Pairbreaking Without Magnetic Impurities in Disordered Superconductors

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(Dated: January 9, 2002)

We study analytically the effects of inhomogeneous pairing interactions in short coherence length superconductors, using a spatially varying Bogoliubov-de Gennes model. Within the Born approximation, it reproduces all of the standard Abrikosov-Gor’kov pairbreaking and gaplessness effects, even in the absence of actual magnetic impurities. For pairing disorder on a single site, the T-matrix gives rise to bound states within the BCS gap. Our results are compared with recent scanning tunneling microscopy measurements on Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ with Zn or Ni impurities.

PACS numbers: 74.20.-z, 74.40.+k, 74.80.-g

The effect of disorder in superconductors has long been a subject of considerable interest. A generally accepted physical picture is that magnetic impurities destroy superconductivity by locally breaking the pairs, whereas non-magnetic impurities are not pairbreaking, according to Anderson’s theorem. This is true for an isotropic s-wave BCS superconductor, in which the order parameter is uniform and momentum independent. Since in most high transition temperature $T_c$ cuprates, the suppression of $T_c$ with Zn or Ni doping is comparable, there were proposals to explain this in terms of $d$-wave superconductivity. However, nuclear magnetic resonance (NMR) experiments indicated that the nominally non-magnetic Zn$^{++}$ ions polarize the spin background in the CuO$_2$ planes upon substitution of the nominally S = 1/2 Cu$^{++}$ ions. Moreover, recent scanning tunneling microscopy (STM) measurements directly above the Zn or Ni impurity sites observed strong resonance peaks. Very recently, several groups noticed from STM measurements that underdoped Bi$_2$Sr$_2$CuO$_{8+δ}$ (BSCCO) and Bi$_2$-2$_{x}$ Pb$_{2}$Sr$_{2}$Cu$_{2}$O$_{8+δ}$ are extremely disordered on a scale of a few nm. This disorder is characterized by two gaps, one corresponding to the superconducting gap, with characteristic superconducting peaks, and a non-superconducting gap.

There is now a large body of evidence that the pseudogap observed in cuprates above $T_c$ is not superconducting. The most convincing of these experiments determined that the magnetic field dependence of the resistivity, NMR spin-lattice relaxation rate, magnetization, and the gaps observed in intrinsic tunneling experiments for the superconducting and pseudogaps are qualitatively different. In particular, the pseudogap regime is field independent until one reaches the Zeeman field for breaking up chargeless spin zero pairs. This is precisely consistent with the pseudogap being particle-hole pairs, which could be either of the charge-density wave (CDW) or spin-density wave (SDW) form. As in one dimension, such excitations are expected to arise from repulsive interactions between like charges, whereas superconductivity can arise when the interactions between like charges are attractive.

Thus, if indeed the disorder involves a percolation problem between superconducting and density-wave regions on a nanometer scale, then the phase coherence can only arise from Josephson coupling of the superconducting grains. In addition, one would expect the c-axis tunneling to be very incoherent, as inferred in BSCCO from c-axis twist Josephson junction experiments.

In this letter, we assume the superconductor is electronically disordered on the scale of the coherence length. We further assume the essential ingredient in the disorder is not one of impurities, but rather disorder in the pairing interaction itself. Thus, we expect that $T_c$ varies from site to site, as does the resulting order parameter amplitude. We treat this type of disorder using a Bogoliubov-deGennes procedure, assuming that the order parameter amplitude varies locally.

Here we show that in the Born approximation, this problem maps exactly onto that of pairbreaking in a superconductor, with all of the features of that model, including gapless superconductivity. At a particular defect site, the T-matrix gives rise to bound states within the gap, even without magnetic impurities.

