Time Reversal Breaking Superconducting State in the Phase Diagram of the Cuprates

G. Sangiovanni, M. Capone, S. Caprara
Dipartimento di Fisica, Università di Roma “La Sapienza”, and
INFM Center for Statistical Mechanics and Complexity, Piazzale Aldo Moro 2, I-00185 Roma, Italy

We review and extend a previous study on the symmetry of the superconducting state, stimulated by recent tunneling and Andreev reflection measurements giving robust evidences for the existence of a $d_{x^2-y^2} + id_{xy}$ order parameter in the overdoped regime of two different cuprates. Looking for a possible second-order phase transition from a standard $d_{x^2-y^2}$ to a mixed and time reversal breaking state, we confirm the results of our previous analysis on La$_2-x$Sr$_x$CuO$_4$. In the case of Y$_{1-x}$Ca$_x$Ba$_2$Cu$_3$O$_{7-x}$ as well, among all the allowed symmetries, the $d_{x^2-y^2} + id_{xy}$ is the most favored one and the unconventional state is likely to occur in a small dome of the phase diagram located in the optimal-overdoped region and at very low temperatures.

I. INTRODUCTION

Recent tunneling and Andreev reflection experiments[1, 2] on high-$T_c$ cuprate superconductors (HTCS) have shown small deviations from the pure $d_{x^2-y^2}$ symmetry of the superconducting gap[3]. Deutscher and co-workers have determined the doping dependence of the zero-bias conductance peak in tunneling experiments on (110) oriented Y$_{1-x}$Ca$_x$Ba$_2$Cu$_3$O$_{7-x}$ (YBCO) films and have shown that this peak, which is associated to the $d_{x^2-y^2}$ symmetry[4], is spontaneously splitted in some of the measured samples signaling the presence of a small secondary component of the bulk superconducting gap[5]. This secondary component, which removes the nodal lines of the $d_{x^2-y^2}$ phase has been subsequently confirmed by Gonnelli and co-workers who performed a re-analysis of their Andreev reflection data on La$_2-x$Sr$_x$CuO$_4$. In the case of Y$_{1-x}$Ca$_x$Ba$_2$Cu$_3$O$_{7-x}$ as well, among all the allowed symmetries, the $d_{x^2-y^2} + id_{xy}$ is the most favored one and the unconventional state is likely to occur in a small dome of the phase diagram located in the optimal-overdoped region and at very low temperatures.

In the past Balatsky[6] has studied the properties of the magnetic-field-induced transition to the $d_{x^2-y^2} + id_{xy}$ state proposed by Laughlin[7] to explain the thermal conductivity plateaux in Bi$_2$Sr$_2$CaCu$_2$O$_{8}$[8]. More recently a quantum critical point separating a $d_{x^2-y^2} + id_{xy}$ from a pure $d_{x^2-y^2}$ phase has been suggested[9]. Recently we have given, in collaboration with other authors, a simple analysis of the gap equation based on general symmetry arguments that indicates the existence of a $d_{x^2-y^2} + id_{xy}$ superconducting region in the phase diagram of the cuprates[10]. In accordance with the recent experimental results[11, 12] we have found that the unconventional pairing state should be stable in the optimal-overdoped regime and at very low temperatures.

II. SYMMETRY ANALYSIS AND BCS EQUATION

In order to describe the transition between two different superconducting phases, as the one from a pure $d_{x^2-y^2}$ to a mixed $d_{x^2-y^2} + id_{xy}$ state, we can use the classification of the superconducting classes based on the symmetry properties under crystal point transformations[13].

We start by imposing two constraints on the order parameter:

i. $|\Delta_{g\mathbf{k}}| = |\Delta_{\mathbf{k}}|$ where $g\mathbf{k}$ denotes the vector obtained from $\mathbf{k}$ after the action of one of the $N_G$ group operators $O_g$.

ii. $\Delta_{\mathbf{k}+\mathbf{K}} = \Delta_{\mathbf{k}}$ where $\mathbf{K}$ is a reciprocal lattice vector.

