

Using the results of Appendix A, Eq. (B2) reduces to

$$F_0(t) = \sum_{j=1}^N \frac{1}{3} I(I+1)(2I+1) \prod_k' \left(\frac{\sin[(2I+1)B_{jkt}/2\hbar]}{\sin(B_{jkt}/2\hbar)} \right) \left(\frac{1}{3} I(I+1)(2I+1)(2I+1)^{N-1} N \right)^{-1} \\ = \frac{1}{N} \sum_{j=1}^N \prod_k' \left(\frac{\sin((2I+1)B_{jkt}/2\hbar)}{(2I+1) \sin(B_{jkt}/2\hbar)} \right). \quad (\text{B3})$$

Effects of Nonmagnetic Impurities upon Anisotropy of the Superconducting Energy Gap*

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The influence of the presence of nonmagnetic impurities upon the anisotropy of the superconducting energy-gap parameter is considered. Using a factorable BCS-like model for the effective electron-electron matrix element, $V_{pp'} = (1+a_p)V(1+a_{p'})$, within the context of an earlier theory by Markowitz and Kadanoff, it is shown that when impurities are present the wave-vector-dependent gap parameter Δ_p is replaced by a complex, wave-vector- and energy-dependent gap parameter $\Delta(\mathbf{p}, \omega) = \Delta_i(\omega) + a_p \Delta_a(\omega)$. The behavior of $\Delta_i(\omega)$ and $\Delta_a(\omega)$ is extensively examined as a function of impurity concentration; it is found, for example, that the magnitude of the anisotropic part $\Delta_a(\omega)$ of the gap parameter tends to zero in the limit of large impurity concentration. A model calculation, assuming a rectangular shape for the anisotropy distribution function $P(a)$, illustrates the behavior for small and moderate impurity concentrations. The behavior for large impurity concentrations is found to depend, to lowest order, only upon the mean-squared anisotropy $\langle a^2 \rangle$. The behavior of the effective density of states is also examined; it is shown to become isotropic as the impurity concentration increases. The precise shape of the effective density of states for energies near the gap is obtained for the large-impurity-concentration limit. Experimental manifestations of the reduction of the anisotropy by impurity scattering are briefly discussed.

I. INTRODUCTION

THE presence of impurities in a superconductor has an interesting influence upon the effects of anisotropy of the superconducting energy gap. An important result of the addition of ordinary nonmagnetic chemical or physical impurities is the reduction—or “washing out”—of the anisotropy of the energy gap. Such a reduction of the anisotropy has been observed in specific heat,¹⁻³ nuclear spin-lattice relaxation,⁴ tunneling,⁵ infrared absorption,⁶ and surface resistance⁷ experiments. Similarly, the observed initial

decrease in the transition temperature as small amounts of impurities are added⁸⁻¹¹ is also a result of anisotropy reduction.

The theory of the reduction of anisotropy by impurity scattering, suggested by the work of Anderson,¹² has been successfully applied to the latter problem by several groups.¹³⁻¹⁹ When impurities are present, the essential modification of the theory of the superconduct-

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ing state is the replacement of the wave-vector-dependent energy-gap parameter Δ_p by a complex, impurity concentration-, wave vector-, and energy-dependent gap parameter $\Delta(\mathbf{p}, \omega)$. (Here, \mathbf{p} and ω denote wave-vector and energy.) The influence of the impurity scattering upon the anisotropy of $\Delta(\mathbf{p}, \omega)$ is contained within the structure of a certain set of rather complicated integral equations.

In order to make a careful study of the behavior of $\Delta(\mathbf{p}, \omega)$ as a function of impurity concentration, we shall in this paper make use of the theoretical framework provided by Markowitz and Kadanoff.¹³ Accordingly, we assume that a factorable BCS-like model for the effective electron-electron matrix element $V_{pp'}$ (Ref. 20) of the form

$$V_{pp'} = (1 + a_p)V(1 + a_{p'}), \quad (1.1)$$

is appropriate for the case of a pure, single-crystal superconductor. The anisotropy function a_p , defined for quasimomenta \mathbf{p} near the Fermi surface and assumed to depend only upon the direction of \mathbf{p} with respect to the crystal axes, is defined to have zero average over the Fermi surface. The gap parameter, which has the form $\Delta_p = \epsilon_0 + a_p \epsilon_0$ in the absence of impurities, may then, as we shall see later, be expressed as $\Delta(\mathbf{p}, \omega) = \Delta_i(\omega) + a_p \Delta_a(\omega)$ in the presence of impurities. (Here, the subscripts i and a label the isotropic and anisotropic parts of the gap parameter.) The complex functions $\Delta_i(\omega)$ and $\Delta_a(\omega)$ may then be obtained by solving the above mentioned integral equations. We shall find for small impurity concentrations that $\Delta_i(\omega) \simeq \Delta_a(\omega) \simeq \epsilon_0$; the behavior is much the same as in the absence of impurities. However, for large impurity concentrations, although the isotropic part $\Delta_i(\omega)$ of the gap parameter remains at nearly its original value ϵ_0 , the coefficient $\Delta_a(\omega)$ of the anisotropy function a_p becomes small; thus, the energy-gap parameter becomes essentially isotropic.

In the following sections we shall first briefly discuss Markowitz and Kadanoff's derivation of the anisotropy equations—the equations which govern the behavior of $\Delta_i(\omega)$ and $\Delta_a(\omega)$ in the presence of impurity scattering. We shall employ the anisotropy distribution function $P(a)$ to obtain these equations in a form convenient for further study. We shall next discuss the solutions of the anisotropy equations in various cases, proceeding as far as possible without assuming a definite form for $P(a)$. Particularly interesting results will be obtained in the limit of large impurity concentrations. We shall then make use of a simple model for $P(a)$ in order to demonstrate the behavior of $\Delta(\mathbf{p}, \omega)$ where it is sensitive to the details of the anisotropy distribution. Finally, after examining the behavior of the effective density of states as a function of impurity concentration, we shall briefly discuss the experimental manifestations of the “washing out” of the anisotropy by impurity scattering.

II. ANISOTROPY IN THE PRESENCE OF NONMAGNETIC IMPURITIES

A. The Anisotropy Equations

Our description of the superconducting state in the presence of impurities will follow that of Markowitz and Kadanoff,¹³ who make use of the matrix Green's function $g(\mathbf{p}, \omega)$ and include anisotropy by means of the factorable model (1.1) discussed earlier. For isotropic impurity scattering their result for the impurity-averaged Green's function may be written in the form

$$g(\mathbf{p}, z) = \frac{zZ(z)\tau_0 + \Delta(\mathbf{p}, z)Z(z)\tau_1 + \epsilon_p\tau_3}{[zZ(z)]^2 - [\Delta(\mathbf{p}, z)Z(z)]^2 - \epsilon_p^2}, \quad (2.1)$$

where z is a complex energy variable, ϵ_p is the energy of the Bloch state of wave vector \mathbf{p} , and

$$\tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.2)$$

are Pauli matrices. The wave-function renormalization factor $Z(z)$ is found to be

$$Z(z) = 1 \pm i \langle [z^2 - \Delta^2(\mathbf{p}', z)]^{1/2} \rangle_{\text{av}}' / 2\tau, \quad (2.3)$$

where, in this and in later expressions, the upper (lower) sign applies when z is in the upper (lower) half plane, and the square root denotes that branch which obeys $[z^2 - \Delta^2(\mathbf{p}, z)]^{1/2} \rightarrow z$ as $z \rightarrow \infty$. The angular brackets $\langle \rangle_{\text{av}}$ denote a Fermi-surface average. The prime appearing as a superscript to these brackets refers to \mathbf{p}' and reminds us that the quantity within the brackets is to be averaged by moving \mathbf{p}' (not \mathbf{p}) over the Fermi surface. The collision time τ is given by the usual expression, $\tau = (n_I v_F \sigma)^{-1}$, relating the number of impurities per unit volume n_I , the Fermi velocity v_F , and the total cross section σ . The energy-gap parameter $\Delta(\mathbf{p}, z)$ is determined from

