Crossover behavior for complex order parameter in high-$T_c$ superconductors

E. V.L. de Mello
Departamento de Física, Universidade Federal Fluminense, Av. Litorânia s/n, Niterói, R.J., 24210-340, Brazil
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A number of recent experiments have suggested the presence of either real or complex components in the gap symmetry of high-$T_c$ superconductors (HTSC). In this paper we introduce a novel approach to study the competition of such complex order parameter mixtures by varying the position of the two-body attractive potential in a two dimensional extended Hubbard Hamiltonian. We show that this procedure explain a number of experimental results and on the theoretical side, it may be related with certain HTSC microscopic models like the spin fluctuation theory. Following current trends we concentrate on the study of $d_{x^2−y^2}$ order parameter with a component of the type $d_{xy}$ or a s-wave like $s_{x^2+y^2}$ and $s_{xy}$ symmetry. We show that the position of the optimal s-component peak changes with the position parameter $b$ while the d-component occurs always in the optimally region around hole content $\rho \approx 0.39$. These studies may be useful to interpret some experimental data and to explain why similar experiments yield different gap symmetries.

74.20.-z,74.25.Dw,74.72.-h

I. INTRODUCTION

In order to understand the fundamental mechanism for high-$T_c$ superconductors (HTSC), many experiments have attempted to find out the properties of the superconductors pair wave function. Notwithstanding this effort the nature of the orbital order parameter symmetry (or energy gap) has not yet been settled, despite increasing evidences toward a major $d_{x^2−y^2}$ symmetry as it explains a number of different experimental results [1,2]. Furthermore the d-wave state has also theoretical support from weak and strong-coupling approaches [3] and from Monte Carlo and numerical studies on a two dimensional Hubbard model [4]. On the other hand several experiments have also suggested the presence of complex mixture of order parameters. For instance, c-axis Josephson tunneling data between twinned YBCO and a s-wave superconductor were interpreted by a condensate containing a mixture of $d_{x^2−y^2}$ and s order parameter [5,6]. This type of order parameter symmetry was argued to be a consequence of the orthorhombicity of the YBCO crystal structure [6]. Recently, Klemm at al [7] have studied the symmetry operation of the crystal groups relevant to Hg1001, YBCO and BSCCO to analyze the possibility of different order parameter symmetry combinations for these HTSC and their results agree with the c-axis Josephson tunneling experiments. Furthermore the possibility of complex mixtures of different symmetries has also been suggested [8] as it would induce time reversal symmetry breaking in connection with magnetic defects or small fractions of a flux quantum $\Phi_0 = \hbar c/2e$ observed in YBCO powders. Similarly a complex admixture of $d_{x^2−y^2}$ and s symmetry was also proposed [9] to explain the ab-oriented YBCO/I/Cu tunnel junctions data [10]. They proposed an interesting and very simple physical picture: Andreev scattering near the YBCO surface causes strong pair dissociation. The resulting quasiparticles may then be paired again also by a subdominant s-channel that is less sensitive to surface pair breaking then the dominant $d_{x^2−y^2}$-channel. Calculations minimizing the free energy show [1] that such complex mixture can coexist at low temperatures. Using a tight binding model in a mean field treatment Honerkamp et al [11] have arrived at a similar conclusion that a surface phase transition towards a time-reversal symmetry breaking surface state carrying an $s + id_{x^2−y^2}$ state may appear (below $T_c$). Recently [12] a complex mixture of $d_{x^2−y^2} + id_{xy}$ was also proposed in order to explain a phase transition characterized by magnetic field plateaus or kinks in the thermal conductivity [13] of $\mathrm{Bi}_2\mathrm{Sr}_2\mathrm{CaCu}_2\mathrm{O}_8$ compounds.

