Anisotropy and magnetism of high temperature oxides superconductors

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Abstract

Phonon or electron mediated weak BCS attraction is enough to have high critical temperature if a van Hove anomaly is at work. This could apply to electron doped compounds and also to compounds with CuO\textsubscript{2} planes overdoped in holes, where $T_{c}$ decreases with increasing doping. If phonons dominate, it should lead to an anisotropic but mainly $s$ superconductive gap, as observed recently in overdoped LaSrCuO, and probably also in electron doped compounds. If electrons dominate, a $d$ gap should develop as observed in a number of cases. In the underdoped range, the observed decrease of $T_{c}$ with hole doping can be related in all cases to the development of antiferromagnetic fluctuations which produces a magnetic pseudogap, thus lowering the density of states at the Fermi level. The observed mainly $d$ superconductive gap then can be due to a prevalent superconductive coupling through antiferromagnetic fluctuations; it could also possibly be attributed to the same phonon coupling as in the overdoped range, now acting on Bloch functions scattered in the magnetic pseudogap. More systematic studies of superconductive gap anisotropy and of magnetic fluctuations would be in order.

74.20.-z, 74.20.Fg
I. INTRODUCTION

Since the discovery of the perovskite copper oxides with superconducting critical temperature $T_c$ between 30 and 40K \cite{1}, the high $T_c$ copper oxides with parallel CuO$_2$ layers have been much studied because of the hope, soon realised, of increasing $T_c$ still further and also because such high value of $T_c$ did not fit a ‘classical’ BCS formula. Indeed $T_c$ is then related to the Debye temperature $T_D$ by \cite{2}

$$T_c \simeq T_D \exp(-1/\lambda),$$

where the exponential is very small for a weak relative coupling

$$\lambda = V n(E_F) \simeq V/E_F,$$

in which $V$ is the phonon mediated electron-electron coupling, $n(E_F)$ is the electron density of states, $E_F$ the Fermi energy. With $T_D \leq 300K$ and $\lambda \ll 1$, $T_c$ up to 25K should be very exceptional. Classical corrections for larger phonon coupling $\lambda$ or for effective Coulomb repulsion $\mu^*$ \cite{3-5} do not significantly alter conclusions.

It is then natural to examine specific properties of HTSC:

– quasi two-dimensionality, with weakly coupled CuO$_2$ layers.
– antiferromagnetic(AF) fluctuations. The mother materials of HTSC are insulators with AF order below $T_N$.
– anisotropic superconductive gaps.

The phase diagram with doping and temperature is indeed very rich, with the antiferromagnetic ordered phase, the superconductive phases – underdoped and overdoped –, a pseudo AF gap region as well as a ‘normal’ metallic range as shown schematically in Fig. 1 for the usual hole doped compounds. Electron doped compounds show a similar succession of AF, superconductive and normal metallic phases, with smaller critical temperatures.

Finally, in common with the classical BCS case, the superconductive state occurs through condensation of cooper singlet pairing ($\mathbf{k} \uparrow, -\mathbf{k} \downarrow$).

Our purpose is first to stress again that a usual BCS weak coupling scheme of delocalised electrons is enough to explain the high value of $T_c$ observed. The observed anisotropy of the superconductive gap might tell us whether its coupling is predominantly through electrons or through phonons. But the possible variation of this anisotropy with doping must take into account the scattering of the Fermi wave functions in the presence of AF fluctuations. It is then clear that the nature of the superconductive coupling, whether by phonons or electrons, is more directly related to the anisotropy of the gap in the overdope range of ‘normal’ metallic behavior.

II. CUO$_2$ LAYERS

We will use a well-known simplified picture restricted to positive holes of the $2p^6$ of the oxygen and of the $3d^{10}$ of the copper, moving in a CuO$_2$ plane. Only the orbitals O$_{2p}$ and Cu$_{3d}$ orbitals occupied by these holes are considered.
A. Electronic structure

The three essential energies are

\( U \): the positive energy of repulsion for two electrons on the same site.

\( \Delta \): the energy of promotion \( 3d \to 2p \) for a hole.