$$\Delta(\mathbf{p}, z) = (1 + a_p)\epsilon_0 \pm \frac{i}{2\tau} \left\langle \frac{\Delta(\mathbf{p}', z) - \Delta(\mathbf{p}, z)}{[z^2 - \Delta^2(\mathbf{p}', z)]^{1/2}} \right\rangle_{\text{av}}', \quad (2.4)$$

where ϵ_0 must be determined self-consistently from the equation

$$\epsilon_0 = N(0)V \int_{-\omega_D}^{\omega_D} \frac{d\omega'}{2} \tanh\left(\frac{\beta\omega'}{2}\right) \times \left\langle (1 + a_{p'}) \operatorname{Re} \left(\frac{\Delta(\mathbf{p}', z')}{[z'^2 - \Delta^2(\mathbf{p}', z')]^{1/2}} \right) \right\rangle_{\text{av}}' \quad (2.5)$$

with

$$z' = \omega' \pm i0^+.$$

[Equation (2.4) is equivalent in content to similar expressions derived by Tsuneto¹⁴ and Hohenberg.¹⁷] We remark that for nonspherical Fermi surfaces the density of Bloch states of one spin in energy at the Fermi surface is actually anisotropic and depends upon the position of the quasimomentum \mathbf{p} on the Fermi surface.

²⁰ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

Therefore, this effect should be included if the procedure of converting the sum over wave vectors to an integral over Bloch energies plus an average over the Fermi surface is to be correct. However, since this anisotropy here plays a role secondary to that of the angular dependence of $V_{pp'}$, we have suppressed it by replacing the density of states by a corresponding isotropic average $N(0)$.

The dependence of the gap parameter upon \mathbf{p} is quite simple in this treatment, for $\Delta(\mathbf{p}, z)$ may be written in terms of the anisotropy function a_p as

$$\Delta(\mathbf{p}, z) = \Delta_i(z) + a_p \Delta_a(z). \quad (2.6)$$

When we insert this form into Eq. (2.4) and average over the Fermi surface, recalling that the Fermi surface average of the anisotropy function vanishes by definition (i.e., $\langle a_p \rangle_{\text{av}} = 0$), we find

$$\Delta_i(z) = \epsilon_0 \pm i \Delta_a(z) \langle a_{p'} / (z^2 - \Delta^2(\mathbf{p}', z))^{1/2} \rangle_{\text{av}} / 2\tau. \quad (2.7)$$

If we multiply Eq. (2.4) by a_p before we average over the Fermi surface, we obtain

$$\Delta_a(z) = \epsilon_0 \mp i \Delta_a(z) \langle 1 / (z^2 - \Delta^2(\mathbf{p}', z))^{1/2} \rangle_{\text{av}} / 2\tau. \quad (2.8)$$

We see that the integral equations (2.7) and (2.8) determine $\Delta_i(z)$ and $\Delta_a(z)$ in terms of the variables ϵ_0 , τ , and z . Before we examine the solutions of these equations, we shall first make a few simplifications.

The expressions obtained above involve the complex energy z , which lies in either the upper or the lower half plane, but not on the real axis. However, since physically measurable quantities involve only the values of $\Delta(\mathbf{p}, z)$ and related functions as z approaches the real axis, we shall restrict our attention to the complex energies $z = \omega \pm i0^+$, infinitesimally above or below the real axis. (The argument $\omega \pm i0^+$ will be suppressed wherever possible.) We note that when the gap parameter is separated into its real and imaginary parts,

$$\Delta(\mathbf{p}, \omega) = \Delta_1(\mathbf{p}, \omega) + i \Delta_2(\mathbf{p}, \omega), \quad (2.9)$$

the real part is an even function of the energy ω , and the imaginary part is an odd function of ω :

$$\begin{aligned} \Delta_1(\mathbf{p}, \omega \pm i0^+) &= \Delta_1(\mathbf{p}, -\omega \pm i0^+), \\ \Delta_2(\mathbf{p}, \omega \pm i0^+) &= -\Delta_2(\mathbf{p}, -\omega \pm i0^+). \end{aligned} \quad (2.10)$$

Because of this symmetry we shall henceforth consider only non-negative values of ω .

It is also convenient at this point to introduce a dimensionless quantity $y = (2\epsilon_0\tau)^{-1}$, which, since it is proportional to the impurity concentration, may be regarded as a "dirtiness" parameter. When $y \ll 1$, a condition we call "small impurity concentration," we will see that the effects of anisotropy are quite pronounced, whereas for $y \gg 1$, a condition we call "large impurity concentration," these effects are largely washed out. The value $y \simeq 1$ (or perhaps $y \simeq \langle a^2 \rangle^{1/4} \simeq \frac{1}{3}$ for typical superconductors) is roughly the boundary between these impurity concentration regimes.

Since the integrands of the Fermi-surface averages

appearing in Eqs. (2.5), (2.7), and (2.8) depend upon the distribution of the various values of a_p over the Fermi surface, it is convenient to introduce an anisotropy distribution function $P(a)$. We define $P(a)da$ to be the fraction of the Fermi surface for which a_p has a value in the interval a to $a+da$. The above Fermi surface averages may then be converted into one-dimensional integrals, yielding

$$\Delta_i = \epsilon_0 \pm i \epsilon_0 y \Delta_a \int da \frac{a P(a)}{[\omega^2 - (\Delta_i + a \Delta_a)^2]^{1/2}}, \quad (2.11)$$

$$\Delta_a = \epsilon_0 \mp i \epsilon_0 y \Delta_a \int da \frac{P(a)}{[\omega^2 - (\Delta_i + a \Delta_a)^2]^{1/2}}, \quad (2.12)$$

and

$$\begin{aligned} \epsilon_0 &= N(0) V \int_{-\omega_D}^{\omega_D} \frac{d\omega}{2} \tanh\left(\frac{1}{2}\beta\omega\right) \\ &\times \int da P(a) (1+a) \operatorname{Re} \left(\frac{\Delta_i + a \Delta_a}{[\omega^2 - (\Delta_i + a \Delta_a)^2]^{1/2}} \right). \end{aligned} \quad (2.13)$$

In these expressions the square root denotes that branch which obeys the relation

$$[\omega^2 - (\Delta_i + a \Delta_a)^2]^{1/2} \rightarrow \omega \quad \text{as} \quad |\omega| \rightarrow \infty. \quad (2.14)$$

If we employ a different form of the square root defined by the relation

$$[(\Delta_i + a \Delta_a)^2 - \omega^2]^{1/2} = \mp i [\omega^2 - (\Delta_i + a \Delta_a)^2]^{1/2}, \quad (2.15)$$

then we have

$$[(\Delta_i + a \Delta_a)^2 - \omega^2]^{1/2} \rightarrow \Delta_i(0) + a \Delta_a(0) \quad \text{as} \quad \omega \rightarrow 0. \quad (2.16)$$

With this definition Eqs. (2.11) and (2.12) may be rewritten in an alternate form more convenient for small energies ω :

$$\Delta_i = \epsilon_0 + \epsilon_0 y \Delta_a \int da \frac{a P(a)}{[(\Delta_i + a \Delta_a)^2 - \omega^2]^{1/2}}, \quad (2.17)$$

$$\Delta_a = \epsilon_0 - \epsilon_0 y \Delta_a \int da \frac{P(a)}{[(\Delta_i + a \Delta_a)^2 - \omega^2]^{1/2}}. \quad (2.18)$$

The anisotropy equations (2.11), (2.12), [or (2.17) and (2.18)], and (2.13) are of considerable importance for the examination of the interplay between anisotropy of the superconducting energy gap and impurity scattering. Within these equations are contained the details of the manner in which the addition of impurities causes the anisotropy effects to be washed out. It is thus important that we study the solutions of these equations in some detail.

