\omega}_{n}) \rangle \ll 1/\tau_{1} + 2c \, (\hat{\omega}_{n}) \Gamma, \tag{1.44}$$

this becomes

$$\frac{1}{1/\tau_1 + 2c(\hat{\omega}_n)\Gamma} \frac{(v_F q)^2}{3} = \tau(\hat{\omega}_n) \frac{(v_F q)^2}{3} . \tag{1.45}$$

Using the above definitions we have, in the dirty limit

$$2\pi N(0)k_{B}T\sum_{n}'\operatorname{Re}\left(\frac{1-c(\hat{\omega}_{n})[1-\tau_{\operatorname{res}}(\hat{\omega}_{n})/\tau_{\mathfrak{s}}(\hat{\omega}_{n})]d+i\langle\hat{\omega}_{n}/2\tau_{\mathfrak{s}}(\hat{\omega}_{n})v\Gamma\rangle d}{2[1+c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{\mathfrak{s}}(\hat{\omega}_{n})^{-1}+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}+i\langle P(\hat{\omega}_{n})\rangle}\right) = \frac{1}{|g|}, \qquad (1.46)$$

$$2\pi N(0)k_{B}T\sum_{n}'\operatorname{Re}\left(\left\{\left[c(\hat{\omega}_{n})\left(1-\frac{\tau_{\operatorname{res}}(\hat{\omega}_{n})}{\tau_{\mathfrak{s}}(\hat{\omega}_{n})}\right)-i\langle\frac{\hat{\omega}_{n}}{2\tau_{\mathfrak{s}}(\hat{\omega}_{n})v\Gamma}\right\rangle\right]\right\}$$

$$\times\left[1-c(\hat{\omega}_{n})\left(1-\frac{\tau_{\operatorname{res}}(\hat{\omega}_{n})}{\tau_{\mathfrak{s}}(\hat{\omega}_{n})}\right)d+i\langle\frac{\hat{\omega}_{n}}{2\tau_{\mathfrak{s}}(\hat{\omega}_{n})v\Gamma}\right\rangle\right]\right\}$$

$$\times\left\{2[1-c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{\mathfrak{s}}(\hat{\omega}_{n})+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}+i\langle P(\hat{\omega}_{n})\rangle\}^{-1}\right]=\frac{n_{I}(2l+1)}{U_{eff}}d, \qquad (1.47)$$

where

$$1/\tau_{res}(\hat{\omega}_n) \equiv 2c \, (\hat{\omega}_n) \Gamma \quad . \tag{1.48}$$

Using the definitions of $c(\hat{\omega}_n)$, $1/\tau_s(\hat{\omega}_n)$, [(1.36) and (1.37)] and $P(\hat{\omega}_n)$ [(1.41)], it may be shown that the first of the above equations corresponds exactly to the result of Shiba¹³ [Eq. (3.13) in his paper] if q^2 is set equal to zero in (1.46) and (1.47).

Using the fact that the sum over Matsubara frequency in (1.46) and (1.47) is symmetric, we find the real parts

$$2\pi N(0)k_{B}T\sum_{n}'\frac{\{1-c(\hat{\omega}_{n})[1-\tau_{res}(\hat{\omega}_{n})/\tau_{s}(\hat{\omega}_{n})]d\}\{2[1+c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{s}(\hat{\omega}_{n})^{-1}+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}\}}{\{2[1+c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{s}(\hat{\omega}_{n})^{-1}+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}\}^{2}+\langle P(\hat{\omega}_{n})\rangle^{2}}=\frac{1}{|g|}, \qquad (1.49)$$

$$2\pi N(0)k_{B}T\sum_{n}'\left\{c(\hat{\omega}_{n})\left(1-\frac{\tau_{res}(\hat{\omega}_{n})}{\tau_{s}(\hat{\omega}_{n})}\right)\left[1-c(\hat{\omega}_{n})\left(1-\frac{\tau_{res}(\hat{\omega}_{n})}{\tau_{s}(\hat{\omega}_{n})}\right)d\right]+d\left\langle\frac{\hat{\omega}_{n}}{2\tau_{s}(\hat{\omega}_{n})v\Gamma}\right\rangle^{2}\right\}$$

$$\times\frac{\{2[1+c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{s}(\hat{\omega}_{n})^{-1}+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}\}}{\{2[1+c(\hat{\omega}_{n})]|\omega_{n}|+\tau_{s}(\hat{\omega}_{n})^{-1}+\frac{1}{3}\tau(\hat{\omega}_{n})(v_{F}q)^{2}\}^{2}+\langle P(\hat{\omega}_{n})\rangle^{2}}=\frac{n_{I}(2l+1)}{U_{eff}}d . \qquad (1.50)$$

The term $1 - c(\hat{\omega}_n)[1 - \tau_{\text{res}}(\hat{\omega}_n)/\tau_s(\hat{\omega}_n)]d$ in Eq. (1.49) is a pair-weakening term. In the nonmagnetic case v = 0, so this reduces to $1 - c(\hat{\omega}_n)d$, while in the magnetic case there arises a new term due to exchange scattering. This will be discussed subsequently.

In Appendix C the ω_n dependences of $c(\hat{\omega}_n)$, $[\tau_s(\hat{\omega}_n)]^{-1}$, and $P(\hat{\omega}_n)$ are considered. There, it is found that for

$$\frac{\Gamma}{\Gamma^2 + (|E_I| - |v|)^2} \ll \frac{1}{2\omega_D} , \qquad (1.51)$$

 $(\omega_D = \text{Debye energy})$ the ω_n dependence of these quantities is negligible.

II. CALCULATION OF d

Assuming condition (1.51), the sums may be performed in the standard way¹⁴ to obtain a transcendental equation involving the digamma function ψ :

$$\ln(2\gamma \theta_{D}/\pi T) + \psi(\frac{1}{2}) - \frac{1}{2} [\psi(\frac{1}{2} + \rho^{*}) + \psi(\frac{1}{2} + \rho^{-})] \\ = \langle 1 + c \rangle / (1 - ad) \lambda , \quad (2.1) \\ \frac{a}{|g|} \left[1 + \lambda d \left\langle \frac{1}{2\tau_{s}v} \right\rangle^{2} 2\pi k_{B} T \sum_{n}^{\prime} \left(\frac{\hat{\omega}_{n}}{\Gamma} \right)^{2} \\ \times \frac{2(1 + c) |\omega_{n}| + \tau_{s}^{-1} + \frac{1}{3}\tau(v_{F}q)^{2}}{[2(1 + c) |\omega_{n}| + \tau_{s}^{-1} + \frac{1}{3}\tau(v_{F}q)^{2}]^{2} + \langle P \rangle^{2}} \right] = \frac{n_{I}(2l + 1)d}{U_{eff}}$$
(2.2)

Here $\gamma = 1.78$,



FIG. 1. Diagrammatic equations for the conductionelectron vertex function (Λ_s) and the localized-electron vertex function (Λ_l) to be used in calculating the kernels $K_s(q)$ and $K_l(q)$, represented by the "bubble diagrams."

$$a \equiv c \left(1 - \tau_{\rm res} / \tau_{\rm s}\right) , \qquad (2.3)$$

$$\rho^{\pm} \equiv \frac{1}{4\pi k_{B}T} \left(\frac{\tau_{s}^{-1}}{1+c} + \frac{\frac{1}{3}\tau(v_{F}q)^{2}}{1+c} \pm i \frac{\langle P \rangle}{1+c} \right)$$
$$\equiv \rho^{0} \pm i \frac{\langle P \rangle}{4\pi k_{B}T(1+c)} , \qquad (2.4)$$

and λ is the coupling constant |g|N(0).

