

### Theory of positron annihilation in superconductors

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A theory of positron annihilation in Cooper-pair superconductors is presented. It is assumed that the positron and electrons are not correlated. It is argued that a comparison of positron data with density-of-states measurements might be used to test the hypothesis that superconductivity in the high-temperature superconductors results from pair formation. The prospects for the observation of the effects of the superconductive transition are briefly reviewed.

Within the past year or so there have been numerous angular-resolved positron-annihilation experiments reported on  $\text{YBa}_2\text{Cu}_3\text{O}_7$ .<sup>1</sup> Under suitable circumstances, such measurements yield a projection, onto one or two dimensions, of the Fermi-sea distribution function,  $\rho(\mathbf{p})$ , in momentum space and, indeed, there are already reports that indicate the existence of a Fermi surface in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  in the normal state.<sup>1</sup> Given realistic limits of resolution, there is little hope,<sup>2</sup> with earlier conventional superconductors, that the changes in the momentum distribution which accompany the transition to the ordered state can be detected. However, because of the rather small Fermi velocity and, depending upon which measurements one trusts, the possibility of, at least, an order of magnitude larger gap, there is some reasonable hope that such changes might be observed in these new materials. In the superconducting state the Fermi edge in momentum space is broadened by an amount  $\delta p$ , which can be estimated from  $\delta p = \Delta/\hbar v_F$ , i.e.,  $\delta k/k_F \sim 2/\pi \xi_0 k_F \sim 10^{-1}$  for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  or the newer Bi and Tl compounds. State of the art technique permits the resolution of a few percent of the Fermi momentum.

Despite the relative simplicity of the calculation, a theory of the momentum distribution seen in positron-annihilation experiments on superconductors does not appear to have been previously presented; in this paper the simplest such theory will be developed. The approach is based upon the BCS theory, however, as the calculation will demonstrate, the basic assumption is that the superconductivity is associated with pairs described by the usual two parameters  $u_k$  and  $v_k$  (see later for definitions). In turn these two same parameters determine, or are determined by, the density of states which might be measured in tunneling experiments, etc. Positron measurements, if they can be realized, therefore represent a rather direct check of the hypothesis that superconductivity is associated with pair formation and not, e.g., with the condensation of Bose particles such as holons<sup>3</sup> (if in fact the holons are bosons<sup>4</sup>). The theory will not account for the dynamic correlation between the positron and electrons.

The simplest considerations have been given, many years ago, by de Gennes.<sup>5</sup> He observed that probability of finding an electron in a state with wave vector  $\mathbf{k}$ , in the BCS ground state, is

$$\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = v_{\mathbf{k}}^2 = \frac{1}{2} \left[ 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right], \tag{1}$$

where  $E_{\mathbf{k}} = (\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2}$  and where  $\Delta$  is the energy gap. As stated earlier, in the condensed state, this implies a smearing of the Fermi distribution  $\delta k \sim \Delta/\hbar v_F$ . De Gennes noted that *ideally*  $v_{\mathbf{k}}^2$  could be measured via the Compton effect or positron annihilation.

The only formal theory aimed at positron annihilation in superconductors is that of Brovetto *et al.*<sup>6</sup> In order to obtain a momentum associated with the quasiparticles in the superconducting state, they assume that the energy of such a quasiparticle is purely kinetic, i.e., in terms of a momentum  $\mathbf{P}$ , the energy, measured relative to the normal-state Fermi energy, is  $(P^2 - p_F^2)/2m$ . They then equate this to the energy of an *occupied* quasiparticle state

$$E_{\mathbf{k}} = -[(\epsilon_{\mathbf{k}} - \epsilon_F)^2 + \Delta^2]^{1/2}$$

which results in

$$P^2 = p_F^2 - \{[(\hbar\mathbf{k})^2 - p_F^2]^2 + (2m\Delta)^2\}^{1/2}, \tag{2}$$

from which they calculate a momentum distribution function. This approach predicts the existence of a Fermi edge in the superconducting state *and* also predicts a reduction in the momentum of all occupied states and therefore a *narrowing* of the momentum distribution. This conclusion is evidently not in agreement with de Gennes's elementary considerations and warrants examination.