Before proceeding, we pause to note that y and ϵ_0 enter the anisotropy equations (2.11) and (2.12) merely as parameters. The quantity y measures the importance of the impurity scattering, whereas ϵ_0 sets the scale of the magnitudes of Δ_i , Δ_a , and ω . In fact, if we measure these quantities in units of ϵ_0 by introducing reduced quantities

$$\bar{\Delta}_i = \Delta_i / \epsilon_0, \quad \bar{\Delta}_a = \Delta_a / \epsilon_0, \quad \bar{\omega} = \omega / \epsilon_0, \quad (2.19)$$

then ϵ_0 completely disappears from the resulting equations for $\bar{\Delta}_i$ and $\bar{\Delta}_a$, which then depend only upon y and $\bar{\omega}$. (We shall not, however, make further use of these reduced quantities.)

B. Approximate Solutions of the Anisotropy Equations

It is evident from the structure of Eqs. (2.11) and (2.12) that the solutions $\Delta_i(\omega)$ and $\Delta_a(\omega)$ may depend rather sensitively upon the details of $P(a)$, especially for energies ω near ϵ_0 . However, when the square root is a slowly varying function of a , as is the case, for example, when ω is not too close to ϵ_0 , the solutions depend only upon the gross properties, such as $\langle a^2 \rangle \equiv \langle a_p^2 \rangle_{av}$, of the anisotropy distribution function. By expanding the square root in powers of a , performing the resulting integrals, and neglecting terms of order $\langle a^3 \rangle$, we obtain the following equations, which depend upon $\langle a^2 \rangle$ but upon none of the finer structure of $P(a)$:

$$\Delta_i = \epsilon_0 \pm i\epsilon_0 \langle a^2 \rangle y \frac{\Delta_i \Delta_a^2}{(\omega^2 - \Delta_i^2)^{3/2}}, \quad (2.20)$$

$$\Delta_a = \epsilon_0 \mp i\epsilon_0 y \frac{\Delta_a}{(\omega^2 - \Delta_i^2)^{1/2}} \mp i\epsilon_0 \langle a^2 \rangle y \frac{\Delta_a^3 (\omega^2 + 2\Delta_i^2)}{(\omega^2 - \Delta_i^2)^{5/2}}. \quad (2.21)$$

The above equations are valid when $y \gg 1$ or, for $y \lesssim 1$, when ω is not too close to ϵ_0 .

One way to solve these equations is by means of a perturbative approach, using $\langle a^2 \rangle$ as the small parameter. Let us assume that Δ_i and Δ_a may be expanded in powers of $\langle a^2 \rangle$. Then the first terms in this expansion are:

$$\begin{aligned} \Delta_i &= \Delta_i^0 + \langle a^2 \rangle \delta_i \\ \Delta_a &= \Delta_a^0 + \langle a^2 \rangle \delta_a. \end{aligned} \quad (2.22)$$

When we insert these expressions into Eqs. (2.20) and (2.21), expand all quantities in powers of $\langle a^2 \rangle$, and

equate the coefficients of the zeroth and first powers of $\langle a^2 \rangle$, we may solve the resulting equations to find the quantities Δ_i^0 , δ_i , Δ_a^0 , and δ_a . The solutions $\Delta_{i1}(\omega - i0^+)$ and $\Delta_{i2}(\omega - i0^+)$ obtained in this manner are plotted in Fig. 1 for various values of y ; the corresponding solutions $\Delta_{a1}(\omega - i0^+)$ and $\Delta_{a2}(\omega - i0^+)$ are plotted in Fig. 2. We note that this method of solution breaks down as ω approaches ϵ_0 , as is seen from Figs. 1 and 2.

In the limit as the impurity concentration goes to zero, the above solutions reduce, of course, to

$$\Delta_i(\omega) = \Delta_a(\omega) = \epsilon_0, \quad (y = (2\epsilon_0\tau)^{-1} = 0), \quad (2.23)$$

whereas in the limit as the impurity concentration becomes very large, the solutions become

$$\Delta_i(\omega) = \epsilon_0, \quad \Delta_a(\omega) = 0, \quad (y = \infty). \quad (2.24)$$

We see then, that the complex energy gap parameter, $\Delta(\mathbf{p}, \omega) = \Delta_i(\omega) + a_p \Delta_a(\omega)$, which can be quite anisotropic in the absence of impurities, becomes isotropic in the limit of large impurity concentration.

We may use this property of the gap parameter to estimate the change in ϵ_0 arising from the addition of impurities. By substituting the results (2.23) or (2.24) into the Eq. (2.13) from which ϵ_0 is determined, we obtain for $y=0$

$$\begin{aligned} \frac{1}{N(0)V} &= \int da P(a)(1+a)^2 \\ &\times \int_{\epsilon_0(1+a)}^{\omega_D} d\omega \frac{\tanh(\frac{1}{2}\beta\omega)}{[\omega^2 - \epsilon_0^2(1+a)^2]^{1/2}}, \end{aligned} \quad (2.25)$$

and for $y = \infty$

$$\frac{1}{N(0)V} = \int_{\epsilon_0}^{\omega_D} d\omega \frac{\tanh(\frac{1}{2}\beta\omega)}{(\omega^2 - \epsilon_0^2)^{1/2}}. \quad (2.26)$$

At zero temperature, the ω integrals can easily be performed. By expanding the result for $y=0$ in powers

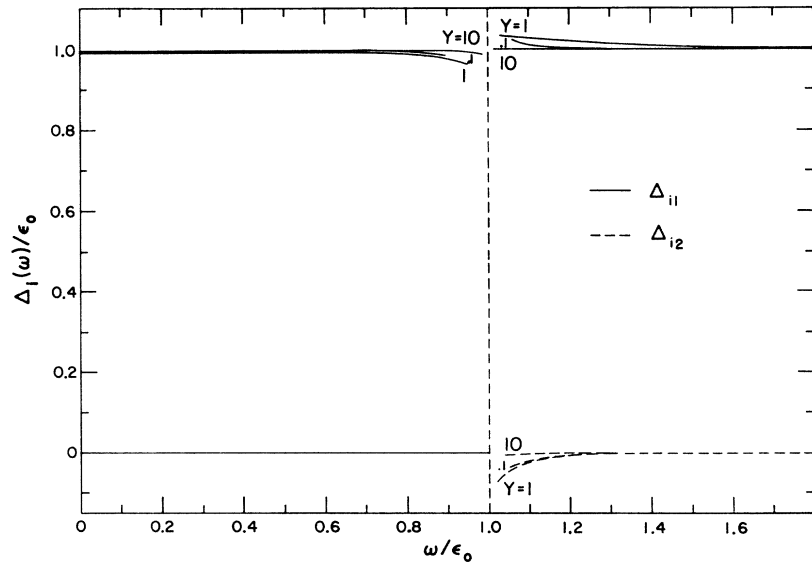


FIG. 1. Approximate solutions for the real and imaginary parts of the isotropic part of the gap parameter, $\Delta_{i1}(\omega - i0^+)/\epsilon_0$ and $\Delta_{i2}(\omega - i0^+)/\epsilon_0$, versus ω/ϵ_0 for various values of $y = (2\epsilon_0\tau)^{-1}$, using $\langle a^2 \rangle = 0.02$. Note that, for all values of y , Δ_{i1} differs little from ϵ_0 , and Δ_{i2} differs little from zero.

