Superconducting order parameters with sign changes: The density of states and impurity scattering

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We compute $N_s(E)$ for a family of superconducting order parameters with sign changes at the Fermi surface, and find surprising results. We consider all $\Delta(\hat{\mathbf{k}})$ such that $\Delta(\hat{\mathbf{k}})=+\Delta_0$ on part of the Fermi surface, and $\Delta(\hat{\mathbf{k}})=-\Delta_0$ on the rest, yielding an average of $\langle\Delta(\hat{\mathbf{k}})\rangle=r\Delta_0$, where $0\leqslant r\leqslant 1$. For $0<r<1$, as the impurity concentration increases, the number of low-lying states increases, and the superconductor becomes gapless. As the impurity concentration is further increased, the gap in the spectrum is restored, and $N_s(E)$ approaches the pure limit BCS form, with a renormalized gap. [S0163-1829(96)04829-1]

I. INTRODUCTION

Much theoretical work has been recently devoted to superconductors with an order parameter $\Delta(\hat{\mathbf{k}})$ that is a nontrivial function of $\hat{\mathbf{k}}$.[1–3] Both the heavy Fermion and the high-T_c superconductors may have such an order parameter, and there is an effort to see if their experimental properties can be understood in terms of such a $\Delta(\hat{\mathbf{k}})$.[4]

If the order parameter is unconventional, and so transforms according to a nonidentity representation of the crystal point group, then $\Delta(\hat{\mathbf{k}})$ must indeed have a strong $\hat{\mathbf{k}}$ dependence; for example, the Fermi-surface average must vanish: $\langle\Delta(\hat{\mathbf{k}})\rangle=0$.

However, models involving conventional order parameters with an interesting $\hat{\mathbf{k}}$ dependence have also been proposed. In these models, $\Delta(\hat{\mathbf{k}})$ has the complete rotational symmetry of the crystal, but can change sign as a function of $\hat{\mathbf{k}}$.[5–9]

Thus $\langle\Delta(\hat{\mathbf{k}})\rangle$ need not vanish, but will be reduced by cancellation effects. Recent theory has shown that superconductors with such conventional order parameters can be quite sensitive to scattering by ordinary, nonmagnetic impurities.

In order to focus on the effects due to a sign change on the Fermi surface, in this paper we consider a particular family of order parameters; for this family, we are able to compute the density of states $N_s(E)$ for an arbitrary Fermi surface, in the presence of impurity scattering. Our family of order parameters satisfies the following condition: $\Delta(\hat{\mathbf{k}})=+\Delta_0$ or $\Delta(\hat{\mathbf{k}})=-\Delta_0$ for all $\hat{\mathbf{k}}$, such that $\langle\Delta(\hat{\mathbf{k}})\rangle=r\Delta_0$, with $0\leqslant r\leqslant 1$. Thus, $\Delta(\hat{\mathbf{k}})$ is equal to $+\Delta_0$ on part of the Fermi surface, and is equal to $-\Delta_0$ on the rest of the Fermi surface, with a net average value of $r\Delta_0$.

The virtues of our model are several. First, the order parameters we consider have no nodes, so that any interesting structure in $N_s(E)$ at low energy is due to the sign change in $\Delta(\hat{\mathbf{k}})$ combined with the impurity scattering. A second advantage of our model is that it permits the determination of several analytical results. In fact our analytic results are not limited to the Born limit, but can be derived for arbitrary impurity scattering potential v.

We note that in two cases—(a) $r=1$, so that $\Delta(\hat{\mathbf{k}})=\Delta_0$ for all $\hat{\mathbf{k}}$, with any amount of impurity scattering; (b) any value of r, with no impurity scattering—the density of states is simply given by the usual BCS answer:

$$\frac{N_s(E)}{N(0)}=\theta(E-\Delta_0)\ \frac{E}{\sqrt{E^2-\Delta_0^2}}. \tag{1}$$

We also note that the $r=0$ case, which covers the possibility of an unconventional order parameter, has been extensively discussed in a previous paper.[10]

One particularly interesting result we find, is that when $0<r<1$, the effects of impurity scattering can be surprisingly nonmonotonic.[5–9] For example, as $1/\tau$ is increased, the superconductor becomes gapless at a certain critical value of $1/\tau\Delta_0$; as $1/\tau$ is further increased, an energy gap in the spectrum is restored at a higher value of $1/\tau\Delta_0$. Finally as $1/\tau\Delta_0\to\infty$ the density of states approaches that given by Eq. (1) except that Δ_0 is replaced by $r\Delta_0$.

