Properties of anisotropic superconductors with approximately neutral electron-electron interaction

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A Bardeen-Cooper-Schrieffer-type theory of superconductivity, in which the attractive electron-electron interaction is represented by a separable anisotropic term and the repulsion by an isotropic term, is extended to calculations of a variety of properties of the pure material and of the effects of both normal and paramagnetic impurities on the transition temperature, T_c. The goals are (1) the identification of properties which are likely to be quite different for materials with an approximately neutral interaction as compared with the usual regime in which the attraction dominates and (2) the estimation of maximum impurity concentrations which can be tolerated. For the pure material, the main conclusions are that the mean-squared anisotropy of the energy gap, the ratios of twice the Fermi-surface average of the gap to T_c, and of the zero-temperature critical magnetic field, $H_c(0)$, to T_c, the jump in the specific heat at T_c, the isotope effect, and the quasiparticle density of states can all be quite different, whereas the reduced temperature-dependent quantities $\Delta_{\vec{k}}(t)/\Delta_{\vec{k}}(0)$ and $H_c(t)/H_c(0)$ are not. Although very sensitive to the value of the mean-squared anisotropy, it is estimated that the maximum tolerable concentrations of both kinds of impurities are on the order of $10^{-2}\%$ to $10^{-4}\%$.

I. INTRODUCTION

In a recent paper, Whitmore and Carbotte[1] investigated the behavior of the superconducting transition temperature T_c of anisotropic materials in which the effective electron-electron interaction is, on the average, approximately neutral or even slightly repulsive. Without referring to any particular material, they pointed out that systems in which this could arise are found in the alkalis in which the electron-phonon mass-enhancement parameter $\lambda \sim 0.11-0.19$ (or perhaps higher for Li), and in the noble metals in which $\lambda \sim 0.16-0.21$; as well, the effects of paramagnons can be simulated by an effective Coulomb parameter $\mu^*_{\rm eff}$ which can be as high as about 0.3, and by an effective $\lambda_{\rm eff}$ which is reduced from λ by about 30%.

With the use of a Bardeen-Cooper-Schrieffer (BCS) type theory, the interaction was modeled by a separable, attractive part[2] and by an isotropic repulsion,

$$V_{\vec{k}\vec{k}'}=(1+a_{\vec{k}})V_{ep}(1+a_{\vec{k}'})-V_c \ . \tag{1}$$

Here V_{ep} and V_c are assumed to be positive, and the anisotropy is incorporated via the $a_{\vec{k}}$ which is assumed to be independent of energy in the energy range of interest, and to have zero Fermi-surface average, i.e., $\langle a \rangle = 0$. The double Fermi-surface average of $V_{\vec{k}\vec{k}'}$ is $V_{ep}-V_c$, from which it is seen that in this model the average interaction is attractive, neutral, or repulsive depending on whether $V_{ep}-V_c$ is positive, zero, or negative.

Physically, the first term in (1) can be interpreted as being due to the electron-phonon interaction, and V_c to the direct Coulomb interaction, but this is not necessary. An alternative, less specific, model interaction would be

$$V_{\vec{k}\vec{k}'}=\bar{V}+\delta V[(1+a_{\vec{k}})(1+a_{\vec{k}'})-1] \ , \tag{2}$$

which is equivalent to (1) if $\bar{V}$, the average of $V_{\vec{k}\vec{k}'}$, is chosen to be $V_{ep}-V_c$, and δV is V_{ep}.

This model leads to a closed expression for T_c, namely

$$T_c=1.13\omega_D e^{-f} \ , \tag{3}$$

with f given by

$$f=\frac{-[N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*]+\{[N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*]^2+4N(0)V_{ep}\mu^*\langle a^2\rangle\}^{1/2}}{2N(0)V_{ep}\mu^*\langle a^2\rangle} \ . \tag{4}$$

In these expressions ω_D is the Debye frequency, $N(0)$ the Fermi-energy density of states, $\langle a^2 \rangle$ a measure of the mean-squared anisotropy of $V_{\vec{k}\vec{k}'}$, and $N(0)V_c$ has been identified as μ^*, consistent with the physical interpretation of $V_{\vec{k}\vec{k}'}$ in the preceding paragraph. Here and throughout this paper atomic units with $\hbar = e = m_e = 1$ are used. In these units a temperature of 1.16 K corresponds to 1 meV.

The most remarkable property of this solution for T_c is its existence for all nonzero V_{ep} and μ^* as long as $\langle a^2 \rangle \neq 0$, which implies, within the separable model, that a finite T_c will exist no matter how large the repulsion is, as long as there is some anisotropy. A related important feature is the fact that when $N(0)V_{ep} \simeq \mu^*$, the anisotropy enters the solution not as $\langle a^2 \rangle$ but rather as $\langle a^2 \rangle^{1/2}$. This results in a larger T_c than would otherwise have been the case. In fact, the simple estimates suggested that at $\mu^* = N(0)V_{ep}$, and for $\langle a^2 \rangle = 0.1$, T_c could be on the order of 50 mK or larger, remaining above 1 mK well into the range $\mu^* > N(0)V_{ep}$. Of course, these values can be taken as no more than approximate guides.

Because of the essential role played by the anisotropy, it was anticipated that normal impurities would have a very important effect on T_c, since they are known to eliminate the anisotropy,[3] reducing T_c to the isotropic value. An investigation of their effect led to the conclusion that T_c was indeed reduced to a very small value, say below 1 mK, by relatively low-impurity concentrations.[4]

The quantitative results, and even, as Leavens *et al.*[5] have pointed out, the existence of a finite T_c for all μ^*, are dependent on the two major approximations used, namely, the BCS-type theory and the separable interaction. By expanding $V_{\vec{k}\vec{k}'}$ in Fermi-surface harmonics, those authors considered a simple but nonseparable anisotropy, and showed that the normal state is not necessarily unstable at $T = 0$ K. They also emphasized that quantitative investigation of superconductors, especially if the coupling is very weak, cannot be based on the BCS gap equation with a symmetric, temperature-independent interaction. Finally, they considered the effect of normal impurities within their model, concluding that for the parameters they used, for which $\mu^* \simeq N(0)V_{ep}/2$, the use of the separable model can exaggerate the impurity-induced reduction in T_c.

However, the present model does provide a tractable means of exploring a variety of properties of superconductors for which the average interaction is about neutral, which is the purpose of the present work. It is not the present intention to obtain quantitative predictions. Rather, it is hoped only to identify and provide some insight into those properties which are qualitatively different in this case, compared with the isotropic case or the intermediate one, in which the anisotropy is a small perturbation on the average interaction. This latter case has been treated in depth by Clem,[6,7] who used the model interaction of Markowitz and Kadanoff,[2] which is Eq. (1) with $V_c = 0$.

Many of the results will be presented as a function of the ratio $\mu^*/N(0)V_{ep}$, which will be denoted by

$$S \equiv \frac{\mu^*}{N(0)V_{ep}} . \tag{5}$$

Clearly, $S = 0$ is the case treated by Clem, in which $\mu^* = 0$. The situation $0 < S \ll 1$ implies the presence of a relatively small μ^*, as is the case for most known superconductors in which the anisotropy is relatively unimportant. $S = 1$ corresponds to the case of an interaction which is, on average, exactly neutral; when $S \simeq 1$ the anisotropy plays an essential role in that it can greatly enhance T_c above the isotropic value. The interest of this paper is focused primarily on this regime.

In the next section the basic theory and equations are specified in a little more detail, and two distribution functions for the anisotropy are introduced. In Sec. III properties of the pure metal are examined, namely the mean-squared anisotropy of the energy gap, the ratio $2\Delta_0(0)/T_c$, where $\Delta_0(0)$ is the Fermi-surface average of the zero-temperature gap, the temperature dependence of the gap, the specific-heat jump at T_c, the zero-temperature critical magnetic field and the deviation function, the isotope effect, and the quasiparticle density of states. Section IV is devoted to the effects of normal and paramagnetic impurities on T_c, and in Sec. V the results are summarized.

II. ANISOTROPY MODEL AND BASIC EQUATIONS

As indicated, a BCS-type theory is used for all calculations, with the effective electron-electron interaction given by (1). For the pure-metal properties the standard BCS gap equation[8] is used, which, combined with (1), is

$$\Delta_{\vec{k}}=\sum_{\vec{k}'}{}'[(1+a_{\vec{k}})V_{ep}(1+a_{\vec{k}'})-V_c]\times\Delta_{\vec{k}'}\frac{\tanh\beta E_{\vec{k}'}/2}{2E_{\vec{k}'}}\ , \tag{6}$$

where $E_{\vec{k}'}=(\epsilon_{\vec{k}'}^2+\Delta_{\vec{k}'}^2)^{1/2}$, $\beta=1/T$, $\Delta_{\vec{k}}$ is the energy gap, ω_D the Debye frequency, and the prime on the sum indicates it is to be restricted to the range $|\epsilon_{\vec{k}}|\le\omega_D$, $|\epsilon_{\vec{k}'}|\le\omega_D$.