\( t \): the absolute value of the transfer integral of \( 3d \leftrightarrow 2p \), which gives the frequency at which a positive hole can transfer between a Cu and a neighboring O.

In HTSC compounds, X rays absorption data for the inner \( s \) shells of O show that the \( 2p \) holes exist in appreciable number for undoped as well as for doped samples \([6]\). The same conclusion can be drawn from the observed shift of the NMR line of Y in YBaCuO \([7]\). These fundamental observations are only compatible with

\[ |\Delta| \leq t. \tag{2.1} \]

If we neglect for the moment the possible effect of \( U \) in the AF compounds, the positive holes are then in a band of extended states with a width \( w \) of the order of \( t \) \([6]\).

The \( 3d \) holes are correlatively fewer than if all the holes were concentrated on the Cu ions. They will be less than 1 on average on each copper in the undoped samples, and their short range repulsion \( U \) cannot lead to any Verwey-Mott Coulomb localisation. In the absence of the magnetic effects discussed later, the holes should form, independently of doping, a fermi liquid, with a Fermi surface and a band structure, responsible for metallic conduction.

More precisely, if \( U \gg w \simeq t \), the situation would recall that of heavy fermion compounds, where \( U \) acts mostly by increasing the effective mass in energy.

If \( U \simeq w \simeq 2t \), the situation is analogous to that of transition metals, where the essential effects of correlation due to \( U \) can be treated by perturbation \([11]\).

The position of the X rays satellite emission line due to double excitation on Cu in these compounds in fact compares with that observed in a metal like Ni \([3]\); this suggest that, although sizable, the effects of \( U \) can be usefully computed with a perturbing scheme, i.e. \( U \simeq w \). The study of the limits of stability (in temperature and in doping) of the observed AF phase, as discussed later, agree with this conclusion. This is what will be done in this paper, although there is no essential difference in the metallic phase when \( U \gg w \).

B. Approximate band structure \([6]\)

In the tight binding approximation used here, the Fermi level falls near the middle of the antibonding \( \text{CuO}_2 \) band which couples the \( 3d_{x^2-y^2} \) orbitals of Cu and the \( 2p_x \) orbitals of O (Fig. 2). The one particle band structure should depend on \( t, t' \) (transfer integrals in the \( x \) and \( y \) directions). Comparison with more exact band structure calculations lead, for typical HTSC' like LaSrCuO and YBaCuO to the following order of magnitude:

\[ \Delta \simeq 1\text{eV}, \]

\[ t \simeq 2\text{eV}, \]

\[ |t - t'| \simeq 10^{-2}\text{eV} \quad (\text{in orthorhombic YBaCuO}), \tag{2.2} \]

and thus the total band width of the band is
This leads to an effective tight binding picture between Cu atoms

\[ E_k \simeq -2t_\parallel \cos k_x a - 2t'_\parallel \cos k_y b, \]  

with

\[ t_\parallel \simeq \frac{t}{2\sqrt{2}}, \]  

and

\[ w \simeq 8t_\parallel. \]  

For undoped compounds, the Fermi level is then a square in the tetragonal phase \( t' = t \) and very near to it in the orthorhombic one \( t' \neq t \). Doping by electrons and by holes produce almost square Fermi surfaces with nearly symmetric deviations from the undoped square surface (Fig. 3). This fundamental symmetry between electron and hole dopings fits well the general symmetry of the phase diagram observed for electron and for hole doped compounds.

The Fermi surface has the obvious property of exact or nearly exact nesting by a translation \( \mathbf{Q} \) equal to or nearly equal to the reciprocal lattice period \( \mathbf{Q}_R \), at the origin of the AF instability discussed later. But the Fermi level sits also near a strong peak in the density of states, which diverges logarithmically at \((\pm \pi, 0), (0, \pm \pi)\) for the undoped compounds (Fig. 4). This van Hove anomaly is characteristic of the (quasi) two-dimensional compounds, where it is much stronger than in more isotropic 3d compounds.

\[ \boxed{2V = \int_{E_F - k_BT_D}^{E_F + k_BT_D} \tanh \left( \frac{E - E_F}{2k_BT_\parallel} \right) n(E) \frac{dE}{E - E_F},} \]  

leads to values of \( T_\parallel \) much larger than \( (1.1) \), obtained with \( n(E) \) constant.