The work presented in our paper is closely related to several very recent publications.[5–9] These authors all consider order parameters which change sign on the Fermi surface, and yet have a nonzero average; in contrast to our work these papers are mostly concerned with order parameters with nodes. These papers all agree in finding that an increase in the impurity concentration can induce a gap in the spectrum.

II. BASIC EQUATIONS

To do our calculations, we use the Gor'kov equations, in their quasiclassical form.[3,11] The key quantity is then the propagator $\hat{g}(\hat{\mathbf{k}},\epsilon)$, which is a 2×2 matrix in particle-hole space. Here $\hat{\mathbf{k}}$ is a unit vector on the Fermi surface, and ϵ is a Matsubara frequency. The solution for $\hat{g}(\hat{\mathbf{k}},\epsilon)$ is given by

$$\hat{g}(\hat{\mathbf{k}},\epsilon)=\frac{-\pi\{i(\epsilon+ia_3)\hat{\tau}_3-i[\Delta(\hat{\mathbf{k}})-ia_2]\hat{\tau}_2\}}{\{(\epsilon+ia_3)^2+[\Delta(\hat{\mathbf{k}})-ia_2]^2\}^{1/2}}=g_3\hat{\tau}_3+g_2\hat{\tau}_2. \tag{2}$$

The impurity self-energy $\hat{a}(\epsilon)$ is given by

$$\hat{a}(\epsilon)=c\hat{t}(\epsilon), \tag{3}$$

where c is the density of impurities, and $\hat{t}(\epsilon)$ is the t matrix, given in terms of $\hat{g}$ by the following equation:

$$\hat{t}(\epsilon)=v+N(0)v\int_{\mathrm{FS}}d^2\hat{\mathbf{k}}n(\hat{\mathbf{k}})\hat{g}(\hat{\mathbf{k}},\epsilon)\hat{t}(\epsilon). \tag{4}$$

For simplicity, we have taken the impurity potential to be the s wave of strength v. Here $N(0)$ is the density of states at the Fermi surface in the normal state, and $n(\hat{\mathbf{k}})d^2\hat{\mathbf{k}}$ is the partial density of states in $d^2\hat{\mathbf{k}}$, normalized to one:

$$\int_{\mathrm{FS}}d^2\hat{\mathbf{k}}n(\hat{\mathbf{k}})=1. \tag{5}$$

Equations (2)–(4) along with the gap equation, must be solved self-consistently. The density of states is then computed using the $\hat{\tau}_3$ component of $\hat{g}$:

$$N_s(E)=\frac{N(0)}{\pi}\,\mathrm{Im}\int_{\mathrm{FS}}d^2\hat{\mathbf{k}}n(\hat{\mathbf{k}})g_3(i\epsilon\rightarrow E-i\eta,\hat{\mathbf{k}}). \tag{6}$$

For our family of order parameters, the equations can be analyzed in quite a bit of detail, since the $\hat{\mathbf{k}}$ integrals can be done. First, we note that $\hat{g}(\hat{\mathbf{k}},\epsilon)$, for a given value of ϵ has only two different values, depending on $\hat{\mathbf{k}}$. Then we write

$$g_{3+}(\epsilon)=\frac{-\pi i(\epsilon+ia_3)}{[(\epsilon+ia_3)^2+(\Delta_0-ia_2)^2]^{1/2}}, \tag{7}$$

$$g_{3-}(\epsilon)=\frac{-\pi i(\epsilon+ia_3)}{[(\epsilon+ia_3)^2+(-\Delta_0-ia_2)^2]^{1/2}}, \tag{8}$$

$$g_{2+}(\epsilon)=\frac{\pi i(\Delta_0-ia_2)}{[(\epsilon+ia_3)^2+(\Delta_0-ia_2)^2]^{1/2}}, \tag{9}$$

$$g_{2-}(\epsilon)=\frac{\pi i(-\Delta_0-ia_2)}{[(\epsilon+ia_3)^2+(-\Delta_0-ia_2)^2]^{1/2}}. \tag{10}$$