Based on the above discussion, we study in this paper the competition of the $d_{x^2−y^2}$ and others subdominants complex symmetries of the gap function. We develop in these calculations a novel approach based on a change in the position of the attractive potential $V$ from its usual nearest neighbor position in the extended Hubbard Hamiltonian. As it is well known, the on-site Coulomb correlations may explain the antiferromagnetism of the low doping regime, the large magnetic fluctuations and the semiconductor like properties of the metallic phase [14,15]. Furthermore the presence of a small attractive interaction leads to phase separation and, on a square lattice, yields a superconducting phase with a $d_{x^2−y^2}$ symmetry [14]. Thus, the Hubbard Hamiltonian with such phenomenological attraction is a natural candidate to deal with the HTSC. The idea to change the position of the attractive potential in the extended Hubbard Hamiltonian was originally motivated by the experimental fact that different compounds have different $T_c \times n$ phase diagram and the optimal doping values may vary according the compound. This fact can be physically interpreted due to a possible change in the range of the attrac-
tive interaction that leads to pair formation \([19,20]\); for compounds with short range correlations the carrier density must be larger than those compounds with a longer ranged interaction in order to undergo a superconducting phase transition. The same type of physical argument can be used to interpret the measured different values of the coherence length \(\xi\) for different family of compounds since a short range interaction requires larger densities than a long range one in order to produce the coherence motion that leads to superconductivity. Furthermore, the typical parameter which characterizes the strength of the attractive interaction \([21]\). \(\chi = m_\alpha a^2 V/2\hbar^2\), when estimated for most of HTSC, varies between 10-3000 and such high values indicate that the size of the bound states (or Cooper pairs) are indeed related to the size of the minimum of the attractive potential.

Another interesting aspect from the theoretical point of view is that this parametric change of the attractive potential can be related with the order parameter \([23]\) and the typical parameter which characterizes the strength of the attractive interaction, \(\Delta_0 = V\). Taking a close look at this expansion, one can easily verify that it contains terms like \((\cos k_x a - \cos k_y a)\) which are proportional to \((\cos(2k_x a) - \cos(2k_y a))\) and what can be seen as a type of d-wave gap symmetry that arises from a potential like \(V(\vec{k}) = V_0(\cos(2k_x a) + \cos(2k_y a))\). By the same token, we can find terms proportional to \((\cos(3k_x a) - \cos(3k_y a))\) which can be originated by a potential \(V(\vec{k}) = V_0(\cos(3k_x a) + \cos(3k_y a))\) and so on. There will also be crossed terms proportional to \((\cos(k_x a) \times \cos(k_y a))\) that may be associated to a next-nearest potential. Thus, we see that the gap expression proposed by the spin-fluctuation theory contains several terms and some may be associated to a potential of the form \(V(\vec{k}) = V_0(\cos(bk_x a) + \cos(bk_y a))\), where \(b = 1, 2, 3, \ldots\) is a parameter related to the position of the attractive potential (\(b = 1\) leads to the usual nearest-neighbor expression). Consequently we have studied in this paper the phase diagram of complex admixtures of a d-wave like order parameter with some minor complex component with this parameterized change of the potential position, that is, with different values of \(b\). These calculations are made with the extended Hubbard model on a square lattice of side \(a\), which describes a tight binding model with the strong correlations taken into account and is defined by

\[
H = - \sum_{ij} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - V \sum_{ij} n_in_j.
\]

(1)

where \(t_{ij}\) is the hopping integral between sites \(i\) and \(j\) and are estimated by comparison with either band structure calculations or Fermi surface measurements, \(U\) is the on-site correlated repulsion and \(V\) is an attractive phenomenological interaction which in principle can be due to spin fluctuations, as mentioned above or any other type of mechanism. In order to obtain quantitative results, we have used the tight-binding dispersion relation derived from Fermi surface measurements by Norman et al \([22]\) for \(Bi_2Sr_2CaCu_2O_8\) but this choice is not a fundamental requirement, another studies have used different dispersion \([24]\) with small quantitative changes.

II. The Method

We used a BSC mean-field approximation \([23,24]\) to study the superconducting phase associated with the Hamiltonian of Eq. (1) described above. In this model the superconducting state is characterized by a gap order parameter, which at a finite temperature \(T\) satisfies the BCS self-consistent equation

\[
\Delta_{k} = - \sum_i V_{ki} F_{i\bar{k}}
\]

(2)

where \(V_{ki}\) is the Fourier transform of the potential of Eq. (1) and

\[
F_{k} = \frac{\Delta_{k}}{2E_k \tanh \frac{E_k}{2k_BT}}.
\]

