Temperature dependent gap anisotropy in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ as evidence for a mixed-symmetry ground state

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(September 17, 2018)

Abstract

In a recent experiment, Ma et al. measured the temperature dependence of the gap anisotropy of oxygen-annealed Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$. Their measurements were taken along the two directions $\Gamma - M$ and $\Gamma - X$. They found that the gap along both directions is nonzero at low temperatures and that the ratio is strongly temperature dependent. We show, using Ginzburg-Landau theory, that this behavior can be obtained if one assumes the existence of s-wave and d-wave components for the order parameter. Our theory predicts orthorhombic anisotropy in the gap and anomalous behavior for the electronic specific heat below $T_c$.

PACS numbers: 74.20.Mn, 74.25.Nf, 74.72.Bk, 74.25.Bt
The most central issue in high-\(T_c\) superconductivity at the present time is the nature of the order parameter. Many experiments have attempted to clarify the form and symmetry of the order parameter, with the most conclusive being of the phase-sensitive tunneling variety \([1,2]\). These indicate that the gap function changes sign when rotating by \(\pi/2\) in momentum space. This suggests a d-wave order parameter in the system studied, namely \(\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\) with small \(\delta\). Spin-fluctuation models of high-\(T_c\) lead to d-wave superconductivity \([4,5]\). Strong correlation models have a similar instability to d-wave pairing \([6,7]\). Thus the experiments on \(\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\) may be taken as a confirmation of the magnetic mechanism in general. To distinguish between the two models is not an easy problem. However, variational Monte Carlo (VMC) calculations on a strong correlation model, the extended t-J model, have suggested that, while a d-wave is the dominant instability, s-wave and d-wave mixing may be the favored ground state for higher doping levels \([8]\) and certain band structure parameters \([9]\). From this point of view, not all high-\(T_c\) systems are alike, and it becomes crucial to perform experiments on different systems and, most importantly, at different doping levels.

Apart from the tunneling technique, the most direct measurement (although not phase-sensitive) is angle-resolved photoemission (ARPES). A recent experiment by Ma et al. \([10]\) used ARPES to investigate the gap in \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}\) single crystals. In particular this group has measured the gap at two points on the Fermi surface: \(\Delta(\Gamma - M)\) or \(\Delta(k_x = 0)\) in our coordinate system (along the Cu-O bond) and \(\Delta(\Gamma - X)\) or \(\Delta(k_x = k_y)\). This was done as a function of temperature. The basic features of the experimental results are: (i) the gap \(\Delta(\Gamma - M)\) opens up quickly below \(T_c\) and \(\Delta(\Gamma - M) > \Delta(\Gamma - X)\) for all temperatures; (ii) \(\Delta(\Gamma - X)\) is small or even zero for \(T > 0.8 T_c\) and then increases gradually as \(T\) is further reduced, leading to a strongly temperature-dependent gap anisotropy; (iii) there are indications of upward curvature in \(\Delta(\Gamma - X)\); (iv) the temperature dependence of \(\Delta\) is weak in both directions for a wide range of temperatures (from \(T=0\) K to \(T=0.7 T_c\) approximately). These data are different from results obtained by other workers on \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}\) \([11,12]\) in that the gap along \(\Gamma - X\) is not always small. This is due to annealing in an oxygen
atmosphere, leading to higher oxygen content and the presumably to a higher hole doping level in the CuO$_2$ planes. [10]

We do not possess a detailed microscopic theory of s-d mixing and the VMC calculations are restricted to T=0. Thus we work within the framework of Ginzburg-Landau theory. The point group symmetry of the CuO$_2$ planes in the temperature range of interest is orthorhombic C$_{2v}$, due to buckling of the planes [13]. In this symmetry the interesting thing is that an order parameter with d-wave symmetry transforms according to the identity representation. [These symmetry issues are discussed in detail in Ref. [8]]. So from a strict symmetry point of view a d-wave and an s-wave are indistinguishable. The concept of a two-component order parameter, where one component has an s-wave symmetry and the other a d-wave symmetry is thus well-defined only in the tetragonal case. In the present orthorhombic case we can regard the s-d mixing as a strong temperature dependent anisotropy which nevertheless never actually breaks the crystalline symmetry. If we write the Ginzburg-Landau free energy density as follows:

$$f = \alpha_0^s(T - T_s)|\Psi_s|^2 + \alpha_0^d(T - T_d)|\Psi_d|^2 + \beta_s|\Psi_s|^4 + \beta_d|\Psi_d|^4 + \beta|\Psi_s|^2|\Psi_d|^2$$

$$+ \beta_{sd} \left( \Psi_s^2 \Psi_d^2 + c.c. \right) + \gamma (\Psi_s \Psi_d^* + c.c.),$$

the difference from the case of tetragonal symmetry is the addition of the final bilinear term. In fact the coupling constant $\gamma$ is proportional to the orthorhombic distortion $b - a$ where $b$ and $a$ are the lattice constants in the Cu-O plane. Note that in our case, the gradient terms are not necessary due to the absence of external fields and the assumed homogeneity of the material (translational invariance). We minimize the free energy with respect to $|\Psi_s|$ and $|\Psi_d|$ and the phase difference of the two components $\phi$. The phase difference is crucially important. If it is zero then the resulting state is s+d: the gap function is real (except for the overall phase related to gauge freedom). If $\phi$ is nonzero the state is more similar to s+id: it breaks time reversal symmetry and has no nodes.

The minimization leads to coupled equations which we have solved numerically. The result of the calculations is that, according to the sign of the parameter $\beta_{sd}$ in the above
functional, there are two possibilities for the value of $\phi$. It is either zero or there is a transition from a continuous value (temperature dependent) to zero. We attempted to fit the data with a temperature dependent phase shift without success. The data therefore point to the $s+d$ state. So we adopted the case $\phi = 0$ for the phase difference between the two components of the order parameter. We chose $\beta_{sd} < 0$ (which then essentially adds to $\beta$) and $\gamma < 0$. The equations we have to solve in order to get the order parameters become:

$$\alpha_{s,d} |\Psi_{s,d}| + 2\beta_{s,d} |\Psi_{s,d}|^3 + (\beta + \beta_{sd}) |\Psi_{d,s}|^2 |\Psi_{s,d}| + \frac{\gamma}{2} |\Psi_{d,s}| = 0.$$  \hfill (2)

The gap function we consider is of the form:

$$\Delta(k) = |\Psi_d| f_d(k) + |\Psi_s| f_s(k),$$  \hfill (3)

where $k$ lies on the Fermi surface. The assumed forms of the $k$-dependence are:

$$f_d(k_x = k_y) = 0, f_d(k_x = 0, k_y) = 1$$  \hfill (4)

$$f_s(k_x = k_y) = f_s(k_x = 0, k_y) = 1$$  \hfill (5)

Accordingly, the gap along the $\Gamma-X$ direction is the solution $|\Psi_s|$ whereas along the $\Gamma-M$ direction it is $|\Psi_s| + |\Psi_d|$. In order to compare the data over the whole temperature range to experiment we used the approximation $\alpha_{s,d}/\beta_{s,d} \propto [\tanh(\nu(T_F - 1)^{1/2})]^2$. For $\nu = 1.74$ this form gives a good fit to the weak-coupling BCS temperature dependence of the gap. Increasing $\nu$ is a way of mocking up strong-coupling effects. In Fig. [1] we show the results of the fitting to experimental data. Several features of the fit are noteworthy. A strong-coupling value of the parameter $\nu$ must be used in order to represent feature (i) mentioned above. $T_s$ must be lower than $T_d$ by about 15 K so that the s-component is suppressed near $T_c$, feature (ii) above. The upward curvature in $\Delta(\Gamma-X)$ [feature (iii)] is only produced by having a nonzero value of $\gamma$, the bilinear coupling of the two components. Finally, the tangent function in the coefficients of the quadratic terms in the free energy produces a temperature independent gaps at low $T$, as in ordinary BCS theory, [feature (iv)]. There is only one second order transition.
Near $T_c$ the gap is pure d-wave, with gap zeros in the diagonals and maxima along the axes. As the temperature is reduced, the s-wave component grows, the nodes move towards the $k_y$ axis and the gap along this axis become smaller while the gap along the $k_x$ axis becomes larger. Thus it is a temperature-dependent orthorhombic anisotropy. We take, for illustration purposes only, a circular Fermi surface with $f_d = \cos(2\theta_k)$, $f_s = 1$. Then the zeros of the gap move from a value of $\theta_k = \pi/4$ close to $T_c$ to a value which is temperature dependent ($\theta_k = -1/2 \arccos(-\Psi_s/\Psi_d)$). This is shown in Fig. 2. In this extreme example the zeros of the gap move all the way to the $k_y$ axis and then disappear. We stress that this disappearance is a highly model-dependent phenomenon, depending, for example on the detailed momentum dependence of the s-wave component. On the other hand, the qualitative result that the zeros of the gap will move as the temperature is varied is a firm prediction of the two-component theory as long as the components have different temperature dependences, as is indicated by the experiments. Note also that experiments such as the reported in Ref.1 which depend only on the relative phase change under a $\pi/2$ rotation in k-space and will not be affected by a small movement of the nodes.