Using these definitions in Eq. (4) we can then derive two complex, coupled equations for $a_3(E)$ and $a_2(E)$:

$$ia_3(E)=\frac{icv^2N(0)\{[(1+r)/2]g_{3+}(E)+[(1-r)/2]g_{3-}(E)\}}{1-N(0)^2v^2(\{[(1+r)/2]g_{2+}(E)+[(1-r)/2]g_{2-}(E)\}^2+\{[(1+r)/2]g_{3+}(E)+[(1-r)/2]g_{3-}(E)\}^2)}, \tag{11}$$

$$ia_2(E)=\frac{icv^2N(0)\{[(1+r)/2]g_{2+}(E)+[(1-r)/2]g_{2-}(E)\}}{1-N(0)^2v^2(\{[(1+r)/2]g_{2+}(E)+[(1-r)/2]g_{2-}(E)\}^2+\{[(1+r)/2]g_{3+}(E)+[(1-r)/2]g_{3-}(E)\}^2)}. \tag{12}$$

These equations are the basis of our calculations.

Instead of c and v it is convenient to calibrate impurity effects in terms of two other parameters, defined as follows:[12]

$$\frac{1}{2\tau}=\frac{c\pi N(0)v^2}{1+[\pi N(0)v]^2}, \tag{13}$$

$$\sigma=\frac{[\pi N(0)v]^2}{1+[\pi N(0)v]^2}. \tag{14}$$

Here τ is the normal-state collision time, and σ measures the strength of v. Finally, we note that many of our answers are expressed in terms of Δ_0, which is itself a function of T, σ, and τ.

$$\Delta_0=\Delta_0(\sigma,\tau,T). \tag{15}$$

The gap equation which determines Δ_0 will be discussed in Sec. VI.

III. DISCUSSION OF $N_s(E=0)$

One particularly interesting question to study is the following: for what values of τ and σ is $N_s(E=0)\neq 0$, so that the superconductor is gapless?[5–9] In this section we derive, for our family of order parameters, an analytic answer to this question.

At $E=0$, we can rewrite Eqs. (11) and (12) in the following way. Define $z=ia_3/\Delta_0$, and $y=ia_2/\Delta_0$. We then can write

$$z=\frac{1}{2\tau\Delta_0}\times\frac{\frac{1}{1-\sigma}z\frac{\frac{1+r}{2}\sqrt{z^2+(1+y)^2}+\frac{1-r}{2}\sqrt{z^2+(1-y)^2}}{\sqrt{z^2+(1-y)^2}\sqrt{z^2+(1+y)^2}}}{1+\frac{\sigma}{1-\sigma}\frac{z^2\left(\frac{1+r}{2}\sqrt{z^2+(1+y)^2}+\frac{1-r}{2}\sqrt{z^2+(1-y)^2}\right)^2+\left(\frac{1+r}{2}(1-y)\sqrt{z^2+(1+y)^2}-\frac{1-r}{2}(1+y)\sqrt{z^2+(1-y)^2}\right)^2}{(z^2+(1-y)^2)(z^2+(1+y)^2)}}, \tag{16}$$

$$y=-\frac{1}{2\tau\Delta_0}\times\frac{\frac{1}{1-\sigma}\frac{\frac{1+r}{2}(1-y)\sqrt{z^2+(1+y)^2}-\frac{1-r}{2}(1+y)\sqrt{z^2+(1-y)^2}}{\sqrt{z^2+(1-y)^2}\sqrt{z^2+(1+y)^2}}}{1+\frac{\sigma}{1-\sigma}\frac{z^2\left(\frac{1+r}{2}\sqrt{z^2+(1+y)^2}+\frac{1-r}{2}\sqrt{z^2+(1-y)^2}\right)^2+\left(\frac{1+r}{2}(1-y)\sqrt{z^2+(1+y)^2}-\frac{1-r}{2}(1+y)\sqrt{z^2+(1-y)^2}\right)^2}{(z^2+(1-y)^2)(z^2+(1+y)^2)}}. \tag{17}$$