The maximum of \( T_\parallel \) in this approximation occurs when the Fermi level sits on the van Hove anomaly, thus for a half filled conduction band, at zero doping. For large enough value of \( T_D \), \( (2.7) \) then gives, from \( (2.4) \)

\[ k_BT_\parallel \simeq 2t_\parallel \exp \left( -\sqrt{\pi t_\parallel / V} \right). \]  

\textbf{C. High value of } T_c \text{ in the overdoped metal range}

We can reasonably neglect possible effects of AF thermal fluctuations in this 'normal' metallic range (Fig. 1). A high critical temperature \( T_\parallel \) can then be obtained in the mean field BCS approximation.

This can be seen assuming an isotropic coupling \( V \) and an anisotropic \( s \) gap \( [12,13] \). Then, if the Fermi level \( E_F \) is near enough to a van Hove anomaly of the density of states \( n(E) \), the BCS equation

\[ \boxed{2V = \int_{E_F - k_BT_D}^{E_F + k_BT_D} \tanh \left( \frac{E - E_F}{2k_BT_\parallel} \right) n(E) \frac{dE}{E - E_F},} \]  

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\[ k_BT_\parallel \simeq 2t_\parallel \exp \left( -\sqrt{\pi t_\parallel / V} \right). \]  

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This is much larger than (1.1), both because \( \lambda \) is replaced by \( \sqrt{\lambda} \) in the exponential and because \( k_BT_D \) is replaced by an electron energy \( t_\| \) in front of the exponential: the cutoff in (2.7) is provided by the fast fall of the wings of the van Hove anomaly more than by \( T_D \).

With \( t_\| \simeq 1eV \), (2.8) then leads easily to large value of \( T_\| \), larger than of those observed, even for small value of \( \lambda \). Indeed

\[
\lambda \simeq V/4t_\| \simeq 0.1 \text{ gives } T_\| \simeq 1000K. \quad (2.9)
\]

Two major corrections should appreciably reduce this upper limit [8]:

– in the overdoped normal metal range discussed here \( c > c_M \), Fig. 1), the Fermi level is appreciably shifted from its optimum value at zero doping.

– because of the weak coupling between the electronic structures of neighboring \( \text{CuO}_2 \) planes, superconductive fluctuations should reduce somewhat \( T_c \) from \( T_\| \).

Very rough estimates of then two effects lead, in the optimum doping range \( c \simeq c_M \), to

\[
T_c \leq 100K. \quad (2.10)
\]

Minor corrections affecting the core of the van Hove anomaly and discussed in [6] are not changing such estimate. The possibility of anisotropic gap, discussed below, should increase \( T_\| \), thus \( T_c \) but little.

In conclusion \( T_c \) up to 100K are easily compatible, in the overdoped metallic range, with a weak coupling schemes, as could be obtained by standard phonon or electron couplings. Even higher values of \( T_c \) could be obtained in similar compounds with no AF instability.

### III. ANTIFERROMAGNETISM AND SUPERCONDUCTIVITY

#### A. Covalent antiferromagnetism [6]

In the model of delocalised electrons which follows from (2.1), the only magnetism possible is a band magnetism. The classical motor of such a magnetism is, following Stoner and Lomer, the Coulomb interaction \( U \) (except in the limit of infinite \( U \)’s, where one should consider the exchange interaction \( J - tS \) \( (J \) exchange, \( S \) overlap, cf. [14]) and/or direct transfers between \( \text{O} 2p \) orbitals (Barisic, priv. comm.).

In fact, if \( U \) is treated in perturbation, one expects for the undoped compounds, an antiferromagnetism with a wave vector \( Q_R \) which is the side of the square, Fig. 3; and the value obtained for \( T_N \), including corrections for thermal fluctuations, is compatible with \( U \leq w \). Because only a fraction of holes is found on the Cu, of the order of 1/2 if \( |\Delta| \leq w \), we can interpret in this way the observed magnetic moments; quantum fluctuations of these moments are expected to be weak because, in this description, each atomic moment on a copper ion interacts in perturbation with many others, through the long range spin oscillation it produces.