Before performing the formal calculation it is perhaps useful to review a few pertinent results of the BCS pairing theory. Independent of the pairing mechanism the reduced Hamiltonian will be of the form

$$\mathcal{H} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\downarrow}) - V \sum'_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger c_{-\mathbf{k}\downarrow} c_{\mathbf{k}'\uparrow}, \tag{3}$$

where the prime indicates that the sum is over all  $\mathbf{k}$  values such that  $\xi_{\mathbf{k}}$  lies within some limited range, usually denoted  $\omega_D$ , about the Fermi surface. This energy interval is determined by the region where the pairing interac-

tion is attractive. The order parameter, or gap function, is defined by

$$\Delta = V \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle, \quad (4)$$

and the following equations of motion are obtained:

$$\omega_{\mathbf{k}} c_{\mathbf{k}\uparrow} = \xi_{\mathbf{k}} c_{\mathbf{k}\uparrow} - \Delta c_{-\mathbf{k}\downarrow}^{\dagger} \quad (5a)$$

and

$$\omega_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} = -\xi_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} - \Delta^* c_{\mathbf{k}\uparrow}. \quad (5b)$$

The secular determinant for these equations is

$$\begin{vmatrix} \omega_{\mathbf{k}} - \xi_{\mathbf{k}} & \Delta \\ \Delta & \omega_{\mathbf{k}} + \xi_{\mathbf{k}} \end{vmatrix} = 0 \quad (6)$$

and results in an eigenenergy

$$E_{\mathbf{k}} \equiv \omega_{\mathbf{k}} = (\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2}. \quad (7)$$

The corresponding eigenvectors are

$$\alpha_{\mathbf{k}\uparrow} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} \quad (8a)$$

and

$$\alpha_{-\mathbf{k}\downarrow} = u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger}, \quad (8b)$$

where

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left[ 1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right]; \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left[ 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right]. \quad (9)$$

In terms of these operators the Hamiltonian is of the form

$$\mathcal{H} = E_{g.s.} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^{\dagger} \alpha_{\mathbf{k}\sigma}, \quad (10)$$

where  $E_{g.s.}$  is the ground-state energy. Recall that although the sum in this expression runs over  $\mathbf{k}$  vectors which lie above *and* below the original Fermi surface, the excitations which correspond to  $\alpha_{\mathbf{k}\sigma}^{\dagger}$  all have *positive* energies, i.e., this standard form of the Hamiltonian does *not* have a set of quasiparticle states which are full in the ground state and which might evolve from the occupied Fermi sea as  $\Delta$  is adiabatically turned on. (In order to make a connection of this sort, it would be necessary, e.g., for the usual Fermi sea, to effect a particle to hole transformation for those levels which lie below the Fermi surface but *not* for those above the Fermi sea). Trivially  $E_{\mathbf{k}} = [\xi_{\mathbf{k}\sigma} / (1 - 2v_{\mathbf{k}}^2)]$  and so, if  $\xi_{\mathbf{k}\sigma}$  is determined from normal-state data, the density of states of the superconductor is determined once  $v_{\mathbf{k}}^2$  is known.

Inverting Eqs. (8) gives for an electron (as opposed to a quasiparticle) destruction operator

$$c_{\mathbf{k}\sigma} = u_{\mathbf{k}} \alpha_{\mathbf{k}\sigma} + v_{\mathbf{k}} \alpha_{-\mathbf{k}-\sigma}^{\dagger}. \quad (11)$$

The first term on the left-hand side represents the amplitude associated with the possibility that the destruction of an electron will result in the destruction of a quasiparticle. Since there are no quasiparticles excited, such a process is *not* possible at  $T=0$ . The second term contains a hidden destruction operator for a pair (see Tink-

ham<sup>7</sup>) and hence corresponds to the amplitude for a process in which the positron annihilates half a pair leading to the *creation* of a  $\alpha_{-\mathbf{k}-\sigma}^{\dagger}$  quasiparticle. This latter process is possible for  $T=0$  and it is therefore the amplitude  $v_{\mathbf{k}}$  which is important for positron annihilation in this limit. The definition, Eq. (9), of this amplitude gives  $v_{\mathbf{k}}^2 \sim 1$  for  $\mathbf{k}$  vectors which would correspond to states well below the conventional Fermi surface and, because the admixture of creation into destruction operators becomes small, falls to zero, for vectors which have  $k \lambda$  values which are much more than  $\delta k$  larger than  $k_F$ .

