## Strong-coupling theories for superconductors containing local spin fluctuations

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Theories for isotropic and anisotropic superconductors containing transition-metal impurities which give rise to local spin fluctuations are developed by use of the Migdal-Eliashberg formalism. The multiplicative renormalization method is used to obtain the normal and anomalous *d*-electron propagators. The decreases in the transition temperatures of the isotropic and anisotropic superconductors due to the local spin fluctuations are obtained within the framework of the square-wellmodel version of the Midgal-Eliashberg formalism. Different approaches are used to obtain the decreases for the two cases. The effects of the local spin fluctuations on the jump in the specific heat at  $T_c$  of the strong-coupling anisotropic superconductors are also calculated.

## I. INTRODUCTION

For certain transition-metal (TM) impurities dissolved in host metals, the Coulomb repulsion between the d electrons of opposite spins which are localized about an impurity site may not be strong enough to cause the formation of long-lived magnetic moments, or the widths of the impurity states may be so broad as to delocalize the moments. For these impurities, the localized spins may, instead, fluctuate in time with a frequency  $1/\tau_{\rm SF}$  where  $\tau_{\rm SF}$ is the localized spin-fluctuation lifetime. If this lifetime is greater than the thermal fluctuation lifetime, the TM impurities will still give rise to magnetic behaviors. However, if the spin fluctuation lifetime is smaller than the thermal lifetime, the impurities will give rise to nonmagnetic behavior. The resistivity of the metals containing these types of spin fluctuations will vary as 1  $-(T/T_{LDF})^2$  where  $T_{LSF}$  is the temperature equivalent of  $\tau_{\rm SF}$ .

When the host metal is in the superconducting phase, the local spin fluctuations (LSF's) will cause the transition temperature to decrease almost exponentially.<sup>1</sup> The observed decrease of  $T_c$  due to the LSF's appears to follow the modified exponential decrease predicted by Kaiser<sup>2</sup> for superconductors containing nonmagnetic localized excited states, the precursors of the LSF's. Most of the earlier attempts<sup>3,4</sup> to develop a theory for the LSF's in the superconductors were based on the random-phase approximation (RPA) treatment of the Coulomb repulsion term in the Anderson Hamiltonian used to describe the TM impurities in the host system. A more successful attempt was by Schlottmann<sup>5</sup> who applied the multiplicative renormalization technique of Iche<sup>6</sup> which is known to provide for an exact treatment of the LSF's in the normal metal. In a series of papers,<sup>7-9</sup> I was able to obtain expressions for several transport properties of superconductors containing LSF's. I showed that the observed thermal conductivity<sup>10</sup> and transverse attenuation coefficient<sup>11</sup> of the dilute ZnMn superconductors could be fitted by the expressions derived in Refs. 8 and 9.

All of the theoretical studies mentioned above are based on the weak Bardeen-Cooper-Schrieff<sup>12</sup> (BCS) theory of superconductivity. The rather large electron-phonon mass enhancement seen in certain metals indicates the need of taking into account the renormalization of the diagonal part of the self-energy corrections due to the electronphonon interaction (in the BCS theory, only the offdiagonal part of the self-energy correction due to the interaction is considered) when formulating a theory for the superconducting phase of these metals. The Eliashberg<sup>13</sup> theory, which is an extension of the Migdal theory<sup>14</sup> for phonons in a normal metal, treats in an explicit manner both the strong electron-phonon interactions and the Coulomb repulsion between the opposite spin electrons forming the Cooper pair when calculating the diagonal and off-diagonal parts of the self-energy corrections. Therefore, the Eliashberg theory<sup>13</sup> should be used to describe the strong-coupling superconductors. This formulation of superconductivity has been used to calculate the transition temperatures of several strong-coupling superconductors<sup>15-17</sup> using only measured information about the normal phases of the metals.

Recently, much interest has been drawn to strongcoupling (SC) superconductors containing magnetic and nonmagnetic impurities. Allen<sup>18</sup> and Carbotte and coworkers<sup>19,20</sup> have studied the decrease in  $T_c$  of the SC superconductors due to normal scattering by nonmagnetic impurities and to the spin-flip scattering by weakly interacting paramagnetic impurities. Schachinger and Carbotte<sup>21</sup> and Yoksan and Nagi<sup>22</sup> have studied the effects due to strongly interacting paramagnetic impurities. The Shiba-Rusinov<sup>23</sup> treatment of the spin-flip scattering was used in both of these studies. Both studies found interesting behaviors due to the formation of impurity states within the energy gap of the superconductor. Recently, Yoksan and Nagi<sup>24</sup> studied the effects due to Kondo impurities in the SC superconductors. The purpose of the present paper is to formulate a strong-coupling theory for superconductors containing transition-metal impurities which give rise to local spin fluctuations. The multiplicative renormalization method of Schlottmann<sup>5</sup> is used to treat the Coulomb repulsion between the d electrons of opposite spins which are localized about the impurity sites. In order to avoid the need to numerically solve the Eliashberg equations and to be able to obtain analytical expressions, the square-well model  $\lambda^{\Theta\Theta}$  for the spectral distribution function will be used. Both isotropic and anisotropic superconductors will be considered. Expressions for the transition temperatures of the isotropic and anisotropic supercondcutors containing the LSF will be obtained. An expression for the jump in the specific heat at  $T_c$  for the anisotropic superconductor will also be obtained.

