S and D Wave Mixing in High $T_c$ Superconductors

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(February 1, 1995)

Abstract

For a tight binding model with nearest neighbour attraction and a small orthorhombic distortion, we find a phase diagram for the gap at zero temperature which includes three distinct regions as a function of filling. In the first, the gap is a mixture of mainly $d$-wave with a smaller extended $s$-wave part. This is followed by a region in which there is a rapid increase in the $s$-wave part accompanied by a rapid increase in relative phase between $s$ and $d$ from 0 to $\pi$. Finally, there is a region of dominant $s$ with a mixture of $d$ and zero phase. In the mixed region with a finite phase, the $s$-wave part of the gap can show a sudden increase with decreasing temperature accompanied with a rapid increase in phase which shows many of the characteristics measured in the angular resolved photoemission experiments of Ma et al. in Bi$_2$Sr$_2$CaCu$_2$O$_8$

PACS numbers: 74.20.Fg, 74.70.Vg
Many experiments in the last few years have been interpreted in terms of a gap with \(d_{x^2-y^2}\) symmetry in the CuO\(_2\) planes. Among these is the penetration depth experiment of Hardy et al.\(^1\) which show a linear dependence over a large temperature range down to the lowest temperatures measured. This is illustrative of a large class of experiments indicating that the gap goes to zero on the Fermi surface but which are not sensitive to its phase. Many new experiments have been devised specifically to test the phase\(^2\) of the gap over the Brillouin zone with mixed results. Some favour \(d_{x^2-y^2}\) symmetry, others extended s-wave. Perhaps the most detailed information on the momentum dependence of the gap has come from a variety of angular resolved photoemission data.\(^7\)–\(^12\) Recently, Ding et al.\(^13\) have found that the zero’s in the gap are displaced somewhat from the main diagonals to either side of the \((\pi, \pi)\) direction. This can arise if the gap is not pure \(d_{x^2-y^2}\) but has an additional small s-wave component with zero relative phase between the two. This can be achieved if a small orthorhombic distortion is introduced in the CuO\(_2\) plane\(^4\) and in addition the bilayer nature of Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\) is taken into account to give nodes on both sides of the diagonal. In the experiment of Ma et al.,\(^17\) the temperature variation of the gap is investigated in different directions in the Brillouin zone. In particular, the gap is found small and perhaps zero near \(T_c\) in the \((\pi, \pi)\) direction and to increase rapidly below a reduced temperature of \(T/T_c = 0.8\). In the \((0, \pi)\) direction, the gap is large and follows more closely a BCS behaviour.

In this paper, we investigate the phase diagram for simple BCS model with first nearest neighbour attraction with a view at understanding its phase diagram as a function of filling \(n\) and of making connections with the experimental situation described above. For the band structure, we employ a tight binding model with first and second nearest neighbour hopping. For tetragonal symmetry, we find at zero temperature, as a function of decreasing filling a region of pure \(d_{x^2-y^2}\) symmetry which is followed by one of mixed \(d_{x^2-y^2}\) plus an extended \(s_{x^2+y^2}\) part with relative phase of \(\pi/2\) between the two pieces. Finally at yet lower filling, there is a region of pure \(s_{x^2+y^2}\) gap. If some small but finite orthorhombic distortion is introduced into the CuO\(_2\) plane, the situation changes considerably in the sense that no
pure \( d_{x^2-y^2} \) region remains. Instead, it is replaced by a mixture of mainly \( d_{x^2-y^2} \) but with a small admixture of \( s_{x^2+y^2} \) with no relative phase so that in this region, the nodes in the gap are shifted somewhat off the \((\pi, \pi)\) direction. As the filling is lowered at some particular critical value of \( n \), the relative phase starts growing sharply from 0. In this regime there are only point nodes in the gap at \((\pm \pi/2, \pm \pi/2)\) in the Brillouin zone of the CuO\(_2\) plane. This increase in relative phase is accompanied by a rapid increase in the \( s_{x^2+y^2} \) part and similar sharp decrease in \( d_{x^2-y^2} \). When the phase has increased to \( \pi \), the \( s \)-wave part dominates and the gap will again have zeros on the Fermi surface. Adding an on site repulsion to the model changes the range of the various regions somewhat but more distinctively adds a small constant component to the gap which can be of the same or opposite sign as the \( s_{x^2+y^2} \) part.