We use the Nambu representation,

$$
\Psi(r) = \begin{pmatrix}
  c_\uparrow(r) \\
  c_\downarrow(r) \\
  c_\uparrow^\dagger(r) \\
  c_\downarrow^\dagger(r)
\end{pmatrix},
$$

$$
\Psi^\dagger(r) = \begin{pmatrix}
  c_\downarrow^\dagger(r) \\
  c_\uparrow^\dagger(r) \\
  c_\uparrow(r) \\
  c_\downarrow(r)
\end{pmatrix}, \quad (1)
$$

where $c_\uparrow(r)$ [$c_\downarrow^\dagger(r)$] annihilates [creates] a quasiparticle with spin eigenstate $\downarrow$ [$\uparrow$] at the position $r$. We set $\hbar = c = k_B = 1$. The Hamiltonian under study is $H = H_0 + H_1 + H_2 + H_3$, where

$$
H_0 = \int d^3 r \Psi^\dagger(r) [\xi(r) \rho_3 \sigma_0 + \Delta_0 \rho_2 \sigma_2] \Psi(r), \quad (2)
$$

$$
H_1 = \frac{1}{2} \int d^3 r \Psi^\dagger(r) \tilde{V}(r) \Psi(r), \quad (3)
$$

$$
\tilde{V}(r) = U_1(r) \rho_3 \sigma_0, \quad (4)
$$

$$
\tilde{V}(r) = U_1(r) \rho_3 \sigma_0.
$$
\[ \hat{V}_2(\mathbf{r}) = U_2(\mathbf{r}) \mathbf{S} \cdot \hat{\sigma} / [S(S+1)]^{1/2} \]
\[ \hat{\sigma} = \hat{x} \rho_3 \sigma_1 + \hat{y} \rho_0 \sigma_2 + \hat{z} \rho_3 \sigma_3, \]  
(5)
\[ \hat{V}_3(\mathbf{r}) = U_3(\mathbf{r}) \rho_2 \sigma_2, \]  
(6)

where \( \rho_j \sigma_{j'} \equiv \rho_j \otimes \sigma_{j'} \) is a rank 4 tensor composed of two Pauli matrices for \( j, j' = 1, 2, 3 \) and \( \rho_0, \sigma_0 \) are rank 2 identity matrices, respectively. \( H_0 \) is the Bogoliubov-de Gennes version of the BCS Hamiltonian, with momentum space quasiparticle energy dispersion \( \xi_k \) relative to the Fermi energy \( \mu \). \( \Delta_0(T) \) is the real bare uniform BCS order parameter, and \( H_1 \) and \( H_2 \) are the interactions due to scattering off random non-magnetic and magnetic impurities with effective potentials \( U_1(\mathbf{r}) \) and \( U_2(\mathbf{r}) / [S(S+1)]^{1/2} \), respectively. \( H_3 \) with effective potential \( U_3(\mathbf{r}) \) is the new interaction arising from random variations in the pairing interaction.\[ \] In \( H_2 \), \( \mathbf{S} \) and \( S \) are the spin vector and quantum number of the magnetic impurities, respectively, and \( \hat{\sigma} \) represents the quasiparticle spin eigenvector. We assume the spatial averages of all of the random potentials vanish, \( \langle U_i(\mathbf{r}) \rangle = 0 \) for \( i = 1, 2, 3 \). In the absence of all defects, the order parameter \( \Delta_0(T) = V(c_\uparrow(\mathbf{r}) c_\downarrow(\mathbf{r})) \) satisfies the standard BCS gap equation,
\[ \Delta_0 = -V T \sum_{|\omega_n| \leq \omega_0} \int \frac{d^2 \mathbf{k}}{(2\pi)^3} \text{Tr} [\rho_2 \sigma_2 \hat{G}_0(\mathbf{k}, \omega_n)], \]
(7)
\[ \hat{G}_0^{-1}(\mathbf{k}, \omega_n) = i\omega_n \rho_0 \sigma_0 - \xi_k \rho_3 \sigma_0 - \Delta_0 \rho_2 \sigma_2, \]
where \( \hat{G}_0 \) is the bare Green’s function matrix, \( V < 0 \) is the uniform (BCS) part of the pairing interaction, \( N(0) \) is the single-spin quasiparticle density of states, \( \omega_0 \) is a BCS-like cutoff, and \( \omega_n \) are the Matsubara frequencies.