### **II. FORMALISM**

## A. d-electron propagators

As is well known, the Hartree-Fock treatment of the Coulomb repulsion between the d electrons of opposite spins which are localized at the impurity sites, breaks down close to the magnetic-to-nonmagnetic transition region, and so, other treatments must be used in this region. Iche<sup>6</sup> has pointed out that in the random-phase approximation, many diagrams in the perturbative expansion of the self-energy correction due to the Coulomb interaction are neglected in the summations of the ladder and bubble diagrams which lead to the local spin fluctuations. Iche has developed a new approach, the multiplicative renor-

malization method, to treat the Coulomb interaction in the region close to the nonmagnetic-to-magnetic transition point. This method is based on the requirement that many quantities in nature should be invariant under a change in the energy scales. This requirement would then guide one in deciding which diagrams should be kept in the summation. Iche showed that the diagrams which should be kept would be those which gave an expression which satisfied a Lie differential equation. Schlottmann<sup>5</sup> extended the multiplicative renormalization method so that it could be applied to the superconducting phase. He realized that a scale invariant anomalous d-electron propagator could be achieved by separating the diagrams of the perturbative expansion of the anomalous propagator into two subsets and then requiring each subset to obey the multiplicative renormalization requirement (i.e., each set be the solution of an appropriate Lie differential equation).

Following the steps used by Schlottmann<sup>5</sup> (see also Ref. 25), I obtain

$$G_d(i\omega_n) = \frac{|\omega_n| + \Gamma_d}{(|\omega_n| + \Gamma_d)^2 + E_d^2}, \qquad (1)$$

$$F_{d}(i\omega_{n}) = -\frac{U_{\text{eff}}\chi(0)}{(|\omega_{n}| + \Gamma_{d})^{2} + E_{d}^{2}} \frac{\Gamma_{d}^{2}}{\Gamma_{d}^{2} + E_{d}^{2}} 2\pi k_{B}T \times \sum_{m} \int \frac{d\Omega'}{4\pi} \frac{\Delta_{m}(\Omega')}{[|\omega_{m}|^{2} + \Delta_{m}^{2}(\Omega')]^{1/2}} + \frac{\Gamma_{d}}{\pi[(\omega_{n}| + \Gamma_{d})^{2} + E_{d}^{2}]} \int \frac{d\Omega'}{4\pi} \frac{\Delta_{n}(\Omega')}{[|\omega_{n}|^{2} + \Delta_{n}^{2}(\Omega')]^{1/2}}, \quad (2)$$

where  $E_d$  is the energy of the *d* electrons and is taken to be zero in all further calculations,  $\Gamma_d$  is the half-width of the impurity state and is equal to  $\pi N(0) |V|^2$  with N(0)being the density of states at the Fermi surface of the host metal, and *V* is the potential which leads to the mixing of the conduction electrons and the *d* electrons.  $U_{\text{eff}}$  is the effective Coulomb energy defined as

$$U_{\rm eff} = U / [1 + N_d(0)U]$$
(3)

with  $N_d(0)$  being the density of states of the *d* electrons at the Fermi surface.  $\chi(0)$  is the static susceptibility due to rapid spin fluctuations and is taken to be equal to the normal state expression obtained by Iche,<sup>6</sup> i.e.,

$$\mathcal{K}(0) = \exp(U/\pi\Gamma_d)/\pi\Gamma_d . \tag{4}$$

In writing down Eqs. (1) and (2), I have left the integrations over the solid angles undone in order to allow for the possible dependence of the renormalized energy gaps in the solid angle. My results are slightly different from those of Schlottman in that I have not identified the summation

$$2\pi k_B T \sum_{m} \frac{\Delta_m}{\mid \omega_m \mid}$$

appearing on the right-hand side of Eq. (2) as being proportional to the order parameter  $\Delta_{ph}$  defined in the BCS theory.<sup>12</sup> Since the propagators are invariant under a

change in the g scale, they should be the proper propagators for the d electrons in the region close to the nonmagnetic-to-magnetic transition point.

#### B. Eliashberg formalism

The basic Eliashberg equations<sup>13</sup> result from the explicit treatment of the electron-phonon interaction and the Coulomb interaction between the electrons belonging to the Cooper pair when calculating both the diagonal and off-diagonal part of the self-energy corrections of the propagators for the superconducting phase. The Eliashberg equations for the superconductors containing transition-metal impurities which give rise to local spin fluctuations (LSF's) are obtained by adding to the basic equations, the corrections due to the mixing of the impurity electrons with the host system's electrons. The modified Eliashberg equations (written on the imaginary axis) are

$$\widetilde{\omega}_{n} = \omega_{n} + \pi k_{B} T \sum_{m} \int \frac{d\Omega'}{4\pi} \lambda_{kk'}(n-m) \frac{\omega_{m}}{[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega')]^{1/2}} + \frac{1}{2\tau} \int \frac{d\Omega'}{4\pi} \frac{\omega_{n}}{[\omega_{n}^{2} + \Delta_{n}^{2}(\Omega')]^{1/2}} + n_{i} |V|^{2} G_{d}(i\omega_{n})$$
(7)

and

(5)

$$\phi_{S}(\omega_{n}) = \pi k_{B}T \sum_{m} \int \frac{d\Omega'}{4\pi} [\lambda_{kk'}(n-m) - \mu^{*}] \frac{\Delta_{m}(\Omega')}{[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega')]^{1/2}} + \frac{1}{2\tau} \int \frac{d\Omega'}{4\pi} \frac{\Delta_{n}(\Omega')}{[\omega_{n}^{2} + \Delta_{n}^{2}(\Omega')]^{1/2}} + n_{i} |V|^{2} F_{d}(i\omega_{n}) ,$$
(6)

where  $\phi_S(\omega_n)$  is the unrenormalized energy gap,  $\Delta_n(\Omega)$  is the renormalized energy gap,  $\mu^*$  is the pseudopotential describing the Coulomb repulsion between the electrons of opposite spins forming the Cooper pair. The electronphonon coupling parameter  $\lambda_{k,k'}(n-m)$  is defined as

$$\lambda_{k,k'}(n-m) = 2 \int \omega \, d\omega \frac{[\alpha^2 F(\omega)]_{k,k'}}{\omega^2 + (\omega_n - \omega_m)^2} , \qquad (7)$$

where  $[\alpha^2 F(\omega)]_{kk'}$  is the electron-phonon spectral density for the scattering of an electron pair (k, -k) into the pair (k', -k') due to the virtual exchange of a phonon of energy  $\omega$ .  $\tau$  is the lifetime due to the normal scattering by the nonmagnetic impurities. In writing out Eqs. (5) and (6), I have again left the integration over the solid angle undone to allow for the presence of anisotropy in the superconductor.