To determine the impurity effects on T_c it is more convenient to use the linearized Eliashberg equations[9] in the imaginary-frequency-axis representation. Considerable simplification is achieved by assuming isotropic scattering[2,7,9,10]; the impurities are described by two parameters, $t_+=1/2\pi\tau_N$ and $t_-=1/2\pi\tau_p$, where τ_N and τ_p are the lifetimes of electronic excited states due, respectively, to normal impurity scattering and spin-flip scattering. The anisotropy enters through the electron-phonon function $[\alpha^2F(\omega)]_{\vec{k}\vec{k}'}$, leading to anisotropic $\lambda_{\vec{k}\vec{k}'}(m-n)$, which are defined by the usual integrals involving the $[\alpha^2F(\omega)]_{\vec{k}\vec{k}'}$. The BCS-type theory is obtained by neglecting the renormalization of the Matsubara frequencies by the electron-phonon interaction, replacing $\lambda_{\vec{k}\vec{k}'}(m-n)$ by $N(0)V_{ep\vec{k}\vec{k}'}$, and restricting the range of m in the remaining sum to $\pm N$, where $(2N+1)\pi T_c=\omega_D$. This results in

$$\tilde{\Delta}_{\vec{k}}(n)=\pi T_cN(0)\sum_m\left\langle[(1+a_{\vec{k}})V_{ep}(1+a_{\vec{k}'})-V_c]\frac{\tilde{\Delta}_{\vec{k}'}(m)}{|\tilde{\omega}_{\vec{k}'}(m)|}\right\rangle'+\pi(t_+-t_-)\left\langle\frac{\tilde{\Delta}_{\vec{k}'}(n)}{|\tilde{\omega}_{\vec{k}'}(n)|}\right\rangle'\ , \tag{7}$$

$$\tilde{\omega}_{\vec{k}}(n)=\omega_n+\pi(t_++t_-)\mathrm{sgn}(\omega_n)\ . \tag{8}$$

Here, $i\omega_n=i\pi T_c(2n-1)$ are the Matsubara frequencies ($n\epsilon I$), and $\tilde{\Delta}_{\vec{k}}(n)$ is a generalization of the energy gap to the imaginary axis. It is clear from (8) that $\tilde{\omega}_{\vec{k}}(n)$ is independent of $\vec{k}$, and can therefore be written $\tilde{\omega}(n)$. When $t_+=t_-=0$, the pure-metal T_c equation is recovered.

The effect of the anisotropy on some of the properties to be considered can be characterized by its mean-squared value $\langle a^2\rangle$ independent of any further details. However, in other cases it is necessary to assume a distribution function $P(a)$. Two different choices have been made:

$$P_1(a)=\tfrac{1}{2}[\delta(a-A)+\delta(a+A)] \tag{9}$$

and

$$P_2(a)=\frac{1}{2A}\Theta(A-a)\Theta(A+a)\ . \tag{10}$$

Each of these is normalized to unity, and for each $\langle a\rangle=0$. Note however that for $P_1(a)$, $\langle a^2\rangle=A^2$, whereas for $P_2(a)$, $\langle a^2\rangle=A^2/3$. For the cases in which this step is necessary, both $P_1(a)$ and $P_2(a)$ have been employed as a test of the sensitivity of the particular property to the choice.

Many of the quantities considered here are, for an isotropic BCS superconductor, universal in that they do not depend on the values of the parameters $N(0)V$ or ω_D. This is not necessarily the case when the interaction is modeled by Eq. (1). Therefore, all calculations have been done for the two sets of parameters used in the previous work.[1,4] One choice is $N(0)V_{ep}=0.285$ and $\omega_D=32$ meV, leading to a T_c of about 1 K when $\langle a^2\rangle=0.04$ and $\mu^*=0.13$; this corresponds approximately to Al. The second choice is $N(0)V_{ep}=0.41$ and $\omega_D=21$ meV, so $T_c\simeq10$ K when $\langle a^2\rangle=0.04$ and $\mu^*=0.12$, as is roughly the case for Nb. This latter choice is clearly outside the weak-coupling region, but it is still of interest to explore the predictions of the theory in this region, and, in particular, to see to what extent the results are independent of $N(0)V_{ep}$.

III. PURE-METAL PROPERTIES

The mean-squared anisotropy of the gap, denoted by R^2, is defined by

$$R^2=\frac{\langle\Delta_{\vec{k}}^2\rangle-\langle\Delta_{\vec{k}}\rangle^2}{\langle\Delta_{\vec{k}}\rangle^2}\ . \tag{11}$$

With the use of the present model $V_{\vec{k}\vec{k}'}$, $\Delta_{\vec{k}}$ has the form $\Delta_{\vec{k}}=\Delta_0+a_{\vec{k}}\Delta_1$, which, since $\langle a\rangle=0$, implies $R^2=\langle a^2\rangle r^2$, where r is the (temperature-dependent) ratio $r=|\Delta_1/\Delta_0|$. The gap equation can be converted into two equations in two unknowns, r and the ratio of twice the average gap to T_c, $2\Delta_0/T_c$. The first step in doing so is the conversion of the sum over $\vec{k}'$ to averages over constant-energy surfaces, and an energy integral with the density of states replaced by its Fermi-energy value $N(0)$. The resulting equation is averaged over the Fermi surface (in the $\vec{k}$ variable), and then multiplied by $a_{\vec{k}}$ and averaged. After dividing the second result by $\langle a^2\rangle$, the two following coupled equations are obtained:

$$\Delta_0=\Delta_1-\mu^*\langle(\Delta_0+a_{\vec{k}'}\Delta_1)I(\Delta_{\vec{k}'})\rangle' , \tag{12}$$

$$\Delta_1=N(0)V_{ep}\langle(1+a_{\vec{k}'})(\Delta_0+a_{\vec{k}'}\Delta_1)I(\Delta_{\vec{k}'})\rangle' , \tag{13}$$

where

$$I(\Delta_{\vec{k}'})=\int_{-\omega_D}^{\omega_D}\frac{\tanh(\beta E_{\vec{k}'}/2)}{E_{\vec{k}'}}dE_{\vec{k}'} . \tag{14}$$

At $T=0$ this integral is approximately $\operatorname{arcsinh}(\omega_D/|\Delta_{\vec{k}'}|)$, which in the weak-coupling limit of $|\Delta_{\vec{k}'}|\ll\omega_D$ becomes $\ln(2\omega_D/|\Delta_{\vec{k}'}|)$.

If the anisotropy were a small effect, then the $\Delta_{\vec{k}'}$ could be written $\Delta_0[1+a_{\vec{k}'}(\Delta_1/\Delta_0)]$, and the logarithm expanded in terms of the small parameter $a_{\vec{k}'}\Delta_1/\Delta_0$, as was done by Clem.[6] However, the primary interest in the present case is precisely the situation in which this parameter is not necessarily small; the expansion is not appropriate and so to evaluate the averages the distribution functions are employed. With the use of $P_1(a)$, eliminating ω_D in favor of T_c through the T_c equation (3), and further rearranging the result, (12) and (13) are transformed into

$$1=r+\mu^*\left[\ln\left|\frac{e^{-f}}{3.53}\frac{2\Delta_0}{T_c}\right|+\tfrac{1}{2}\ln|1-A^2r^2|-\tfrac{1}{2}Ar\ln\left|\frac{1-Ar}{1+Ar}\right|\right.$$
$$\left.-\tfrac{1}{2}(1+Ar)F(\beta\Delta_0(1+Ar))-\tfrac{1}{2}(1-Ar)F(\beta\Delta_0(1-Ar))\right] , \tag{15}$$

$$r=-N(0)V_{ep}\left[(1+A^2r)\ln\left|\frac{e^{-f}}{3.53}\frac{2\Delta_0}{T_c}\right|+\tfrac{1}{2}(1+A^2r)\ln|1-A^2r|-\tfrac{1}{2}A(1+r)\ln\left|\frac{1-Ar}{1+Ar}\right|\right.$$
$$\left.-\tfrac{1}{2}[1+A(1+r)+A^2r]F(\beta\Delta_0(1+Ar))-\tfrac{1}{2}[1-A(1+r)+A^2r]F(\beta\Delta_0(1-Ar))\right] , \tag{16}$$

$$F(\beta\Delta_{\vec{k}})=2\int_0^{\omega_D}d\epsilon_{\vec{k}}\left[\frac{\partial}{\partial\epsilon_{\vec{k}}}f(E_{\vec{k}})\right]\sinh^{-1}\frac{\epsilon_{\vec{k}}}{|\Delta_{\vec{k}}|} . \tag{17}$$

Similar, albeit somewhat more complicated, equations arise when $P_2(a)$ is used.