The first condition assures that the dispersion $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$ that enters the physical observables is a total symmetric function with respect to the lattice symmetry[14], while the second is simply to preserve the crystal periodicity. Given the strong evidence of singlet pairing in HTCS we require that

iii. $\Delta_{-\mathbf{k}} = \Delta_{\mathbf{k}}$

This further requirement imposes us to work with even functions of $\mathbf{k}$, because of the antisymmetric spin part of the wave function.

Due to the strong anisotropy of the copper oxides we take a two-dimensional square lattice described by the non abelian $\mathbb{C}_4$ point group. This group has eight elements ($N_G = 8$): the identity operator $E$, one 2-fold
rotation $C_4^2$ and two 4-fold rotations $C_4$ about the Z axis perpendicular to the $XY'$ lattice plane and four reflections $\sigma_v$ and $\sigma_d$ in the four vertical planes.

We can write the order parameter as
\[
\Delta_k = \sum_{\mu} \Delta_k^{(\mu)}
\]
where the sum over $\mu$ runs over all the irreducible representations. Using standard methods of group theory, one can determine the expressions for the various $\Delta_k^{(\mu)}$ in (1):
\[
\Delta_k^{(\mu)} = \sum_{r'} \Delta_k^{(\mu)\nu} w_{r'}^{(\mu)}(k)
\]
where the primed sum is restricted to non-equivalent sites of the lattice, that is sites $r = (x, y)$ that cannot be obtained by means of the action of any of the $O_4$ operators on another site $r'$. We deal, in this way, only with gap amplitudes on a particular lattice distance while the sign relation between all the equivalent sites is entirely accounted for by the harmonics $w_{r'}^{(\mu)}(k)$

\[
\begin{align*}
    w_{r'}^{s^+}(k) &= \cos k_xx \cos k_yy + \cos k_xy \cos k_xx \\
    w_{r'}^{s^-}(k) &= -\sin k_xx \sin k_yy + \sin k_xy \sin k_xx \\
    w_{r'}^{d^+}(k) &= \cos k_xx \cos k_yy - \cos k_xy \cos k_xx \\
    w_{r'}^{d^-}(k) &= -\sin k_xx \sin k_yy - \sin k_xy \sin k_xx
\end{align*}
\]

For $r = 0$, the only non-zero harmonic belongs to the $s^+$ representation, and corresponds to the isotropic s-wave. For $r = (\pm 1, 0); (0, \pm 1) \equiv 1$ the $s^+$ and $d^+$ representations are associated with the extended $s_{xy}^{s^2+}$ and $d_{xy}^{2-}y^2$ waves, respectively. For $r = (\pm 1, \pm 1) \equiv 2$, the non-vanishing harmonics are related to the $s_{xy}$ and $d_{xy}$ waves ($s^+$ and $d^-$ representations). In (1) we have not included the basis functions for the two-dimensional representation E because requirement iii. rules out odd functions of $k$. This is a peculiarity of the bi-dimensional square lattice. The $D_{4h}$ group for instance, proper to a system in which the coupling between the different Cu-O planes is not negligible, possesses a two dimensional representation which is even with respect to inversion and in that case it must be considered.

It can be seen that, using the expansion defined by Eq. (1) and (2), the BCS equation becomes
\[
\Delta_k^{(\mu)} = -\frac{2}{\lambda_r} \tilde{V}(r) \sum_r \Delta_k^{(\mu)} \sum_k w_{r'}^{(\mu)}(k) w_{r'}^{(\mu)}(k') K(k')
\]

where the kernel $K(k)$ is defined as
\[
K(k) = \frac{\tanh \frac{\beta \xi}{2}}{2} \frac{\sqrt{\xi^2 + \left| \sum_{r'} \sum_{\nu} \Delta_k^{(\nu)} w_{r'}^{(\nu)}(k) \right|^2}}{2 E_k}
\]