The spectral distribution function  $[\alpha^2 F(\omega)]_{kk'}$  is presently treated as an experimental input. It is not possible at the present time to calculate the form of this function from first principles. The form of the spectral distribution function for a particular metal is obtained from the study of the current-voltage characteristics of proximity effect tunnel junctions.<sup>26</sup> Since these studies do not yield an analytical form for the distribution functions, the Eliashberg equations have to be solved numerically. To avoid the need for having to do numerical calculations and in order to be able to obtain analytical expressions, the coupling parameter is often approximated by a square-well model  $\lambda^{\Theta\Theta}$ 

$$\lambda_{k,k'}(n-m) = \lambda_{k,k'} \Theta(\omega_D - |\omega_n|) \Theta(\omega_D - |\omega_m|) .$$
(8)

This approximation would correspond to the weakcoupling limit of the Eliashberg theory of superconductivity. This limit is not equivalent to the weak-coupling BCS theory of superconductivity due to the presence of the additional term in Eq. (5) arising from the inclusion of the electron-phonon contribution to the diagonal part of the self-energy correction.

### **III. ISOTROPIC SUPERCONDUCTORS**

Using the BCS formulation of superconductivity, Schlottman<sup>5</sup> showed that the decrease in the transition temperature due to TM impurities which give rise to local spin fluctuations follows a modified exponential decrease of the form

$$\frac{T_c}{T_{c0}}\Big|_{wc} = \exp\left[-n_i \left[\frac{N_d(0)}{N(0)}\right] \frac{1}{N(0)g_{eff}} \frac{1 + U_{eff}\chi(0)/N(0)g_{eff}}{1 - n_i \left[\frac{N_d(0)}{N(0)}\right] U_{eff}\chi(0)/N(0)g_{eff}}\right].$$
(9)

This decrease is similar to the decrease in  $T_c$  predicted by Kaiser<sup>2</sup> for superconductors containing TM impurities which form into nonmagnetic resonant states. The similarity is not unexpected since the nonmagnetic resonant states are the precursors of the local spin fluctuations. This similarity explains why it was possible to fit the observed decreases in the transition temperatures of the LSF superconductors, RuFe,  $^1$  AlMn, and  $Th\overline{U}$  (Ref. 27) to Kaiser's expression.

If the electron-phonon mass enhancement in the normal phase of the superconductor is large, the BCS formalism would no longer be appropriate for describing the superconducting state of the metal containing the TM impurities which give rise to the LSF's. Instead the Eliashberg formalism should be used. To obtain the transition temperatures of these superconductors, only the linearized versions of the Eliashberg equations are needed, i.e.,

$$\widetilde{\omega}_{n} = \omega_{n} + \pi k_{B}T \sum_{m} \lambda(n-m) \operatorname{sgn}\omega_{m} + \frac{1}{2\tau} \operatorname{sgn}\omega_{n}$$
$$+ n_{i} |V|^{2} \frac{|\omega_{n}| + \Gamma_{d}}{(|\omega_{n}| + \Gamma_{d})^{2} + E_{d}^{2}}$$
(10)

and

$$\phi_{s}(\omega_{n}) = \pi k_{B} T \sum_{m} \left[ \lambda(n-m) - \mu^{*} \right] \frac{\Delta_{S}(\omega_{n})}{|\omega_{m}|} + \frac{1}{2\tau} \frac{\Delta_{S}(\omega_{n})}{|\omega_{n}|} + n_{i} |V|^{2} \left[ -\frac{U_{\text{eff}}\chi(0)}{(|\omega_{n}| + \Gamma_{d})^{2} + E_{d}^{2}} - \frac{\Gamma_{d}^{2}}{\Gamma_{d}^{2} + E_{d}^{2}} 2\pi k_{B} T \sum_{m} \frac{\Delta_{S}(\omega_{m})}{|\omega_{m}|} + \frac{\Gamma_{d}^{2}}{\pi [(|\omega_{n}| + \Gamma_{d})^{2} + E_{d}^{2}]} \frac{\Delta_{S}(\omega_{n})}{|\omega_{n}|} \right].$$
(11)

In the square-well approximation, only the phonons of frequencies less than the Debye frequency play a role in determining the nature of the superconducting state. Assuming that  $\Gamma_d$  is greater than  $\hbar\omega_D$ , Eqs. (10) and (11) can be simplified and be combined to give

$$\begin{bmatrix} 1+\lambda+n_i \left[\frac{N_d(0)}{N(0)}\right] \end{bmatrix} \Delta_S(\omega_n) \\ = \begin{bmatrix} \lambda-\mu^*-n_i \left[\frac{N_d(0)}{N(0)}\right] U_{\text{eff}}\chi(0) \end{bmatrix} \\ \times 2\pi k_B T \sum_m \frac{\Delta_S(\omega_m)}{|\omega_m|} .$$
(12)

Defining an "effective Coulomb pseudopotential  $\mu_{eff}$ ,"

$$\mu_{\rm eff} = \mu^* + n_i \left[ \frac{N_d(0)}{N(0)} \right] U_{\rm eff} \chi(0) , \qquad (13)$$

I can rewrite Eq. (12) as

$$\frac{1+\lambda+\bar{n}}{\lambda-\mu_{\rm eff}} = 2\pi k_B T \sum_m \frac{1}{\mid \omega_m \mid} , \qquad (14)$$

where  $\overline{n} = n_i N_d(0) / N(0)$ . Evaluating the summation, I get

$$T_{c} = 1.13\hbar\omega_{D} \exp\left[-\frac{1+\lambda+\overline{n}}{\lambda-\mu_{\rm eff}}\right].$$
(15)