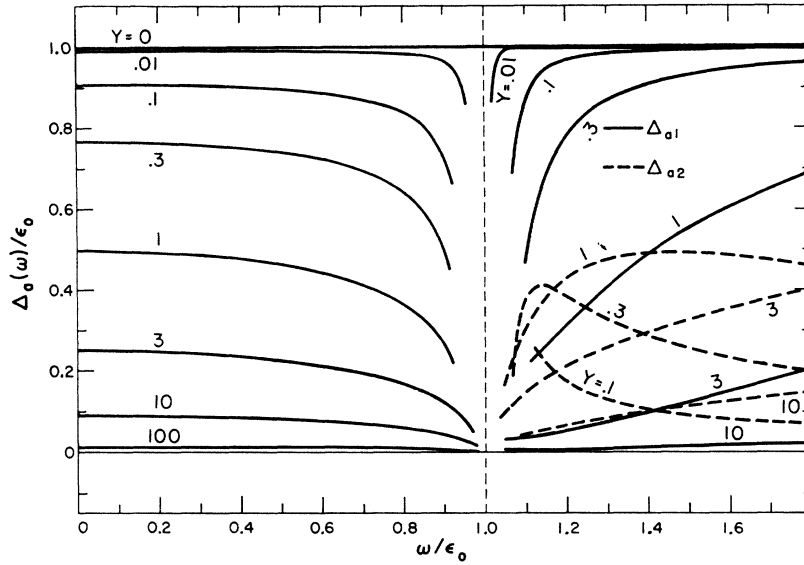


FIG. 2. Approximate solutions for the real and imaginary parts of the anisotropic part of the gap parameter, $\Delta_{a1}(\omega - i0^+)/\epsilon_0$ and $\Delta_{a2}(\omega - i0^+)/\epsilon_0$, versus ω/ϵ_0 , for various values of $y = (2\epsilon_0\tau)^{-1}$, using $\langle a^2 \rangle = 0.02$. Note that as y increases, the magnitude of Δ_a decreases from ϵ_0 to zero.

of a and by retaining only terms of order $\langle a^2 \rangle$, we find, in the weak-coupling ($\omega_D \gg \epsilon_0$) limit,

$$\epsilon_0(0) = 2\omega_D [1 + \langle a^2 \rangle (1/N(0)V - \frac{3}{2})] \times \exp[-1/N(0)V]. \quad (2.27)$$

For $y = \infty$ we have

$$\epsilon_0(0) = 2\omega_D \exp[-1/N(0)V]. \quad (2.28)$$

Let us temporarily assume that ω_D , $N(0)$, and V remain constant as impurities are added to the superconductor. Then, as y increases from zero to ∞ , we expect $\epsilon_0(0)$ to decrease from its maximum in (2.27) to its minimum in (2.28). The corresponding fractional reduction in $\epsilon_0(0)$, given by

$$\frac{\delta\epsilon_0(0)}{\epsilon_0(0)} \equiv \frac{\epsilon_0(0, y=0) - \epsilon_0(0, y=\infty)}{\epsilon_0(0, y=\infty)} = \langle a^2 \rangle \left(\frac{1}{N(0)V} - \frac{3}{2} \right), \quad (2.29)$$

is of the order of 5%, assuming $1/N(0)V \simeq 4$ and $\langle a^2 \rangle \simeq 0.02$ for typical weak-coupling superconductors. This reduction arises solely from the washing out of the anisotropy by the impurity scattering.

For intermediate impurity concentrations we expect that $\epsilon_0(0)$ may be written as

$$\epsilon_0(0) = 2\omega_D [1 + \langle a^2 \rangle (1/N(0)V - \frac{3}{2})\lambda] \times \exp[-1/N(0)V], \quad (2.30)$$

where ω_D , $N(0)$, V , and λ are all functions of the impurity concentration. We expect λ to decrease monotonically from its maximum value of unity at $y=0$, to about one half at $y \simeq 1$, and to zero at $y = \infty$.

C. The Threshold Energy

In the preceding section we derived by an approximate method some expressions for $\Delta_i(\omega)$ and $\Delta_a(\omega)$. For

$\omega < \epsilon_0$, the resulting solutions of Eqs. (2.22) are pure real quantities. This reality of $\Delta_i(\omega)$ and $\Delta_a(\omega)$ for small values of ω is not just an accidental result of certain approximations. When we examine the anisotropy equations (2.17) and (2.18) more closely, we see that the exact solutions $\Delta_i(\omega)$ and $\Delta_a(\omega)$ have vanishing imaginary parts for all values of ω less than some energy ω_0 . We shall call ω_0 the threshold energy for the imaginary parts of $\Delta_i(\omega)$ and $\Delta_a(\omega)$. As we shall see later, ω_0 is also the threshold energy for the effective density of states, which becomes nonzero only for $\omega > \omega_0$.

We wish to estimate the value of ω_0 . We anticipate that, since $\Delta_i(\omega) \simeq \Delta_a(\omega) \simeq \epsilon_0$ for small impurity concentrations, the threshold energy ω_0 should then be approximately $\epsilon_0 + a_{\min}\epsilon_0$, where a_{\min} is the minimum value of a_p on the Fermi surface. For large impurity concentrations, since $\Delta_a(\omega) \simeq 0$, we expect to find $\omega_0 \simeq \epsilon_0$. Thus, depending upon the impurity concentration, the threshold energy ω_0 should obey the condition

$$\epsilon_0(1 + a_{\min}) \leq \omega_0 \leq \epsilon_0. \quad (2.31)$$

One estimate, which we call ω_1 , of the threshold energy may be calculated, as suggested by Hohenberg,¹⁷ from the definition

$$\Delta_i(\omega_1) + a_{\min}\Delta_a(\omega_1) = \omega_1. \quad (2.32)$$

We have carried out this calculation in the Appendix. For small impurity concentrations we find that

$$\omega_1 = \epsilon_0(1 + a_{\min}) + \epsilon_0 y \frac{(C_a |a_{\min}| - C_i)}{(1 + a_{\min})^{1/2} \sqrt{2}}, \quad (y \ll \langle a^2 \rangle^{1/4}), \quad (2.33)$$

where C_a and C_i are integrals, defined in the Appendix, which depend upon the details of the anisotropy distribution function $P(a)$. For large impurity concentrations the estimate ω_1 tends not to ϵ_0 , but to a smaller value, $[1 - (C_i/C_a)]\epsilon_0$. Though the estimate ω_1 may

yield the correct threshold energy in this limit, the behavior of ω_1 nevertheless gives negligible information about the behavior of the density of states function for large impurity concentrations.

In the next section we shall derive another estimate, ω_2 , for the threshold energy. This estimate gives, for large impurity concentrations, the energy at which the density of states and the imaginary parts of the gap parameter rise sharply from zero. The result is

$$\omega_2 = \epsilon_0 [1 - \frac{3}{2} \langle a^2 \rangle / y]^{2/3}, \quad (y \gg \langle a^2 \rangle^{1/4}). \quad (2.34)$$

It is evident from Eqs. (2.33) and (2.34) that the impurity concentration given by $y = (2\epsilon_0\tau)^{-1} \simeq \langle a^2 \rangle^{1/4} \simeq 0.3-0.4$ is roughly the dividing point between the small and large impurity concentration regimes.

D. Behavior for Large Impurity Concentrations

In the preceding sections we have discussed the behavior of $\Delta_i(\omega)$ and $\Delta_a(\omega)$ for small ω , for $\omega = \omega_0$, and for large ω . We have anticipated that the solutions will depend rather sensitively upon $P(a)$ for $\omega \simeq \epsilon_0$. This is indeed the case for $y \lesssim 1$, as we shall see in the following section. However, it is quite remarkable that for $y \gg 1$, the solutions depend only upon $\langle a^2 \rangle$, even for $\omega = \epsilon_0$. It is this latter state of affairs which we wish to examine in the present section.