Turning to the straightforward, but less transparent, formal derivation, the cross section that a positron will annihilate and produce two  $\gamma$ 's is given accurately by the golden rule. However, because there is no energy resolution for the outgoing photons, it is possible to integrate out the energy delta function and so there is a free sum over all possible final states, i.e., the probability,  $\rho(\mathbf{p})$ , that a pair of  $\gamma$ 's with a net (real) momentum of  $\mathbf{p}$  will be created is given by<sup>8</sup>

$$\rho(\mathbf{p}) \sim \frac{2\pi}{\hbar} \left[ \frac{e^2}{mc^2} \right]^2 \times \sum_f \left| \int d\mathbf{r} \langle 0 | e^{-i\mathbf{p}\cdot\mathbf{r}} \Phi_e(\mathbf{r}) \Phi_p(\mathbf{r}) | f \rangle \right|^2, \quad (12)$$

where  $\langle 0 |$  and  $| f \rangle$  correspond, respectively, to the (here superconducting) ground state and final state and where  $\Phi_e(\mathbf{r})$  and  $\Phi_p(\mathbf{r})$  are the local destruction operators for electrons and positrons, respectively. The square of the integral can be written as the product of two integrals and the sum over final states extracted using the completeness relation to give the definition

$$\rho(\mathbf{p}) = \sum_{\sigma} \int d\mathbf{x} \int d\mathbf{y} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \times \langle \Phi_{e\sigma}^{\dagger}(\mathbf{x}) \Phi_{e\sigma}(\mathbf{y}) \rangle \langle \Phi_{p\sigma}^{\dagger}(\mathbf{x}) \Phi_{p\sigma}(\mathbf{y}) \rangle, \quad (13)$$

where, in order to factor the electron and positron expectation values, it has been assumed that these entities are uncorrelated and where a thermally weighted sum over initial states has been substituted for the ground-state wave function so that, now, the angular brackets  $\langle \dots \rangle$  imply that the thermal average is to be taken. In order to easily evaluate  $\rho(\mathbf{p})$ , it is necessary to express the local creation and destruction operators in terms of similar operators but for which the effect on the superconducting eigenstates is known.

First, we transform the electron expectation value to real momentum space, i.e., write

$$\Phi_e^{\dagger}(\mathbf{x}) = \frac{1}{\sqrt{L}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} c_{\mathbf{k}\sigma}^{\dagger} \quad (14)$$

so that

$$\langle \Phi_{e\sigma}^{\dagger}(\mathbf{x}) \Phi_{e\sigma}(\mathbf{y}) \rangle = \frac{1}{L} \sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{y}} \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma} \rangle. \quad (15)$$

If we are to be concerned with real crystalline materials, the  $c_{\mathbf{k}\sigma}^{\dagger}$  do not create energy eigenstates. *In the normal*

state, such eigenstates are created by a set of Bloch wave creation operators  $b_{l\mathbf{k}\sigma}^\dagger$  where  $\mathbf{k}$  is assumed to lie in the first Brillouin zone and  $l$  is a band index. The momentum creation operator may be decomposed in terms of these operators:

$$c_{\mathbf{k}+\mathbf{G}\sigma}^\dagger = \sum_l a_{\mathbf{G}}^{l*}(\mathbf{k}) b_{l\mathbf{k}\sigma}^\dagger, \quad (16)$$

where  $a_{\mathbf{G}}^{l*}(\mathbf{k})$  are complex coefficients and  $\mathbf{G}$  is a lattice vector in the reciprocal lattice.<sup>9</sup> Using this we have

$$\langle \Phi_{e\sigma}^\dagger(\mathbf{x}) \Phi_{e\sigma}(\mathbf{y}) \rangle = \frac{1}{L} \sum_{l', \mathbf{k}, \mathbf{G}} \sum_{k', \mathbf{G}'} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}} e^{-i(\mathbf{k}'+\mathbf{G}')\cdot\mathbf{y}} a_{\mathbf{G}}^{l'*}(\mathbf{k}) a_{\mathbf{G}'}^{l'*}(\mathbf{k}') \langle b_{l\mathbf{k}\sigma}^\dagger b_{l'\mathbf{k}'\sigma} \rangle, \quad (17)$$