It should be remembered that the dependence of  $T_c$  on the impurity concentration enters in two places in the exponential factor appearing in Eq. (15), through the  $\bar{n}$  in the numerator and  $\mu_{\rm eff}$  in the denominator. Combining Eq. (15) with the expression for the transition temperature of the pure strong-coupling superconductor

$$T_{c0} = 1.13\hbar\omega_D \exp\left[-\frac{1+\lambda}{\lambda-\mu^*}\right], \qquad (16)$$

I get

$$\frac{T_c}{T_{c0}} = \exp\left[-\overline{n}\left[\frac{1+\lambda}{\lambda-\mu^*}\right]\frac{\frac{1}{1+\lambda} + \frac{1}{\lambda-\mu^*}U_{\text{eff}}\chi(0)}{1-\overline{n}\frac{1}{\lambda-\mu^*}U_{\text{eff}}\chi(0)}\right].$$
(17)

In the limit of small electron-phonon mass enhancement,  $1+\lambda \rightarrow 1$  and Eq. (17) reduces to the result obtained by Schlottman, Eq. (9).

## **IV. ANISOTROPIC SUPERCONDUCTORS**

#### A. Formalism

Comparing the expressions for the transition temperature and the specific-heat jump at  $T_c$  of the pure anisotropic superconductors and of the anisotropic superconductors containing (normal) nonmagnetic impurities obtained on the basis of the BCS formalism<sup>28,29</sup> with the expressions obtained on the basis of the Migdal-Eliashberg formalism,<sup>30,31</sup> one sees that the two sets of expressions differ only in the replacement of the mean-square pairing anisotropy  $\langle a^2 \rangle$  in the BCS-based expressions by the mean-square energy gap anisotropy  $\langle a^2 \rangle$  defined as

$$\langle \alpha^2 \rangle = \langle a^2 \rangle \frac{\lambda^2 (\mu^* + 1)^2}{(1 + \lambda)^2 (\lambda - \mu^*)^2}$$
 (18)

in the Migdal-Eliashberg expressions. It was hoped<sup>32</sup> that the strong-coupling expressions for these properties in anisotropic superconductors which contained magnetic impurities could be obtained by simply replacing the  $\langle a^2 \rangle$ factor in the equivalent BCS expression by  $\langle \alpha^2 \rangle$  since the BCS expressions are much more easily obtained. This hope was not realized. Ashraf and Carbotte<sup>33</sup> and Zarate and Carbotte<sup>34</sup> showed that the strong-coupling expressions for the anisotropic superconductors containing weakly interacting paramagnetic impurities contained modifications to the BCS expressions that go beyond the simple substitution given by Eq. (18). Yoksan and Nagi<sup>35</sup> found that the strong-coupling expressions for the anisotropic obtained within the framework of the Shiba-Rusinov<sup>23</sup> treatment of the spin-flip scattering by the paramagnetic impurities could not be obtained from the BCS expression<sup>36</sup> by the above substitution.

To see if a connection exists if the nonmagnetic impurities in an anisotropic superconductor give rise to local spin fluctuations, I will now calculate the strong-coupling expressions for  $T_c$  and the specific-heat jump at  $T_c$  for the superconductor. Since I am interested in the specificheat jump, I will need to work with the complete (nonlinear) forms of the Eliashberg equations, Eqs. (5) and (6). To represent the anisotropy, I have taken the spectral distribution function to be of the separable form

$$[\alpha^{2}F(\omega)]_{kk'} = [1 + a_{k}(\Omega)]\alpha^{2}F(\omega)[1 + a_{k'}(\Omega')].$$
(19)

Other dependences of  $[\alpha^2 F(\omega)]_{kk'}$  on  $a_k(\Omega)$  and  $a_{k'}(\Omega')$  have been proposed.<sup>37</sup> Equation (19) is the most commonly used form.

Substituting Eq. (19) into the nonlinear Eliashberg equations and then using the square-well approximation, I get

$$\phi_{S}(\omega_{n}) = [1 + a_{k}(\Omega)]\lambda 2\pi k_{B}T \sum_{m=0} \left\langle (1 + a_{k'}(\Omega')) \frac{\Delta_{m}(\Omega')}{[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega')]^{1/2}} \right\rangle' - \mu_{\text{eff}}2\pi k_{B}T \sum_{m} \left\langle \frac{\Delta_{m}(\Omega')}{[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega')]^{1/2}} \right\rangle + \frac{1}{2\tau_{\text{eff}}} \left\langle \frac{\Delta_{n}(\Omega')}{[\omega_{n}^{2} + \Delta_{n}^{2}(\Omega')]^{1/2}} \right\rangle'$$

$$(20)$$

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and

$$z = \widetilde{\omega}_n / \omega_n = 1 + n_i \left( \frac{N_d(0)}{N(0)} \right) + [1 + a(\Omega)]\lambda$$
$$+ \frac{1}{2T_{\text{eff}}} \left\langle \frac{1}{[\omega_n^2 + \Delta_n^2(\Omega')]^{1/2}} \right\rangle', \qquad (21)$$

where  $\langle \cdots \rangle'$  denotes an average over the solid angle. The effective Coulomb pseudopotential  $\mu_{\text{eff}}$  is the same as before, i.e., Eq. (13), and  $\tau_{\text{eff}}$  is the new electronic lifetime defined as

$$\frac{1}{2\tau_{\rm eff}} = \frac{1}{2\tau} + n_i \left[ \frac{N_d(0)}{N(0)} \right] \Gamma_d . \tag{22}$$