We assumed a real bare uniform order parameter \( \Delta_0 \), and restricted our consideration in \( H_3 \) to spatial fluctuations of the amplitude of \( \Delta_0 \). The model can also treat spatial fluctuations of the phase of \( \Delta_0 \) by letting \( \Delta_0 \rho_1 \sigma_2 \) and \( U_3(\mathbf{r}) \rho_2 \sigma_2 \) be generalized to \( \Delta_0 \rho_1 \sigma_2 + \Delta_0 \rho_2 \sigma_2 \) and \( U_3(\mathbf{r}) \rho_1 \sigma_2 + U_3(\mathbf{r}) \rho_2 \sigma_2 \), respectively.

Our main interest lies in studying \( H_3 \). Using quantum Monte Carlo techniques to study a two-dimensional square lattice with an on-site attractive Hubbard pairing interaction in \( H_0 \),\[ \] Ghosal et al. obtained interesting results in excellent qualitative agreement with those obtained from STM measurements.\[ \] We also consider \( H_1 \) and \( H_2 \) for comparison, because the combination of one or both of them with \( H_3 \) can lead to interesting novel behavior. In the Born approximation, these interactions add or subtract in a simple fashion. However, in the T-matrix approximation for a single defect site, these interactions interact in a highly non-trivial manner.

In the self-consistent Born approximation, the quasiparticle self-energy \( \hat{\Sigma} = \hat{\Sigma}_1 + \hat{\Sigma}_2 + \hat{\Sigma}_3 \), where
\[ \hat{\Sigma}_1(\mathbf{k}, \omega_n) = n_i \sum_{\mathbf{k}'} \hat{V}_i(\mathbf{k} - \mathbf{k}') \hat{G}(\mathbf{k}', \omega_n) \hat{V}_i(\mathbf{k}' - \mathbf{k}), \]
\[ \hat{\Sigma}_2(\mathbf{k}, \omega_n) = \hat{\Sigma}_0^{-1}(\mathbf{k}, \omega_n) - \hat{\Sigma}(\mathbf{k}, \omega_n), \]
\[ \hat{\Sigma}_3(\mathbf{k}, \omega_n) = \hat{\Sigma}_2(\mathbf{k}, \omega_n) \]
\( \hat{V}_i(\mathbf{k}), U_i(\mathbf{k}) \) are the spatial Fourier transforms of \( \hat{V}_i(\mathbf{r}), U_i(\mathbf{r}) \), respectively. Neglecting any possible anisotropy arising from Fermi surface integrations, the effective rates of the three processes are
\[ 1/\tau_i = 2\pi n_i N(0)|U_i(\mathbf{k}_F)|^2, \]
(10)
where \( n_i \) is the density of defects of type \( i \).

As in the usual pairbreaking theory, \[ \] the same form as does \( \hat{G}_0 \), except that \( \omega_n \) and \( \Delta_0 \) are replaced by their renormalized equivalents \( \tilde{\omega}_n \) and \( \tilde{\Delta} \), respectively. We then obtain the standard equations for the renormalized gap and Matsubara frequency,
\[ \tilde{\omega}_n = \omega_n + (1/\tau_1 + 1/\tau_{pb}) \frac{\tilde{\omega}_n}{2[\tilde{\omega}_n^2 + \Delta^2]^{1/2}}, \]
(11)
\[ \tilde{\Delta} = \Delta_0 + (1/\tau_1 - 1/\tau_{pb}) \frac{\tilde{\Delta}}{2[\tilde{\omega}_n^2 + \Delta^2]^{1/2}}, \]
(12)
\[ 1/\tau_{pb} = 1/\tau_2 + 1/\tau_3 \]
(13)
is the total pairbreaking rate. The new physics arises from \( H_3 \). Evidently, within the self-consistent Born approximation, the effects of the random interactions are exactly equivalent to those of magnetic impurities.