If there is no magnetic field, the averages are

$$\langle P \rangle = 2n_{I}(2l+1) |V|^{2} \frac{(\Gamma^{2} + E_{II}) \langle v \rangle}{(\Gamma^{2} + E_{II})^{2} + 4\Gamma^{2} v^{2}} = 0, \quad (2.5)$$

$$\left\langle \frac{1}{2\tau_s v} \right\rangle = 2n_I (2l+1) \left| V \right|^2 \Gamma \frac{\langle v \rangle}{(\Gamma^2 + E_I, E_I)^2 + 4\Gamma^2 v^2} = 0.$$
(2.6)

If it is true that $\Gamma \gtrsim \omega_n$ over the entire range of the sum in (2.2), then as an *upper* estimate of this summation, we may replace $(\hat{\omega}_n/\Gamma)^2 = [(\omega_n/\Gamma) + 1]^2$ by a number on the order of at most 4 to find

$$\frac{a}{|g|} \left(1 + 4 \left\langle \frac{1}{2\tau_s v} \right\rangle^2 \frac{d}{1 - ad} \right) = \frac{n_I (2l+1) d}{U_{eff}} \quad (2.7)$$

This equation is easily solved to obtain *d*:

$$d = \{1 + ad_0 - 4\langle 1/2\tau_s v \rangle^2 - [(4\langle 1/2\tau_s v \rangle^2 - (1 + ad_0))^2 - 4 ad_0]^{1/2} \} (2a)^{-1}, \qquad (2.8)$$

where

$$d_0 = \frac{aU_{eff}}{n_I(2l+1)|g|} \quad . \tag{2.9}$$

Supposing that

$$4 \langle 1/2\tau_s v \rangle^2 \ll 1 + ad_0, \qquad (2.10)$$

we find that

$$d = d_0$$
 . (2.11)

In the following work, we shall assume that Eq. (2.10) is true. It is certainly correct if there is no magnetic field since then $\langle v \rangle = 0$. If $\langle v \rangle \neq 0$, we find (taking $E_t = 0$)

$$\left\langle \frac{1}{\tau_s v} \right\rangle^2 = \left(\frac{n_I (2l+1)}{\pi N(0)} \right)^2$$
$$= \begin{cases} 16 \langle v \rangle^2 / \Gamma^4, \ \Gamma \gg v \\ 1 / \Gamma^2, \ \Gamma \approx v \\ 16 \Gamma^4 / v^6, \ \Gamma \ll v \end{cases}$$

The only questionable case is that of $E_1 = 0$, $\Gamma \sim v$, when Γ is small. However, here it is obvious (see Fig. 2) that the localized electron density of states can *not* be considered slowly varying within the width ω_D of the Fermi surface; hence (1.51) rules out this possibility. Thus, (2.10) is consistent with (1.51).

Equation (2.1) can be rewritten

$$\ln\left(\frac{T}{T_{c0p}}\right) + \frac{c + ad_0}{(1 - ad_0)\lambda} + \frac{1}{2} \left[\psi(\frac{1}{2} + \rho^*) + \psi(\frac{1}{2} + \rho^*)\right] - \psi(\frac{1}{2}) = 0$$
(2.12)

where T_{c0p} is the critical temperature of the pure host in zero magnetic field. The critical temperature of the alloy in zero field is found by setting $T = T_{c0}$ and $q^2 = 0$ and solving. The upper critical field for a bulk sample is found by setting q^2 $= 2eH_{c2}$, and for a parallel thin film by setting q^2 $= 4 \langle [eA(x)]^2 \rangle$, where A(x) is the vector potential and the brackets indicate a spatial average.¹⁵

The parameter c represents the dilution effect discussed in the introduction. It describes the fractional amount of admixture at the Fermi level:

$$c = n_{I}(2l+1) |V|^{2} \frac{\Gamma^{2} + E_{I}^{2} + v^{2}}{(\Gamma^{2} + E_{I}, E_{I})^{2} + 4\Gamma^{2}v^{2}}$$

= $\frac{n_{I}(2l+1)}{N(0)} \frac{1}{2} [N_{I}(0) + N_{I}(0)] = n_{I}(2l+1) \frac{\overline{N}_{I}(0)}{N(0)}$.
(2.13)

 $\overline{N}_{l}(0)$ is the spin-averaged density of localized states at the Fermi level. We can rewrite Eq. (2.9) as



FIG. 2. Illustration of the appearance of the virtual states. States are occupied up to the last horizontal line. E is the average of the energies of the spin-up and spin-down localized states, and 2v is the energy splitting, giving a measure of the localized moment at the impurity site.

where $\tau_{\rm res}$ is given by Eq. (1.48):

$$1/\tau_{res} = 2n_{I}(2l+1)[\overline{N}_{l}(0)/N(0)]\Gamma$$

$$= 2n_{I}(2l+1)\pi \overline{N}_{l}(0) |V|^{2} . \qquad (2.15)$$

Using Eq. (2.13) and

$$\frac{1}{\tau_s} = n_I (2l+1) \left| V \right|^2 \frac{4\Gamma v^2}{(\Gamma^2 + E_I, E_I)^2 + 4\Gamma^2 v^2} , \qquad (2.16)$$

the ratio

$$\frac{\tau_{\rm res}}{\tau_{\rm s}} = \frac{2v^2}{\Gamma^2 + E_l^2 + v^2} \quad , \tag{2.17}$$

hence

$$1 - \frac{\tau_{\text{reg}}}{\tau_s} = \frac{\Gamma^2 + E_1^2 - v^2}{\Gamma^2 + E_1^2 + v^2} . \qquad (2.18)$$

 $1/\tau_{\rm res}$ is the rate at which conduction electrons are scattered by the resonance, while $1/\tau_{\rm s}$ measure the rate of "spin-flip" scattering. Note, in (2.17), that in the magnetic limit, $U + 2lJ \gg \Gamma$, we have (choosing J = 0)

$$\frac{\tau_{\rm res}}{\tau_{\rm s}} = \frac{2}{(E_{\rm I}/v)^2 + 1} ,$$

which has a maximum value of 2 ($E_1 = 0$) and a minimum value of ($E_1/v \sim 0$)

$$\frac{2}{(4l+1)^2+1} = \begin{cases} \frac{1}{41} , & l=2\\ \frac{1}{85} , & l=3 \end{cases}$$

Of course, outside of the magnetic limit, the minimum value of (2.17) is obtained for v = 0. The fact that τ_{res}/τ_s is always nonzero for $v \neq 0$ is a manifestation of the interdependence of the "resonant" and "spin-flip" scattering of conduction electrons from the localized impurity states. In fact, the spin-flip scattering occurs via the same process as resonant scattering.