Equations (20) and (21) can be combined into a single equation for the renormalized energy gap, i.e.,

$$\Delta_{n}(\Omega) = \frac{\phi_{0}' + a(\Omega)\phi_{1}' + \frac{1}{2\tau_{\text{eff}}}\phi_{n}'}{1 + \lambda + \overline{n} + a(\Omega)\lambda + \frac{1}{2\tau_{\text{eff}}}C_{n}'}, \qquad (23)$$

where

$$\phi_{0}^{\prime} = \lambda 2\pi k_{B}T \sum_{m=0}^{\infty} \left\langle \left[1 + a(\Omega^{\prime})\right] \frac{\Delta_{m}(\Omega^{\prime})}{\left[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega^{\prime})\right]^{1/2}} \right\rangle^{\prime} -\mu_{\text{eff}}2\pi k_{B}T \sum_{m=0}^{\infty} \left\langle \frac{\Delta_{m}(\Omega^{\prime})}{\left[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega^{\prime})\right]^{1/2}} \right\rangle^{\prime}, \quad (24)$$

$$\phi_{1}' = \lambda 2\pi k_{B}T \sum_{m=0} \left\langle \left[1 + a(\Omega')\right] \frac{\Delta_{m}(\Omega')}{\left[\omega_{m}^{2} + \Delta_{m}^{2}(\Omega')\right]^{1/2}} \right\rangle',$$
(25)

$$\phi_n' = \left\langle \frac{\Delta_n(\Omega')}{\left[\omega_n^2 + \Delta_n^2(\Omega')\right]^{1/2}} \right\rangle', \qquad (26)$$

and

$$C'_{n} = \left\langle \frac{1}{\left[\omega_{n}^{2} + \Delta_{n}^{2}(\Omega')\right]^{1/2}} \right\rangle' .$$
(27)

Dividing the numerator and denominator of Eq. (23) by  $(1 + \lambda + \overline{n})$ , I get

$$\Delta_n(\Omega) = \frac{\phi_0 + a(\Omega)\phi_1 + \frac{1}{2\tau_{\text{eff}}}\phi_n}{1 + \frac{1}{2\tau_{\text{eff}}}C_n + \frac{\lambda}{1 + \lambda + \bar{n}}a(\Omega)}, \qquad (28)$$

where the lack of the primes on the  $\phi$ 's and  $C_n$  indicates that the division of Eqs. (24)–(27) by  $(1+\lambda+\overline{n})$  has been performed.

Following Zarate and Carbotte,<sup>34</sup> I now make the approximation that

$$\Delta_{n}(\Omega) = A_{n0} + a(\Omega)A_{n1} + a^{2}(\Omega)A_{n2}.$$
<sup>(29)</sup>

I now identify  $\phi_0$  as being the pseudo-order-parameter  $\epsilon$ . Substituting Eq. (29) into Eq. (28) and after expanding the denominator in powers of  $a(\Omega)$ , I find

$$A_{n0} = \frac{\phi_0 + \frac{1}{2\tau_{\text{eff}}}\phi_n}{1 + \frac{1}{2\tau_{\text{eff}}}C_n} , \qquad (30)$$

$$A_{n1} = \frac{\phi_1}{1 + \frac{1}{2\tau_{\text{eff}}}C_n} - \frac{\lambda}{1 + \lambda + \overline{n}}A_{n0}, \qquad (31)$$

and

$$A_{n2} = -\frac{\lambda}{1+\lambda+\overline{n}} \frac{A_{n1}}{1+\frac{1}{2\tau_{\text{eff}}}c_n} .$$
(32)

Substituting Eq. (29) into the definitions of  $\phi_0$ ,  $\phi_1$ ,  $\phi_n$ , and  $C_n$ , Eqs. (24)–(27), and then substituting the resulting expressions into Eqs. (30)–(32), I get

$$A_{no} = \left[ 1 - \langle a^2 \rangle \rho \frac{\lambda}{1 + \lambda + \overline{n}} \frac{h |\omega_n|}{(|\omega_n| + \rho)^2} \right] \epsilon$$
$$+ \frac{1}{2} \langle a^2 \rangle H_{2n} \epsilon^3 , \qquad (33)$$

where

$$H_{2n} = -\left[\frac{\lambda}{1+\lambda+\bar{n}}\right] \left[\frac{\rho h}{(|\omega|+\rho)^3}\right] \left[\frac{\rho}{|\omega_n|}-1\right] - \frac{2\rho h^2}{|\omega_n|(|\omega_n|+\rho)^2}$$
(34)

with  $\rho = 1/2\tau_{\rm eff}$  and

$$h = \lambda \frac{1 + \overline{n} + \mu_{\text{eff}}}{(1 + \lambda + \overline{n})(\lambda - \mu_{\text{eff}})} .$$
(35)

The coefficients  $A_{nl}$  and  $A_{n2}$  are obtained by substituting Eq. (35) into Eqs. (31) and (32). Since these coefficients, when they appear in the expressions for  $T_c$  and the specific-heat jump, are multiplied by  $\langle a^2 \rangle$ , only the isotropic part of these coefficients need to be known. They are

$$A_{n1}^{(i)} = \frac{h |\omega_n|}{|\omega_n| + \rho} \epsilon + \frac{1}{2} \rho \frac{h}{(|\omega_n| + \rho)^2 |\omega_n|} \epsilon^3 \qquad (36)$$

and

$$A_{n2}^{(i)} = -\frac{\lambda}{1+\lambda+\overline{n}} \left[ \frac{h |\omega_n|^2}{(|\omega_n|+\rho)^2} \epsilon + \rho \frac{h}{(|\omega_n|+\rho)^3} \epsilon^3 \right].$$
(37)

Substituting Eqs. (35), (36), and (37) into Eq. (29) and then substituting the resulting expression into the definition of the pseudo-order-parameter, a self-consistent equation for the pseudo-order-parameter is obtained.