(3)

where \(\varepsilon_k\) is the dispersion relation taken from Ref. \([23]\) and \(\mu\) is the chemical potential. Following along the lines of Ref. \([24]\), one can easily show that \(V_{ki}\) may be written in a "separable" form, \(V_{ki} = U - 2V \cos(k_x a) \cos(l_x a) + \cos(k_y a) \cos(l_y a)\) which leads to the usual d and s-wave. This procedure can easily be generalized for the case of \(b = 2, 3, \ldots\) discussed above and will be developed below in order to study the superconducting transition with respect to the position of the attractive potential. For a two-component order parameter with a separable form, the corresponding gap equations may be written as \([27]\)

\[
V_{ki} = \sum_{j=1}^2 V_{ij} f_{k\bar{i}}^j, \quad \Delta_{k} = \sum_{j=1}^2 \Delta_{j} f_{k\bar{i}}^j
\]

(4)

Here, since we want to study the competition between the \(d_{x^2-y^2}\) and others symmetries, we have always taken \(V_{1} = V_{d_{x^2-y^2}}, f_{k}^1 = (\cos(bk_x a) - \cos(bk_y a))\) and \(\Delta_1 = \Delta_{d_{x^2-y^2}}\) and the complex component can either be \(V_{2} = V_{d_{xy}}, V_{s_{x2+y2}}\) or \(V_{s_{xy}}\) with \(f_{k}^2 = 2\sin(bk_x a)\sin(bk_y a),\cos(bk_x a) + \cos(bk_y a)\) or \(2\cos(bk_x a)\cos(bk_y a)\) and the gap functions are \(\Delta_1 = i\Delta_{d_{xy}}, \Delta_{s_{x2+y2}}, \Delta_{s_{xy}}\) respectively. Now, separating the real and imaginary parts and combining Eq. (3) and Eq. (4) we obtain the following two gap equations.
\[ \Delta_j = \sum_k V_j f_k^2 \tanh \left( \frac{E_k}{2k_BT} \right), \quad j = 1, 2 \]  

These two equations has to be solved with the density of carriers \( \rho \) equation which is given by [26]

\[ \rho(\mu, T) = \frac{1}{2} \sum_k \left( 1 - \frac{\varepsilon_k}{E_k} \tanh \frac{E_k}{2k_BT} \right) \]  

Thus we solve self-consistently the above 3 equations (Eq.5 and Eq.6) in order to study the phase diagram of a complex admixture of the order parameter. These equations are general in the sense that they can be applied to any type of two component symmetry mixtures. The results will be discussed below.

III. RESULTS AND DISCUSSIONS

![Graph showing critical temperatures for the s and d-channels for b = 1.](image)

FIG. 1. The critical temperatures for the s and d-channels for \( b = 1 \). The continuous line is the calculations described in the paper and the diamonds are the experimental points from Ref. 28

We start with the analysis for the complex mixing with the two most relevant symmetries, The \( d_{x^2-y^2} \) and the \( s_{x^2+y^2} \) which we write as \( d_{x^2-y^2} + is_{x^2+y^2} \). We have solved the above self consistent equations with fixed \( V_d/t = 0.11 \) and \( V_{s_{x^2+y^2}}/t = 0.18 \), which these values were chosen in order to obtain reasonable values for the critical temperatures \( T_c \) in the range of parameters studied. In this way we obtain a maximum \( T_c \approx 94K \) for \( b=1 \) and by the dominant \( d_{x^2-y^2} \) symmetry near the optimum doping. In Fig.1 we show the results for the values of \( T_c \propto \rho \) in order to compare with the experimental results of Allgier et al [29] on Bi(2)Sr2CaCu2O8+δ (Bi2212). Notice that their maximum \( T_c \) occur at \( \rho \approx 0.32 \) while our calculations yield a maximum \( T_c \) at \( \rho \approx 0.39 \) and this discrepancy is probably due the dispersion relation that we used since a similar BCS mean field calculation using the Hubbard Hamiltonian (for \( b=1 \)) gives a maximum which agrees with the experimental result [24].