We begin by recalling the approximate anisotropy equations (2.20) and (2.21). Let us assume that the solutions of these equations are such that the third term on the right-hand side of Eq. (2.21) can be neglected. The quantity Δ_a can then be solved in terms of Δ_i and inserted into Eq. (2.20), yielding

$$\Delta_i = \epsilon_0 [1 \mp i \langle a^2 \rangle / y \Delta_i / (\omega^2 - \Delta_i^2)^{1/2}], \quad (2.35)$$

which can now be solved for Δ_i in terms of ω .

For the purpose of the solution of Eq. (2.35) it is convenient to introduce an auxiliary variable θ , the phase angle of the square root:

$$(\omega^2 - \Delta_i^2)^{1/2} \equiv r e^{\pm i\theta}, \quad 0 \leq \theta \leq \frac{1}{2}\pi. \quad (2.36)$$

Under the condition that $\langle a^2 \rangle / y \ll \theta$, we obtain the following approximate solutions:

$$\Delta_{i1} = \epsilon_0 [1 - \langle a^2 \rangle / y]^{2/3} \sin^{4/3} \theta, \quad (2.37)$$

$$\Delta_{i2} = \mp \epsilon_0 \langle a^2 \rangle / y]^{2/3} \sin^{1/3} \theta \cos \theta, \quad (2.38)$$

$$\Delta_{a1} = \epsilon_0 (1/y) \langle a^2 \rangle / y]^{1/3} \sin^{2/3} \theta, \quad (2.39)$$

$$\Delta_{a2} = \mp \epsilon_0 (1/y) \langle a^2 \rangle / y]^{1/3} \sin^{-1/3} \theta \cos \theta, \quad (2.40)$$

and

$$\omega = \epsilon_0 [1 + \langle a^2 \rangle / y]^{2/3} (1 - 4 \sin^2 \theta) / 2 \sin^{2/3} \theta]. \quad (2.41)$$

All the approximations which lead to the above results are satisfied for large impurity concentrations ($y \gg 1$) when $\omega \simeq \epsilon_0$. We note that the solutions $\Delta_i(\omega)$ and $\Delta_a(\omega)$ for such a case depend upon $\langle a^2 \rangle$ but upon none of the finer details of the anisotropy distribution function $P(a)$.

Under the conditions that $\langle a^2 \rangle / y]^{1/3} \ll 1$ and $\omega \simeq \epsilon_0$, the reduced effective density of states and the related

function involving $\Delta(\mathbf{p}, \omega)$ are approximately equal and are given by

$$\begin{aligned} n(\mathbf{p}, \omega) &= \text{Re}[\omega / (\omega^2 - \Delta^2(\mathbf{p}, \omega))^{1/2}] \\ &\simeq \text{Re}[\Delta(\mathbf{p}, \omega) / (\omega^2 - \Delta^2(\mathbf{p}, \omega))^{1/2}] \\ &\simeq \text{Re}[\epsilon_0 / (\omega^2 - \Delta_i^2(\omega))^{1/2}] \\ &= (y / \langle a^2 \rangle)^{1/3} \sin^{1/3} \theta \cos \theta. \end{aligned} \quad (2.42)$$

This quantity has its maximum value,

$$n_{\max} = \frac{1}{2} (3^{1/2} / 2^{1/3}) (y / \langle a^2 \rangle)^{1/3}, \quad (2.43)$$

at $\theta = \frac{1}{6}\pi$, which, as is seen from Eq. (2.41), corresponds to the energy $\omega = \epsilon_0$. The threshold for $n(\mathbf{p}, \omega)$ as well as for the imaginary parts Δ_{i2} and Δ_{a2} of the gap parameter, is given by the value $\theta = \frac{1}{2}\pi$. The corresponding threshold energy, which we call ω_2 in this approximation, is then found from Eq. (2.41) to be

$$\omega_2 = \epsilon_0 [1 - \frac{3}{2} \langle a^2 \rangle / y]^{2/3}. \quad (2.44)$$

In terms of the reduced quantities

$$\tilde{n} \equiv n(\mathbf{p}, \omega) / n_{\max}, \quad (2.45)$$

$$\tilde{\omega} \equiv (\omega - \epsilon_0) / (\epsilon_0 - \omega_2), \quad (2.46)$$

the effective density of states is then seen to have a shape which is independent of both the impurity concentration and the anisotropy; it is described by the parametric equations

$$\tilde{n} \equiv 2(2^{1/3} / 3^{1/2}) \sin^{1/3} \theta \cos \theta, \quad (2.47)$$

$$\tilde{\omega} \equiv (1 - 4 \sin^2 \theta) / (3 \sin^{2/3} \theta). \quad (2.48)$$

We note that we may write

$$\tilde{n} \simeq 2(2^{1/3} / 3^{1/2}) (\tilde{\omega} + 1)^{1/2}, \quad (\theta \simeq \frac{1}{2}\pi), \quad (2.49)$$

$$\tilde{n} \simeq \frac{2}{3} 2^{1/3} (\tilde{\omega})^{-1/2}, \quad (\langle a^2 \rangle / y \ll \theta \ll 1). \quad (2.50)$$

The curve of \tilde{n} versus $\tilde{\omega}$ is plotted in Fig. 3.

E. Behavior for Small and Moderate Impurity Concentrations

We have postponed until now a discussion of the behavior of $\Delta_i(\omega)$ and $\Delta_a(\omega)$ for energies ω near ϵ_0 and for impurity concentrations such that $y \lesssim 1$. For this case the structure of the anisotropy distribution function $P(a)$ is important; the nature of the solutions of the anisotropy equations then depends in detail upon the particular model chosen for $P(a)$. The main features of these solutions for $\omega \simeq \epsilon_0$ are qualitatively as follows: For small impurity concentrations ($y \ll 1$) the imaginary parts, Δ_{i2} and Δ_{a2} , are small, and the real parts are given by $\Delta_{i1} \simeq \Delta_{a1} \simeq \epsilon_0$. For larger impurity concentrations the imaginary parts are larger in magnitude, and the ω dependence of all the quantities, Δ_{i1} , Δ_{i2} , Δ_{a1} , and Δ_{a2} , reflects the detailed shape of the anisotropy distribution function. As the impurity concentration is further increased, this structure becomes obscured and is pulled in towards ϵ_0 . At the same time, the magnitude of Δ_a decreases. For large impurity concentrations

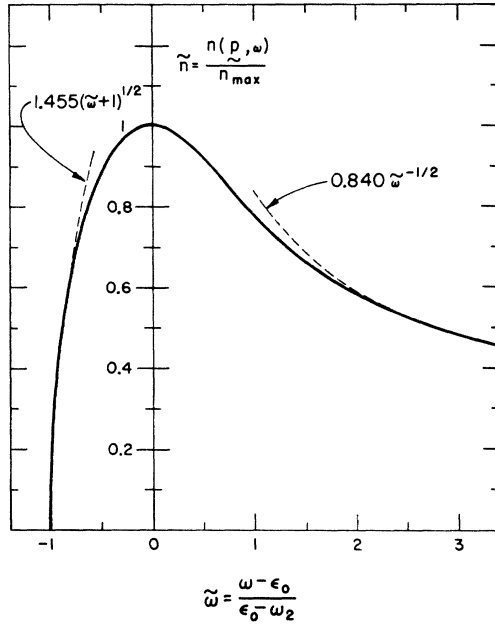


FIG. 3. The shape of the reduced effective density of states under the conditions $\langle a^2 \rangle / y^{1/2} \ll 1$ and $\omega \simeq \epsilon_0$: $\tilde{n} \equiv n(\mathbf{p}, \omega) / n_{\max}$ versus $\tilde{\omega} \equiv (\omega - \epsilon_0) / (\epsilon_0 - \omega_2)$.