The zero-temperature values of these properties, R^2 and $2\Delta_0(0)/T_c$, are examined first. In this limit, $F(\beta\Delta_{\vec{k}})=0$, so the relevant equations are just (15) and (16), but without the last two terms of each. As will be the case for each property to be considered, the two special cases of $\mu^*\ll N(0)V_{ep}$ (or zero), and $\mu^*\simeq N(0)V_{ep}$, will be examined in particular, as well as general results presented throughout the range $0<\mu^*\lesssim 1.25N(0)V_{ep}$ where appropriate. In the first case, the anisotropy represents a small effect, and these equations can be solved approximately with the result that, to lowest order in $\langle a^2\rangle$,

$$R^2\simeq\frac{\langle a^2\rangle}{(1-S)^2} \tag{18}$$

and

$$\frac{2\Delta_0(0)}{T_c}\simeq 3.53(1-\tfrac{3}{2}R^2) . \tag{19}$$

The last result is that obtained by Clem,[6] with the qualification that in his case, with $\mu^*=0$, $R^2=\langle a^2\rangle$.

In the region $S\simeq 1$, similar expressions are more difficult to obtain, primarily because of the functions $\ln|1\pm Ar|$, since Ar is not small. However, with the use of $P_1(a)$ it can be shown that $R^2=1$ when $S=1-\langle a^2\rangle$, which is a slightly attractive potential. With the use of $P_2(a)$, the nearly identical result of $R^2=1$ occurs when

$$S=1-\langle a^2\rangle[1+0.08N(0)V_{ep}] .$$

An expansion of r in μ^* can be made about this point, with the result that in the region of $S\simeq 1$, to low order in $\langle a^2\rangle$,

$$r \simeq \frac{1}{\langle a^2\rangle^{1/2}} + \left[\frac{1}{2}\frac{(S-1)}{\langle a^2\rangle^{1/2}} - \frac{0.21N(0)V_{ep}(S-1)}{\langle a^2\rangle^{1/2}} + \{\tfrac{1}{2} + 0.04\mu^* + 0.09[N(0)V_{ep}]^2(S-1)\} \right], \tag{20}$$

leading to the special case that at $S=1$

$$R^2 = 1 + \langle a^2\rangle^{1/2}[1 + 0.08N(0)V_{ep}] . \tag{21}$$

A similar expansion cannot be made for $P_1(a)$ because of a singularity at $S=1$. The derivative $(\partial r/\partial \mu^*)_{S=1}=0$, but the second derivative, $(\partial^2 r/\partial \mu^{*2})_{S=1}$, is discontinuous and divergent, with values $\pm\infty$, rendering an expansion impossible. In either case R^2 is found to be one for an interaction which is slightly attractive, and somewhat greater than one when $S=1$. This is very different from the usual case in which $R^2 \simeq \langle a^2\rangle$ or slightly larger.

Approximate expressions for $2\Delta_0(0)/T_c$ can also be obtained. For example, at $S=1$ using $P_2(a)$,

$$\frac{2\Delta_0(0)}{T_c} \simeq \frac{3.53}{1.91}\exp\left\{ -\langle a^2\rangle \left[0.44 \left[1 + 0.08N(0)V_{ep} - \frac{1}{8N(0)V_{ep}} \right] \right] \right\} . \tag{22}$$

It is clear from this equation that the ratio is significantly reduced from the value of 3.53. However, it should be emphasized that this expression must be considered as quite approximate because neglect of relatively small terms of higher order in $\langle a^2\rangle$ in the arguments of the exponential could lead to large effects on the value of the complete expression.

The numerical results are illustrated in Figs. 1 and 2. In agreement with Eq. (18), R^2 starts off at the value of $\langle a^2\rangle$, remaining within a factor of 2 of this value until $S \simeq 0.3$, after which it increases rapidly, becoming 1 at $S \simeq 1-\langle a^2\rangle$ as predicted earlier, and increasing beyond that. The illustrated curves were obtained using $P_1(a)$ and $N(0)V_{ep}=0.285$. The results using $P_2(a)$ are indistinguishable from these for $0 \lesssim S \lesssim 1$, and differ by about 4% at the most up to $S=1.25$. Clearly, the general behavior is independent of this choice. Furthermore, although the relevant equations do depend on $N(0)V_{ep}$, choosing $N(0)V_{ep}=0.41$ resulted in differences too small to be seen on this graph.

As seen from Fig. 2, $2\Delta_0(0)/T_c$ does begin at approximately $3.53(1-3/2R^2)$, and is reduced to just about 3.53/2 when $S=1$, with further reductions for larger S. This exhibits the qualitative predictions of Eq. (22) which in fact turns out to be surprisingly accurate. In this case changing to $P_2(a)$ has a slightly larger effect but in no way alters the general behavior. As with R^2, the effect of altering $N(0)V_{ep}$ is negligible. It is apparent that in this region both R^2 and $2\Delta_0(0)/T_c$ are also rather independent of $\langle a^2\rangle$, depending primarily on the fact that $S \simeq 1$.

The temperature dependence of Δ_0 and Δ_1 can be investigated by returning to the finite-temperature equations (15)–(17), for which the function F is

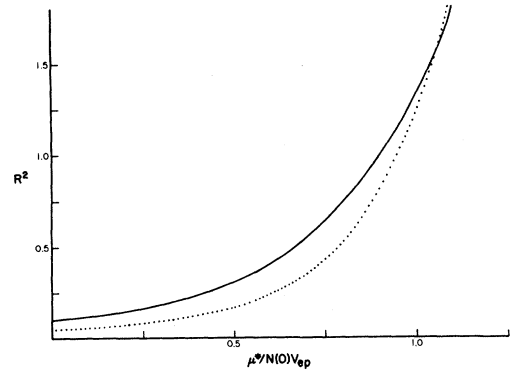

FIG. 1. Mean-squared anisotropy of the gap R^2 as a function of $\mu^*/N(0)V_{ep}$, for $\langle a^2\rangle$ equal to 0.05 (· · ·) and 0.1 (——). These curves were derived using $N(0)V_{ep}=0.285$ and $P_1(a)$. The minor effects of changing $N(0)V_{ep}$ and $P(a)$ are described in the text.

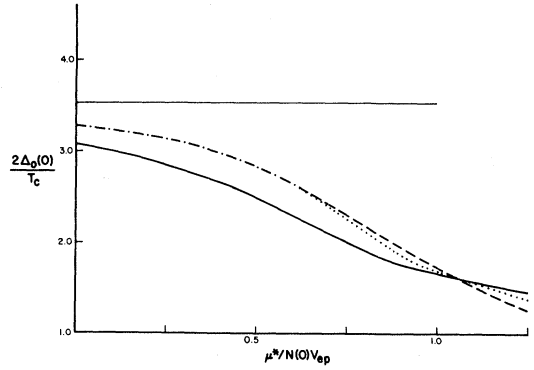

FIG. 2. Ratio $2\Delta_0(0)/T_c$, as a function of $\mu^*/N(0)V_{ep}$, for $\langle a^2\rangle$ equal to 0.05 (· · ·) and 0.1 (——) using $P_1(a)$, and $\langle a^2\rangle=0.05$ using $P_2(a)$ (— — —). In each case $N(0)V_{ep}=0.285$, but the effect of changing to 0.41 is too small to be seen on this graph. The BCS value, illustrated by the top horizontal line, is 3.53 up to $\mu^*=N(0)V_{ep}$.

evaluated numerically. Typical results are illustrated in Fig. 3 where $\Delta_0(t)/\Delta_0(0)$ has been plotted as a function of the reduced temperature $t=T/T_c$. It is clear that although there is some deviation from the isotropic result, choosing $\mu^*\simeq N(0)V_{ep}$ does not alter the general behavior. There is also a slight dependence on the choice of $P(a)$, but no significant dependence on the value chosen for $N(0)V_{ep}$. The ratio $r(T)$ is nearly independent of temperature, resulting in $\Delta_1(t)/\Delta_1(0)$ being not much different from $\Delta_0(t)/\Delta_0(0)$, and so this is not shown. As pointed out by Markowitz and Kadanoff, this is consistent with early experiments on Al by Masuda and Redfield[11] and by Masuda.[12]