The BCS gap equation determines the energy gap or order parameter \( \Delta_k \) as a function of momentum \( k \) in the reciprocal lattice. To describe electrons in a 2-dimensional CuO\(_2\) plane, we will use a tight binding dispersion relation with up to second nearest neighbours of the form

\[
\varepsilon_k = -2t [\cos(k_x a) + (1 + \delta) \cos(k_y a)] - 2B \cos(k_x a) \cos(k_y a) - (2 - 2B - \mu) \tag{1}
\]

with \( t \) the first nearest neighbour hopping parameter which is often assumed to be 100meV, \( B \) second neighbour hopping in units of \( t \) often taken to be \( B = 0.45 \) for Y\(_1\)Ba\(_2\)Cu\(_3\)O\(_7\) and \( \mu \) is the chemical potential. The final parameter \( \delta \) in equation (1) is an orthorhombic distortion introduced into the CuO\(_2\) plane which could be thought of as roughly modeling the existence of chains in YBaCuO. It has almost become conventional to eliminate the chemical potential in Eq. [1] in favour of the filling factor \( n \) defined as

\[
n = \frac{2}{\mathcal{N}} \sum_k \left[ 1 - \frac{\varepsilon_k}{E_k} \tanh \left( \frac{1}{2} \beta E_k \right) \right], \tag{2}
\]

where the sum over \( k \) is over the first Brillouin zone of the CuO\(_2\) plane and \( \mathcal{N} \) is a normalization factor so that half filling corresponds to \( n = 1 \).
In momentum space, the BCS gap equation is given in terms of the pairing potential $V_{k-k'}$ and the temperature $\beta^{-1} = k_B T$ by

$$\Delta_k = \frac{1}{N} \sum_{k'} \left[ V_{k-k'} \frac{\Delta_{k'}}{2E_{k'}} \tanh \left( \frac{1}{2} \beta E_{k'} \right) \right],$$  \hspace{1cm} (3)

with $E = \sqrt{\varepsilon_k^2 + \Delta_k^2}$ the quasiparticle energies in the superconducting state.

The nearest neighbour part of the pairing potential has the form:

$$V_{k-k'}^{(nn)} = 2g_x \cos(k_x - k'_x) + 2g_y \cos(k_y - k'_y),$$ \hspace{1cm} (4)

where $a_x$ and $a_y$, the lattice parameters, are both taken to be $a$. In Eqs. (3) and (4) it can be set equal to one if the momentum is measured in units of $2\pi/a$. In Eq. (4), $g_x$ and $g_y$ are coupling constant taken to be equal and their value set by the desired value of critical temperature $T_c$ or of gap amplitude. With the form in Eq. (4) for the pairing potential, the BCS equation, Eq. (3), can be solved by convolution using fast Fourier transform techniques using

$$\Delta_k = \frac{1}{N} \sum_{k'} V_{k-k'} F_{k'} = \mathcal{F}^{-1} \left[ \mathcal{F} [V_k] \cdot \mathcal{F} [F_{k'}] \right],$$ \hspace{1cm} (5)

where $\mathcal{F}[x_k] \equiv \sum_k e^{i k \cdot r_k} x_k$ is the Fourier transform operator and $F_k \equiv \Delta_k \tanh (\beta E_k/2) / 2E_k$.

Another technique for solving the gap equation, Eq. (3), with the pairing potential of Eq. (4) is to expand the interaction in terms of separable functions:

$$V_{k-k'}^{(nn)} = 2g_x \left\{ \cos(k_x') \cos(k'_x) - \sin(k_x) \sin(k'_x) \right\}$$

$$+ 2g_y \left\{ \cos(k_y') \cos(k'_y) - \sin(k_y) \sin(k'_y) \right\},$$ \hspace{1cm} (6)

The $\sin(k_{x,y})$ terms do not contribute for singlet pairing. For a general separable interaction of the form:

$$V_{k-k'}^{(sep.)} = \sum_{n,m} v_{n,m} \hat{n}_{k}^n \hat{n}_{k'}^m$$ \hspace{1cm} (7)

of which Eq. (6) is a special case, we can write Eq. (4) as:

4
\[ \Delta_k = \sum_n \eta^n_k \sum_m \nu_{n,m} \frac{1}{N} \sum_{k'} \eta^{m}_{k'} F_{k'}, \quad (8) \]

and we see that \( \Delta_k \) has no more components \( \eta^n_k \) than there are in the interaction. We will assume the \( \eta^n_k \) to be an orthonormal set and only a few are needed to represent Eq. 8. The fast Fourier transform technique for solving Eq. 8 serves as a check on the alternate method represented in Eq. 8 which involves a set of coupled integral equations which can be solved by vector integration. Before presenting results (similar work can be found in references 18–20) for the solution of the gap equation, we present, for completeness, the expression for the penetration depth \( \lambda^{-2}_{i,j}(T) \) which is a tensor. Results for this quantity will be given in the next section. The expression for \( \lambda^{-2}_{i,j}(T) \) is:

\[ \lambda^{-2}_{i,j} \propto \sum_{k} \frac{\partial \varepsilon_{k}}{\partial k_i} \frac{\partial \varepsilon_{k}}{\partial k_j} \left[ \frac{\partial f(E_k)}{\partial E_k} - \frac{\partial f(\varepsilon_k)}{\partial \varepsilon_k} \right] \quad (9) \]

where the \( \frac{\partial \varepsilon_{k}}{\partial k_i} \) are related to Fermi velocities and the overall constant in Eq. 9 is of no interest here.

In Fig. 1, we show a phase diagram for the gap at zero temperature as a function of filling \( n \) (see Eq. 3) for a case \( t = 100 \text{meV}, B = 0.45, T = 0 \) and \( g_{x,y} = 0.75t \). A small orthorhombic distortion \( \delta = 0.1 \) is also included in the calculations. Throughout the phase diagram, only the two components \( d_{x^2-y^2} \propto (\cos(k_x) - \cos(k_y)) \) and \( s_{x^2+y^2} \propto (\cos(k_x) + \cos(k_y)) \) appear in the gap. The amplitude multiplying these two functions are denoted by solid circles (\( d_{x^2-y^2} \) part) and solid square (\( s_{x^2+y^2} \) part). The relative phase \( \phi \) between the two basis functions is also given. We note that in the region down to approximately \( n = 0.45 \), the solution at zero temperature \( T = 0 \) is mainly \( d \)-wave with a small admixture of extended \( s \)-wave. The relative phase between these two components is zero throughout this region which means that the zero line nodes of the gap will be displaced somewhat off the main diagonals. This is seen in the angular resolved photoemission data of Ding et al.(13) although our model includes a single plane and nodes are found only on one side of the diagonals and not on both sides as seen in the experiments. This can be understood, however, quite naturally if a bilayer model were used to model \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \) instead of the single plane model.
used here. The small admixture of \( s_{x^2+y^2} \) just described is due entirely to our use of a small orthorhombic distortion in the electronic dispersion and the amplitude of this component would be zero in a pure tetragonal case so that we would get instead, in this case, a region of pure \( d_{x^2-y^2} \) in our phase diagram.

Next, we note in Fig. that below approximately \( n = 0.45 \) up to about 0.28, we have a region of admixture of extended s-wave and \( d_{x^2-y^2} \) coexistence but with a finite relative phase of \( \phi \). For \( \phi = \pi/2 \), the admixture is roughly of equal proportion while a small relative phase corresponds to a small amount of extended s and a phase near \( \pi \) a small amount of \( d_{x^2-y^2} \). Below \( n \approx 0.28 \), we recover a region of zero relative phase but with the two amplitudes having opposite signs and the \( s_{x^2+y^2} \) part dominating. If an orthorhombic distortion was not included in our calculation the phase would always be \( \pi/2 \) but the \( s_{x^2+y^2} \) component would only set in at some critical hole concentration \( n_{c1} \) and the \( d_{x^2-y^2} \) component would drop to zero sharply at some other smaller critical concentration \( n_{c2} \) with \( n_{c1} \) and \( n_{c2} \) dependent on the parameters of the theory such as details of the pairing potential and the underlying band structure.