and substituting, we easily find

$$\rho(\mathbf{p}) = \frac{1}{L} \sum_{l', \mathbf{k}, \mathbf{G}} \sum_{k', \mathbf{G}'} \int d\mathbf{x} \int d\mathbf{y} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{x}} e^{-i(\mathbf{k}'+\mathbf{G}')\cdot\mathbf{y}} \langle \Phi_{p\sigma}^\dagger(\mathbf{x}) \Phi_{p\sigma}(\mathbf{y}) \rangle a_{\mathbf{G}}^{l'*}(\mathbf{k}) a_{\mathbf{G}'}^{l'*}(\mathbf{k}') \langle b_{l\mathbf{k}\sigma}^\dagger b_{l'\mathbf{k}'\sigma} \rangle. \quad (18)$$

In order to obtain an expression appropriate for a superconductor, only one more step is required. It is necessary to express the normal-state Bloch states in terms of the Bogoliubov-Valatin quasiparticle operators  $\alpha_{\mathbf{k}\sigma}^\dagger$  which can be written in terms of the Bloch operators and which correspond to energy eigenstates of the superconductor. For simplicity it will be assumed that only a single band is involved in the superconductivity and so dropping the band index,  $l$ , we write

$$b_{\mathbf{k}\sigma}^\dagger = u_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^\dagger + v_{\mathbf{k}} \alpha_{-\mathbf{k}-\sigma}. \quad (19)$$

We need

$$\begin{aligned} \langle b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}'\sigma} \rangle &= \langle (u_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^\dagger + v_{\mathbf{k}} \alpha_{-\mathbf{k}-\sigma}) (u_{\mathbf{k}'} \alpha_{\mathbf{k}'\sigma}^\dagger + v_{\mathbf{k}'} \alpha_{-\mathbf{k}'-\sigma}^\dagger) \rangle \\ &= (u_{\mathbf{k}}^2 \langle \alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} \rangle + v_{\mathbf{k}}^2 \langle \alpha_{-\mathbf{k}-\sigma} \alpha_{-\mathbf{k}-\sigma}^\dagger \rangle) \delta_{\mathbf{k}\mathbf{k}'}. \end{aligned} \quad (20)$$

The integral over the real-space variables can be eliminated by defining the squared (temperature-dependent) Fourier transform of the positron wave function as

$$|\Phi_p(\mathbf{p})|^2 = \frac{1}{L} \int d\mathbf{x} \int d\mathbf{y} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \langle \Phi_{p\sigma}^\dagger(\mathbf{x}) \Phi_{p\sigma}(\mathbf{y}) \rangle. \quad (21)$$

This is a delta function,  $\delta(\mathbf{p})$ , if the positron wave function is assumed constant.

Finally, substituting into the foregoing gives the result

$$\begin{aligned} \rho(\mathbf{p}) &= \sum_{\mathbf{k}, \mathbf{G}} \sum_{\sigma} |\Phi(\mathbf{p}-\mathbf{k}+\mathbf{G})|^2 |a_{\mathbf{G}}(\mathbf{k})|^2 \\ &\quad \times [u_{\mathbf{k}}^2 (1-n_{\mathbf{k}}) + v_{\mathbf{k}}^2 n_{\mathbf{k}}], \end{aligned} \quad (22)$$

where  $n_{\mathbf{k}} \equiv [1/(e^{-\beta E_{\mathbf{k}}} + 1)]$  is the thermal distribution function for quasiparticles in the superconductor. It should be noted that at  $T=0$ ,  $\langle \alpha_{\mathbf{k}\sigma} \alpha_{\mathbf{k}\sigma}^\dagger \rangle = n_{\mathbf{k}} = 1$ , for all  $\mathbf{k}$ , while  $\langle \alpha_{\mathbf{k}\sigma}^\dagger \alpha_{\mathbf{k}\sigma} \rangle = 1 - n_{\mathbf{k}} = 0$ . This reflects the fact that none of the  $\alpha_{\mathbf{k}\sigma}^\dagger$  states are occupied at zero temperature.