Using standard pairbreaking theory, \[ \] one finds
\[ \frac{\tilde{\omega}_n}{\Delta_0} = u(1 - \frac{\zeta}{\sqrt{1 + u^2}}), \]
(14)
\[ u = \frac{\tilde{\omega}_n}{\tilde{\Delta}}, \]
(15)
\[ \zeta = 1/(\tau_{pb} \Delta_0). \]
(16)

The spatial average gap \( \Delta(T) \) is then
\[ \Delta = |V| T \sum_{|\omega_n| \leq \omega_0} \int \frac{d^2 \mathbf{k}}{(2\pi)^3} \text{Tr} [\rho_2 \sigma_2 \hat{G}(\mathbf{k}, \omega_n)], \]
(17)
\[ = \pi |V| N(0) T \sum_{|\omega_n| \leq \omega_0} \frac{1}{\sqrt{1 + u^2}} \]
leading to the standard equation for \( T_c/T_{c0} = t \),
\[ 0 = \ln(t) + \psi \left( \frac{1}{2} + \frac{\alpha_{pb}}{2\pi t} \right) - \psi \left( \frac{1}{2} \right), \]
(18)
\[ \alpha_{pb} = 1/(\tau_{pb} T_{c0}). \]
(19)
where \( \psi(x) \) is the digamma function. For small \( \alpha_{pb}, T_c \approx T_{c0} - \pi/4\tau_{pb} \). We note that \( T_c/T_{c0} \) can be suppressed to zero even without any magnetic impurities, for \( 1/\tau_3 \geq 1/\tau_3c = \pi T_{c0}/2\gamma \), where \( \gamma = 1.781 \) is the exponential of Euler’s constant. In addition, the superconductivity becomes gapless for \( 1 > \tau_{3c}/\tau_3 \geq 12e^{-\pi/4} \approx 0.912 \). Thus, even an isotropic, s-wave superconductor can become gapless, as observed in the cuprates with STM.\[ \]

This can only occur in short coherence length superconductors with strong local inhomogeneities in the pairing interaction, as is a likely explanation for the vanishing
of the $T_c$ in the highly underdoped region of the cuprate phase diagram, although that region is also complicated by the simultaneous appearance of local SDW/CDW order at the non-superconducting regions not included in this calculation.

In order to make direct comparison with STM experiments, we solve the T-matrix for a single defect site. We assume the site has all three types of defects associated with it. We approximate the effects of the magnetic impurity by assuming that its spin behaves classically. Then, the T-matrix equation can be solved exactly,

$$
\hat{T}(\omega_n) = \frac{\hat{V}(0)}{1 - \hat{g}_0(\omega_n)\hat{V}(0)},
$$

(20)

$$
\hat{V}(0) = \sum_{i=1}^{3} \hat{V}_i(0),
$$

(21)

$$
\hat{g}_0(\omega_n) = -\frac{\pi N(0)}{|\omega_n + \Delta_0^2|^{1/2}}[i\omega_n\rho_\sigma_0 + \Delta_0\rho_\sigma_2],
$$

(22)

is the bare Green’s function at the origin, $\hat{I} = \rho_\sigma_0$ is the rank 4 identity matrix, and the effects of a finite quasiparticle energy bandwidth have been neglected. Bound states within the gap at $T = 0$ at the frequency $\omega$ are obtained from

$$
\det[\hat{I} - \hat{g}_0(i\omega)\hat{V}(0)] = 0.
$$

(23)

Solving Eqs. (21) - (23) exactly, we generally obtain four bound states within the gap at $\omega = \overline{\omega}_0\Delta_0$, where

$$
\overline{\omega}_0 = \pm[A + sR]^{1/2}/B,
$$

(24)

$$
A = 16\nu_3^2 \nu_3^2 + a_+^2(a_-^2 + 4\nu_1^2),
$$

(25)

$$
B = a_+^2 + 4\nu_2^2,
$$

(26)

$$
C = a_+^2 - 4\nu_3^2,
$$

(27)

$$
R = [A^2 - B^2C^2]^{1/2},
$$

(28)

$$
a_{\pm} = \nu_3^2 + \nu_3^2 - \nu_3^2 \pm 1,
$$

(29)

$$
\nu_1 = \pi N(0)\nu_1(0),
$$

(30)

and $s = \pm 1$.