Consider the pair-weakening term

$$ad_0 = \frac{\overline{N}_I(0) U_{eff}}{\lambda} c \left(1 - \frac{\tau_{res}}{\tau_s}\right)^2. \qquad (2.19)$$

This represents the total effect of the pair weakening via conduction-electron admixture into the localized levels which are correlated by the Coulomb repulsion $U_{\rm eff}$. The pair weakening is controlled by the balance between resonant and spinflip scattering, $1/\tau_{\rm res}$ and $1/\tau_s$, respectively. When these two types of scattering are indistinguishable, in the sense that they occur at the same rate, the effects of $U_{\rm eff}$ on the pairing are totally given by the pair-breaking term. When spin-flip and resonance scattering are distinguishable, occurring at different rates, then two distinct effects on T_{c0} (and H_{c2}) become distinguishable: opposition of the pairing by U_{eff} (pair weakening) and pair breaking. In a superconductor, this interdependence of pair-breaking and pair-weakening mechanisms is a basic feature of the Anderson model.

Comparing (2.17) with the requirement of (1.51), we see that

$$\tau_{\rm res}/\tau_s \ll 2v^2/\omega_D \Gamma \quad . \tag{2.20}$$

For the magnetic limit $U + 2lJ \gg \Gamma$, this is not very restrictive.

In the magnetic limit, *c* and *ad* are negligible since $U + 2lJ \gg \Gamma$ so (2.12) becomes

$$\ln\left(\frac{T}{T_{c0p}}\right) + \frac{1}{2} \left[\psi\left(\frac{1}{2} + \frac{1}{4\pi k_B T \tau_s} + \frac{v_F^2 \tau}{12\pi k_B T} q^2 + i \frac{\langle P \rangle}{4\pi k_B T}\right) + \psi\left(\frac{1}{2} + \frac{1}{4\pi k_B T \tau_s} + \frac{v_F^2 \tau}{12\pi k_B T} q^2 - i \frac{\langle P \rangle}{4\pi k_B T}\right)\right] - \psi\left(\frac{1}{2}\right) = 0, \quad (2.21)$$

which is the Abrikosov-Gorkov result if $q^2 = 0$, $\langle P \rangle = 0$, and the Fulde-Maki result if $q^2 = 2eH_{c2}$ and $\langle P \rangle \neq 0$ (see Sec. III).

In the nonmagnetic limit v = 0, so (2.12) is

$$\ln\left(\frac{T}{T_{c0p}}\right) + \frac{c(1+d_0)}{(1-cd_0)\lambda} + \psi\left(\frac{1}{2} + \frac{v_F^2 \tau q^2}{12\pi k_B T(1+c)}\right) - \psi(\frac{1}{2}) = 0, \quad (2.22)$$

which is (for q = 0) Kaiser's result. Note that this equation also gives H_{c2} at all temperatures and concentrations for a nonmagnetic localized impurity.

If

$$\rho^{0} \gg \langle P \rangle / 4\pi k_{B} T (1+c)$$
 (2.23)

(negligible exchange field polarization) then (2.12) may be written

$$\ln\left[\left(\frac{T}{T_{c0p}}\right)\exp\left(\frac{c+ad_{0}}{(1-ad_{0})\lambda}\right)\right]+\psi\left(\frac{1}{2}+\frac{\alpha}{4\gamma(T/T_{c0p})}\right)$$
$$+\frac{\tau H_{c2}(T)}{\tau^{0}H_{c2}^{0}(0)}\frac{1}{4\gamma(T/T_{c0p})(1+c)}-\psi(\frac{1}{2})=0, \quad (2.24)$$

where

$$\begin{aligned} \alpha &= \frac{\gamma}{\pi k_B T_{c0p} \tau_s(1+c)} , \quad \text{for } \gamma = 1.78 \\ H_{c2}^0(0) &= \frac{3\pi k_B T_{c0p}}{2e \gamma v_B^2 \tau^0} . \end{aligned}$$

Also, τ^0 and $H^0_{c2}(0)$ refer to the host without the localized impurities.

(3.1)

III. COMPARISON WITH EXCHANGE MODEL

The Fulde-Maki¹⁶ expression for the critical temperature and upper critical field of an alloy with magnetic impurities described by the exchange model is

$$\ln (T/T_{c0\phi}) + \frac{1}{2} [\psi(\frac{1}{2} + \rho_{FM}^{*}) + \psi(\frac{1}{2} + \rho_{FM}^{-})] - \psi(\frac{1}{2}) = 0,$$

where

$$\rho_{\rm FM}^{\pm} \equiv \frac{1}{4\pi k_B T} \left(\frac{2}{\tau_2} \left\langle \frac{\langle S_z^2 + S_x^2 \rangle}{S^2} + \frac{v_F^2}{3} \tau 2 e H_{c2} \right. \right. \\ \left. \pm i 2n_I J_{\rm ex}(0) \left\langle S_z \right\rangle \right) \quad . \tag{3.2}$$

(We have taken $1/\tau_{so} \rightarrow 0$ in their expression.)

Comparing the above with Eq. (2.21), we make the identifications

$$\frac{1}{\tau_s} = \frac{2}{\tau_2} \frac{\langle S_z^2 + S_x^2 \rangle}{S^2}$$
$$= 2n_I \pi N(0) J_{ex}^2 \langle S_z^2 + S_x^2 \rangle, \qquad (3.3)$$

$$\langle P \rangle = 2n_I J_{\text{ex}} \langle S_{\text{e}} \rangle . \tag{3.4}$$

Recalling (2.16) and (1.41), as well as the definition of v (1.10) we have

$$\langle S_{z}^{2}+S_{x}^{2}\rangle = \frac{1}{2}(\langle n_{\star}\rangle - \langle n_{\star}\rangle)^{2}(2l+1), \qquad (3.5)$$

$$J_{ex}^{2} = |V|^{4} \left[(U + 2lJ)^{2} / (E_{l}, E_{l})^{2} \right], \qquad (3.6)$$

$$\langle S_{z} \rangle = \frac{1}{2} (2l+1) (\langle n_{*} \rangle - \langle n_{*} \rangle), \qquad (3.7)$$

$$J_{ex} = -|V|^{2}(U+2lJ)/E_{l} E_{l}$$
(3.8)

(for $U + 2lJ \gg \Gamma$).