The region of finite phase (not zero or \( \pi \)) in Fig. is very interesting and was investigated further. For a fixed value of filling \( n \) taken to be 0.36, we show in Fig. our results for the two components of the gap as a function of temperature. At high temperatures near the critical temperature \( T_c \), we have a sharply rising \( d_{x^2-y^2} \) (solid circles) component as \( T \) is reduced and a small \( s_{x^2+y^2} \) (solid squares) component. There is zero phase between these two components. But abruptly at \( T \approx 36K \) to be compared with a critical temperature of approximately 68K the phase switches on and the \( s_{x^2+y^2} \) component starts rising quite rapidly. Our results are in qualitative agreement on these points with the angular resolved photoemission data of Ma et al. Of course our phase diagrams only roughly approximate the observed doping dependance. In view of this we make no attempt to fit the data since our model is quite simplified and, in particular, does not include the bilayer nature of the CuO\(_2\) planes in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_8\), and so in the high temperature regime, our gap nodes fall only on one side of the diagonals. At lower temperature, once there is a finite relative
phase between the two components, the line node in the gap at the Fermi surface is lost, of course, because it is no longer real and both real and imaginary components would need to vanish simultaneously. For a $d_{x^2-y^2}$ and $s_{x^2+y^2}$ mixture, this can happen only at four points $(\pm \pi/2, \pm \pi/2)$ which, in general, will not fall on the Fermi surface. This can be seen in much more detail in Fig. 3, but before doing so, we point out the insert in Fig. 2 in which we show the unnormalized penetration depth in the two principles in plane directions as a function of temperature. Since $\delta \neq 0$ in our calculations, $\lambda_{xx}^{-2}$ and $\lambda_{yy}^{-2}$ will be different although, as can be seen from the figure, their temperature dependence tracks each other fairly well and both show a clear change in slope at $T = 36K$, the point at which the relative phase $\phi$ becomes finite.

In Fig. 3, we show contour plots of the gap in the two dimensional CuO$_2$ plane Brillouin zone as well as a plot of the Fermi surface. Four frames are shown. Two correspond to the region above the second critical temperature $T_{c2} \approx 36K$ and two below. Above $T_{c2}$, the phase between the two components of the gap is zero and so the order parameter is real and its value can be plotted as a function of $k_x$ and $k_y$. We see in Fig. 3 (frame b) positive and negative contours for $\Delta(T = 40K)$ and that the zero contour is not a straight line along the diagonal as it would be for pure $d_{x^2-y^2}$ wave. Instead, it is displaced below the diagonal around $(\pi, \pi)$ and above it around $(0, 0)$. Only at $(\pi/2, \pi/2)$ is it exactly on the diagonal. Referring again to Fig. 2, it is clear that the amount the node in the gap at the Fermi surface will have moved off the main diagonals will depend on temperature. In frame (d) of Fig. 3, we show $|\Delta(T = 40K)|$ rather than its actual value. This graph differs from frame (b) only in as much as all contours are for positive values of the gap. It is to be used for easier comparison with the data of frame (a) which is for $|\Delta(T = 30K)|$. In this case, the gap is complex and there is no zero contour for $|\Delta(T = 30K)|$. The amount of change in the contours as compared to the previous frame (d) is not large, however, since the temperature has not been changed by much. The final set of contours shown in frame (c) are for low temperature and now these are quite different. We note, in particular, that $|\Delta(T = 1K)|$ has a value near 6meV at the Fermi surface in the direction $(\pi, \pi)$ and about
16meV for the (0, π) direction in rough agreement with the experimental situation found in Bi$_2$Sr$_2$CaCu$_2$O$_8$.\(^{(17)}\)

Using a simple tight binding model for the electron dispersion relation and a pairing potential involving a nearest neighbour attraction, we have calculated a phase diagram for the gap as a function of filling including in the calculation a small orthorhombic distortion. At high filling, the gap is found to be mainly of $d_{x^2-y^2}$ symmetry with a small admixture of extended s-wave ($s_{x^2+y^2}$) less than 10\% in our work. The phase between the two components at zero temperature is zero so that in this region of phase space there are line nodes and the zeros of the gap in the Brillouin zone are slightly displaced off the diagonal. The degree of displacement increases with decreasing filling. In our work, the $s_{x^2+y^2}$ component is completely due to the orthorhombic distortion and disappears in a tetragonal system. At some critical filling $n_{c1}$, a phase develops between $d_{x^2-y^2}$ and $s_{x^2+y^2}$ components. As the phase grows rapidly with decreasing filling, the amount of $d_{x^2-y^2}$ component decreases rapidly and the amount of $s_{x^2+y^2}$ increases. At some lower critical filling $n_{c2}$ not so different from $n_{c1}$, the phase becomes $\pi$ and remains at this value for $n \leq n_{c2}$ in which case the state is mainly $s_{x^2+y^2}$ with a smaller admixture of $d_{x^2-y^2}$. In a tetragonal system, the concentrations $n_{c1}$ and $n_{c2}$ would be between the boundary of pure $d_{x^2-y^2}$ and mixture $d+is$ and between $d+is$ region and pure s wave respectively with the phase in the mixed region exactly $\pi/2$.