#### **B.** Transition temperature

Carrying out the substitution mentioned above, I obtain after lengthy algebra

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$$\frac{1+\lambda+\overline{n}}{\lambda-\mu_{\text{eff}}} = \pi k_B T \sum_{|\omega_n| (<\omega_D)} \frac{1}{|\omega_n|} - \pi k_B T \sum_{|\omega_n| (<\omega_D)} \frac{\epsilon^2}{|\omega_n|^3} + \langle a^2 \rangle h^2 \left[ \pi k_B T \sum_{|\omega_n| (<\omega_D)} \frac{1}{|\omega_n| + \rho} - \pi k_B T \sum_{|\omega_n| (<\omega_D)} \frac{3 |\omega_n| + 2\rho}{|\omega_n|^2 (|\omega_n| + \rho)^2} \right].$$
(38)

Since the pseudo-order-parameter vanishes at  $T = T_c$ , I find that Eq. (38) at  $T = T_c$  becomes

$$\frac{1+\lambda+\bar{n}}{\lambda-\mu_{\rm eff}} = \sum_{n=0}^{n_D-1} \frac{1}{n+\frac{1}{2}} + \langle a^2 \rangle h^2 \sum_{n=0}^{n_D-1} \frac{1}{n+\frac{1}{2}+\frac{\rho}{2\pi k_B T_c}}, \qquad (39)$$

where the summations over  $\omega_n$  have been converted to summations over the *n* appearing in  $\omega_n = (2n+1)\pi k_B T$ . The upper limit in the summations is  $n_D - 1$  where  $n_D = \hbar \omega_D / 2\pi k_B T_c$ . Performing the summation, I get

$$\frac{1+\lambda+\overline{n}}{\lambda-\mu_{\text{eff}}} = \psi \left[ \frac{\hbar\omega_D}{2\pi k_B T_c} + \frac{1}{2} \right] - \psi(\frac{1}{2}) + \langle a^2 \rangle h^2 \left[ \psi \left[ \frac{\hbar\omega_D}{2\pi k_B T_c} + \frac{\rho}{2\pi k_B T_c} + \frac{1}{2} \right] - \psi \left[ \frac{\rho}{2\pi k_B T_c} + \frac{1}{2} \right] \right], \quad (40)$$

where  $\psi(x)$  is the digamma function. If  $\rho$  (=1/2 $\tau_{eff}$ ) is small (much less than  $2\pi k_B T_c$ ), I can expand the digamma functions in powers of  $\rho/2\pi k_B T_c$  to get

$$\frac{1+\lambda+\overline{n}}{\lambda-\mu_{\rm eff}} = (1+\langle a^2\rangle h^2) \left[ \psi \left[ \frac{\hbar\omega_D}{2\pi k_B T_c} + \frac{1}{2} \right] - \psi(\frac{1}{2}) \right] \\ + \langle a^2\rangle h^2 \left[ \frac{\rho}{2\pi k_B T_c} \right] \left[ \psi' \left[ \frac{\hbar\omega_D}{2\pi k_B T_c} + \frac{1}{2} \right] \\ - \psi'(\frac{1}{2}) \right], \qquad (41)$$

where  $\psi'$  is the trigamma function. In the limit  $\hbar\omega_D \gg 2\pi k_B T_c$ ,  $\psi(\hbar\omega_D/2\pi k_B T_c + \frac{1}{2}) - \psi(\frac{1}{2})$  varies as  $\ln(2e^C \hbar\omega_D/\pi k_B T_c)$  where C is the Euler constant. Combining Eq. (41) with the expressions for the transition temperature  $T_{c0}$  of the pure anisotropic superconductor

$$(1 + \langle \alpha^2 \rangle) \ln \left[ \frac{2e^C \hbar \omega_D}{\pi k_B T_{c0}} \right] = \frac{1 + \lambda}{\lambda - \mu^*} , \qquad (42)$$

where  $\langle \alpha^2 \rangle$  is the mean-square energy gap anisotropy defined by Eq. (18), I get

$$\ln \frac{T_c}{T_{c0}} = \frac{1+\lambda}{\lambda-\mu^*} \left[ \frac{1}{1+\langle \alpha^2 \rangle} \right] - \frac{1+\lambda+\bar{n}}{\lambda-\mu_{\text{eff}}} \left[ \frac{1}{1+\langle a^2 \rangle h^2} \right] + \frac{\langle a^2 \rangle h^2}{1+\langle a^2 \rangle h^2} \left[ \frac{\rho}{2\pi k_B T_c} \right] \left[ \psi' \left[ \frac{\hbar\omega_D}{2\pi k_B T_c} + \frac{1}{2} \right] - \psi'(\frac{1}{2}) \right].$$
(43)

The dependence of  $T_c$  on the impurity concentration enters in three ways, through its explicit appearance, through the dependence of  $\frac{1}{2}\tau_{\rm eff}$  on  $\overline{n}$  and through the dependence of  $\mu_{\rm eff}$  (leading in turn to the dependence of h) on  $\overline{n}$ .