The AF order leads to the opening of an antiferromagnetic gap around the Fermi level (Fig. 5), leading to a band insulator in the AF state. For \( T \) slightly larger than \( T_N \), we expect strong AF fluctuations, inducing an effect of antiferromagnetic ’pseudogap’, as described initially by Mott in another context: without vanishing completely, the density of
states should decrease around the Fermi level $E_F$, between rounded bonding B (i.e. antiferromagnetic) and antibonding AB (i.e. ferromagnetic) peaks, as pictured in Fig. 5. For strong enough fluctuations, i.e. near enough to $T_N$, one expects a localisation of all the states in the pseudogap, thus an insulator by disorder, à la Anderson.

For weakly doped compounds, the observed AF order preserves a periodicity coherent with that of the crystal: this can be expected if there is interference of spin density waves on the CuO$_2$, an ordinary phenomenon, to be expected here especially by the fact that the faces of the square, Fig. 3, nest exactly by the translation $Q_R$ (cf. Appendix A). From the fact that $Q_R$ does not superpose the opposite faces of the Fermi surface in weakly doped samples, a rapid decrease of $T_N$ is expected with increasing doping. This is just what is observed (Fig. 1), and the value of the maximum doping of the AF phase corresponds again to a modest value of $U \approx w$.

Finally in the more strongly doped compounds, the intensity of the AF fluctuations decrease with increasing temperature or doping. The limit of notable fluctuations is marked by $T_f$ in Fig. 1: they disappear in fact beyond the peak of superconductivity $T_c(c_M)$, by smoothly joining $T_c$ around $c_t$ slightly larger than than $c_M$. Depending on the compound considered, the average wave vector of these fluctuations remains at $Q_R$ (YBaCuO) or varies with doping like the nesting vector $Q$ of the Fermi surface (Fig. 3, LaSrCuO): such variation, in agreement with the Lomer criterion, confirms the role of the Fermi surface in a weakly perturbed band structure. One expects also, below $T_f$, the appearance of an AF pseudogap (Fig. 5), with a density of states at the Fermi level decreasing with temperature and with doping. This phenomenon this phenomenon first observed by NMR [7– 9] in underdoped YBaCuO, i.e. for $c < c_t$, Fig. 1 (by study of both the Knight shift and the relaxation rate of Y, little sensitive to magnetic effects). Note that, in this region, the magnetic fluctuations seem to be too small to localise strongly by disorder the Fermi electrons.

**B. Superconductivity and density of states at the Fermi level [6]**

In reducing the density of states at the Fermi level, the AF pseudogap lowers the critical superconductive temperature $T_c$. This effect is the more important the lower the doping; it is prolonged continuously in the region of AF gap, with vanishing density of states and no $T_c$ at all. This explains naturally the rapid decrease of $T_c$ with doping in the underdoped range ($c < c_M$, Fig.1); this effect is independent of the nature of the coupling, if it is of the BCS type [8]; it has recently been taken into account in models of superconductive coupling through AF waves [10].

It must be stressed that many authors have wanted to see in the pseudogap appearing at $T_f$ an effect of superconductive fluctuations. It seems a priori not very reasonable to try to explain by the same physical phenomenon two curves, $T_f(c)$ and $T_c(c)$ so different in behavior in the phase diagram. One can also remark that $T_f(c)$ varies as expected for the AF fluctuations, as observed e.g. by neutron scattering. Finally the superconductive gap as measured by the Andreev reflection varies quasiparabolically with $c$, as $T_c(c)$; but the gap observed by normal tunnel effect or optically varies like $T_f(c)$, as expected for a gap due to AF fluctuations [14].

If this interpretation is correct, the AF fluctuations are much more developed than the superconductive ones in the underdoped range, at least in the compounds discussed here such
as YBaCuO or LaSrCuO. This might at least partly be due to a weakness of the magnetic interplane couplings compared with the superconductive interplane couplings. Other HTSC compounds might deviate from the phase diagram sketched Fig. 1.