We should point out that the comparison with a HTSC experimental phase diagram, as in Fig.1, has only meaning if the material has a BCS type behavior, that is, when the appearance of the superconducting gap and phase coherence occur simultaneously at the onset of superconductivity. On the other hand, angle-resolved photoemission spectroscopy (ARPES) on underdoped Bi2212 has revealed the presence of a "pseudogap" above \( T_c \) [29,30,23] which has also been confirmed by recently Fermi surface ARPES measurements [32]. This unusual behavior may be an indication of non-BCS behavior which \( T_c \) is controlled by the doping level, at underdoped regime, rather then by phase coherence with a single particle gap \( \Delta_F [23] \). Nevertheless this is not a completely settled scenario which only more experiments will give the correct interpretation specially because the pseudogap has not yet been seen in several cuprate superconductors [34].

![Graph showing results for the zero temperature gap amplitudes \( \Delta_{d_{x^2-y^2}} \) (continuous lines) and \( \Delta_{s_{x^2+y^2}} \) (dashed lines) as function of the hole density \( \rho \) for \( b=1(a),2(b) \) and 3(a). \( \rho = 0 \) is the half-filling density.](image)

FIG. 2. Results for the zero temperature \( \Delta_{d_{x^2-y^2}} \) (continuous lines) and \( \Delta_{s_{x^2+y^2}} \) (dashed lines) in units of \( t = 0.26eV \) as function of the hole density \( \rho \) for \( b=1(a),2(b) \) and 3(a). \( \rho = 0 \) is the half-filling density.

In the Fig.2 we show the results for the zero temperature gap amplitudes \( \Delta_{d_{x^2-y^2}} \) (continuous line) and \( \Delta_{s_{x^2+y^2}} \) (dashed line) as function of the density \( \rho \) for three values of the parameter \( b \), namely \( b = 1, 2 \) and 3. Where there is superconductivity region, the values of \( \Delta \) have their maxima at zero temperature and vanishes at \( T_c \) in agreement with the BCS method. In fact, the self-
consistent calculations yields the temperature, the density $\rho$ and the value of the gap as one solves Eqs. 5 and 6 simultaneously. In Fig.3 we show how the gap changes with the temperature. The zero temperature gap value is proportional to $T_c$ and the constant of proportionality differs slightly from one channel to the other. We get $\Delta(0)/k_BT_c \approx 2.6$ in the optimally region.

There are very interesting differences from the $s$ and $d$ channels which arises as we vary the parameter $b$. For $b = 2$, the values of $\Delta_{d_{x^2-y^2}}$ are basically suppressed while for $b = 3$ its strength is decreased by about half of its value for $b = 1$ (which agrees with the calculations of Ref. [24]) and does not move appreciably from the optimum doping value of hole content $\rho = 0.39$ ($\rho$ is the fraction of holes per Cu atom in the CuO$_2$ sheet). This result is a little higher then the experimental result [28] which yields $\rho = 0.32$ for the Bi optimum doping value. The maximum $T_c$ is related with the envelope of the curve shown in Fig.2. On the other hand, for the extended $s$, $\Delta_{s_{x^2+y^2}}$, the change in $b$ causes the value of the corresponding optimum doping density to change continuously; it is at $\rho \approx 0.41$ for $b = 2$ and and about $\rho = 0.32$ for $b = 3$ as it is seen in Figs.2a, 2b and 2c. At $b = 1$ (Fig.2a), the s-wave has the optimum doping at $\rho \approx 0.05$, for $b = 2$ the maximum $T_c$ occurs at $\rho \approx 0.40$ and it dominates over $\Delta_d$ which is almost entirely suppressed. For $b = 3$ the competition between the two channels becomes very interesting; the maximum of $\Delta_s$ has moved to $\rho \approx 0.33$ while the maximum of $\Delta_d$ remains fixed at $\rho \approx 0.42$ which gives rise to a completely novel doubled crossover phenomena; up to $\rho \approx 0.35$ the self-consistent equations yields pure extended s-wave solutions. Between $\rho \approx 0.35 - 0.37$ the mixing of order parameters starts at low temperatures but with the s-channel dominating over the d-channel as its critical temperature $T_c$ is larger as shown in Fig.2c and at Fig.3a for $\rho = 0.37$.