In the region of finite phase $\phi$ for the zero temperature gap, the temperature variation of the gap is complicated. At high temperature near $T_c$ (equal to 68K for the case considered), the gap is real and is an admixture of mainly $d_{x^2-y^2}$ with a small amount of $s_{x^2+y^2}$ so that the zero gap contours are displaced from the main diagonals. At some critical temperature equal to 36K in our example, a finite phase develops between the s and d components. While the $d_{x^2-y^2}$ component changes little at this temperature and shows an overall temperature dependence that is similar to that of an isotropic superconductor, the $s_{x^2+y^2}$ abruptly increases with decreasing temperature as observed in the angular resolved photoemission experiments of Ma et al.\(^{(17)}\) In this temperature region, the gap shows no zeros on the Fermi surface and in our model ends up at $T = 0$ with $s_{x^2+y^2}$ part roughly half the $d_{x^2-y^2}$ part. These
ratios depend on the parameters used of course. Calculation of the temperature dependent penetration depth show a clear change in slope of both the $x$ and $y$ components of the in plane penetration depth, $\lambda_{xx}^{-2}$ and $\lambda_{yy}^{-2}$, at $T = 36$K.

Research supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC) and by the Canadian Institute for Advanced Research (CIAR). We thank P. Soininen for discussions and interest.
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FIGURES

FIG. 1. Phase diagram for the gap at zero temperature as a function of hole concentration with \(n = 1\) corresponding to half filling. The parameters used in the calculations are \(t = 100\) meV for the nearest neighbour hopping parameter, \(B = 0.45\) for next nearest neighbour hopping, \(\delta = 0.1\) for the orthorhombic distortion in the dispersion curves and \(g_{x,y} = 0.75t\) for the nearest neighbour pairing potential. The solid circles give the amplitude of the \(d_{x^2-y^2}\) component and the solid squares the extended \(s_{x^2+y^2}\) component. The gap in meV is given by the left hand side vertical axis while the phase between the two components is given by the open circles and the scale is shown on the right hand side vertical axis. It varies from 0 to \(\pi\).

FIG. 2. The temperature dependence \((T)\) of the gap for a case with filling \(n = 0.36\) which falls in the region of finite phase \(\phi\) and complex gap in the phase diagram of Fig. 1. The other parameters are as given in Fig. 1. The critical temperature is 68K. The amplitude of the \(d_{x^2-y^2}\) component is given by the solid circles and that of the \(s_{x^2+y^2}\) by the solid squares. The phase which sets in abruptly at \(T = 36\)K is shown as the open circles. Again, the scale for the gap is on the left hand side in meV and for the phase on the right hand vertical axis in degrees from (0 to 90). The inset shows the temperature dependance of the x and y penetration depths.

FIG. 3. Contours of the gap as a function of momentum in the first Brillouin zone of the CuO\(_2\) plane. Also shown is the Fermi line for filling \(n = 0.36\). Because of the orthorhombic distortion included in our work through the parameter \(\delta\) in the dispersion curve, the Fermi surface does not have tetragonal symmetry and is open in the horizontal direction and crosses the gap contours. Frame (a) is for \(|\Delta(T = 30\)K|\), frame (b) for \(\Delta(T = 40\)K\), frame (c) for \(|\Delta(T = 1\)K|\) and frame (d) for \(|\Delta(T = 40\)K|\). Note that the value of the basis functions at \((0, \pi)\) is two times the amplitude in Fig. 2.
(a) $|\Delta(T = 30\, \text{K})|$

(b) $\Delta(T = 40\, \text{K})$

(c) $|\Delta(T = 1\, \text{K})|$

(d) $|\Delta(T = 40\, \text{K})|$