The Schrieffer-Wolff transformation gives, for $N(0) J_{\rm ex} \ll 1$, the result (3.8) for $J_{\rm ex}$. Note that a comparison of the Fulde-Maki expression with the more general equation (2.12) is not possible since this equation contains an extra contribution due to pair weakening. We can only make unambiguous contact with the Fulde-Maki result in the magnetic limit, where the pair-weakening effects are negligible.

IV. RESULTS FOR T_{c0} AND H_{c2}

Let

$$\boldsymbol{\zeta} \equiv \left(\boldsymbol{\alpha} + \frac{\tau H_{c2}(T)}{\tau^0 H_{c2}^0(0)} \; \frac{1}{1+c} \right) \exp\left(\frac{c + ad_0}{(1-ad_0)\lambda}\right) \tag{4.1}$$

in Eq. (2.24). The solutions for ζ as a function of

$$t' \equiv \frac{T}{T_{c0p}} \exp\left(\frac{c + ad_0}{(1 - ad_0)\lambda}\right)$$
(4.2)

are tabulated¹⁷ so that we may write

$$\boldsymbol{\zeta} = \boldsymbol{U}(\boldsymbol{t}'), \qquad (4.3)$$

instead of $\ln t' + \psi(\frac{1}{2} + \zeta/4\gamma t') - \psi(\frac{1}{2}) = 0$.

When no magnetic field is present the critical

temperature is given by

$$T_{c0} = T_{c0\phi} \exp\left(\frac{-c - ad_0}{(1 - ad_0)\lambda}\right) U^{-1} \left[\alpha \exp\left(\frac{c + ad_0}{(1 - ad_0)\lambda}\right)\right].$$
(4.4)

The initial slope of T_{c0}/T_{c0p} with respect to concentration n_I is [using (2.24)]

$$\frac{d(T_{c0}/T_{c0p})}{dn_{I}}\Big|_{n_{I}=0} = -\frac{1}{\lambda} \left. \frac{c+ad_{0}}{n_{I}} \right|_{n_{I}=0} -\frac{\psi^{(1)}(\frac{1}{2})}{4\pi k_{B}T_{c0p}} \left. \frac{\tau_{s}^{-1}}{n_{I}} \right|_{n_{I}=0}, \quad (4.5)$$

where $\psi^{(1)}(\frac{1}{2})$ is the trigamma function. Using Eqs. (2.3), (2.13), (2.16), (2.18), and (2.19) this may be written

$$\frac{d(T_{c0}/T_{c0b})}{dn_{I}}\Big|_{n_{I}=0} = -\frac{b+D(1-x)^{2}}{\lambda} - \frac{\pi^{2}b\Gamma}{4\gamma\Delta_{00}}x,$$
(4.6)

where we have introduced the concentration-independent parameters

$$b \equiv c/n_{I} = (2l+1) N_{I}(0)/N(0) , \qquad (4.7)$$

$$D \equiv \frac{c}{n_{I}} \frac{U_{eff} \overline{N}_{I}(0)}{\lambda}$$

$$= \frac{c}{n_{I}} \frac{\overline{N}_{I}(0)}{\lambda}$$

$$\times \frac{U}{1 + (U/2E) [\arctan(E_{II}/\Gamma) + \arctan(E_{II}/\Gamma)]} , \qquad (4.8)$$

$$x \equiv \tau_{\rm res} / \tau_s , \qquad (4.9)$$

$$\Delta_{00} = \pi k_B T_{c0p} / \gamma . \qquad (4.10)$$

Note from Eq. (2.17) that x ranges from 0 to 2 as v varies.

In terms of the above parameters

$$\alpha = \frac{1}{(1 + n_I b) \Delta_{00} \tau_{res}} x$$

= $\frac{2n_I b \Gamma}{(1 + n_I b) \Delta_{00}} x \equiv \frac{n_I \alpha_0 x}{1 + n_I b}$, (4.11)

$$\boldsymbol{\zeta} = \begin{pmatrix} n_{I} \alpha_{0} x \\ 1 + n_{I} b \end{pmatrix} + \frac{\tau H_{c2}(T)}{\tau^{0} H_{c2}^{0}(0)} \frac{1}{1 + n_{I} b} \\ \times \exp\left(n_{I} \frac{b + D(1 - x)^{2}}{[1 - n_{I} D(1 - x)^{2}]\lambda}\right) .$$
(4.12)

For $x \ll 1$, Eq. (4.6) is

$$\frac{d(T_{c0}/T_{c0b})}{dn_{I}}\Big|_{n_{I}=0} = -\frac{b+D}{\lambda} - 1.38 \frac{b\Gamma}{\Delta_{00}} x . \quad (4.13)$$

In Fig. 3 we have displayed the quantity T_{c0}/T_{c0p} as a function of concentration for b = 30, D = 30, $\lambda = 0.2$, and various values of $\alpha_0 x$, where $x \ll 1$ is satisfied. Values for α_0 probably range up from $\alpha_0 = 1000$. For $\alpha_0 = 5000$, an x as small as x = 0.025



FIG. 3. Solid lines: Graphs of the critical temperature of the alloy (no magnetic field) divided by the critical temperature of the pure host (T_{c0}/T_{c0p}) for $\alpha_0 = 1000$, $\Gamma = 16\frac{2}{3}\Delta_{00}$, and various values of x. Dashed lines: Graphs of the same for $\alpha_0 = 5000$, $\Gamma = 83\frac{1}{3}$ Δ_{00} .

gives rise to a substantial deviation from any prediction based on Kaiser's theory. There is also a substantial difference between results for x at this value and the Abrikosov-Gorkov result.