By analyzing the behavior of the gap near T_c, an expression for the discontinuity in the specific heat at the transition can be derived. The first step is obtaining a limiting expression for the function $F(\beta\Delta_{\vec{k}})$ for small $\beta\Delta_{\vec{k}}$. Using

$$f(E_{\vec{k}})=\tfrac{1}{2}[1-\tanh(\beta E_{\vec{k}}/2)]$$

and the well-known expansion of $\tanh(\beta E_{\vec{k}}/2)$ in terms of the Matsubara frequencies, one can obtain by standard methods[13] the first two terms in the expansion. Employing these in (15) it can be shown that for $t\lesssim 1$, to lowest order in $1-t$,

$$\Delta_0(t)\simeq\left[\frac{8}{7\zeta(3)}\right]^{1/2}\frac{\pi T_c}{[1+3A^2r^2]^{1/2}}\times\left[\frac{1-r}{\mu^*}+f+(1-t)\right]. \tag{23}$$

At $T=T_c$ ($t=1$), r has the value $r_c=1+\mu^*f$, ensuring $\Delta_0(1)=0$. With the use of the expansion in (16) instead of (15) an expression analogous to (23) can be derived, which can be combined with it to show that, to lowest order in $1-t$,

$$r\simeq r_c+\alpha(1-t)\,, \tag{24}$$

where

$$\alpha=\frac{2\langle a^2\rangle\mu^* r_c^2(1-\langle a^2\rangle r_c^2)}{1+6\langle a^2\rangle r_c^2+(\langle a^2\rangle r_c^2)^2}\,. \tag{25}$$

This result can then be inserted into (23) to obtain

$$\Delta_0(t)\simeq 3.06T_c\left[\frac{1+\langle a^2\rangle r_c^2}{1+6\langle a^2\rangle r_c^2+(\langle a^2\rangle r_c^2)^2}\right]^{1/2}\times(1-t)^{1/2}\,. \tag{26}$$

The corresponding behavior for $\Delta_1(t)$ is easily related to Eq. (26) through the fact that, to lowest order, $\Delta_1(t)\simeq r_c\Delta_0(t)$. It should be pointed out here that r_c and hence $\Delta_0(t)$, do not depend separately on $N(0)V_{ep}$, but only on S (as well as $\langle a^2\rangle$). This expression is based on the use of $P_1(a)$, but the dependence on this choice was seen to be small in Figs. 2 and 3.

The calculation of the specific heat differs only slightly from the standard procedure, coming from $C_v=-(\partial S/\partial\beta)$ with the entropy S given by

$$S=2\left\langle\int N(\epsilon_{\vec{k}})d\epsilon_{\vec{k}}\left[\frac{\beta E_{\vec{k}}}{1+e^{\beta E_{\vec{k}}}}+\ln(1+e^{-\beta E_{\vec{k}}})\right]\right\rangle, \tag{27}$$

with $E_{\vec{k}}=|\epsilon_{\vec{k}}|$ above T_c and $E_{\vec{k}}=(\epsilon_{\vec{k}}^2+\Delta_{\vec{k}}^2)^{1/2}$ below. The discontinuity in C_v at T_c is found to be

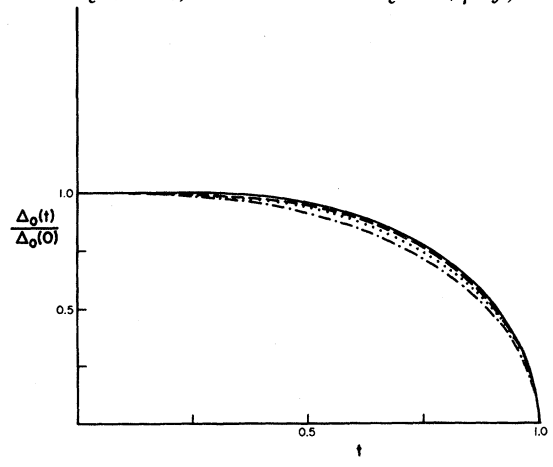

FIG. 3. $\Delta_0(t)/\Delta_0(0)$ as a function of reduced temperature t, for the isotropic BCS case (——), and the anisotropic case with $\langle a^2\rangle=0.1$ using $P_1(a)$ with $\mu^*=0$ (· · ·), and $\mu^*=N(0)V_{ep}$ (— — —), and $\langle a^2\rangle=0.1$, $\mu^*=N(0)V_{ep}$, using $P_2(a)$ (—·—·—·). The choice of $N(0)V_{ep}$ has no significant effect.

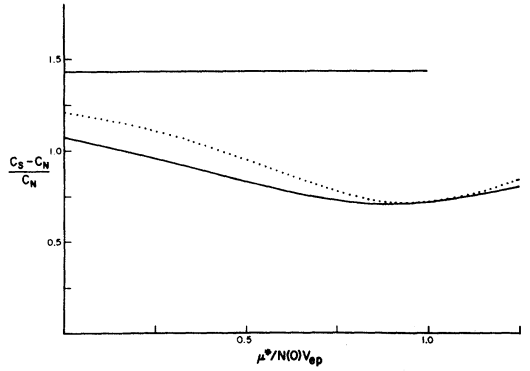

FIG. 4. Specific-heat jump $(C_S-C_N)/C_N$ at T_c as a function of $\mu^*/N(0)V_{ep}$. The upper solid curve is the isotropic BCS result of 1.43. The other two curves are for $\langle a^2\rangle=0.05$ (· · ·) and $\langle a^2\rangle=0.1$ (——), using Eq. (42) which is based on $P_1(a)$.

$$C_S-C_N=2\beta_c^3\left\langle \int N(\epsilon_{\vec{k}})d\epsilon_{\vec{k}}\frac{1}{2}\left[\frac{\partial\Delta_0^2}{\partial\beta}+2a_{\vec{k}}\frac{\partial}{\partial\beta}(\Delta_0\Delta_1)+a_{\vec{k}}^2\frac{\partial\Delta_1^2}{\partial\beta}\right]\right|_{\beta_c}\frac{e^{\beta|\epsilon_{\vec{k}}|}}{(1+e^{\beta|\epsilon_{\vec{k}}|})^2}\Bigg\rangle . \tag{28}$$

In these expressions C_S and C_N are the specific heat of the superconducting and normal states, respectively, and $\beta_c=1/T_c$. Because the $\epsilon_{\vec{k}}$ are free-electron energies, the Fermi-surface average involves only the functions $a_{\vec{k}}$; with the use of $\langle a\rangle=0$, Eq. (26) for $\Delta_0(t)$, and the related expression for $\Delta_1(t)$, a procedure similar to the standard one yields

$$\frac{C_S-C_N}{C_n}=1.43\left[\frac{(1+\langle a^2\rangle r_c^2)^2}{1+6\langle a^2\rangle r_c^2+(\langle a^2\rangle r_c^2)^2}\right], \tag{29}$$

which, like $\Delta_0(t)$ and $\Delta_1(t)$ near T_c, does not depend separately on $N(0)V_{ep}$. This reduces to the usual value of 1.43 in the isotropic case, and, to lowest order in $\langle a^2\rangle$, to $1.43(1-4\langle a^2\rangle)$ in the anisotropic case with $\mu^*=0$, in agreement with Clem.[6] When $\mu^*=N(0)V_{ep}$, the jump is reduced to just about one-half this value,

$$\frac{C_S-C_N}{C_N}\simeq\frac{1.43}{2}\left[1+\frac{\langle a^2\rangle}{8}\right]. \tag{30}$$

Although this is only to first order in the anisotropy, it is very close to the full result, as seen from Fig. 4. The solid curve indicates a continual reduction in this jump up to $S\simeq1$, followed by an increase as μ^* is increased beyond $N(0)V_{ep}$. This reflects the very rapid increase in R^2, and hence in Δ_1^2, as μ^* is increased beyond about $S=1$. It is also apparent that, as for R^2 and $2\Delta_0(0)/T_c$ in the region $S\simeq1$, the value of the specific-heat jump is determined primarily by simply being in the regime $S\simeq1$.

The critical magnetic field $H_c(T)$ is, as usual, obtained from the difference between the free energies of the normal and superconducting states. The result can be expressed

$$\frac{H_c(T)^2}{4\pi N(0)}=\Delta_0^2(1+R^2)-\frac{2\pi^2}{3}T^2+2\left\langle\int_{-\infty}^{\infty}(\epsilon_{\vec{k}}^2+E_{\vec{k}}^2)\frac{f(E_{\vec{k}})}{E_{\vec{k}}}d\epsilon_{\vec{k}}\right\rangle . \tag{31}$$

At zero temperature only the first term remains. This can be combined with Eqs. (18) and (19) for small S, and with (21) and the observation that $2\Delta_0(0)/T_c$ is very nearly 3.53/2 for $S=1$, to show that in these limiting cases

$$\frac{H_c(0)}{\sqrt{4\pi N(0)}T_c}\simeq\begin{cases}1.77(1-R^2), & S\ll1\\ \dfrac{1.77}{\sqrt{2}}, & S=1 .\end{cases} \tag{32}$$

These have a slight dependence on the choice of $P(a)$ through R^2 and $2\Delta_0(0)/T_c$. The first result is that of Clem with the earlier noted qualification that $R^2=\langle a^2\rangle$ in his case, which is the same behavior which occurred in the present calculation of $2\Delta_0(0)/T_c$. When $S\simeq1$ it is apparent that, relative to T_c, $H_c(0)$ is reduced by a factor of $\sqrt{2}$.