and $\lambda_r$ is a multiplicity factor equal to 1 for a generic $r$, 2 for a site on the axis or on the bisectors of the lattice and 8 for $r = (0, 0)$. It must be noted that the form (1) represents the mean-field equation for a system described by a generic static pairwise interaction between the electrons $V_{kk'}$ (with $V(r)$ the corresponding real space Fourier transform) and it is obtained without any previous decoupling of the interaction term in a given symmetry channel. It consists of an infinite dimension homogeneous problem which, in general, will be of difficult solution. Nevertheless it can be observed that the appearance of a harmonic labeled by $r$ is always controlled by the corresponding $V(r)$. If the attractive potential is therefore a rapidly decreasing function of $r$ we can restrict ourselves to the smallest distances bonds. We introduce the short-hand notations $V_0, V_1, V_2, \ldots$ for the on-site, nearest-neighbor (nn), next-to-nearest-neighbor (nnn), \ldots components of $V(r)$. Due to the repulsive character of the local interaction $V_0$ in the HTCS, the isotropic s-wave is ruled out. We consider here attractive (negative) nn ($V_1$) and nnn ($V_2$) interactions. For the following discussion we do not take into account longer range terms.

We have not yet made use explicitly of the first requirement on the invariance of the gap amplitude $|\Delta_k|$ under point group transformations. Its effect is to force the gap function to transform either like a single representation, or like a complex (time-reversal breaking) combination of the form $\Delta_k^n + i \Delta_k^z$, with $\Delta_k^n$ and $\Delta_k^z$ belonging to different representations of the point group. To describe this latter possibility, in the case of $V_0 > 0$, $V_1 < 0$, $V_2 < 0$, we take the complex combination $\Delta_k^n w_1^n(k) + i \Delta_k^z w_2^n(k)$, with both $\Delta_k^n$ and $\Delta_k^z$ real. Each gap parameter affects the other only through the quasi-particle spectrum and the BCS equations read
\[
\frac{1}{|V_1|} = \int \frac{dk}{4\pi^2} \left( w_1^n(k) \right)^2 \frac{\tanh(\beta E_k/2)}{2 E_k}
\]
\[
\frac{1}{|V_2|} = \int \frac{dk}{4\pi^2} \left( w_2^n(k) \right)^2 \frac{\tanh(\beta E_k/2)}{2 E_k}
\]

where $\beta$ is the inverse temperature and $E_k = \xi_k^2 + (\Delta_k w_1^z(k))^2 + (\Delta_k w_2^z(k))^2)^{1/2}$

| $C_{4v}$ | $E$ | $C_4$ | $C_2$ | $C_4(2)$ | $\sigma_x$ | $\sigma_z(2)$ | $\sigma_y(2)$ |
|-------|-----|------|------|---------|---------|---------|---------|
| A1    | 1   | 1    | 1    | 1       | 1       | 1       | s^+     |
| A2    | 1   | 1    | 1    | -1      | -1      | 1       | s^-     |
| B1    | 1   | 1    | -1   | 1       | -1      | 1       | d^+     |
| B2    | 1   | 1    | -1   | -1      | 1       | 1       | d^-     |
| E     | 2   | -2   | 0    | 0       | 0       | e       | e       |
with η = s⁺, d⁺, ζ = s⁺, d⁻ (η ≠ ζ). For typical values of
the particle density in the HTCS, the Van Hove singularity
(VHS) of the two-dimensional DOS strongly favors the
dₓ²−y² symmetry, which thus represents the principal
component of the superconducting gap, in agreement
with the phenomenology[13]. We take henceforth η = d⁺
in Eqs. (3), (4).