Now, at $E=0$, the solution for z is either purely real or purely imaginary. When z is real, $N_s(E=0)>0$, while when z is purely imaginary, $N_s(E=0)=0$. These two solutions are separated by the $z=0$ solution, which occurs when σ, τ, and r [recall $\langle\Delta(\hat{\mathbf{k}})\rangle=r\Delta_0$] are related in a certain way. These considerations lead to the following result.

Imagine we start increasing the value of $1/2\tau$ from zero. When $1/2\tau\Delta_0$ reaches the following value:

$$\frac{1}{2\tau\Delta_0}=\frac{1+N(0)^2\pi^2v^2r^2}{1+N(0)^2\pi^2v^2}=1-\sigma+\sigma r^2, \tag{18}$$

the superconductor becomes gapless so that $N_s(E=0)>0$. However, as we further increase $1/2\tau$, the superconductor remains gapless only up to a critical value, given by

$$\frac{1}{2\tau\Delta_0}=\frac{1}{r}. \tag{19}$$

For the unitarity limit ($\sigma=1$) the two curves bounding the gapless region are given by

$$\frac{1}{2\tau\Delta_0}=r^2, \tag{20}$$

$$\frac{1}{2\tau\Delta_0}=\frac{1}{r}. \tag{21}$$

For the Born limit ($\sigma=0$), the curves are given by

$$\frac{1}{2\tau\Delta_0}=1, \tag{22}$$

$$\frac{1}{2\tau\Delta_0}=\frac{1}{r}. \tag{23}$$

In Fig. 1 we plot, in the $1/\tau-r$ plane, the gapless region for the Born and unitarity limits.

We should stress several points concerning these results:

(1) At $r=0$, as $1/\tau$ is increased a gap is never restored. This result was derived in our previous paper,[10] which dealt with the $r=0$ case.

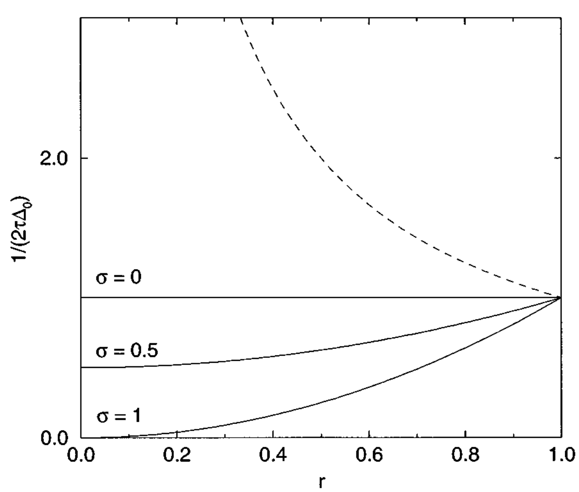

FIG. 1. Lines bounding the region in which $N_s(E=0)>0$. The upper bounding curve is given by the dashed line, $1/2\tau\Delta_0=1/r$; the lower boundary curve depends on σ [defined in Eq. (14)], and we show the curve for three different cases. Recall the definition of the parameter r: $\langle\Delta(\hat{\mathbf{k}})\rangle=r\Delta_0$.