It is useful to rewrite Eq. (24) for the three special cases of two defects only. For non-magnetic defects, $\nu_2 = 0$, there are only two bound states symmetric about zero bias,

$$
\overline{\omega}_0 \to \pm \sqrt{|(1 + \nu_3^2)(1 - \nu_3^2)(1 + \nu_3^2)|^{1/2} / (1 + \nu_3^2)},
$$

(31)

For the trivial case of a site with just a non-magnetic impurity, Eq. (31) shows that there are no poles inside the gap. However, for a pairing interaction defect alone, there are poles at $\overline{\omega}_0 = \pm |1 - \nu_3^2|/(1 + \nu_3^2)$.

For impurities alone, $\nu_3 = 0$, there are also only two bound states symmetric about zero bias, at

$$
\overline{\omega}_0 \to \pm \frac{|1 + u + u|}{|(1 + u^2)/2|^{1/2}},
$$

(32)

where $u_{\pm} = \nu_1 \pm \nu_2$. For $\nu_1 = 0$, this reduces to the result of Shiba for a classical magnetic impurity, $\overline{\omega}_0 = \pm |1 - \nu_2^2|/(1 + \nu_2^2)$, even though we did not average over the classical spin direction before summing the T-matrix.

The most interesting case arises when both $\nu_2, \nu_3 \neq 0$ and $\nu_2 \neq \nu_3$. In the limit $\nu_1 = 0$, there are four bound states symmetric about zero bias at

$$
\overline{\omega}_0 \to \pm \frac{(\nu_2^2 - \nu_2^2 + s|1 - \nu_2^2\nu_3^2|)}{(1 + \nu_2^2)(1 + \nu_2^2)},
$$

(33)

where $s = \pm 1$, $v_{\pm} = \nu_2 \pm \nu_3$. For $\nu_2, \nu_3 \neq 0$ and $\nu_2 \neq \nu_3$, there are four bound states, exhibiting reflection symmetry about zero bias. Otherwise, if either $\nu_2$ or $\nu_3 = 0$, or if $\nu_2 = \nu_3$, there are only two bound states that are symmetric about zero bias. We note that Eq. (33) for either $\nu_1 = 0$ or $\nu_3 = 0$ reduces to Eq. (31) and (24) with $\nu_1 = 0$, respectively. In addition, for $\nu_2 = \nu_3$, it reduces to Eq. (31) if $\nu_1 = 0$ and $\nu_2 \to 2\nu_2$, etc. Moreover, setting $\nu_2 = \nu_3$ in Eq. (31) with $\nu_1$ arbitrary leads to only two bound states symmetric about zero bias, at $\overline{\omega}_0 = \pm \sqrt{|b+/b_-|^{1/2}}$, where $b_{\pm} = (1 + \nu_1^2)^2 \pm 4\nu_3^2$. Thus, we conclude that in order to obtain four bound states, two on each side of zero bias, one requires $0 \neq \nu_2 \neq \nu_3 \neq 0$.

When the defect is a quantum spin with a single component normal to the surface, the spin operator $S_z$ commutes with the Hamiltonian, and the spin states are easily described by $|SM\rangle$, with $S_z|SM\rangle = M|SM\rangle$. Then the magnetic impurity in the presence of the non-magnetic potential and the pairing disorder can all be solved exactly. There are bound states for each of the $2S + 1$ eigenstates.