Near the critical concentration $(T_{c0}/T_{c0\rho}|_{n_{cr}}=0)$ the digamma function in (1.24) behaves like the logarithm, thus

$$n_{\rm cr} \alpha_0 x = 4\gamma (1 + n_{\rm cr} b) \exp\left(-n_{\rm cr} \frac{b + D(1 - x)^2}{[1 - n_{\rm cr} D(1 - x)^2]\lambda}\right).$$
(4.14)

For x = 0 this gives Kaiser's result.

$$n_{\rm cr} = 1/D$$
 . (4.15)

For $x \neq 0$ but $x \ll 1$ we have

$$n_{\rm er} = \frac{1}{\alpha_0 x - 4\gamma b \exp[-n_{\rm er}(b+D)/(1-n_{\rm er}D)\lambda]} \times 4\gamma \exp\left(-n_{\rm er}\frac{b+D}{(1-n_{\rm er}D)\lambda}\right) . \tag{4.16}$$

If $n_{\rm cr}$ is slightly less than 1/D, this is approximately

$$n_{\rm cr} \approx \frac{4\gamma}{\alpha_0 x} \exp\left(-n_{\rm cr} \frac{b+D}{(1-n_{\rm cr}D)\lambda}\right)$$
 (4.17)

Of course, for this $n_{\rm cr}$, x is quite small. Thus the critical concentration varies initially quite rapidly with x. From (4.16) it can be seen that for $n_{\rm cr} \ll 1/D$ and $n_{\rm cr}(b+D)/\lambda \ll 1$,

$$n_{\rm cr} \approx 4\gamma / \alpha_0 x$$
, (4.18)

the Abrikosov-Gorkov result. Note that this requires

$$(2 b \Gamma / \Delta_{00}) x = \alpha_0 x \gg (4 \gamma / \lambda) (b + D) , \qquad (4.19)$$

which means that the initial slope (4.13) will also follow the Abrikosov-Gorkov result. Note that Fig. 1, however, considers the opposite case

$$\alpha_0 x \ll (4\gamma/\lambda)(b+D) , \qquad (4.20)$$

as well as $\alpha_0 x \sim (4\gamma/\lambda)(b+D)$.

Identifying $\alpha_0 x$ as the pair-breaking parameter and $(4\gamma/\lambda)(b+D)$ as the pair-weakening parameter, from Fig. 3 we conclude that for pair weakening, which is much stronger than pair breaking, one may observe a situation where the shape of the T_{c0} vs- n_I curve may retain the exponential-type variation which is characteristic of nonmagnetic impurity down to very low temperatures. That is to say, an impurity with a small magnetic moment may appear to behave as one with no magnetic moment even down to $T_{c0}/T_{c0p} \sim 0.1$. For larger $\alpha_0 x$, the curve may appear linear down to such a value (as for $\alpha_0 x = 250$).

The lesson of Fig. 3 is that there exists a "transition region" between the nonmagnetic impurity (Kaiser) result for the shape of the T_{c0}/T_{c0p} -vs- n_I curve, and the magnetic (Abrikosov-Gorkov) result for the shape, where neither limiting theory gives an adequate description of the results.

The upper critical field (for a bulk sample) may be calculated as a function of temperature using

$$\frac{\tau H_{c2}(T)}{\tau^0 H_{c2}^0(0)} = (1 + n_I b) \exp\left(-n_I \frac{b + D(1 - x)^2}{[1 - n_I D(1 - x)^2]\lambda}\right)$$
$$\times U(t') - n_I \alpha_0 x \qquad (4.21)$$



FIG. 4. Graph of $\tau H_{c2}/\tau^0 H_{c2}^0(0)$ vs reduced temperature (T/T_{c0}) for x = 0 and various concentrations.

[t' is defined in Eq. (4.2)].

In Figs. 2 and 3 the results for $\tau H_{c2}(T)/\tau^0 H_{c2}^0(0)$ vs T/T_{c0} are given at various values of concentration for $\alpha_0 x = 0$ and $\alpha_0 x = 78$, respectively. Here T_{c0} is the critical temperature of the alloy at the concentration and value of x indicated in zero magnetic field, i.e., the solution of Eq. (4.4). All other parameters are as they were in Fig. 3. At low concentrations (~250 ppm) the increase in pair breaking is not very evident. However, the effect of approaching the critical concentration is clearly evident in Fig. 5 for concentrations greater than 2000 ppm. From Fig. 3 we observe that the critical concentration for $\alpha_0 x = 78$ is slightly greater than 4000 ppm, which explains the intercept of the 4000 ppm curve in Fig. 5. In Fig. 5 one observes the expected result of a larger α_0 , a more rapid decrease in H_{c2} with increasing concentration.

The lesson of Figs. 4 and 5 is much the same as that of Fig. 3. Even a small amount of exchange scattering has drastic effects on the superconducting alloy. These effects, however, may not be strongly in evidence until one attains concentrations nearing the critical concentration, since the major effect of small pair breaking (compared to pair weakening) is the rapid reduction in critical concentration.

One may conclude that an exponential decline of

 T_{c0} with concentration does *not* necessarily imply that the impurity is nonmagnetic, but that, far enough away from the critical concentration, the description in terms of the Kaiser model is probably quite good, and will break down only as the critical concentration is approached. However, there also exists a "transition region" between Kaiser and Abrikosov-Gorkov behavior in which the alloy is best described in terms of an amalgam of the two theories, with the phase boundary determined by Eq. (2. 24). In this case, both pair breaking and pair weakening must be included. The influence of pair breaking is strongest at the higher concentrations, while the pair weakening has its greatest influence for smaller concentrations.

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FIG. 5. Solid lines: Graphs of $\tau H_{c2}/\tau^0 H_{c2}^0(0)$ vs T/T_{c0} for x = 0.078, $\alpha_0 = 1000$, and $\Gamma = 16\frac{2}{3}\Delta_{00}$. Dashed lines: Graphs of same for x = 0.078, $\alpha_0 = 5000$, and $\Gamma = 83\frac{1}{3}\Delta_{00}$.

G. B. ARNOLD

APPENDIX A: SELF-ENERGIES

Prior to configuration averaging, the self-energy for a conduction electron is given to second order as

$$\Sigma(\vec{k}, \vec{k}'', i\omega_n)_{\alpha} = \sum_{k'} \frac{1}{N} \sum_{i=1}^{N_I} e^{-i(\vec{k}-\vec{k}')\vec{R}_i} W(\vec{k}-\vec{k}') G^{(0)}(\vec{k}', i\omega_n)_{\alpha} \frac{1}{N} \sum_{n=1}^{N_I} e^{-i(\vec{k}'-\vec{k}'')R_j} W(\vec{k}'-\vec{k}'') + \sum_{m} \frac{1}{N} \sum_{i=1}^{N_I} e^{-i(\vec{k}+\vec{k}'')R_i} V_m(\vec{k}) V_m(\vec{k}'') C_i^{(0)}(i\omega_n)_{\alpha}^m,$$
(A1)

where $C_i^{(0)}(i_{\ell_i})_{\alpha}^m = 1/(i\omega_n - E_i - v_i\alpha)$ and N is the total number of lattice points.