($y \gg 1$) the quantities Δ_{a1} , Δ_{a2} , and Δ_{i2} become small, while Δ_{i1} remains close to the value ϵ_0 ; the gap parameter thus becomes essentially isotropic. The ω dependence then no longer reflects details of $P(a)$, and the behavior is as discussed in the preceding section.

For a quantitative description of $\Delta_i(\omega)$ and $\Delta_a(\omega)$, a model for $P(a)$ must be chosen; the resulting Eqs. (2.11) and (2.12) must then be solved numerically. The following iterative procedure may be used to generate such numerical solutions with the aid of a digital computer: For given values of ω , $y = (2\epsilon_0\tau)^{-1}$, and ϵ_0 , trial input

functions Δ_i^{in} and Δ_a^{in} are assumed. Using the equations

$$\Delta_i^{\text{out}} = \epsilon_0 \pm i\epsilon_0 y \Delta_a^{\text{in}} \int da \frac{aP(a)}{[\omega^2 - (\Delta_i^{\text{in}} + a\Delta_a^{\text{in}})^2]^{1/2}}, \quad (2.51)$$

$$\Delta_a^{\text{out}} = \epsilon_0 \mp i\epsilon_0 y \Delta_i^{\text{in}} \int da \frac{P(a)}{[\omega^2 - (\Delta_i^{\text{in}} + a\Delta_a^{\text{in}})^2]^{1/2}}, \quad (2.52)$$

output functions Δ_i^{out} and Δ_a^{out} are computed. If the output quantities are different from the input quantities, new input functions are prepared and inserted back into the equations to obtain new output functions. This process is repeated until the output functions are numerically equal (within predetermined limits) to the corresponding input functions, at which time the iteration procedure is terminated.

Since the functional form of $P(a)$ enters by means of one-dimensional integrals which are performed numerically at each step of the iteration process, it is thus a simple matter to obtain solutions for arbitrary models of the anisotropy distribution function. However, for simplicity we have used the rectangular model

$$P_0(a) \equiv (2a_{\max})^{-1}, \quad a_{\min} < a < a_{\max}, \\ \equiv 0, \quad \text{otherwise}; \quad (2.53)$$

$$a_{\max} = -a_{\min} = (3\langle a^2 \rangle)^{1/2}, \quad (2.54)$$

with $\langle a^2 \rangle = 0.02$ to obtain the results shown in Figs. 4 and 5. In Fig. 4 we have plotted Δ_{i1} and Δ_{i2} (with arguments $z = \omega - i0^+$) versus ω for various values of y , and in Fig. 5 we have plotted similar curves of Δ_{a1} and Δ_{a2} . These results demonstrate the features discussed earlier.

F. The Effective Density of States

The theoretical expressions for a number of physically measurable properties in the absence of impurities may

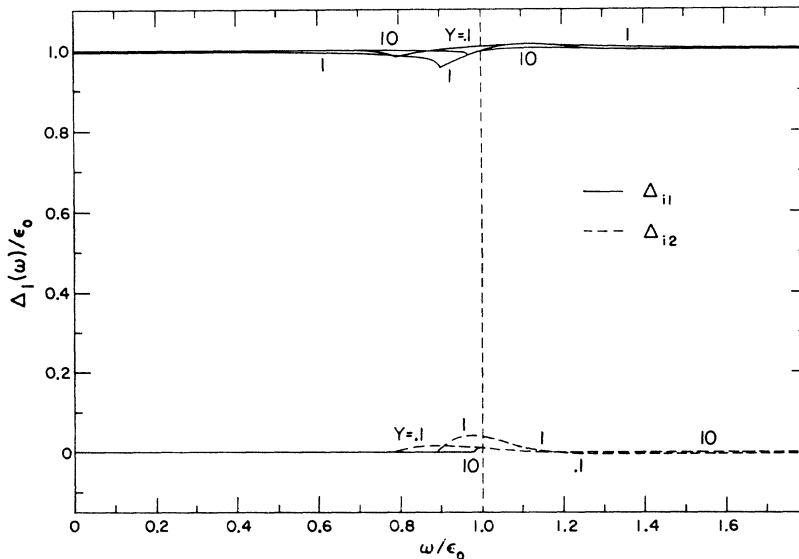
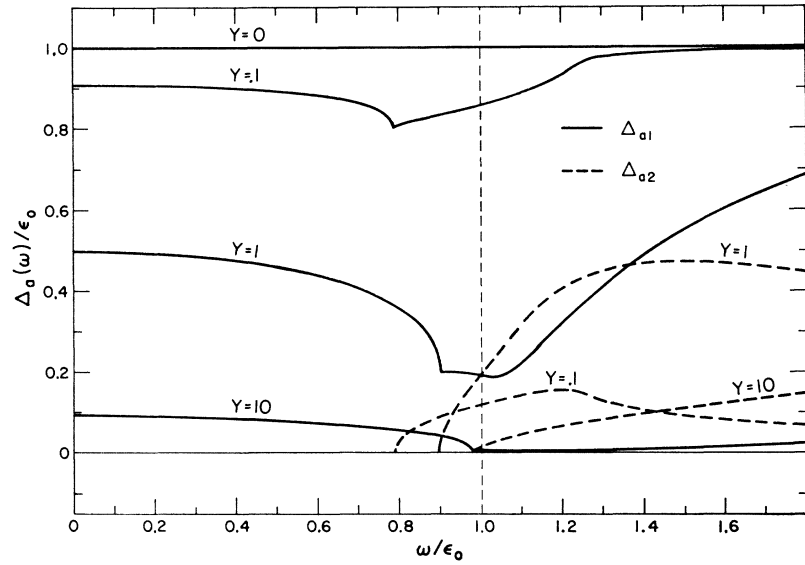


FIG. 4. Numerical solutions for the real and imaginary parts of the isotropic part of the gap parameter, $\Delta_{i1}(\omega - i0^+)/\epsilon_0$ and $\Delta_{i2}(\omega - i0^+)/\epsilon_0$, versus ω/ϵ_0 . These solutions, obtained using a rectangular anisotropy distribution function with $\langle a^2 \rangle = 0.02$, are shown for various values of $y = (2\epsilon_0\tau)^{-1}$. Note that, for all values of y , Δ_{i1} differs little from ϵ_0 , and Δ_{i2} differs little from zero.

FIG. 5. Numerical solutions for the real and imaginary parts of the anisotropic part of the gap parameter, $\Delta_{a1}(\omega - i0^+)/\epsilon_0$ and $\Delta_{a2}(\omega - i0^+)/\epsilon_0$, versus ω/ϵ_0 . These solutions, obtained using a rectangular anisotropy distribution function with $\langle a^2 \rangle = 0.02$, are shown for various values of $y = (2\epsilon_0\tau)^{-1}$. Note that as y increases, the magnitude of Δ_a decreases from ϵ_0 to zero.



be expressed in terms of the reduced, anisotropic, effective density of states, $n(\mathbf{p}, \omega) = \text{Re}[\omega/(\omega^2 - \Delta_p^2)^{1/2}]$. (We neglect energy dependence in the gap parameter arising from strong coupling.) In the presence of impurities, the corresponding effective density of states is given by

$$n(\mathbf{p}, \omega) = \text{Re}[\omega/(\omega^2 - \Delta^2(\mathbf{p}, \omega))^{1/2}], \quad (2.55)$$

where $\Delta(\mathbf{p}, \omega) = \Delta_i(\omega) + a_p \Delta_a(\omega)$ must be determined from the anisotropy equations (2.11), (2.12), and (2.13). It is thus of interest to examine the behavior of $n(\mathbf{p}, \omega)$ as a function of impurity concentration.