# C. Jump in the specific heat at $T_c$

By keeping the higher powers of the order parameter in Eq. (38), we get

$$\left[\frac{\epsilon}{2\pi k_B T}\right]^2 = \frac{(1+\lambda+\overline{n})/(\lambda-\mu_{\rm eff})-A(T)-\langle a^2\rangle h^2 B(T)}{C(T)+\langle a^2\rangle h^2 D(T)}$$

where

$$A(T) = \psi \left[ \frac{\hbar \omega_D}{2\pi k_B T} + \frac{1}{2} \right] - \psi(\frac{1}{2}) , \qquad (45a)$$

$$B(T) = \psi \left[ \frac{\hbar \omega_D}{2\pi k_B T} + \frac{\rho}{2\pi k_B T} + \frac{1}{2} \right] - \psi \left[ \frac{\rho}{2\pi k_B T} + \frac{1}{2} \right],$$
(45b)

$$C(T) + \frac{1}{4} \left[ \psi^{(2)} \left[ \frac{\hbar \omega_D}{2\pi k_B T} + \frac{1}{2} \right] - \psi^{(2)}(\frac{1}{2}) \right], \quad (45c)$$
  
and

$$D(T) = \left[\frac{\rho}{2\pi k_B T}\right]^2 \left[\psi \left[\frac{\hbar\omega_D}{2\pi k_B T} + \frac{\rho}{2\pi k_B T} + \frac{1}{2}\right] - \psi \left[\frac{\rho}{2\pi k_B T} + \frac{1}{2}\right] - \psi \left[\frac{\hbar\omega_D}{2\pi k_B T} + \frac{1}{2}\right] + \psi(\frac{1}{2})\right] + \left[\frac{\rho}{2\pi k_B T}\right] \left[\psi' \left[\frac{\hbar\omega_D}{2\pi k_B T} + \frac{\rho}{2\pi k_B T} + \frac{1}{2}\right] - \psi' \left[\frac{\rho}{2\pi k_B T} + \frac{1}{2}\right] - 2\psi' \left[\frac{\hbar\omega_D}{2\pi k_B T} + \frac{1}{2}\right] + 2\psi'(\frac{1}{2})\right], \quad (45d)$$

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(44)

where  $\psi^{(2)}(x)$  is one of the higher polygamma functions. The explicit dependence of the order parameter on the temperature is obtained by expanding all the functions appearing in Eq. (44) about the transition temperature  $T_c$ . Doing this, I get

$$\epsilon^{2}(T) = \frac{A'(T_{c}) + \langle a^{2} \rangle h^{2} B'(T_{c})}{C(T_{c}) + \langle a^{2} \rangle h^{2} D(T_{c})} 8\pi^{2} k_{B}^{2} T_{c}^{2} \left[ 1 - \frac{T}{T_{c}} \right],$$
(46)

where

$$\mathbf{f}'(T) = -T_c \frac{\partial A(T)}{\partial T} \Big|_{T_c}$$

and

$$B'(T) = -T_c \left. \frac{\partial B(T)}{\partial T} \right|_{T_c}$$

The difference between the free energies of the normal and superconducting phase is given by<sup>38</sup>

$$\frac{\Delta F}{N(0)} = \pi k_B T \left\langle \sum_{n} \left\{ \left[ \widetilde{\omega}_n^2 + \phi_n^2(\Omega') \right]^{1/2} - \widetilde{\omega}_n \right\} \times \left[ 1 - \frac{\widetilde{\omega}_n^0}{\left[ \widetilde{\omega}_n^2 + \phi_n^2(\Omega') \right]^{1/2}} \right] \right\rangle, \quad (47)$$

where  $\tilde{\omega}_n$  and  $\phi_n(\Omega)$  are given by Eqs. (20) and (21).  $\tilde{\omega}_n^0$ is the renormalized frequency in the Migdal theory<sup>14</sup> for the normal phase. Expanding the square-root terms in Eq. (47) in powers of the anisotropy parameter  $a_k(\Omega)$ , I get

$$\frac{\Delta F}{(1+\lambda+\overline{n})N(0)} = \frac{1}{2}\epsilon^4(T)[C(T)+\langle a^2\rangle h^2 D(T)], \quad (48)$$

where  $\epsilon^2$  is given by Eq. (46). Using the definition of the specific-heat jump at  $T_c$ 

$$\Delta C_{NS} = T_c \left. \frac{\partial^2 \Delta F}{\partial T^2} \right|_{T = T_c}, \qquad (49)$$

I get

$$\Delta C_{NS} = (1 + \lambda + \bar{n}) \delta N(0) \pi^2 k_B^2 T_c$$

$$\times \left[ \frac{[A'(T_c) + \langle a^2 \rangle h^2 B'(T_c)]^2}{C(T_c) + \langle a^2 \rangle h^2 D(T_c)} \right].$$
(50)

In the limit  $h\omega_D >> 2\pi k_B T_c$ , the upper limits in the summations in A(T), B(T), C(T), and D(T) can be extended to infinity. With these extensions

$$A'(T_c) = 1$$
, (51a)

$$B'(T_c) = 1 - \left[\frac{\rho}{2\pi k_B T_c}\right] \psi' \left[\frac{\rho}{2\pi k_B T_c} + \frac{1}{2}\right], \quad (51b)$$

and

$$C(T_c) = 8\lambda(3) . \tag{51c}$$

If in addition,  $\frac{1}{2}\tau_{\text{eff}}$  is much less than 2  $k_BT_c$ , then

$$D(T_c) = 6C(T_c) . (51d)$$

With these approximations, I get

$$\Delta C_{NS} = (1+\lambda+\bar{n})8N(0)\pi^2 T_c \left[ \frac{\left[ 1+\langle a^2 \rangle h^2 - \langle a^2 \rangle h^2 \left[ \frac{\rho}{2\pi k_B T_c} \right] \psi' \left[ \frac{\rho}{2\pi k_B T_c} + \frac{1}{2} \right] \right]^2}{8\lambda(3)(1+6\langle a^2 \rangle h^2)} \right].$$
(52)

This expression is very similar to the expression obtained by Yoksan and Nagi<sup>35</sup> for the specific-heat jump at  $T_c$  of a strong-coupling anisotropic superconductor containing *non-transition-metal impurities*. By setting  $N_d(0)$  to zero, Eq. (52) reduces exactly to Yoksan and Nagi's expression.