We have taken $\langle n_{ii} \rangle + \langle n_{ii} \rangle$ to be a *constant* for all *i*, but $\langle n_{ii} \rangle - \langle n_{ii} \rangle$ may vary from site to site. In Eqs. (1.8)-(1.10) we suppressed the index for simplicity of notation.

The average of the above all possible lattice points is introduced formally as

$$\begin{split} \overline{\Sigma}(\vec{k},\vec{k}^{\prime\prime},i\omega_{n})_{\alpha} &= \sum_{k'}^{-1} \frac{1}{N} \sum_{i=1}^{-1}^{-1} \left(\frac{1}{N} \sum_{l=1}^{N} e^{-i(\vec{k}\cdot\vec{k}^{\prime\prime})\vec{R}_{l}} \right) W(\vec{k}-\vec{k}^{\prime}) G^{(0)}(\vec{k}^{\prime},i\omega_{n})_{\alpha} W(\vec{k}^{\prime}-\vec{k}^{\prime\prime}) \\ &+ \sum_{k'}^{-1} \frac{1}{N} \sum_{i=1}^{N} \left(\frac{1}{N} \sum_{l=1}^{N} e^{-i(\vec{k}\cdot\vec{k}^{\prime\prime})\vec{R}_{l}} \right) \frac{1}{N} \sum_{j\neq 1}^{-1} \left(\frac{1}{N} \sum_{l'=1}^{N} e^{-i(\vec{k}^{\prime}-\vec{k}^{\prime\prime})\vec{R}_{l'}} \right) W(\vec{k}-\vec{k}^{\prime}) G^{(0)}(\vec{k}^{\prime},i\omega_{n})_{\alpha} W(\vec{k}^{\prime}-\vec{k}^{\prime\prime}) \\ &+ \sum_{m}^{-1} \frac{1}{N} \sum_{i=1}^{N} \left(\frac{1}{N} \sum_{l=1}^{N} e^{-i(\vec{k}\cdot\vec{k}^{\prime\prime})\vec{R}_{l}} \right) V_{m}(\vec{k}) V_{m}(\vec{k}^{\prime\prime}) C_{i}^{(0)}(i\omega_{n})_{\alpha}^{m} \\ &= n_{I} \sum_{k'} \left| W(\vec{k}-\vec{k}^{\prime}) \right|^{2} G^{(0)}(\vec{k}^{\prime},i\omega_{n})_{\alpha} \delta_{kk''} + n_{I} \left(n_{I} - \frac{1}{N} \right) W(0) W(\vec{k}-\vec{k}^{\prime\prime}) \delta_{k,k''} G^{(0)}(\vec{k},i\omega_{n})_{\alpha} \\ &+ n_{I} \sum_{m}^{-1} \left| V_{m}(\vec{k}) \right|^{2} \langle C^{(0)}(i\omega_{n})_{\alpha}^{m} \delta_{k,k''} , , \end{split}$$

where

$$\langle C^{(0)}(i\omega_n)^m_{\alpha} \rangle \equiv \frac{1}{n_I N} \sum_{i=1}^{N_I} C^{(0)}_i (i\omega_n)^m_{\alpha} .$$
 (A3)

In the last term of Eq. (A2), it has been reasoned that the exponential may be averaged separately from the localized electron propagator. We believe this assumption is justified because the site dependence of the propagator is such that the actual spatial *configuration* of impurities has little influence on the spatial variation of the localized electron propagator. For the propagator, only the variation of $\langle n_{ii} \rangle$ and $\langle n_{ii} \rangle$ from site to site is important, not the actual *configuration* of these sites.

The *proper* self-energy is easily identified in (A2) as

$$\begin{split} n_{I} \sum_{k'} & \left| W(\vec{\mathbf{k}} - \vec{\mathbf{k}}') \right|^{2} G^{(0)}(\vec{\mathbf{k}}', i\omega_{n})_{\alpha} \delta_{k,k'}, \\ & + n_{I} \sum_{m} \left| V_{m}(\vec{\mathbf{k}}) \right|^{2} \langle C^{(0)}(i\omega_{n})_{\alpha}^{m} \rangle \delta_{k,k''}. \end{split}$$

The site index i will be deleted in v_i and all quantities depending thereon, with the agreement that any quantity depending on v implicitly depends on the site.

The theory we employ reduces to Anderson's Hartree-Fock theory in the normal state.¹⁷ In this

theory there are two possible values of $\langle n_{ii} \rangle$ - $\langle n_{ii} \rangle$, equal in magnitude but opposite in sign. Thus v_i^2 is independent of *i*. Thus, the spin-orientation average is relevant only to quantities containing odd powers of v_i .

Using the above averaging technique, the selfenergy for conduction and localized electrons is calculated self-consistently from the coupled equations

$$\Sigma(\vec{\mathbf{k}}, i\omega_n)_{\alpha} = n_i \sum_{k'} |W(\vec{\mathbf{k}} - \vec{\mathbf{k}}')|^2 G(\vec{\mathbf{k}}', i\omega_n)_{\alpha}$$
$$+ n_I \sum_{m} |V_m(\vec{\mathbf{k}})|^2 C(i\omega_n)_{\alpha}^m, \qquad (A4)$$

$$\Sigma (i\omega_n)^m_{\alpha} = \sum_{\mathbf{k}} |V_m(\mathbf{k})|^2 G(\mathbf{k}, i\omega_n)_{\alpha}, \qquad (A5)$$

using the ansatz

$$G(\vec{k}, i\omega_n)_{\alpha} = \frac{1}{i\omega_n Z_{\alpha}(\omega_n) - \epsilon_k - \phi_{\alpha}(\omega_n)} , \qquad (A6)$$

$$C(i\omega_n)^m_{\alpha} = \frac{1}{i\omega_n Z_I(\omega_n) - E_{I\alpha} - \phi_I(\omega_n)} \quad , \tag{A7}$$

where Z_{α} , Z_{1} , ϕ_{α} , and ϕ_{1} are *real*. $G(\bar{k}, i\omega_{n})_{\alpha}$ and $C(i\omega_{n})_{\alpha}^{m}$ are the conduction- and localized-electron propagators, respectively:

$$\Sigma(\mathbf{k}, i\omega_n)_{\alpha} = i\omega_n - \epsilon_k - [G(k, i\omega_n)_{\alpha}]^{-1}$$

$$=i\omega_n[1-Z_{\alpha}(\omega_n)]-\epsilon_k-\phi_{\alpha}(\omega_n),\qquad (A8)$$

$$= i\omega_n \left[1 - Z_I(\omega_n) \right] - E_{I\alpha} - \phi_I(\omega_n) .$$
 (A9)