In Figs. 1 and 2, we have illustrated how this solution can aid in understanding the STM results ob-
FIG. 2: Sketch of the two positive bias bounds states obtained with \( v = (0, \pm 0.51, \pm 1.01) \), along with the data of Ref. (10) obtained above the Ni site in BSCCO.

Thus, we solved the T-matrix in this modified BCS model of a local, on-site attractive pairing interaction with three types of defects on a site. For a superconductor with local, near-neighbor pairing of \( d_{x^2-y^2} \)-wave symmetry, the local gap \( \Delta_{ij} \) at the site \((i, j)\) on a tetragonal lattice is coupled hierarchically to the \( \Delta_{i'j'} \) at every site \((i', j')\). Hence, a generalization of our results to \( d \)-wave superconductors would not be straightforward.

In summary, we have shown that disordered short coherence length superconductors can exhibit pairbreaking from spatial fluctuations in the pairing interaction, in a manner very similar to that found with magnetic impurities. We studied the effects of a single site with up to three types of defects using the T-matrix approximation, and found bound states within the superconducting gap arising from either pairing fluctuations or magnetic impurities. Our best fits to the scanning tunneling microscopy data above the sites of Zn and Ni impurities suggest that Zn behaves either as a strong pairing fluctuation defect or as a strong magnetic impurity, whereas Ni behaves as both a strong magnetic impurity and a strong pairing defect.

[1] A. A. Abrikosov and L. P. Gor’kov, Zh. Eksp. Teor. Fiz. 36, 319 (195 [Nov. Phys. JETP 9, 220 (1959)].
[2] P. G. de Gennes, Physik Kondensierten Materie, 3, 79 (1964) and K. Maki, Physics 1, 21 (1964).
[3] V. Ambegaokar and A. Griffin, Phys. Rev. 137, A1151 (1965).
[4] K. Maki in Superconductivity, Vol. II , edited by R. D. Parks, (Marcel Dekker Inc., New York, 1969).
[5] P. W. Anderson, J. Phys. Chem. Solids 11, 26 (1959).
[6] A. V. Mahajan et al., Phys. Rev. Lett. 72, 3100 (1994).
[7] M. I. Salkola, A. V. Balatsky and D. J. Scalapino, Phys. Rev. Lett. 77, 1841 (1996).
[8] M.-H. Julien et al., Phys. Rev. Lett. 84, 3422 (2000).
[9] S. H. Pan et al., Nature (London) 403, 746 (2000).
[10] E. W. Hudson et al., Nature (London), 411, 920 (2000).
[11] S. H. Pan et al., Nature (London) 413, 282 (2001).
[12] K. M. Lang et al., Nature (London) 415, 412 (2002).
[13] C. Howald, P. Fournier, and A. Kapitulnik, Phys. Rev. B 64, 100504(R), (2001).
[14] T. Cren et al., Europhys. Lett. 54, 84 (2001).
[15] T. Shibnau et al., Phys. Rev. Lett. 86, 5763 (2001).
[16] M. Suzuki and T. Watanabe, Phys. Rev. Lett. 85, 4787 (2000).
[17] V. M. Krasnov et al., Phys. Rev. Lett. 86, 2657, 2001; ibid. 84, 5860, (2000).
[18] G.-q. Zheng et al., Phys. Rev. B 60, R9947 (1999); K. Gorny et al., Phys. Rev. Lett. 82, 177 (1999).
[19] R. A. Klemm, Physica C 341, 839 (2000).
[20] Q. Li et al., Phys. Rev. Lett. 83, 4160 (1999).
[21] Yu. N. Ovchinnikov, S. A. Wolf, and V. Z. Kresin, Phys. Rev. B 63, 064524 (2001).
[22] C. Huscroft and R. T. Scalettar, Phys. Rev. Lett. 81, 2775 (1998).
[23] A. Ghosal, M. Randeria, and N. Trivedi, Phys. Rev. Lett. 81, 3940 (1998); Phys. Rev. B 65, 014501 (2001).
[24] H. Shiba, Prog. Theo. Phys. 40, 435 (1968).