C. Nature of superconductive couplings

In the BCS type of approach used here, two types of couplings can be dominating: attractive phonons, or repulsive electrons. As in other compounds, the observation of a possible anisotropy of the superconductive gap and a study of its form \( \Delta_k \) can give some indication on the nature of the couplings \( V_{k,k'} \), as indicated by the BCS gap equation

\[
\Delta_k = - \sum_{k'} \frac{V_{k,k'} \Delta_{k'}}{2 \sqrt{\Delta_{k'}^2 + \varepsilon_{k'}^2}} \tanh \frac{\sqrt{\Delta_{k'}^2 + \varepsilon_{k'}^2}}{2k_BT}.
\]  

(3.1)

where \( \varepsilon_{k'} \) is the one-particle energy measured from the Fermi level.

Following general arguments recalled in Appendix B, it is usually agreed that an \( s \) gap (Fig. 6a) or an anisotropic \( s \) one (e.g. \( s + g \), Fig. 6b) are the signature of phonon attractive couplings, while a \( d \) gap (Fig. 6c) or a \( d + s \) one (Fig. 6d) are due to predominantly electron-electron coupling, as due to AF waves for instance.

Many observations have in fact indicated the presence of \( d \) gaps in many HTSC compounds, thus favoring the idea of coupling through AF waves \[16,17\]. This would not be in disagreement with the general conclusion of this paper that a simple BCS weak coupling scheme could apply to HTSC compounds. In such a scheme, the exact role of the van Hove anomaly would have to be studied, although it was implicitly taken into account into computations \[17\].

Conclusions from experiments have however to be analysed carefully. Thus

–electron doped compounds show few signs of \( d \) gap symmetry, even if they have admittedly lower values of \( T_c \) than the corresponding hole doped ones. (However, there is a report on the existence of \( d \) gap \[18\].)

–recent measurements by Deutscher et al. \[19\] using Andreev reflection techniques, show for LaSrCuO a \( d \) gap for underdoped samples \((c < c_M, \text{Fig.1})\), but an anisotropic \( s \) gap for optimum \((c \simeq c_M)\) and for overdoped sample \((c > c_M)\). These measurements for anisotropic \( s \) gaps can indeed be fitted with computations by Bouvier and Bok \[21\] who, following Abrikosov \[20\], use a coupling by phonons screened in two dimensions. Deutscher’s results agree with Tsuei et al’s \[22\] on the quantification of vortices in grain boundaries giving a \( d \) gap in YBaCuO \((c \leq c_M)\), although a \( d + s \) gap is more likely near \( c_M \) \[23\]. Results by Tsuei and others on a number of HTSC compounds seem generally to obtain a \( d \) gap, but probably mostly on samples where an overdoping is not sure, either in the grains or in the grain boundaries.

It seems therefore that sizable \( T_c \)’s are compatible with observed (anisotropic) \( s \) gaps and phonon coupling. And Eq. (3.1) then leads to such values of \( T_c \), due to the fact that the van Hove anomalies are near the maximum of the gap in \( \mathbf{k} \) space. This is a priori what is to be expected in the overdoped normal metal range.

For the underdoped range \((c < c_M)\), the situation might be more complex. It might well be that a strong AF instability leads to a \( d \) gap. In compounds such as LaSrCuO with \( s \)
gaps for \( c \geq c_M \), one must then go, on reducing doping, through intermediary situations such as Abrikosov’s ([20], Fig. 6e) and Béal and Maki’s ([23], Fig. 6d) where either phonon or AF waves are respectively predominant, but both types of couplings are sizable.