Thus in this limit

$$\rho(\mathbf{p}) = \sum_{\mathbf{k}, \mathbf{G}} \sum_{\sigma} |\Phi(\mathbf{p}-\mathbf{k}+\mathbf{G})|^2 |a_{\mathbf{G}}(\mathbf{k})|^2 v_{\mathbf{k}}^2 \quad (23)$$

and in the limit  $\Delta \rightarrow 0$ , the normal metal result is recovered since  $v_{\mathbf{k}}^2 \rightarrow \Theta(\mathbf{p}_F - \mathbf{p})$ , i.e., becomes a step function. For a finite  $\Delta$ , if free particle wave functions are assumed for both the positron and electron, this final expression reduces to that of de Gennes. It is *not* possible to recover the expression of Brovotto *et al.*, since here the Fermi edge is lost in the superconducting state, and, while the edge of the momentum distribution broadens, the width does not change.

Current technique does not permit the resolution of all three components of the momentum; rather, the experiment yields a one- or two-dimensional projection of  $\rho(\mathbf{k})$ . By way of illustration, the simplest case will be considered, namely, the one-dimensional projection for a free-electron model at zero temperature. In this case  $\rho(\mathbf{k}) = v_{\mathbf{k}}^2$ , and integrating out the perpendicular components of the momentum gives straightforwardly

$$\begin{aligned} \rho(k_z) &\propto \frac{\pi}{2} \left[ \left\{ \left[ \left[ \frac{k_z}{k_F} \right]^2 - 1 \right]^2 + \left[ \frac{\Delta}{\mathcal{E}_F} \right]^2 \right\}^{1/2} \right. \\ &\quad \left. + \left[ 1 - \left[ \frac{k_z}{k_F} \right]^2 \right] \right], \end{aligned} \quad (24)$$

where  $\mathcal{E}_F$  is the Fermi energy and where the normalization still needs to be determined. If  $N = 2 \int_0^\infty \rho(k_z) dk_z$ , then with  $d^2 = 1 + (\Delta^2/\mathcal{E}_F^2)$ ,

$$\frac{dN}{d\Delta^2} = \frac{k_F^3 \pi}{2 \mathcal{E}_F^2 \sqrt{d}} K \left[ \frac{d+1}{2d} \right], \quad (25)$$

where  $K(k)$  is the complete elliptic integral of the first kind. An expansion for this function, valid for small  $(\Delta^2/\mathcal{E}_F^2)$ , results in a now normalized

$$\rho(k_z) = \frac{3}{8} \left[ \frac{(([(k_z/k_F)^2 - 1]^2 + (\Delta/\mathcal{E}_F)^2]^{1/2} + [1 - (k_z/k_F)^2])}{1 + \frac{3}{16} (\Delta/\mathcal{E}_F)^2 [\ln 32 + 1 - 2 \ln(\Delta/\mathcal{E}_F)]} \right]. \quad (26)$$

This function is plotted for several rather large values of the gap in Fig. 1. The solid curve corresponds to the normal state, while the dashed curve reflects a realistic  $\Delta/\mathcal{E}_F=0.1$ . The sharp Fermi edge disappears with an appreciable tail extending out to a  $k_z \sim 1.25$ . The other two values plotted are most likely too large but serve to illustrate the fashion in which this *projected* distribution broadens. In real two- or three-dimensional materials the Fermi *momentum* depends upon the direction, and therefore the normal-state Fermi edge itself becomes rather difficult to observe. It is therefore even more difficult, but perhaps not impossible,<sup>1</sup> to detect the presence of a gap by its effects on this edge. However, reflecting the net broadening of the distribution, the probability of finding small momenta,  $k_z$ , decreases, approximately like

$$1 - \text{const} \left[ \frac{\Delta}{\mathcal{E}_F} \right]^2,$$

where the constant is of order of unity. This few percent effect is insensitive to details of the dispersion relation and will be of a similar magnitude in real materials. This reduction, most likely, represents the simplest fashion in which to detect the appearance of the gap.

Very recently Doniach<sup>10</sup> has considered the momentum distribution in the normal state of the high-temperature superconductors using a model in which the electrons are strongly correlated. He uses the so-called slave-boson method<sup>11</sup> and the mean-field approximation.<sup>12</sup> Within this mean-field approximation, for a nearly half-filled band, there is a very marked narrowing of