At $\rho \approx 0.38$ a crossover arises and the d-channel solutions dominates over the s-channel which becomes the minor component as shown in Fig.2c and Fig.3b. There is always mixing at low temperatures (the continuous curve of the minor s-wave never vanishes completely) but the d-channel is the only one at $T_c$. At $\rho \approx 0.48$ there is a new crossover and the dominant solution changes again as the s-wave becomes the dominant solution and the only one at $T_c$ and the d-wave appears again at low temperatures as the minor components as displayed in Fig.2c and Fig.3c. Notice that the appearance of this subdominant component is exactly as the mechanism proposed to explain the ab-oriented YBCO/I/Cu tunnel junction data [12] discussed in the introduction.

Next we have studied the complex gap function of symmetry $d_{x^2-y^2}+is_{xy}$. The results are quite similar to those above; for $b = 1$ the d-state dominates and has its optimum doping at $\rho = 0.40$ as shown in Fig.4a. For $b = 2$ the d-channel is again suppressed and the $s_{xy}$-state is the only one and its maximum doping is also at $\rho \approx 0.83$ as displayed in Fig.3b. For $b = 3$ there is again the very interesting doubled crossover between these two competing symmetries. For $0.2 < \rho < 0.36$ there is only s-wave
Thus we verified that the states in Fig.4c that, for feature with this type of admixture: we can see from in $\Delta$ ... appears as it becomes the dominant channel and the only channel at $T_c$. Thus we verified that the states $d_{x^2-y^2} + is_{x+y}$ has also the doubled crossover and the dominant regions are similar to those for $d_{x^2-y^2} + is_{x+y}$ however, there is a new feature with this type of admixture: we can see from Fig.4c that, for $b = 3$, one kind of gap symmetry influences the other. One can easily see the abrupt change in $\Delta_{sxy}$ near $\rho \approx 0.33$ and the change in slope for both channels near $\rho \approx 0.48$. The new phenomenon, that is, the slightly suppression on $\Delta(T)$ of the dominant channel can also be seen on Figs.5a, 5b and 5c. This is a new feature not seen in Figs.3c, and this suppression is the cause of the pure d-wave solutions at the optimal region which did not occur for previous studied extended s-wave. This interesting feature may be similar to what happens in Andreev scattering near surfaces as discussed in the introduction.

![Graph](image)

FIG. 5. The display of the doubled crossover. As the density increases we see the solutions change from dominant s-channel in a), to a dominant d-channel as in b) and again a dominant s-channel in c). The temperature T is in Kelvins.

Lastly we have also studied the complex order parameter mixing $d_{x^2-y^2} + id_{xy}$ for the three values of $b$, however we have not found even a single crossover. For $b = 1$, the $d_{x^2-y^2}$ channel dominates and has also its optimum value at $\rho = 0.40$ and the $d_{xy}$ appears only at low temperatures. For $b = 2$ and 3 the $d_{xy}$ dominates completely around the same optimal region and the other channel gives only a very small component at low temperatures. Thus we do not observe any crossover for $d_{x^2-y^2} + id_{xy}$ complex mixture, simply the interchange of dominant symmetry as we change $b$.

IV. CONCLUSIONS

The complex mixtures in superconducting order parameter were studied here as function of hole density in the context of the BCS mean-field calculations for the extended Hubbard model. We have revealed very interesting properties that may be relevant for HTSC; if the interaction is sufficiently short ranged that can be mapped by a nearest neighbor potential, at low doping, the system is described by either pure $d_{x^2-y^2}$ or $s_{x+y}$ order parameter. If the range of the potential is larger the system changes its order parameter symmetry (for $b = 2$) or may admit a mixed state with both $s$ and $d$ components present (for $b = 3$). In this last case the dominant component depends strongly on the density or doping level $\rho$ and may change abruptly the dominant symmetry at $T_c$. Since in most HTSC it is difficult to determine $\rho$ accurately and as our calculations demonstrate, a small change in $\rho$ may be accompanied by a crossover of the dominant component. If we assume an expansion with $b = 1, 2, 3...$ like that of the spin fluctuation theory of Ref. [24], then one must look at their weight to see which one is more important and concomitantly, which symmetry of the order parameter is the dominant one. This present work provides a hint to understand why different order parameter symmetries appear in different experiments performed on the same type of compounds.

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* evandro@if.uff.br

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