Equations (A4) and (A5) may be solved for Z_{α} , Z_{i} , ϕ_{α} , and ϕ_{i} :

$$\omega_{n} Z_{\alpha}(\omega_{n}) = \omega_{n} + n_{I} \left\langle \int \frac{d^{3} k'}{(2\pi)^{3}} \left| W(\vec{k} - \vec{k'}) \right|^{2} \frac{\omega_{n} Z_{\alpha}(\omega_{n})}{[\omega_{n} Z_{\alpha}(\omega_{n})]^{2} + [\epsilon_{k'} + \phi_{\alpha}(\omega_{n})]^{2}} \right\rangle + n_{I} \left\langle \sum_{m} \left| V_{m}(\vec{k}) \right|^{2} \frac{\omega_{n} Z_{I}(\omega_{n})}{[\omega_{n} Z_{I}(\omega_{n})]^{2} + [E_{I\alpha} + \phi_{I}(\omega_{n})]^{2}} \right\rangle , \qquad (A10)$$

$$\omega_n Z_l(\omega_n) = \omega_n + \int \frac{d^3 k}{(2\pi)^3} \left\| V_m(\vec{\mathbf{k}}) \right\|^2 \frac{\omega_n Z_\alpha(\omega_n)}{\left[\omega_n Z_\alpha(\omega_n) \right]^2 + \left[\boldsymbol{\epsilon}_k + \boldsymbol{\phi}_\alpha(\omega_n) \right]^2} \quad , \tag{A11}$$

$$\phi_{\alpha}(\omega_{n}) = -n_{I} \left\langle \sum_{m} |V_{m}(\mathbf{k})|^{2} \frac{E_{I\alpha} + \phi_{I}(\omega_{n})}{[\omega_{n}Z_{I}(\omega_{n})]^{2} + [E_{I\alpha} = \phi_{I}(\omega_{n})]^{2}} \right\rangle,$$
(A12)

$$\phi_{l}(\omega_{n}) = -\int \left| \frac{d^{3}k}{(2\pi)^{3}} \right| V_{m}(\vec{k}) \left|^{2} \frac{\phi_{k} + \phi_{\alpha}(\omega_{n})}{\left[\omega_{n} Z_{\alpha}(\omega_{n})\right]^{2} + \left[\epsilon_{k} + \phi_{\alpha}(\omega_{n})\right]^{2}} \right|$$
(A13)

For energies within ω_D of the Fermi surface, the region of interest here, the momentum dependences of V(k) and W(k - k'') are negligible. The integral for $\phi_1(\omega_n)$ is negligible. In this region the frequency (ω_n) dependence of the other integrals is also negligible.

Making some definitions, we have

 $\sum (i\omega_n)^m_\alpha = i\omega_n - E_{1\alpha} - [C(i\omega_n)^m_\alpha]^{-1}$

$$\begin{split} \tilde{\omega}_{n\alpha} &= \left[1 + C_{\alpha}(\hat{\omega}_{n}) \right] \omega_{n} + \left(\frac{1}{2\tau_{1}} + C_{\alpha}(\hat{\omega}_{n})\Gamma \right) \frac{\tilde{\omega}_{n\alpha}}{|\tilde{\omega}_{n\alpha}|} , \\ \hat{\omega}_{n} &= \omega_{n} + \Gamma \tilde{\omega}_{n\alpha} / \left| \tilde{\omega}_{n\alpha} \right| , \end{split}$$

$$\begin{aligned} \text{(A14)} \\ \text{(A15)} \end{split}$$

$$\phi_{\alpha}(\hat{\omega}_{n}) = - \langle C_{\alpha}(\hat{\omega}_{n}) E_{l\alpha} \rangle = - C_{\alpha}(\hat{\omega}_{n}) E_{l} - C_{\alpha}(\hat{\omega}_{n}) \langle v \rangle_{\alpha},$$
(A16)

where

$$C_{\alpha}(\hat{\omega}_{n}) \equiv n_{I}(2l+1) \left| V \right|^{2} / (\hat{\omega}_{n}^{2} + E_{l\alpha}^{2}) , \qquad (A17)$$

$$1/2\tau_1 = n_I \pi N(0) |V|^2 , \qquad (A18)$$

$$\Gamma \equiv \pi N(0) \left| V \right|^2 . \tag{A19}$$

The dressed conduction- and localized-electron propagators are therefore

$$G(\vec{k}, i_{\mathcal{W}_n})_{\alpha} = \frac{1}{i\bar{\omega}_{n\alpha} - \epsilon_k - \phi_{\alpha}(\hat{\omega}_n)} \quad , \tag{A20}$$

$$C(i\omega_n)_{\alpha} = \frac{1}{\hat{i\omega}_n - E_{I\alpha}} \quad . \tag{A21}$$

APPENDIX B: VERTEX FUNCTIONS

Configuration averaging the diagrams of Fig. 1 we get

$$\Lambda_{s}(\mathbf{\bar{q}}, i\omega_{n}, -\omega_{n})_{\pm} = 1 + n_{I}(2l+1) \left| W \right|^{2} \sum_{k} \left\langle G(\mathbf{\bar{k}} + \mathbf{\bar{q}}, i\omega_{n})_{\pm} G(-\mathbf{\bar{k}}, -i\omega_{n})_{\pm} \Lambda_{s}(\mathbf{\bar{q}}, i\omega_{n}, -i\omega_{n})_{\pm} \right\rangle + n_{I}(2l+1) \left| V \right|^{2} \left\langle C(i\omega_{n})_{\pm} C(-i\omega_{n})_{\mp} \Lambda_{I}(\mathbf{\bar{q}}, i\omega_{n}, -i\omega_{n})_{\pm} \right\rangle,$$
(B1)

$$\Lambda_{i}(\mathbf{\ddot{q}}, i\omega_{n}, -i\omega_{n})_{\pm} = -d + |V|^{2} \sum_{k} G(\mathbf{\ddot{k}} + \mathbf{\ddot{q}}, i\omega_{n})_{\pm} G(-\mathbf{\ddot{k}}, -i\omega_{n})_{\mp} \Lambda_{s}(\mathbf{\ddot{q}}, i\omega_{n}, -i\omega_{n})_{\pm}.$$
(B2)