As we mentioned above the spectrum for the ζ component
is (pseudo)gapped by the principal dₓ²−y² gap. As a consequence a critical value |Vₓ²| for the onset of a
mixed order parameter exists, as opposed to the case of
the Cooper instability in the metallic phase. The critical
coupling for both dₓy and sₓy secondary pairing is deter-
mimed by solving the BCS equations (3), (4) with Δζ = 0
and ζ = d − , s + respectively[11]. Numerical solutions
show that the dₓ²−y² + idₓy symmetry is much favored
with respect to the dₓ²−y² + isₓy as one expects from a
qualitative analysis of Eq. (3), (4). Moreover, the contin-
uous transition from dₓ²−y² to dₓ²−y² + isₓy is generally prevented by a first-order transition from pure dₓ²−y²
to pure sₓy, due to the strong competition between the
two harmonics, which makes mixing unfavorable. This
scenario does not find experimental support. The con-
tinuous transition from dₓ²−y² to dₓ²−y² + idₓy is therefore the most natural candidate if a pure dₓ²−y²
is to be modified by a small secondary component, as
suggested by the experiments[15]. As far as the depen-
dence of the dₓy critical coupling on the value of |Vₓ| is
concerned it can be realized that the more |Vₓ| grows the
smaller is the ratio |Vₓ²|/|Vₓ| so as to favor the transition
to the dₓ²−y² + idₓy state in the intermediate-to-strong
coupling regime.

III. RESULTS AND CONCLUSIONS

In this section we show numerical solutions of
Eq. (3), (4) obtained studying the dependence on hole con-
centration (δ) and on band parameters. In a previous
work[11] the phase diagram for the dₓ²−y² + idₓy super-
conducting region for the case of LSCO (closed Fermi
surface) was derived. Here we want to show the case of
bilayer compounds like Bi₂Sr₂CaCuv₂O₈+δ (Bi2212) and
YBCO (open Fermi surface). Our rigid band dispersion
is thus ξₓ² = −2t(cos kₓ + cos kᵧ) + 4′ cos kₓ cos kᵧ ±
4t₁ (cos kₓ - cos kᵧ)² - μ where t and t’ are nn and
nnn hoppings and μ is the chemical potential. We take
w = 200 meV, t’ = 50 meV and t₁ = 35 meV. For the
case of Bi2212, ARPES measurements show a value for
2t₁ that varies from 88 meV to 140 meV. Unfortunately
we are not aware of similar data on YBCO, but the bare
values of t₁ in Bi2212 and YBCO are similar, so that
we can expect similar renormalized values. In addition
we introduce a cut-off ω₀ in the integrals which measures
the typical energy scale of the attractive potential[14].
As shown in Fig. 1 for each doping δ, we fix V₁ such
that the critical temperature for dₓ²−y² pairing coincides with
the pseudogap temperature T∗ (which we interpret as the
temperature for Cooper pair formation without phase co-
erence in the underdoped regime), and smoothly con-
nects to Tc around optimal doping. Then we fix a value
for the ratio V₂/V₁ that never exceeds the physical thresh-
old of 1. The connection between this value and the pres-
ence of a quantum critical point located near optimum
doping is given a previous work[11].

We find that the mixed dₓ²−y² + idₓy order parameter
is then stabilized in a small dome slightly shifted in the
overdoped region, 0.17 < δ < 0.22. The dₓ²−y² + idₓy
transition temperature is always only a small fraction of
the dₓ²−y² one and the same ratio is obtained between
the gap amplitudes. In the extreme overdoped region
the system approaches weak coupling determining the
closure of the dome. On the other hand the vanishing of
the dₓy component in the underdoped region is due to
band structure effects.

We finally summarize the results of this analysis:
1. As found in our previous work[11], a mixed order pa-
rameter of the form dₓ²−y² + idₓy can be stabilized in
a small dome contained in the larger dₓ²−y² region. The
dₓy component does not grow indefinitely with increas-
ing doping and it is always smaller than the dₓ²−y². A
recent re-analysis of the LSCO data with a dₓ²−y² + idₓy
gap parameter[11], clearly displays the closure of the dome
in the overdoped. The confirmation of our prediction in
YBCO calls instead for further measurements at larger
doping in the overdoped region.
2. The intermediate-to-strong coupling regime is a nec-
essary condition for the existence of the mixed order pa-
rameter.
3. dₓ²−y² + idₓy pairing is more likely to occur in closed
Fermi surface materials such as LSCO or electron doped
materials, and in compounds where an interlayer hopping
splts the VHS.
Acknowledgments

We thank Claudio Castellani, Carlo Di Castro and Marco Grilli for their collaboration.

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