#### **V. DISCUSSION**

In Secs. II–IV, I have developed strong-coupling theories for superconductors containing transition-metal impurities which give rise to local spin fluctuations. Using the Migdal-Eliashberg formalism, I have obtained expressions for the decrease in the transition temperatures of both isotropic and anisotropic superconductors due to the LSF's and an expression for the jump in the specific heat at  $T_c$  of anisotropic superconductor containing LSF's. It should be pointed out that the expression for the specific-heat jump does not become the expression for the specific-heat jump of an isotropic superconductor when the mean-square anisotropy parameter  $\langle a^2 \rangle$  is set to zero.

The reason for this is that in the limit  $\langle a^2 \rangle = 0$ , the expansion for the renormalized energy gap, Eq. (29), would not contain sufficient information for the calculation of the specific-heat jump. One would have to use, instead, an expansion of the form  $a_1\epsilon + a_{-1}\epsilon^{-1}$ . I will return to this problem in a future study.

To see what changes to the BCS theory arise when the Migdal-Eliashberg formalism is used, I have plotted in Figs. 1 and 2, the decreases in  $T_c$  of an isotropic superconductor as predicted by the strong-coupling expression, Eq. (17), and by the weak-coupling (Schlottmann's) expression, Eq. (9). In Fig. 1, I show the decreases by different values of  $U_{eff}\chi(0)$ , while in Fig. 2, I show the decreases for different values of the electron-phonon massenhancement parameter  $\lambda$ . For the values of the densities of states N(0) and  $N_d(0)$ , I have used N(0)=0.286states/eV atom (the density of states of aluminum) and  $N_d(0)=0318$  states/eV atom (typical density of states for transition-metal impurities dissolved in aluminum) The value of  $\mu^*$  is taken to be 0.1. The values of the other pa-



FIG. 1. Decrease in  $T_c$  of an isotropic superconductor due to LSF's. The three sets of curves show the decrease in  $T_c$  predicted by the Migdal-Eliashberg based expression, --, and by Schlottmann's expression,  $\cdots$ , for different values of  $U_{\text{eff}}\chi(0)$ . The impurity concentrations appearing in Eqs. (9) and (17) do not include the effects of the orbital degeneracy off the impurities and so the values of  $n_i$  appearing in the figure should be multiplied by 2l + 1 for their use in Eqs. (9) and (17).

rameters are given in the figures. The effective BCS coupling constant  $N(0)g_{eff}$  appearing in Schlottmann's expression for  $T_c$  was set at  $(\lambda - \mu^*)/(1 + \lambda)$  in order for both expressions to predict the same  $T_{c0}$ , the transition temperature of the pure superconductor. Looking at Fig. 1, I see that the decreases in the transition temperatures due to the LSF's become steeper as the LSF parameter  $U_{\rm eff}\chi(0)$  becomes larger. The decreases in the  $T_c$ 's predicted by the Migdal-Eliashberg-based expression, Eq. (17), are less than the decreases predicted by Schlottman's expression, Eq. (9), for a given value of  $U_{\text{eff}}\chi(0)$ . Figure 2 shows the decreases in  $T_c$  to be less steep as the value of the electron-phonon mass-enhancement parameter  $\lambda$  is increased. The difference between the values of  $T_c$  predicted by the two expressions becomes less as the value of  $\lambda$ becomes larger.

To see the effects arising from the presence of an anisotropy in the strong-coupling superconductor containing local spin fluctuations, I have plotted in Fig. 3, the decrease in  $T_c$  predicted by Eq. (43) for three values of the anisotropy parameter  $\langle a^2 \rangle$ , 0.011, 0.18, and 0.32. For the value of the parameter characterizing the LSF's, I have set  $U_{\rm eff}\chi(0) = 1$ . This value is well within the range for which Schlottmann's theory should be valid (i.e., for values giving  $g = U/\pi \Gamma_d < 1$ ). For the values of  $\lambda$  and  $\mu^*$ , I have used  $\lambda = 0.412$  and  $\mu^* = 0.127$ . While these values are those for aluminum superconductors, the curves in Fig. 3 should not be viewed as being those for aluminum superconductors containing transition-metal impurities. In plotting the curves, I assumed that the parameter  $\rho = \frac{1}{2} \tau_{\text{eff}}$  is equal to  $n_i (N_d(0)/N(0)) \Gamma_d$  where  $N_d(0)/N(0) = 1$  and  $\Gamma_d = 80$  MeV. Looking at the curves, I see that the decrease in  $T_c$  becomes steeper for





FIG. 2. Decrease in  $T_c$  for different values of  $\lambda$ . The curves in this figure show the decreases predicted by Eqs. (9),  $\cdots$ , and ----, for different values of the electron-phonon by Eq. (17), mass-enhancement parameter.

FIG. 3. Decrease in  $T_c$  of an isotropic superconductor due to LSF's. The curves show the decrease in  $T_c$  when only the anisotropy parameter  $\langle a^2 \rangle$  is changed. Values of the other parameters are either given in the text or in the figure.

larger values of the anisotropy parameter  $\langle a^2 \rangle$ . Additional computer studies show that for much higher values of  $U_{\rm eff}\chi(0)$  (values such that g > 1 where the Schlottmann's theory is not valid), the anisotropy leading to a softening of the decrease (i.e., increasing the value of  $\langle a^2 \rangle$  leads to less steep decreases of  $T_c$ , the reverse of what is seen in Fig. 3). No attempt was made to fit the data on AlMn to Eq. (43) since the equation is sensitive to the choice of  $N_d(0)$ ,  $\Gamma_d$  and  $U_{\text{eff}}\chi(0)$ . For most 3d transition-metal impurities in aluminum,  $\Gamma_d$  is of the order 1 eV. For Mn in aluminum, however, the experimental data points to  $\Gamma_d$  being of order 0.1 eV. The uncertainties in the value of  $\Gamma_d$  and in the values of  $N_d(0)$  (quoted values range from 9.4 states/eV atom down to 2.13 states/eV atom) would make suspect any determination of  $U_{\text{eff}}\chi(0)$  using Eq. (43) to fit the data.

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