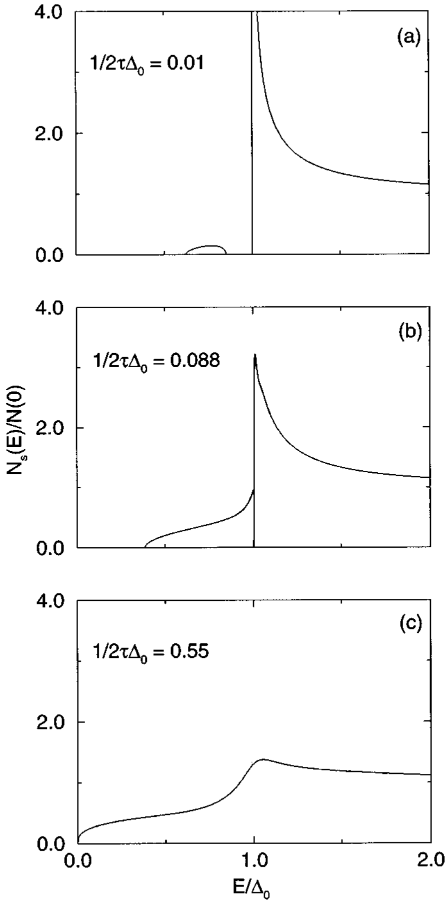

FIG. 2. We show plots of $N_s(E)$, with σ=0.6 and r=0.5, for several values of $1/2\tau$. In (a), the concentration of impurities is low and an impurity band centered on E_b [Eq. (37)] appears. In (b), $1/2\tau$ is just below the value at which the impurity band merges with the continuum, while in (c) $1/2\tau$ is chosen to be the value at which gaplessness begins.

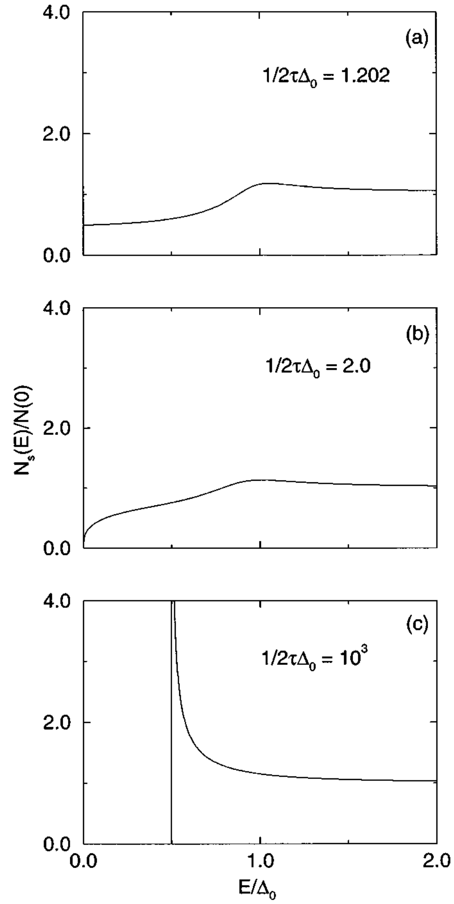

FIG. 3. Plots for $N_s(E)$, for the same values of σ and r as in Fig. 2. In (a), we chose $1/2\tau$ such that $N_s(E=0)$ is a maximum; in (b), $1/2\tau$ is set at the value at which a gap in the spectrum reappears. For (c), we chose $1/2\tau$ to be very large, so that the approach to the pure limit BCS form is apparent.

(2) At $r=1$, there is always a gap in the spectrum, since $N_s(E)$ is given by Eq. (1), regardless of the values of τ and σ.

(3) The upper bounding curve of the gapless region, given by Eq. (19), is the same for any value of σ; in particular, it is the same for the Born and unitarity limits.

We can also derive several other exact results. As $1/2\tau\Delta_0$ increases from the value $(1-\sigma+\sigma r^2)$ to the value $1/r$, the quantity $N_s(E=0)$ attains a maximum at a certain value of $1/2\tau\Delta_0$ between these two limits. The maximum occurs at the following point:

$$\frac{1}{2\tau\Delta_0}=\frac{1-\sigma r(1-r)}{r^{1/2}}. \tag{24}$$

Furthermore, the maximum value of $N_s(E=0)$ is given by

$$\frac{N_s(E=0)}{N(0)}=1-r. \tag{25}$$

Note that this value is independent of σ.

IV. RESULTS FOR $N_s(E)$

In this section, we show numerical results for $N_s(E)$, for typical values of τ, σ, and r. Figures 2 and 3 shows plots of $N_s(E)$ versus E, with the parameters σ and r held fixed at the value σ=0.6 and r=0.5. We show results for six different values of $1/2\tau\Delta_0$, chosen to illustrate the various stages in the behavior of $N_s(E)$ as the concentration of impurity increases.