The existence of an AF pseudogap for underdoped samples suggests however another interpretation of \( d \) gaps. In the case where the AF pseudogap is larger than the superconductive gap, i.e. for large enough underdopings, electronic states coupled by BCS all belong to the AF pseudogap, between the bonding B and the antibonding AB peaks, Fig.6. Each electronic state is then close to a linear combination of the type

\[
|K > = \alpha_k|k > + \beta_k|k - Q > ,
\]

(3.2)

where \( |\alpha_k| \simeq |\beta_k| \). The \( d \) anisotropy of the gap, due to that of \( V_{k,k'} \) can then come from that of the potential of interaction \( V_{k,k'} \). More precisely a coupling \( V_{k,k'} \) as described in \([20,21]\) (with \( V_{k,k'} < 0 \) and the maximum of \( |V_{k,k'}| \) for \( k \simeq k' \)) leads to a \( d \) gap if, near the Fermi level, \( \alpha_k\beta_k < 0 \) on the average. This is expected in hole doped YBaCuO, where \( Q = Q_R > 2k_F \): the Fermi level is then in the lower range of energy in the pseudogap, nearer to B (where \( \beta_k \simeq -\alpha_k \)) than to AB (where \( \beta_k \simeq \alpha_k \)). In a compound such as LaSrCuO, where \( Q \) is less than \( Q_R \), Appendix A shows that the same situation of Fermi level near the lower edge of the pseudogap might apply, with the same result of \( d \) gaps from phonon coupling.

**IV. CONCLUSIONS**

Experimental evidence shows that, at least in compounds such as LaSrCuO and YBaCuO, a delocalised electrons scheme with weak correlations applies to undoped as well as to doped HTSC compounds of the cuprate family; and it would be of interest to extend these X rays and NMR studies, when possible, to other compounds of the same family. It is also clear that, within such scheme, a weak BCS coupling is enough to explain high value of \( T_c \) if one takes into account the presence of (quasi) 2d van Hove anomalies. Exact estimates are however made difficult by the problems of interplane couplings and 2d superconductive fluctuations.

The high anisotropy of the superconductive gap \( \Delta \) explains the large deviations of the observed ratios of \( \Delta/T_c \) from what is expected from the classical isotropic BCS equations. The anisotropic \( s \) gaps observed in electron doped compounds and, more recently, in optimally and overdoped LaSrCuO (\( c \simeq c_M \)) are compatible with a classical phonon coupling. The \( d \) gaps observed in other overdoped compounds can be due to electron coupling; they would then be a signature of larger electron correlations.

The \( d \) gap observed in underdoped LaSrCuO, YBaCuO and a number of the other compounds might be due also to electron couplings which could take the form of coupling by AF waves, especially present in underdoped samples. The AF wave pseudogap, observed in the underdoped samples, decreases the density of states at Fermi level and thus \( T_c \) when it develops, that is for decreasing dopings. This last effect is independent of the nature of superconductive coupling; and indeed the presence of AF pseudogap might possibly explain a phonon coupling leading to \( d \) gap, owing to the special symmetry of the Fermi electrons in the AF pseudogap: this might explain the change of symmetry from \( d \) to \( s \) with increasing.
doping in a compound such as LaSrCuO. Finally this change of gap symmetry with doping, which occurs near maximum of $T_c$, must proceed continuously, in a way that has not been studied completely.

More experiments would be very valuable in this content, especially in three domains:

- anisotropy of the superconductive gap versus doping for hole doped samples in the over-doped and optimum ranges. And also for electron doped sample such as Nd$_{2-x}$Ce$_2$CuO$_4$, the doping dependence of the gap anisotropy might shed a light on the essence of HTSC.

- more systematic relation between AF fluctuations and transport properties in undoped as well as underdoped compounds, in electron doped as well as hole doped compounds.

- more precise properties of phonons in these materials have to be considered. If only intraplane pairings are envisaged, there are six relevant modes of lattice vibrations (there are three atoms CuO$_2$ in a unit cell). Two of them are acoustic and the rest are optical. The considerable complexity of these phonons [24], especially optical ones, should be taken into account. Certainly the simple models considered in [21,22] have to be reexamined.

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APPENDIX A: STABILITY OF AF PHASES

The band contribution to the stability of an AF gap or pseudogap, as pictured Fig. 5, is

$$\delta E = \int_{E_F}^{E_0} n(E)EdE - \int_{E_0}^{E_F} n_0EdE,$$

if $E_F$ and $E_0^F$ are the Fermi levels in presence and in absence of the gap respectively. The Coulomb correction in $U$ to this Hartree approximation is known not to alter qualitatively the conclusions of this typed of analysis.