The full curve is shown in Fig. 5. It is very similar in behavior to $(C_S-C_N)/C_N$; notice in fact that, like this quantity, $[H_c(0)/\sqrt{4\pi N(0)}T_c]^2$ begins at somewhat less than the isotropic value and is reduced to about one-half of that when $S\simeq1$, and then increases beyond that. There is some dependence on the choice of $P(a)$ here, but no significant change is found when $N(0)V_{ep}$ is changed.

A related quantity is the deviation function defined by

$$D(t)=\frac{H_c(t)}{H_c(0)}-(1-t^2) . \tag{33}$$

Because $D(t)$ differs little from the usual case, rather than provide a detailed analysis of this quantity,

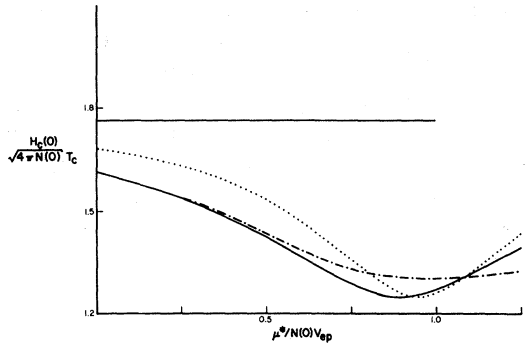

FIG. 5. Zero-temperature critical magnetic field $H_c(0)$ exhibited as a function of $\mu^*/N(0)V_{ep}$. The isotropic BCS result is the upper solid curve, which is 1.77. The results using $P_1(a)$ are exhibited for $\langle a^2\rangle=0.05$ $(\cdots)$ and 0.10 (——), and using $P_2(a)$ for $\langle a^2\rangle=0.1$ $(-\cdot-\cdot-\cdot)$. There is no significant difference for different values of $N(0)V_{ep}$.

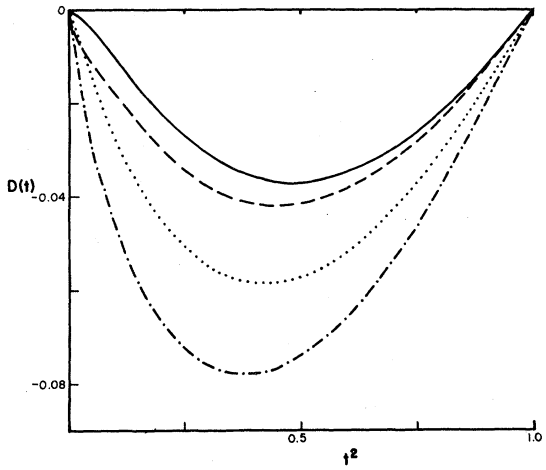

FIG. 6. Deviation function $D(t)$ as a function of t^2. The upper solid curve is the BCS result. The two intermediate curves are found using $P_1(a)$ with $\langle a^2\rangle=0.1$ and $\mu^*=0$ $(\cdots)$ and $\mu^*=N(0)V_{ep}$ $(---)$. The lowest curve corresponds to $P_2(a)$, $\langle a^2\rangle=0.1$, and $\mu^*=N(0)V_{ep}$ $(-\cdot-\cdot-\cdot)$.

only the numerical curves are presented in Fig. 6. The detailed shape is seen to depend somewhat on the choice of $P(a)$, but it is clear that the case $\mu^*=N(0)V_{ep}$ does not change significantly from $\mu^*\simeq 0$. For example, for some strong-coupling materials, $D(t)>0$ throughout, a much larger difference than that found here.

The dependence of T_c on isotopic mass m is described by the isotope parameter β, defined via

$$\beta=\frac{m}{T_c}\frac{\partial T_c}{\partial m}\ . \tag{34}$$

In the T_c equation the variables which could depend on m are ω_D, $N(0)V_{ep}$, and μ^*. The simplest approximations are to assume harmonic phonon frequencies, so that $\omega_D\propto m^{-1/2}$, and to identify $N(0)V_{ep}$ with the electron-phonon mass-enhancement parameter λ, which is independent of m.[14] Following Ref. 14 it is assumed that the mass dependence of μ^* can be approximated through the relationship

$$\mu^*=\frac{\mu}{1+\mu\ln(\epsilon_F/\omega_c)}\ , \tag{35}$$

where ω_c is determined by the phonon frequencies, and so has the same mass dependence as ω_D, and μ is $N(0)$ times the average of the screened Coulomb interaction for scattering at the Fermi surface, which is independent of m. From this it follows that

$$\frac{\partial\mu^*}{\partial m}=-\frac{\mu^{*2}}{2m}\ . \tag{36}$$

With these preliminaries, differentiation of Eq. (3) immediately yields the following result, which is independent of $P(a)$:

$$\beta=-\frac{1}{2}\left[1-(\mu^* f)^2\left[\frac{1-N(0)V_{ep}\langle a^2\rangle f}{1+N(0)V_{ep}\mu^*\langle a^2\rangle f^2}\right]\right], \tag{37}$$

which is exactly $-\frac{1}{2}$ for the isotropic or anisotropic case when $\mu^*=0$, and $-\frac{1}{2}[1-1/(1-S)^2]$ for the isotropic case when $\mu^*\neq 0$, in agreement with Rickayzen.[15] This latter result diverges as $\mu^*\to N(0)V_{ep}$, but in this case T_c vanishes exponentially. When $S=1$, to low order in the anisotropy,

$$\beta\simeq\frac{1}{4\langle a^2\rangle}(1-\tfrac{3}{2}\langle a^2\rangle^{1/2})\ , \tag{38}$$

which again illustrates this divergence for the isotropic case. This equation illustrates the interesting feature of a reduction in β with increasing anisotropy, reflecting the fact that at $S\simeq 1$ there is a delicate balance between μ^* and $N(0)V_{ep}$, which becomes less delicate as the anisotropy becomes more important.

As seen from Fig. 7, β remains close to its usual BCS value of $-\frac{1}{2}$ up until $S\simeq 0.4$, after which it begins to increase, becoming positive in the neigh-

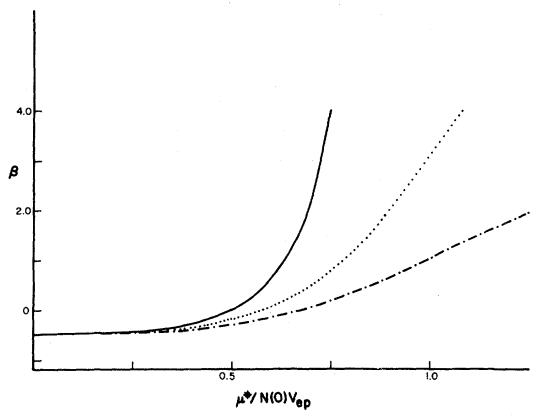

FIG. 7. Isotope-effect parameter β, defined by Eq. (47), as a function of $\mu^*/N(0)V_{ep}$ for the isotropic case $(——)$, $\langle a^2\rangle=0.05$ $(\cdots)$, and $\langle a^2\rangle=0.1$ $(-\cdot-\cdot-\cdot)$.

borhood of $S \simeq 0.5$ to 0.7 depending on $\langle a^2 \rangle$, and then increasing rapidly resulting in a large inverse isotope effect. Consistent with Eq. (38) the actual value of β in this region is a sensitive function of $\langle a^2 \rangle$. Finally, it is pointed out that since both $N(0)V_{ep}f$ and $\mu^* f$ depend only on S, this result is also independent of $N(0)V_{ep}$ except through S.