We see that at small concentration, states at low energy appear, gaplessness setting in at $1/2\tau\Delta_0=0.55$, in agreement with Eq. (18). A gap in the spectrum is reestablished at $1/2\tau\Delta_0=2.0$, as predicted by Eq. (19). Finally, at the largest values of $1/2\tau\Delta_0$ chosen, we can see that $N_s(E)$ is approaching a simple BCS form, with a renormalized gap of $r\Delta_0=0.5\Delta_0$. This large $1/2\tau\Delta_0$ behavior will be discussed in the next section.

We also note that for Fig. 3(a), we have chosen the value of $1/2\tau\Delta_0$ which gives a maximum value for $N_s(E=0)$, in accordance with Eq. (24). As predicted by (25), the value of $N_s(E=0)/N(0)$ is given $1-r=0.5$.

V. $N_s(E)$ IN THE LARGE $1/\tau\Delta_0$ LIMIT

As $1/\tau\Delta_0$ becomes very large, $N_s(E)$ regains its $1/\tau=0$ form with a renormalized value of the gap.[5–9] This was evident in the numerical results presented in the last section; here we discuss an analytic derivation of this result.

As $1/\tau\Delta_0\rightarrow\infty$, an analysis of Eqs. (11) and (12) shows that $ia_2(E)$ and $ia_3(E)$ approach the following limits:

$$ia_2(E)\rightarrow-\frac{1}{2\tau}\frac{r\Delta_0}{[r^2\Delta_0^2-E^2]^{1/2}}, \tag{26}$$

$$ia_3(E)\rightarrow-\frac{1}{2\tau}\frac{iE}{[r^2\Delta_0^2-E^2]^{1/2}}. \tag{27}$$

For a given large value of $1/\tau\Delta_0$, formulas (26) and (27) fail only in a narrow region of E, near the value $E=r\Delta_0$. This region becomes narrower and narrower as $1/\tau\Delta_0\rightarrow\infty$. Using (26) and (27), we obtain for the $1/\tau\Delta_0\rightarrow\infty$ limit of the density of states the following result:

$$\frac{N_s(E)}{N(0)}=\theta(E-r\Delta_0)\ \frac{E}{\sqrt{E^2-r^2\Delta_0^2}}. \tag{28}$$

This formula is quite interesting. It means that as $1/\tau\Delta_0\rightarrow\infty$, the density of states regains the form it had for the pure limit ($1/\tau=0$), except that the gap parameter appearing in (28) has been renormalized to $r\Delta_0$. It seems that the impurities scatter the electrons rapidly about the Fermi surface, so that the electrons effectively see the Fermi-surface average of the order parameter, $\langle\Delta(\hat{\mathbf{k}})\rangle=r\Delta_0$.

One point to be stressed is that the value of Δ_0 appearing in these equations has been reduced by the impurity scattering. Thus, if we denote the value of the order parameter in the pure limit by Δ_{00}:

$$\Delta_{00}(T)=\Delta_0(\sigma,\tau=\infty,T), \tag{29}$$

then we have $\Delta_0<\Delta_{00}$ unless $r=1$ or $1/\tau=0$.

VI. GAP EQUATION AND T_c REDUCTION

With our assumptions for the form of $\Delta(\hat{k})$, the self-consistent equation for the order parameter takes the following form:

$$\Delta(\hat{k})=-\pi TN(0)\sum_{\epsilon}\int d^2\hat{\mathbf{k}}'n(\hat{\mathbf{k}}')V(\hat{\mathbf{k}},\hat{\mathbf{k}}')\times\frac{[\Delta(\hat{\mathbf{k}}')-ia_2]}{\{(\epsilon+ia_3)^2+[\Delta(\hat{\mathbf{k}}')-ia_2]^2\}^{1/2}}. \tag{30}$$