In the small-impurity-concentration limit when $\Delta(\mathbf{p}, \omega) \simeq \epsilon_0(1 + a_p)$, the reduced effective density of states has the form

$$n(\mathbf{p}, \omega) \simeq \text{Re}[\omega/(\omega^2 - \epsilon_0^2(1 + a_p)^2)^{1/2}]. \quad (2.56)$$

This is plotted in Fig. 6 for two directions of \mathbf{p} , one for which $a_p = a_{\min}$ and the other for which $a_p = a_{\max}$. These curves have inverse square-root singularities at energies $\omega = \epsilon_0(1 + a_p)$.

As impurities are added, two important effects occur. First, since both $\Delta_i(\omega)$ and $\Delta_a(\omega)$ take on imaginary parts, the peaks in $n(\mathbf{p}, \omega)$ become rounded and no longer have inverse square-root singularities. Second, since the presence of impurities tends to decrease the magnitude of $\Delta_a(\omega)$, $n(\mathbf{p}, \omega)$ becomes less dependent upon the direction of \mathbf{p} ; the positions of the peaks in energy collapse towards ϵ_0 . Both these effects are demonstrated in Fig. 7 for the same two directions of \mathbf{p} as before. The results have been obtained from the numerical model calculations of the preceding section using the rectangular anisotropy distribution function (2.53).

In the large-impurity-concentration limit the density of states again sharpens but becomes nearly isotropic. It is then given approximately by

$$n(\mathbf{p}, \omega) = \text{Re}[\omega/(\omega^2 - \epsilon_0^2)^{1/2}] \quad (2.57)$$

for $\omega \neq \epsilon_0$. At $\omega = \epsilon_0$, $n(\mathbf{p}, \omega)$ has a maximum given by

$$n_{\max} = \frac{1}{2} (3^{1/2}/2^{1/3}) (y/\langle a^2 \rangle)^{1/3}, \quad (2.58)$$

whereas the precise shape of the effective density of states for $\omega \simeq \epsilon_0$ is given by Eqs. (2.47) and (2.48).

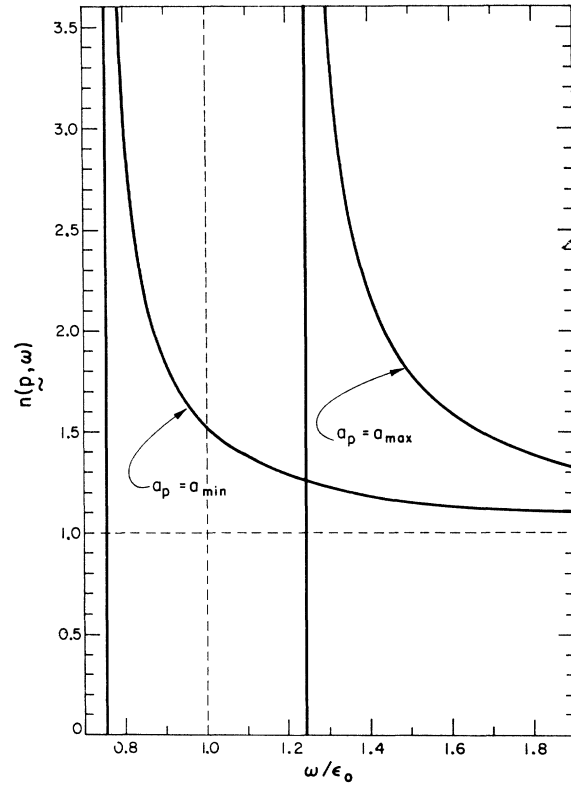


FIG. 6. The reduced, anisotropic, effective density of states, $n(\mathbf{p}, \omega)$, versus ω/ϵ_0 in the absence of impurities, plotted for two directions of \mathbf{p} . Using a rectangular anisotropy distribution function with $\langle a^2 \rangle = 0.02$ and $a_{\max} = -a_{\min} = (3\langle a^2 \rangle)^{1/2} = 0.2449$, one direction of \mathbf{p} corresponds to $a_p = a_{\min}$, and the other direction corresponds to $a_p = a_{\max}$.

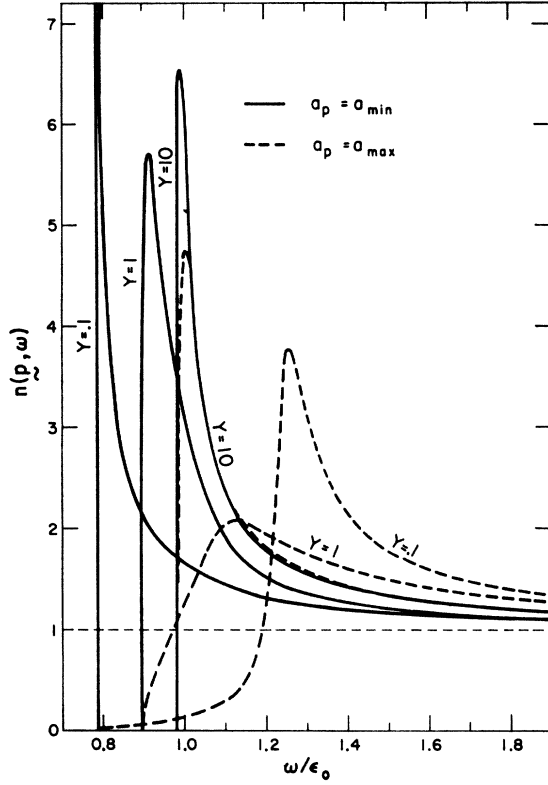


FIG. 7. The reduced, anisotropic, effective density of states, $n(\mathbf{p}, \omega)$, versus ω/ϵ_0 in the presence of impurities, plotted for the same two directions as in Fig. 6. Note that as γ increases, the effective density of states becomes isotropic.

The above results for the effective density of states confirm the behavior suggested by Hohenberg¹⁷ except for certain details in the large-impurity-concentration limit.

Another quantity of some interest is the Fermi surface average of the reduced effective density of states

$$\langle n(\mathbf{p}, \omega) \rangle_{av} = \left\langle \text{Re} \left(\frac{\omega}{[\omega^2 - \Delta^2(\mathbf{p}, \omega)]^{1/2}} \right) \right\rangle_{av} \\ = \int da P(a) \text{Re} \left(\frac{\omega}{[\omega^2 - (\Delta_i + a\Delta_a)^2]^{1/2}} \right). \quad (2.59)$$

In the small-impurity-concentration limit this quantity generally exhibits a considerable amount of broadening and structure, reflecting the form of the anisotropy distribution $P(a)$. As impurities are added, the structure coalesces into a single peak, gradually sharpening to a maximum at $\omega = \epsilon_0$. In the limit of large impurity concentrations ($\gamma \gg 1$), $\langle n(\mathbf{p}, \omega) \rangle_{av}$ is approximately equal to $n(\mathbf{p}, \omega)$, which is discussed above. The numerical calculations of the preceding section, using the rectangular model, have been used to demonstrate the behavior of $\langle n(\mathbf{p}, \omega) \rangle_{av}$ in Fig. 8.