The final function considered in this section is the quasiparticle density of states defined by

$$\frac{N(\omega)}{N(0)} = \int P(a)da \, \mathrm{Re}\left[\frac{\omega}{[\omega^2 - (\Delta_0 + a\Delta_1)^2]^{1/2}} \right] . \tag{39}$$

For the two different distributions rather different results are obtained, which are found simply by analytically performing this integral. With the use of $P_1(a)$, the result is

$$\frac{N(\omega)}{N(0)} = \frac{\omega}{2\Delta_0} \begin{cases} \dfrac{1}{\left[\left[\dfrac{\omega}{\Delta_0}\right]^2 - (1+R^2)\right]^{1/2}} + \dfrac{1}{\left[\left[\dfrac{\omega}{\Delta_0}\right]^2 - (1-R)^2\right]^{1/2}}, & \dfrac{\omega}{\Delta_0} > 1+R \\ \dfrac{1}{\left[\left[\dfrac{\omega}{\Delta_0}\right]^2 - (1-R)^2\right]^{1/2}}, & |1-R| < \dfrac{\omega}{\Delta_0} < 1+R \\ 0, & \dfrac{\omega}{\Delta_0} < |1-R| \end{cases} \tag{40}$$

whereas using $P_2(a)$

$$\frac{N(\omega)}{N(0)} = \frac{1}{2\sqrt{3}R} \frac{\omega}{\Delta_0} \begin{cases} \sin^{-1}\left[\dfrac{1+\sqrt{3}R}{\omega/\Delta_0}\right] - \sin^{-1}\left[\dfrac{1-\sqrt{3}R}{\omega/\Delta_0}\right], & \dfrac{\omega}{\Delta_0} > 1+\sqrt{3}R \\ \dfrac{\pi}{2} - \sin^{-1}\left[\dfrac{1-\sqrt{3}R}{\omega/\Delta_0}\right], & |1-\sqrt{3}R| < \dfrac{\omega}{\Delta_0} < 1+\sqrt{3}R \\ 0, & \dfrac{\omega}{\Delta_0} < |1-\sqrt{3}R| \text{ if } \sqrt{3}R < 1 \\ \pi, & \dfrac{\omega}{\Delta_0} < |1-\sqrt{3}R| \text{ if } \sqrt{3}R > 1 . \end{cases} \tag{41}$$

These are illustrated in Figs. 8 and 9. Large differences for the two different choices of $P(a)$ are clearly seen, and they both differ very much from the isotropic limit. The curves which are shown are for the isotropic case and for the anisotropic cases with $S=0$, $S=1$, and $S=1.2$. The last of these has been included to show the behavior for large R^2. In each case there is a slight dependence on $N(0)V_{ep}$, through the dependence of R.

Consider first the $P_1(a)$ result (Fig. 8). The one singularity at $\omega=\Delta_0$ for the isotropic case is replaced by two singularities at $\omega=\Delta_0|1\pm R|$. When $S\simeq 1$ and $R\simeq 1$, this causes peaks close to $\omega=0$ and out at $\omega\simeq 2\Delta_0$. As μ^* is further increased, the inner singularity is moved back out away from the origin, whereas the outer one is pushed further beyond $2\Delta_0$.

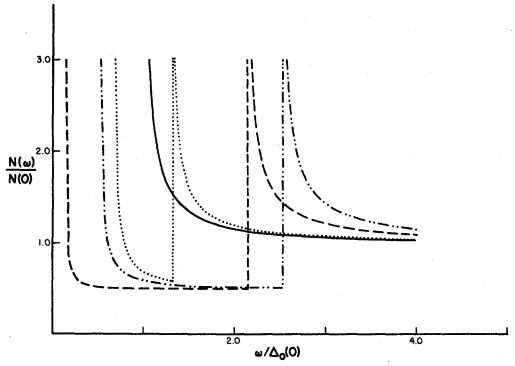

FIG. 8. The quasiparticle density of states $N(\omega)/N(0)$ as a function of $\omega/\Delta_0(0)$ using $P_1(a)$. The solid curve which diverges at $\omega/\Delta_0(0)=1$ is the isotropic BCS result. The rest are all for $\langle a^2 \rangle = 0.1$ with $\mu^*=0$ $(\cdots)$, $\mu^*=N(0)V_{ep}$ $(- - -)$, and $\mu^*=1.2$ $N(0)V_{ep}$ $(-\cdots-\cdots-)$. The value of $N(0)V_{ep}$ has little effect.

At any rate, when $S \simeq 1$ a large value is found when $\omega < \Delta_0$, and a second peak is located at $\omega \simeq 2\Delta_0$.

Turning now to the $P_2(a)$ result (Fig. 9) it is seen that the BCS singularity is replaced by a finite peak when $S=0$ and $\langle a^2 \rangle \neq 0$, and by two peaks when $\mu^* \neq 0$, which are quite small when $S \gtrsim 1$. The outer peaks are well beyond the region of $\omega = 2\Delta_0$, whereas the inner peaks are within $\Delta_0 < \omega < 2\Delta_0$. There is a finite value for $N(\omega)$ down to $\omega = 0$.

From these graphs tentative conclusions can be drawn, first, that although the quasiparticle density of states depends sensitively on $P(a)$, for $S \gtrsim 1$ both choices indicate the presence of a nonzero $N(\omega)$ at frequencies well below $\omega \simeq \Delta_0$, and second, that $N(\omega)/N(0)$ has a two-peak structure with the outer peak at or beyond $\omega \simeq 2\Delta_0$. In passing it is pointed out that for $\omega \gg \Delta_0(1+R)$ an expansion of either result can be made, resulting in the expression obtained by Schachinger and Carbotte[16] for the case $\mu^* = 0$ in a small $\langle a^2 \rangle$ expansion. They then used this for a range of ω, attributing some of the observed structure in $N(\omega)/N(0)$ to the use of this approximation where it is not valid.

IV. IMPURITY EFFECTS ON T_c

The dependence of T_c on normal and paramagnetic impurities is dealt with in the present BCS model through Eqs. (7) and (8). From these it is clear that $\tilde{\Delta}_{\vec{k}}(n)$ has the form

$$\tilde{\Delta}_{\vec{k}}(n) = \tilde{\Delta}_0(n) + a_{\vec{k}} \tilde{\Delta}_1(n) ,$$

analogous to the form for the energy gap $\Delta_{\vec{k}}$. Substituting this form into (7) and (8) it is found that $\tilde{\Delta}_1(n)$ is a constant, say $\bar{\Delta}_1$, as is

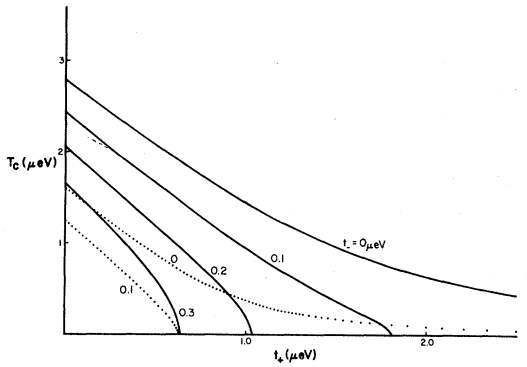

FIG. 10. Reduction of T_c by normal impurity scattering in the presence of paramagnetic impurities. All curves are for $\omega_D = 32$ meV, $N(0)V_{ep} = 0.285$, and $\langle a^2 \rangle = 0.1$, and each is labeled by the value of t_-, describing the paramagnetic impurities. The solid curves (—) correspond to $\mu^* = N(0)V_{ep}$, and the dotted ones (· · ·) to $\mu^* = 1.05N(0)V_{ep}$.

$$\bar{\Delta}_0 = \tilde{\Delta}_0(n) \left[1 - \frac{\pi(t_+ - t_-)}{|\tilde{\omega}(n)|} \right] . \tag{42}$$

Furthermore, they are found to satisfy

$$-N(0)V_{ep}\sigma_2 \bar{\Delta}_0 + [1 - \langle a^2 \rangle N(0)V_{ep}\sigma_1]\bar{\Delta}_1 = 0 , \tag{43}$$

$$(1 + \mu^* \sigma_2)\bar{\Delta}_0 - \bar{\Delta}_1 = 0 , \tag{44}$$

where σ_1 and σ_2 can be expressed in terms of the digamma functions $\psi(x)$ as

$$\sigma_1 = \psi \left[\frac{\omega_D + \pi(t_+ + t_-)}{2\pi T_c} \right] - \psi \left[\frac{\pi T_c + \pi(t_+ + t_-)}{2\pi T_c} \right] \tag{45}$$

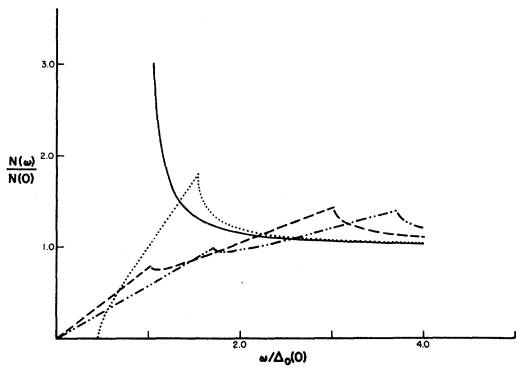

FIG. 9. $N(\omega)/N(0)$ as a function of $\omega/\Delta_0(0)$ using $P_2(a)$. The notation is the same as in Fig. 7.