The pairing interaction and the order parameter can be written as

$$V(\hat{\mathbf{k}},\hat{\mathbf{k}}')=-V_0\phi(\hat{\mathbf{k}})\phi(\hat{\mathbf{k}}'), \tag{31}$$

$$\Delta(\hat{\mathbf{k}})=\Delta_0\phi(\hat{\mathbf{k}}), \tag{32}$$

where $\phi(\hat{\mathbf{k}})=\pm1$ on the Fermi surface, and has an average of r:

$$\int d^2\hat{\mathbf{k}}n(\hat{\mathbf{k}})\phi(\hat{\mathbf{k}})=r. \tag{33}$$

To determine T_c, we work to leading order in Δ_0, obtaining

$$\Delta_0=N(0)V_0\pi T_c\sum_{\epsilon}\frac{(\Delta_0-ia_2r)}{|\epsilon+ia_3|}. \tag{34}$$

Here, ia_2 is evaluated to first order in Δ_0, while ia_3 is evaluated in the normal state. We then arrive at the following equation:

$$\ln\left(\frac{T_c}{T_{c0}}\right)=(1-r^2)\left[\psi\left(\frac{1}{2}\right)-\psi\left(\frac{1}{2}+\alpha\right)\right], \tag{35}$$

where T_{c0} is the transition temperature with no impurities, $\psi(x)$ is the digamma function, and α is a pair-breaking parameter defined as follows:

$$\alpha=\frac{1}{4\pi\tau T_c}. \tag{36}$$

The $r=0$ limit gives the usual result for an unconventional order parameter; when $r=1$, we see that T_c is unchanged by the impurity scattering. We also note that unless $r=0$, T_c is never driven to zero by any finite value of $1/\tau$.

VII. DISCUSSION

The results presented here show that a sign change in the order parameter, together with scattering from nonmagnetic impurities, leads to a complex pattern of behavior in the density of states. In this regard our work agrees with several recent publications.[5–9] For our family of order parameters, the magnitude $|\Delta(\hat{\mathbf{k}})|$ is independent of $\hat{\mathbf{k}}$; in particular, there are no nodes. Then the low-energy structure in $N_s(E)$ is not due to nodes, or to any variation in $|\Delta(\hat{\mathbf{k}})|$.

In the small $1/\tau$ limit, insight into our results can be gained by noting that an isolated impurity, in a superconductor with a $\Delta(\hat{\mathbf{k}})$ satisfying our condition, has a bound state at the following energy:

$$E_b=\Delta_0\left(\frac{1+[\pi N(0)v]^2r^2}{1+[\pi N(0)v]^2}\right)^{1/2}=\Delta_0\sqrt{1-(1-r^2)\sigma}. \tag{37}$$

Thus, for example, in Fig. 2(a) we can understand the location of the small band of states below Δ_0.

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[1] L. P. Gorkov, Sov. Sci. Rev. A **9**, 1 (1987).
[2] M. Sigrist and K. Ueda, Rev. Mod. Phys. **63**, 239 (1991).
[3] P. Muzikar, D. Rainer, and J. A. Sauls, in *The Vortex State*, edited by N. Bontemps, Y. Bruynseraede, G. Deutsher, and A. Kapitulnik (Kluwer, Dordrecht, 1994), pp. 244–264.
[4] Recent articles, containing a large number of references, are J. A. Sauls, Adv. Phys. **43**, 113 (1994), and D. Xu, S. K. Yip, and J. A. Sauls, Phys. Rev. B **51**, 16 233 (1995).
[5] T. Hotta, J. Phys. Soc. Jpn. **62**, 274 (1993).
[6] R. Fehrenbacher and M. R. Norman, Physica C **235–240**, 2407 (1994).
[7] L. S. Borkowski, P. J. Hirschfeld, and W. O. Putikka, Phys. Rev. B **52**, 3856 (1995).
[8] S. V. Pokrovsky and V. L. Pokrovsky, Phys. Rev. Lett. **75**, 1150 (1995).
[9] H. Kim and E. Nicole, Phys. Rev. B **52**, 13 576 (1995).
[10] G. Preosti, H. Kim, and P. Muzikar, Phys. Rev. B **50**, 13 638 (1994).
[11] We follow the notation in G. Preosti and P. Muzikar, Phys. Rev. B **51**, 15 634 (1995).
[12] L. J. Buchholtz and G. Zwicknagl, Phys. Rev. B **23**, 5788 (1981).