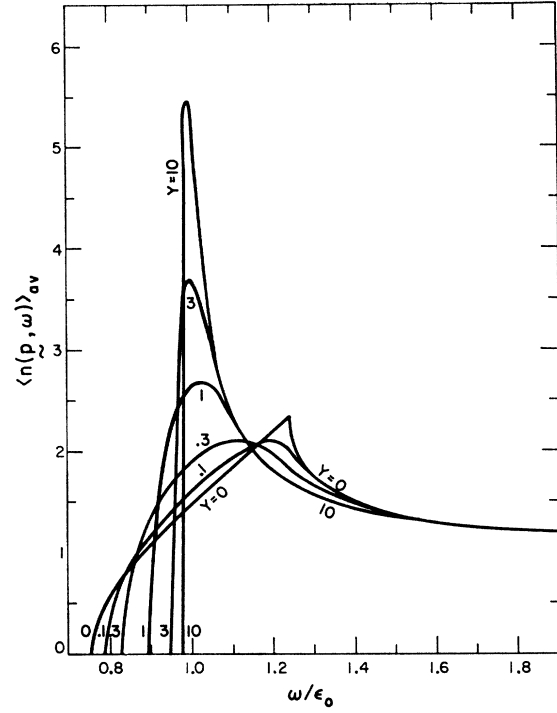


FIG. 8. The Fermi surface average of the reduced, anisotropic, effective density of states, $\langle n(\mathbf{p}, \omega) \rangle_{av}$, versus ω/ϵ_0 , for a rectangular anisotropy distribution function with $\langle a^2 \rangle = 0.02$. As impurities are added and γ increases, the structure in $\langle n(\mathbf{p}, \omega) \rangle_{av}$ coalesces into a single peak, gradually sharpening to a maximum at $\omega = \epsilon_0$. Note that for large impurity concentrations the shape is given by the curve shown in Fig. 3.

The electronic contribution to the specific heat C_s at low temperatures depends upon the Fermi-surface average of the effective density of states $\langle n(\mathbf{p}, \omega) \rangle_{av}$. Any "upward curvature" at the low-temperature end of a curve of $\log C_s$ versus T_c/T arising from small-gap excitations when impurities are absent must gradually disappear as impurities are added, since the Fermi-surface average of the effective density of states then becomes isotropic. Experimental evidence for this sort of behavior has been found previously.¹⁻³

The ratio R_s/R_n of the nuclear spin-lattice relaxation rate in the superconducting state to that in the normal state is proportional to an integral over essentially the square of the Fermi-surface average of the effective density of states. As impurities are added, the above-mentioned sharpening of $\langle n(\mathbf{p}, \omega) \rangle_{av}$ at $\omega = \epsilon_0$ causes the quantity R_s/R_n to increase in magnitude. Such an effect has been observed experimentally by Masuda.⁴ We note that these results should lay the ground work for an improvement of previous calculations¹⁷ of the nuclear spin-lattice relaxation time for large impurity concentrations.

The infrared absorption experiments of Richards⁶ and the surface resistance experiments of Biondi, Garfunkel, and Thompson,⁷ which exhibit anisotropy for samples of high purity, exhibit isotropic behavior for large

impurity concentrations. Since the experimental quantities depend upon $n(\mathbf{p}, \omega)$, which becomes isotropic as impurities are added, the experimental values for the gap parameters thus become independent of direction for large impurity concentrations.

Since superconductive tunneling experiments essentially measure $n(\mathbf{p}, \omega)$ or $\langle n(\mathbf{p}, \omega) \rangle_{av}$ directly, depending upon the preparation of the junctions,^{21,22} it would be interesting to attempt to observe experimentally the effects shown in Fig. 7, which corresponds to single-crystal junctions, and in Fig. 8, which corresponds to a polycrystalline junction.

III. SUMMARY AND DISCUSSION

In this paper we have considered the effects of isotropic impurity scattering upon the anisotropy of the superconducting energy gap. Within the context of a model proposed by Markowitz and Kadanoff,¹³ we have studied the precise manner in which the addition of nonmagnetic impurities decreases the anisotropic part of the energy gap parameter. We then discussed the influence of this "washing out" of the anisotropy upon various experimental quantities.

A detailed comparison with experiment awaits more complete knowledge of the anisotropy distribution functions $P(a)$, which must be obtained from theoretical calculations, such as those by Bennett,²² or from experimental measurements in very pure samples. For example, tunneling, ultrasonic attenuation, specific heat, nuclear spin-lattice relaxation time, and surface resistance measurements all yield information which may be combined to obtain $P(a)$ for a given metal.^{21,22} It is thus hoped that the present results may stimulate further theoretical and experimental research.

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APPENDIX: AN ESTIMATE OF THE THRESHOLD ENERGY

An estimate ω_1 of the threshold energy may be defined by¹⁷

$$\omega_1 = \Delta_i(\omega_1) + a_{\min} \Delta_a(\omega_1). \quad (A1)$$

²¹ J. R. Clem, Ann. Phys. (N. Y.) (to be published).

²² A. J. Bennett, Phys. Rev. **140**, A1902 (1965).

When we insert this definition into Eqs. (2.17) and (2.18), we obtain to good approximation

$$\Delta_i(\omega_1) = \epsilon_0 - \epsilon_0 y (\Delta_a(\omega_1)/2\omega_1)^{1/2} C_i, \quad (A2)$$

$$\Delta_a(\omega_1) = \epsilon_0 - \epsilon_0 y (\Delta_a(\omega_1)/2\omega_1)^{1/2} C_a, \quad (A3)$$

where

$$C_i \equiv - \int_{a_{\min}} da a P(a) (a - a_{\min})^{-1/2}, \quad (A4)$$

$$C_a \equiv \int_{a_{\min}} da P(a) (a - a_{\min})^{-1/2}. \quad (A5)$$

Combining Eqs. (A1), (A2), and (A3), we find the following cubic equation for ω_1 :

$$\omega_1^3 - 2(1 + a_{\min})\epsilon_0\omega_1^2 + [(1 + a_{\min})^2 - 2(C + a_{\min})x^2]\epsilon_0^2\omega_1 + 2(C + a_{\min})(1 - C)x^2\epsilon_0^3 = 0, \quad (A6)$$

where $C \equiv C_i/C_a$ and $x \equiv C_a y/2$. When $y \ll 1$, the solution of this equation may be expressed, to first order in y , as

$$\omega_1 = \epsilon_0(1 + a_{\min}) + \epsilon_0 \frac{(|a_{\min}| - C)}{\sqrt{2}(1 + a_{\min})^{1/2}} C_a y. \quad (A7)$$

When $y \gg 1$, the solution may be expressed, to lowest order in y^{-1} , as

$$\omega_1 = \epsilon_0(1 - C) - \epsilon_0 2(1 - C)(|a_{\min}| - C)(C_a y)^{-2}. \quad (A8)$$

The corresponding values of $\Delta_i(\omega_1)$ and $\Delta_a(\omega_1)$ are obtained from the expressions

$$\Delta_i(\omega_1) = \epsilon_0 - \epsilon_0 C \{ [(1 + \epsilon_0/\omega_1 x^2)^2 - 1]^{1/2} - \epsilon_0/\omega_1 x^2 \}, \quad (A9)$$

$$\Delta_a(\omega_1) = \epsilon_0 \{ (1 + \epsilon_0/\omega_1 x^2) - [(1 + \epsilon_0/\omega_1 x^2)^2 - 1]^{1/2} \}, \quad (A10)$$

which follow from Eqs. (A2) and (A3).

For the case of rectangular model (2.53) for the anisotropy distribution function, using $\langle a^2 \rangle = 0.02$, we obtain $C_i = 0.2333$, $C_a = 2.858$, $C = 0.0816$, and $a_{\min} = -0.2449$. We then find, for $y \ll 1$,

$$\omega_1 \simeq \epsilon_0(0.755 + 0.380y),$$

$$\Delta_i(\omega_1) \simeq \epsilon_0(1 - 0.190y), \quad (A11)$$

$$\Delta_a(\omega_1) \simeq \epsilon_0(1 - 2.325y),$$

and, for $y \gg 1$,

$$\omega_1 \simeq \epsilon_0(0.918 - 0.037y^{-2}),$$

$$\Delta_i(\omega_1) \simeq \epsilon_0(0.918 + 0.018y^{-2}), \quad (A12)$$

$$\Delta_a(\omega_1) \simeq \epsilon_0(0.225y^{-2}).$$