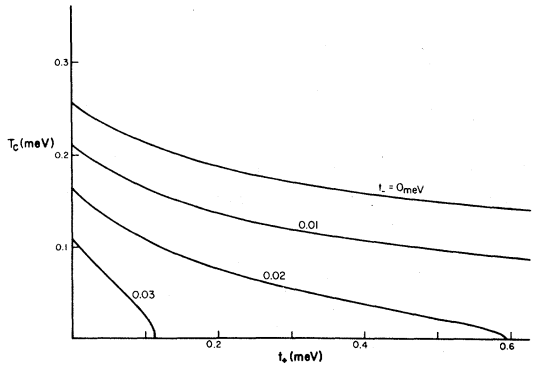

FIG. 11. Reduction of T_c by impurities. The host parameters are as for Fig. 10, except that $\mu^* = 0.13$.

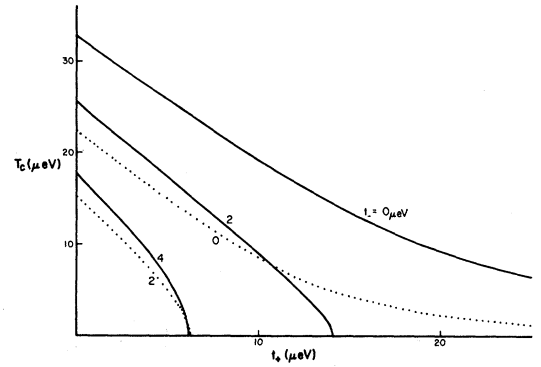

FIG. 12. Reduction of T_c by impurities. All curves correspond to $\omega_D=21$ meV, $N(0)V_{ep}=0.41$, and $\langle a^2\rangle=0.1$. The notation is the same as for Fig. 10.

$$\sigma_2=\psi\left[\frac{\omega_D+2\pi t_-}{2\pi T_c}\right]-\psi\left[\frac{\pi T_c+2\pi t_-}{2\pi T_c}\right]. \tag{46}$$

Nontrivial solutions for the gap occur if the determinant of the coefficients of $\bar{\Delta}_0$ and $\bar{\Delta}_1$ in these equations is zero, leading to the T_c equation

$$\langle a^2\rangle N(0)V_{ep}\mu^*\sigma_1\sigma_2+[N(0)V_{ep}-\mu^*]\sigma_2 +\langle a^2\rangle N(0)V_{ep}\sigma_1-1=0\,. \tag{47}$$

This result for T_c is independent of the choice of $P(a)$, depending on the anisotropy only through $\langle a^2\rangle$. Figures 10–13 illustrate T_c as a function of normal scattering t_+ for different values of the spin-flip scattering parameter t_-. The first two of these both refer to the first representative material in which $\omega_D=32$ meV and $N(0)V_{ep}=0.285$; Fig. 10

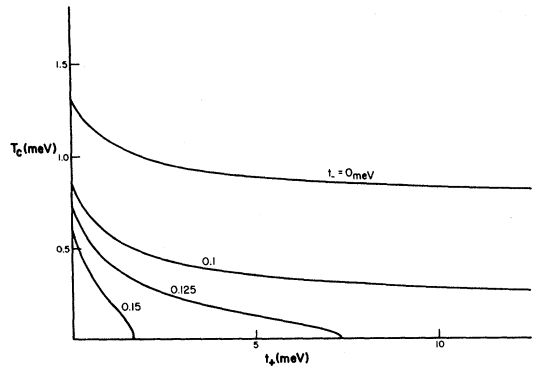

FIG. 13. Reduction of T_c by impurities. The host parameters are as for Fig. 12 except that $\mu^*=0.12$.

is for the case of present primary interest in which $\mu^*\simeq N(0)V_{ep}$, whereas Fig. 11 refers to the usual case of $\mu^*=0.13$. The last two figures are obtained with $\omega_D=21$ meV and $N(0)V_{ep}=0.41$; again the case of $\mu^*\simeq N(0)V_{ep}$ is illustrated first, and then, for comparison, the case of $\mu^*=0.12$ is shown. In all cases $\langle a^2\rangle$ has been chosen to be 0.1 for purposes of illustration.

The most striking features of these graphs are that they all look much the same and that the scales of t_+ and t_- are reduced considerably for the case $\mu^*\simeq N(0)V_{ep}$ as compared with the usual case. Beyond the establishment of the form of these curves in this regime, the most important experimental quantity is the maximum impurity concentrations which can be tolerated. As has been emphasized, because of the various approximations inherent in the calculations, and because only representative parameters are used for the hosts, no accurate quantitative results can be obtained. Instead, the philosopy here is simply that order-of-magnitude estimates of the concentrations are of use as a guide in any attempt to observe the regime focused on in this work.

Comparison of Fig. 10 with 11, and of Fig. 12 with 13, indicates that the scales of t_+ and t_- are reduced by about 2–3 orders of magnitude for the case $\mu^*\simeq N(0)V_{ep}$, as compared with the usual case for the illustrated choice of $\langle a^2\rangle=0.1$, which probably represents an upper limit for the anisotropy. This implies that the maximum allowable concentrations are reduced by about the same factors since t_+ and t_- are proportional to the concentrations.

Experimental work on Fe impurities in In films,[17,18] and Gd in $LaAl_2$,[19,20] La,[21–23] and La_3In,[23] for which the "pure" T_c's are in the range of about 3 to 9 K, indicates that the concentrations of paramagnetic impurities which destroyed superconductivity were in the range of 0.5% to 2%. This suggests then that for the case $\mu^*\simeq N(0)V_{ep}$, with little or no normal scattering ($t_+\simeq 0$), no more than perhaps 0.001% to 0.01% paramagnetic impurities can be tolerated.

If there is even a small amount of paramagnetic impurity present, the figures indicate that normal impurity scattering will drive T_c to zero. Simple estimates of the relevant concentrations can be made in different ways. The first comes from the definition $t_+=1/2\pi\tau_N$ and from the relation

$$\frac{1}{\tau_N}=n_0 v_F\sigma_N c_N\,, \tag{48}$$

where n_0 is the host atomic density, typically about 10^{23} cm^{-3}, v_F is the Fermi velocity, about 10^8

cm s^{-1}, σ_N is the normal scattering cross section per atom, typically 10^{-17} cm^2, and c_N is the concentration of normal impurities relative to host. These parameters lead to values of t_+ per atom in the range of about 1—10 meV, in agreement with data used by Markowitz and Kadanoff.[2] Combining this with the scales of Figs. 10 and 12 implies a range of c_N of about 0.001% to 0.01%. This is also in reasonable agreement with a second approach based on the observation that, in the usual regime, normal concentrations wash out the anisotropy when c_N is a few percent. Comparison of Fig. 10 to 13 indicates that the values of t_+ for which $T_c=0$ when $\mu^*\simeq N(0)V_{ep}$, are roughly 2—3 orders of magnitude smaller than the values of t_+ which essentially eliminate the enhancement of T_c by the anisotropy when $\mu^*\simeq 0.12$ and there are no paramagnetic impurities present. This again leads to values of c_N of about 0.001% to 0.01%. It is thus concluded that the maximum tolerable impurity concentrations of either type are somewhere in the vicinity of 0.001% to 0.01%, but these estimates are only very crude, and also are only for a highly anisotropic material with $\langle a^2\rangle\simeq 0.1$. (Smaller values of $\langle a^2\rangle$ are considered presently.)

An interesting feature of the curves is that T_c vanishes for some finite t_+ in at least some cases. The equations for T_c, (45)—(47), provide a means of determining the conditions for this occurrence and the corresponding critical t_+^c, and alternatively the critical t_-^c for which $T_c\to 0$ in the absence of any normal scattering.

Consider first the case of $t_-\neq 0$. When $T_c\to 0$, the arguments of the digamma functions diverge, so ψ can be replaced by its asymptotic logarithmic approximation, simplifying σ_1 and σ_2. Employing this in (47) one finds

$$t_+^c=\frac{\omega_D}{\pi}\frac{1}{\exp\left[\frac{1}{N(0)V_{ep}\langle a^2\rangle}\left[1-\frac{N(0)V_{ep}\sigma_2}{1+\mu^*\sigma_2}\right]\right]-1} \tag{49}$$

with

$$\sigma_2=\ln\left[\frac{\omega_D+2\pi t_-}{2\pi t_-}\right]. \tag{50}$$

This result indicates that $t_+^c\to\infty$ when the denominator vanishes, so for finite t_+^c the argument of the exponential in the denominator must be positive. This leads to the condition

$$t_-\geq\begin{cases}\dfrac{\omega_D}{2\pi}\dfrac{1}{\exp\left[\dfrac{1}{N(0)V_{ep}-\mu^*}\right]-1}, & S<1\\ 0, & S>1\,.\end{cases} \tag{51}$$

If this condition is satisfied, then t_+^c is given by (49) for $S<1$, and by a simplification of (49) resulting from $\sigma_2\to\infty$ when $t_-=0$ for $S>1$, namely,

$$t_+^c=\frac{\omega_D}{\pi}\frac{1}{\exp\left[\dfrac{\mu^*-N(0)V_{ep}}{N(0)V_{ep}\mu^*\langle a^2\rangle}\right]-1},\quad t_-=0\,. \tag{52}$$

The exact mathematical result is, of course, of little relevance. The interesting result that is obtained is that for a situation in which the average interaction is repulsive, a finite concentration of normal impurities will destroy superconductivity. If $S<1$ some paramagnetic impurities are required, as determined by Eq. (51).