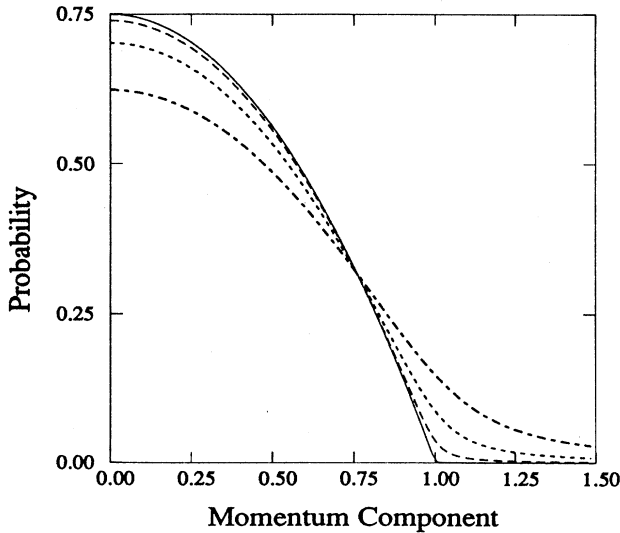


FIG. 1. The probability,  $\rho(k_z)$ , that the  $\gamma$ 's have a center-of-mass momentum component  $k_z$ . The value 1.0 corresponds to  $k_z = k_F$  where  $k_F$  is defined in the normal state. The solid curve corresponds to the normal state while the dashed, dotted, and dash-dotted curves corresponds to increasing values 0.1, 0.25, and 0.5, of the ratio  $\Delta/\mathcal{E}_F$ .

the "coherent" part of the density of states; if  $t$  is the bare hopping matrix element, then the effective such element is  $\delta^2 t$  where  $\delta^2$  is the concentration of holes. This renormalization also enters, as a prefactor, in the expression for the Green's function which determines the density of states and which would be reflected in the positron spectrum. The slave-boson representation of the Green's function is

$$G(\tau) = \langle T \{ f(\tau) b^\dagger(\tau) b(0) f^\dagger(0) \} \rangle$$

which, with the mean-field approximation,

$$\rightarrow \langle b \rangle^2 \langle T \{ f(\tau) f^\dagger(0) \} \rangle \rightarrow \delta^2 \langle T \{ f(\tau) f^\dagger(0) \} \rangle,$$

for the important coherent contribution. The fashion in which  $\delta^2$  enters is equivalent to a renormalization factor  $z$ , i.e., the factor which narrows the bandwidth exactly cancels the prefactor in the Green's function and so the density of the states at the Fermi level remains unchanged. However, this is not so for the *momentum* distribution. The Fermi step in momentum space is reduced by a factor of  $\delta^2$  and so, if  $\delta^2 \sim 0.1 \rightarrow 0.2$ , this represents very important effect. One of the present authors has argued<sup>13</sup> that the mean-field approximation is not justified for the relevant class of models. Also, even if one suspends one's disbelief, it is not clear that the Green's function calculated in this fashion is the one relevant to a positron experiment. Physically, the factor of  $\delta^2$  is associated with the "blocking" of the hopping process in the highly correlated limit, i.e., if there is already an electron on a given site then another electron is blocked from hopping to that site and hence the bandwidth is controlled by the number of holes since this determines the concentration of sites which *are* available for hopping. With this mindset, one observes that the above-mentioned mean-field expression for the Green's function is the one appropriate to the creation of a test *electron*, i.e., to one specific time ordering of the operators. It is the other time ordering, corresponding to the creation of a test *hole*, which is relevant in the positron context. The creation of such a hole requires the site to be *occupied* and the relevant Green's function should therefore contain a prefactor of  $1 - \delta^2$  rather than  $\delta^2$ , and it follows that the renormalization effect is not important for *p*-type superconductors. (Mathematically it is also clear that the operator combination replaced by a  $c$  number is either  $b^\dagger b \rightarrow \delta^2$  or  $bb^\dagger \rightarrow 1 - \delta^2$ , according to the time ordering).

Finally, it might be noted that, if we set  $|\Phi(\mathbf{p} - \mathbf{k} + \mathbf{G})|^2 = \delta(\mathbf{p} - \mathbf{k} + \mathbf{G})$ , Eq. (22) gives the Compton scattering profile.