The average number of electrons per CuO$_2$ in a plane is

$$z = 1 - c = \int_{E_F}^{E_0} n(E)dE - \int_{E_F}^{E_0} n_0dE.$$

This gives

$$\frac{d\delta E}{dz} = E_F - E_0^F, \quad (A3)$$

and

$$\frac{d^2\delta E}{dz^2} = \frac{1}{n(E_F)} - \frac{1}{n_0}. \quad (A4)$$

It is then easy to check that, for a gap due to long range AF order at $Q = Q_R$, $\delta E(Q_R, c)$ has a minimum at zero doping (Fig. A), with a break in the slope $d\delta E/dc$ related to the
gap $E_{AB} - E_B$ (Fig. A), thus to $U$. The symmetry of $\delta E(Q_R, c)$ is related to the symmetry of $n(E)$, itself due to the quasi one dimension of $E_k$ near zero doping (Fig. 3). For an AF order at $Q < Q_R$, the gap of $n(E)$ is expected to be smaller, thus also the stability of the AF phase; the increasing twodimensional nature of $E_k$ produces, for a given $Q$, a stability $\delta E(Q, c)$ less marked and more asymmetrical, which can be reasonably expected to be above $\delta E(Q_R, c)$ in most of the region of stability of the AF order at $Q_R$. This situation, pictured Fig A, could explain that the AF phases with $Q < Q_R$ could only appear, at 0K, outside the region of stability of the AF order at $Q_R$.

In the fluctuating regimes at finite $T$’s, the pseudogap which replaces the gap (Fig. 5) has the effect of diminishing the stability $\delta E(Q, c)$, and of rounding off the angle at the minimum of $\delta E$.

It seems that, for YBaCuO, the commensurate AF phase at $Q_R$ is always the most stable (case $Q$, Fig. A); in LaSrCuO, incommensurate AF phases appear above a finite hole doping (case $Q'$, Fig. A); because their stability decreases fast with decreasing $Q'$, they should appear systematically with a hole doping $c'$ slightly larger than that for the minimum of $\delta E(Q', c)$: Thus, in Fig. A, the phase $Q'(c)$ should only appear for hole concentrations larger than $c'$, where a common tangent touches $Q_R(c)$ and $Q'(c)$: to AB, Fig. 5.

**APPENDIX B: SYMMETRY OF GAP**

The interactions $V_{k,k'}$ obviously have the space group symmetry of the square (dihedral symmetry). The group elements $T$ are unity; rotations by $\pi/2$, $\pi$, and $3\pi/2$; and reflections about $k_x$ and $k_y$ axes and the lines $k_y = k_x$, and $k_y = -k_x$. Then one has

$$V_{Tk,Tk'} = V_{k,k'}.$$  \(\text{(B1)}\)

The gap $\Delta(k)$ created by the interaction $V_{k,k'}$ does not have to have the same symmetry, but it is significantly influenced.

All the reflections and a rotation by $\pi$ have the property $T^2 = \text{unity}$. Therefore even if the gap is not invariant with respect to these transformations there is a possibility that $\Delta(Tk) = -\Delta(k)$. We call this ‘odd parity’ and for $\Delta(Tk) = \Delta(k)$ ‘even parity’.

In order to consider the symmetry of $\Delta(k)$, let us divide the first Brillouin zone into eight octants (Fig. B). For the singlet pairing one has $\Delta(-k) = \Delta(k)$ (the symmetry of rotation by $\pi$ for $V_{k,k'}$). Thus it is enough to consider the gaps in the four regions in $k_y > 0$, $\Delta_1$, $\Delta_2$, $\Delta_3$, and $\Delta_4$ (Fig. B). The four directions $\pm k_x$ and $\pm k_y$ have the van Hove anomalies. The gap will be large in these direction due to the enhanced density of states. Therefore we have even parity for the reflections with respect to $k_x$ and $k_y$ axes. (Note that if one has odd parity, $\Delta = 0$ for the directions of the van Hove anomaly.)