The other question asked here is the value of t_-^c. Anticipating that $t_-^c\ll\omega_D$, one finds that $\sigma_2=\sigma_1-\ln 2$, which can be substituted into (47) leading to a quadratic equation for σ_1. By definition σ_1 and σ_2 must both be non-negative, and this can be used to eliminate one of the two solutions of the quadratic. As long as $N(0)V_{ep}\langle a^2\rangle<1/\ln 2$, which is certainly the case for any sensible values of these parameters, it is found that

$$t_-^c=\frac{\omega_D}{\pi}e^{-\sigma_1} \tag{53}$$

with

$$\sigma_1=\frac{-x+(x^2+4N(0)V_{ep}\mu^*\langle a^2\rangle\{1+[N(0)V_{ep}-\mu^*]\ln 2\})^{1/2}}{2N(0)V_{ep}\mu^*\langle a^2\rangle} \tag{54}$$

and

$$x=N(0)V_{ep}(1+\langle a^2\rangle)-\mu^*-N(0)V_{ep}\mu^*\langle a^2\rangle\ln 2\,. \tag{55}$$

Again, the precise results are of little relevance. However, without exhibiting more figures these equations can be used to provide some indication of how the maximum tolerable impurity concentrations depend on $\langle a^2\rangle$. For example, if $\langle a^2\rangle=0.05$, Eqs. (52) and (53) predict reductions in t_+^c and t_-^c by about 2 orders of

magnitude, implying corresponding reductions in the concentrations. It is again useful to consider the limiting cases of this result, which are

$$t_-^c \simeq \begin{cases} \dfrac{\omega_D}{\pi}\exp\left[-\dfrac{1+N(0)V_{ep}\ln 2}{N(0)V_{ep}(1+\langle a^2\rangle)}\right], & \mu^*=0 \\ \dfrac{\omega_D}{\pi}\exp\left[-\dfrac{1}{N(0)V_{ep}\langle a^2\rangle^{1/2}}\right], & \mu^*=N(0)V_{ep} \end{cases} \tag{56}$$

where the second case has been taken only to lowest order in $\langle a^2\rangle$. Once again, whereas in the usual case of $S \ll 1$ the anisotropy is a small effect appearing in a factor $1+\langle a^2\rangle$, when $S=1$ its dominant effect appears through a term of order $\langle a^2\rangle^{1/2}$, not $\langle a^2\rangle$. This behavior is the same as that of the original expression for T_c for the pure material, in this limit.

V. SUMMARY AND CONCLUSIONS

In this paper a number of properties of superconductors in which the anisotropy plays an essential role have been considered. This is the regime in which the average effective electron-electron interaction is about neutral or even slightly repulsive, and in which T_c would be zero or very tiny in the absence of anisotropy. It has been emphasized that because of the use of a BCS-type theory and a simple separable representation of the anisotropy, the results are in no way to be considered quantitative predictions. The main goal has instead been the identification of pure-metal properties which behave quite differently in this regime as compared with the usual regime in which the interaction is dominated by the attraction and the anisotropy has a relatively minor effect. A second goal was the estimation of the maximum normal and paramagnetic impurity concentrations which can be present without driving T_c to zero.

For all the pure-metal properties studied, there was little or no dependence on $N(0)V_{ep}$ or μ^* separately, but only on their ratio $S=\mu^*/N(0)V_{ep}$. In this sense the quantities are in effect universal; in the isotropic BCS case they are exactly universal, being independent of the BCS parameter $N(0)V$. For the temperature-dependent functions the universality is present in the dependence of the various quantities on the reduced temperature $t=T/T_c$.

The properties which are significantly different are summarized first. The mean-squared anisotropy of the gap, which is normally on the order of $\langle a^2\rangle$, and thus is about 0.05 to perhaps 0.1, is found to be about 1 or larger and, in fact, rather independent of the actual value of $\langle a^2\rangle$. The ratio of twice the average zero-temperature gap to T_c, $2\Delta_0(0)/T_c$, is reduced from slightly less than 3.53 to just about one-half this value when $\mu^* \simeq N(0)V_{ep}$, again nearly independent of $\langle a^2\rangle$.

The relative jump in the specific heat $(C_S-C_N)/C_N$ is also reduced to about one-half the isotropic value of 1.43. This is, however, not as significantly characteristic of this regime as it might appear at first sight, because even when $\mu^*=0$, if $\langle a^2\rangle > 0$ the jump is reduced, for example, to about 1.1 when $\langle a^2\rangle = 0.1$.

The zero-temperature critical magnetic field $H_c(0)$, relative to T_c, is described by the ratio $H_c(0)/\sqrt{4\pi N(0)}T_c$. This is reduced to about $1/\sqrt{2}$ of its isotropic value, or approximately a 30% reduction. However, in a way similar to the specific-heat jump, much of this reduction may be caused by the anisotropy alone, even with $\mu^*=0$.

An inverse isotope effect appears when $\mu^* \simeq 0.5N(0)V_{ep}$ to $0.7N(0)V_{ep}$, becoming very large when $\mu^* \simeq N(0)V_{ep}$. Its magnitude is inversely proportional to $\langle a^2\rangle$, reflecting the fact that as $\langle a^2\rangle$ becomes smaller, the balance between the attractive and repulsive parts of the interaction becomes more delicate, finally resulting in a divergence for the isotropic case when $\mu^*=N(0)V_{ep}$.

The quasiparticle density of states $N(\omega)/N(0)$ differs significantly and as well, it depends on the details of the anisotropy of the interaction. It is tentatively suggested that the characteristics of the regime $\mu^* \simeq N(0)V_{ep}$ are a two-peak structure with the outer peak near or well beyond $\omega \simeq 2\Delta_0(0)$, and a nonzero $N(\omega)/N(0)$ well below $\omega = \Delta_0(0)$.

An additional remark can be made regarding three of these properties. In the isotropic BCS case each of $2\Delta_0(0)/T_c$, $(C_S-C_N)/C_N$, and $[H_c(0)/\sqrt{4\pi N(0)}T_c]^2$ has a universal value for $\mu^* < N(0)V_{ep}$ and is zero for $\mu^* > N(0)V_{ep}$. In the anisotropic case with $\mu^*=N(0)V_{ep}$ each of these is reduced to just about one-half the corresponding isotropic value, nearly independent of the actual

value of $\langle a^2 \rangle$ in each case.

Of the properties considered here those that are not significantly different from the usual case are the reduced quantities $\Delta_0(t)/\Delta_0(0)$, $\Delta_1(t)/\Delta_1(0)$, and the deviation function $D(t)$ which is a measure of $H_c(t)/H_c(0)$. The zero-temperature value of each of Δ_0, Δ_1, and H_c is different, as, of course, is the scale of temperature since T_c is relatively low. But after this overall rescaling the resulting variations with t are not much different from the isotropic BCS result. The mean-squared anisotropy of the gap is nearly independent of t.

Finally, the effects of impurities are summarized. The first observation was that T_c depends on normal and paramagnetic scattering in much the same way whether $\mu^* \simeq 0.12$ or $\mu^* \gtrsim N(0)V_{ep}$, except for a reduction of the energy scales by about 3 orders of magnitude or more. The results were used to suggest that when $\langle a^2 \rangle = 0.1$, for otherwise typical material parameters with typical impurities, the maximum tolerable concentrations of either normal or paramagnetic impurities are about 0.001% to 0.01%. Reducing $\langle a^2 \rangle$ by a factor of 2 caused a further reduction in these numbers by a factor of about 100. This estimate could easily be incorrect by at least 1 order of magnitude due in part to its reliance on the use of typical parameters, but more fundamentally because of the approximations inherent in the model.

In analyzing the conditions under which T_c vanishes, it was found that if $\mu^* > N(0)V_{ep}$ a finite concentration of normal impurities can destroy superconductivity even in the absence of any paramagnetic atoms. If on the other hand $\mu^* < N(0)V_{ep}$, some magnetic atoms are required for T_c to vanish. In all cases a finite concentration of paramagnetic atoms can destroy superconductivity when no normal impurities are present.

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