In summary, it has been shown that the angular correlation of positron-annihilation  $\gamma$  rays, in the absence of electron-positron correlations, is described by

$$\rho(\mathbf{p}) = \sum_{\mathbf{k}, \mathbf{G}} \sum_{\sigma} |\Phi(\mathbf{p} - \mathbf{k} + \mathbf{G})|^2 |a_{\mathbf{G}}(\mathbf{k})|^2 \times [u_{\mathbf{k}}^2 (1 - n_{\mathbf{k}}) + v_{\mathbf{k}}^2 n_{\mathbf{k}}].$$

This result shows that, in the momentum space mapped by positron annihilation, the sharp Fermi edge is lost in the superconducting state. There are two processes. The term proportional to  $v_{\mathbf{k}}^2$  represents a process which can

occur at zero temperature; the positron annihilates, say, the  $\mathbf{k}$  spin  $\sigma$  half of a pair and thereby results in the *creation* of a  $-\mathbf{k}-\sigma$  quasiparticle. On the other hand, that part of the expression which involves  $u_{\mathbf{k}}^2$  reflects the direct *destruction* of a  $k\sigma$  quasiparticle. Since, at zero temperature, there are no quasiparticles excited, this latter process can only occur at finite temperature. It is to be emphasized that this two-fluid-type picture corresponds to one in which the ground state of a superconductor is viewed upon as consisting of condensate in which *all* the relevant electrons, i.e., those within  $\omega_D$  of the Fermi surface, form part of a pair. This is to be contrasted with the semiconductor picture, in which the effect of the superconductivity is to open a gap at the normal-state Fermi surface; in the ground state all the states below the gap are full and all those above empty. With this picture the destruction of a quasiparticle, at  $T=0$ , results in the creation of a quasihole, which is the equivalent of the above-mentioned quasiparticle. However, in using this picture it must be recalled that the process occurs with a reduced amplitude  $v_{\mathbf{k}}$  and that the two pictures must not be mixed, *either*, at  $T=0$ , the positron is viewed upon as destroying half a pair, *or* creating a hole below the gap; there are *not* two distinct processes for the ground state. It has been pointed out that positron-annihilation experiments reflect the distribution of states in momentum space and thereby provide com-

plementary information about the superconductive state to that obtained from, say, tunneling or optical measurements, since these latter reflect the distribution of occupied states in energy space. Should sufficiently accurate data become available for these two methods, it is possible to test rather directly the hypothesis that superconductivity arises through pair formation. In the meantime it is suggested that the change, near  $k_z=0$ , in the one-dimensional projection of the momentum distribution might be the easiest fashion in which to detect the effects of entering the superconductive state; this decreases by a fraction  $\sim(\Delta/\mathcal{E}_F)^2$  with the formation of the gap  $\Delta$ . In principle this few percent effect, illustrated in Fig. 1, should be relatively easy to detect for the new high-temperature superconductors. However, it is imperative that the temperature dependence of the lattice parameters be also determined and, if need be, corrected for. It seems probable that there are lattice anomalies near  $T_c$  and these might easily mimic, or mask, the sought for electronic effect.

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<sup>5</sup>P. G. de Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966); see also L. C. Smedskjaer, B. W. Veal, D. G. Legnini, A. P. Paulikas, and L. J. Nowicki, *Phys. Rev.* **37**, 2330 (1988).

<sup>6</sup>P. Brovetto, A. Delunas, V. Maxia, and G. Spano, *Nuovo Cimento* **9D**, 1325 (1987).

<sup>7</sup>M. Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1975).

<sup>8</sup>R. A. Ferrel, *Rev. Mod. Phys.* **28**, 308 (1956).

<sup>9</sup>This corresponds to the following expansion of a Bloch wave in terms of plane waves:  $\psi_{l\mathbf{k}\sigma}(\mathbf{r}) = \sum_{\mathbf{G}} a_{\mathbf{G}}^l(\mathbf{k}) [(1/\sqrt{V})e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}]$ .

<sup>10</sup>S. Doniach, in *Momentum Distributions*, edited by R. N. Silver and P. E. Sokol (Plenum, New York, 1989).

<sup>11</sup>S. E. Barnes, *J. Phys. F* **6**, 115 (1976); **6**, 1375 (1976); **7**, 2637 (1976); *Adv. Phys.* **30**, 801 (1980); *J. Phys. (Paris)* **39**, C6-828 (1978).

<sup>12</sup>P. Coleman, *Phys. Rev. B* **29**, 3035 (1984).

<sup>13</sup>S. E. Barnes, *Ref. 4*; *Phys. Rev. B* **40**, 723 (1989).