Using the fact that a conduction-electron vertex introduces an energy cutoff, we find

$$\begin{split} \sum_{k} G\left(\vec{k}+\vec{q},i\omega_{n}\right)_{\pm}G\left(-\vec{k},-i\omega_{n}\right)_{\mp} &\approx N(0) \int \frac{d\Omega}{4\pi} \int_{-\infty}^{\infty} d\boldsymbol{\epsilon}_{k} \frac{1}{i\vec{\omega}_{n\pm}-\boldsymbol{\epsilon}_{k}-\vec{v}_{F}\cdot\vec{q}-\boldsymbol{\phi}_{\pm}(\hat{\omega}_{n})} \frac{1}{i\vec{\omega}_{n\mp}+\boldsymbol{\epsilon}_{k}+\boldsymbol{\phi}_{\mp}(\hat{\omega}_{n})} \\ &= N(0) \int \frac{d\Omega}{4\pi} \frac{1}{i\left(\vec{\omega}_{n\pm}+\vec{\omega}_{n\mp}\right)-\left[\boldsymbol{\phi}_{\pm}(\hat{\omega}_{n})-\boldsymbol{\phi}_{\pm}(\hat{\omega}_{n})\right]-\vec{v}_{F}\cdot\vec{q}} \frac{2\pi i}{|\omega_{n}|} \frac{\omega_{n}}{|\omega_{n}|} \\ &\approx 2\pi N(0) \frac{1}{v_{F}q} \left(\frac{v_{F}q}{|\overline{\omega}_{n\pm}|} - \frac{1}{3} \frac{(v_{F}q)^{2}}{|\overline{\omega}_{n\pm}|^{3}}\right) = \frac{2\pi N(0)}{|\overline{\omega}_{n\pm}|} \left[1 - \frac{1}{3} \left(\frac{v_{F}q}{|\overline{\omega}_{n\pm}|}\right)^{2}\right] \equiv 2\pi N(0) B(q^{2}, |\overline{\omega}_{n\pm}|), \end{split}$$
(B3)

where the energy cutoff allows the slowly varying velocity $\vec{\mathbf{v}}_k$ and $N(\xi)$, the density of states, to be approximated by constants, whence the integral over ξ can be extended from $-\infty$ to ∞ , transferring the cutoff to the frequency sum. We define

$$\left|\overline{\omega}_{n\pm}\right| = \left|\widetilde{\omega}_{n\pm}\right| + \left|\widetilde{\omega}_{n\mp}\right| \pm i I(\widehat{\omega}_n) , \qquad (B4)$$

$$I(\hat{\omega}_n) = \phi_+(\hat{\omega}_n) - \phi_-(\hat{\omega}_n), \tag{B5}$$

$$N(0) = mp_{F} / 2\pi^{2} . \tag{B6}$$

With these results, Eqs. (B1) and (B2) are solved to give (1.27) and (1.28) in the text.

APPENDIX C: THE BASIC APPROXIMATION

We are concerned with the frequency variation of

$$c(\hat{\omega}_n), \quad \tau_s(\hat{\omega}_n)^{-1}, \quad P(\hat{\omega}_n)$$

.

[the ω_n variation of $\tau(\hat{\omega}_n)$ is entirely in $c(\hat{\omega}_n)$]. We expand $c(\hat{\omega}_n)$ in a Taylor's series for $\hat{\omega}_n$ about $\hat{\omega}_n = \Gamma$ and require

$$c(\mathbf{\Gamma}) \gg \left| \left[\frac{\partial c(\hat{\omega}_n)}{\partial \hat{\omega}_n} \right]_{\mathbf{\Gamma}} (\hat{\omega}_n - \mathbf{\Gamma}) \right| \quad , \tag{C1}$$

that is,

$$\Gamma^{2} + E_{l}^{2} + v^{2} \gg \frac{\Gamma(\Gamma^{2} + E_{l}^{2})^{2} + \Gamma(\Gamma^{2} + E_{l}^{2})^{2}}{(\Gamma^{2} + E_{l}^{2})(\Gamma^{2} + E_{l}^{2})}$$
(C2)

or

$$\frac{1}{2\pi} \left(\frac{1}{N_{I^{\dagger}}(0)} + \frac{1}{N_{I^{\bullet}}(0)} \right) \gg \left(\frac{N_{I^{\dagger}}(0)}{N_{I^{\bullet}}(0)} + \frac{N_{I^{\bullet}}(0)}{N_{I^{\bullet}}(0)} \right) \left| \hat{\omega}_{n} - \Gamma \right|,$$
(C3)

where

$$N_{I\alpha}(0) \equiv \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + E_{I\alpha}^2}$$
(C4)

is the density of localized states of spin α at the Fermi surface.

We thus need

$$\frac{1}{2\pi |\omega_n|} \gg \frac{N_{II}(0)^2 + N_{II}(0)^2}{N_{II}(0) + N_{II}(0)} , \qquad (C5)$$

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so it is sufficient to have

$$\frac{1}{2|\omega_n|} \gg \frac{\Gamma}{\Gamma^2 + (|E_l| - |v|)^2} \quad . \tag{C6}$$

Now

$$\frac{1}{r_s(\hat{\omega}_n)} \equiv n_I(2l+1) \left| V \right|^2 \frac{4\Gamma v^2}{(\hat{\omega}_n^2 + E_{II} E_{II})^2 + 4\hat{\omega}_n^2 v^2} , \quad (C7)$$

so that, carrying out a procedure similar to that above, we require

$$\frac{1}{\tau_{s}(\Gamma)} \gg \left| \left[\frac{\vartheta \left[1/\tau_{s}(\hat{\omega}_{n}) \right]}{\vartheta \hat{\omega}_{n}} \right]_{\Gamma} (\hat{\omega}_{n} - \Gamma) \right|$$
(C8)

$$1/2 |\omega_n| \gg \pi \left[N_{I^{\dagger}}(0) + N_{I^{\dagger}}(0) \right] .$$
 (C9)

Again, (C6) is sufficient.

Finally

$$P(\hat{\omega}_n) \equiv 2n_I(2l+1) |V|^2 \left(\frac{\Gamma^2 + E_I^2 - v^2 - \omega_n^2}{(\hat{\omega}_n^2 + E_I + E_I)^2 + 4\hat{\omega}_n^2 v^2} \right) v$$
(C10)

is dealt with in the same fashion, yielding the condition

$$1/2 |\omega_n| \gg \pi [N_{l^*}(0) + N_{l^*}(0)] .$$
 (C11)

Thus, if

$$\frac{1}{2\omega_D} \gg \frac{\Gamma}{\Gamma^2 + (|E_1| - |v|)^2} , \qquad (C12)$$

then the functions

$$c(\hat{\omega}_n), \quad \tau_s(\hat{\omega}_n)^{-1}, \quad P(\hat{\omega}_n)$$

may be taken at $\hat{\omega}_n = \Gamma$, neglecting their ω_n dependence.

Condition (C12) may be regarded as equivalent to the requirement that the density of localized states admixed into conduction-electron states (for either spin) be a slowly varying function of energies within the Debye energy of the Fermi surface (see Fig. 2).

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¹³Shiba did not *explicity* calculate the ratio, $d (\phi$ in this notation), nor did he calculate the upper critical field. ¹⁴See, for example, P. G. de Gennes, *Superconductivity*

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