Finally the parity with respect to the lines $k_y = \pm k_x$ will determine the full symmetry of the gap.

i) even parity : isotropic $s$ (Fig. 6(a)), $s + g(\ell = 4)$ (Fig. 6(b)) or something else.

ii) odd parity: $d$ symmetry (Fig. 6(c))

For attractive interactions $V_{k,k'}$ Eq. (B1) shows that the optimum value of $\Delta_k$ has necessary a constant sign, and the even parity follows. For phonon couplings, where $|V_{k,k'}|$ is maximum for $k = k'$ [20,21], the van Hove anomalies lead to a very anisotropic $s$ gap, Fig.6b.
For repulsive interactions, Eq.(3.1) requires the odd parity. For couplings by AF fluctuations, \( V_{k,k'} \) has a large peak at \( k' \approx k - Q_R \) (Fig. B); this leads to odd parity about the line \( k_y = k_x \) and \( k_y = -k_x \), thus to a \( d \) gap, Fig. 6c.
REFERENCES

[1] L.G. Bednorz and K.A. Müller, Z. Phys. B64, 199 (1986).
[2] J. Bardeen, L.N. Cooper, J.R. Schrieffer, Phys. Rev. 106, 162; 108, 1175 (1957).
[3] W.L. McMillan, Phys. Rev. 167, 331 (1968).
[4] P. Morel and P.W. Anderson, Phys. Rev. 125, 1263 (1962).
[5] R. Combescot, Europhys. Lett. 10, 177 (1989).
[6] J. Friedel, Physica C, 153-5, 1610(1988); J. Phys.: Condens. Matter. 1, 7757 (1989); Nato Institute on Condensed Matter, Biarritz (1990).
[7] H. Alloul, T. Ohno, and P. Mendels, Phys. Rev. Lett 38, 1700 (1989).
[8] J. Friedel, L.M. Sayers, J. Phys. (France) 38, 697 (1977).
[9] J.E. Hirsch and D.J. Scalapino, Phys. Rev. Lett. 56, 2732 (1986).
[10] D. Pines, The Gap Symmetry and Fluctuation in High Tc Superconductors edited by J. Bok, G. Deutscher, D. Pavuna and S.A. Wolf, NATO ASI Series, Series B Physics 371 (Plenum Press, New York 1998) p.111.
[11] G. Deutscher, The Gap Symmetry and Fluctuation in High Tc Superconductors edited by J. Bok, G. Deutscher, D. Pavuna and S.A. Wolf NATO ASI Series, Series B Physics 371 (Plenum Press, New York 1998) p.15.
[12] A. Maeda, H. Yasuda and T. Hanaguri, J. Phys. Soc. Jpn. (199), to be published.
[13] G. Deutscher, The Gap Symmetry and Fluctuation in High Tc Superconductors edited by J. Bok, G. Deutscher, D. Pavuna and S.A. Wolf NATO ASI Series, Series B Physics 371 (Plenum Press, New York 1998) p.503.
FIGURES

Fig. 1 Schematic phase diagram of hole doped oxides. AF: antiferromagnetically ordered phase; $T_c$: superconductive transition temperature; $T_f$: below this temperature the AF fluctuations are notable; $S$: superconductive phase; $c_M$: optimal doping; $c_t$: doping for disappearance of AF pseudogap.

Fig. 2 Cu 3$d$ and O 2$p$ orbitals and corresponding transfer integrals $t$, $t'$ in a CuO$_2$ plane.

Fig. 3 Fermi surface.

Fig. 4 Density of states $n(E)$ and van Hove anomaly.

Fig. 5 Symmetry of the anisotropic gap: a. $s$ symmetry; b. ’anisotropic $s$’ symmetry; c. $d$ symmetry; d. $d + s$ symmetry; e. very anisotropic $s$ gap.

Fig. 6 Gap ($T < T_N$) and antiferromagnetic pseudogap($T > T_N$).

Fig. A Stability $\delta E$ of commensurate($Q_R$) and incommensurate ($Q$) AF phases at $OK$ versus hole doping $c$.

Fig. B $\Delta$’s near half-filling.
Fig. 1

Fig. 2
Fig. 3

Fig. 4

Fig. 5
\[ \Delta_{1} \]

\[ \Delta_{2} \]

\[ \Delta_{3} \]

\[ \Delta_{4} \]