In Fig. 3, the anisotropy ratio $\Delta(\Gamma - X)/\Delta(\Gamma - M)$ is plotted as a function of temperature. The dramatic temperature variation of this quantity is well reproduced by the strong-coupling parameters. Also in Fig. 4, the form of the heat capacity (in arbitrary units) is plotted. Since we are interested for values close to $T_c$, we used the linear form of the parameters $\alpha_s$ and $\alpha_d$, in such a way that the first term of the Taylor expansion (with $T_c$ instead of $T$ in the denominator) of the hyperbolic tangent agrees. The hyperbolic tangent form was chosen above in order to compare the data with the theory at much lower temperatures. A somewhat anomalous behaviour of $C_v(T)$ is predicted, with a local maximum around 0.7 $T_c$. This comes from the sharp growth of the second component in the order parameter in this temperature range.

We do not claim that the fit in Fig. 1 is a quantitative confirmation of the two-component theory. The curves are smooth and the numbers of parameters large. It is true, however, that the temperature-dependent anisotropy of the superconducting gap in BSCCO is what
one expects if a two-component order parameter exists. A pure d-wave order parameter alone cannot account for the data. Our main point in this paper is to note that the two-component picture has a number of surprising consequences which may be checked in highly hole-doped BSCCO. These are: the gap energy should have orthorhombic anisotropy at low temperatures; there should be upward curvature in $\Delta(\Gamma - X)(T)$ already suggested by the existing data; the position of the gap nodes should be temperature-dependent; there should be a peak in the electronic specific heat close to $0.7 T_c$.

We would like to thank Marshall Onellion, Ron Kelley, Jian Ma, Christoph Quitmann for valuable discussions. This work was supported by the National Science Foundation under grants No. 9214739 and No. 921047.
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FIGURES

FIG. 1. Shows the gap along the two directions of the Fermi surface in comparison to the experimental data. The solid line is the solution for $\nu = 3.0$ (the values of the parameters are: $\alpha_s/\beta_s = -250[\tanh(3.0(0.8T_c/T - 1)^{1/2})]^2$, $\gamma/\beta_s = \gamma/\beta_d = -100$, $\beta/\beta_s = \beta/\beta_d = 2$, $\alpha_d/\beta_d = -220[\tanh(3.0(T_c/T - 1)^{1/2})]^2$, the dashed line is the solution for $\nu = 1.74$ (the values of the parameters are: $\alpha_s/\beta_s = -340[\tanh(1.74(0.8T_c/T - 1)^{1/2})]^2$, $\gamma/\beta_s = \gamma/\beta_d = -100$, $\beta/\beta_s = \beta/\beta_d = 2$, $\alpha_d/\beta_d = -280[\tanh(1.74(T_c/T - 1)^{1/2})]^2$).

FIG. 2. Shows the zeros of the gap as a function of temperature, for the hypothetical circular Fermi surface. At low temperatures there are no zeros in the gap according to the model and $\Psi_s$ is greater than $\Psi_d$.

FIG. 3. Shows the anisotropy ratio defined as $\Delta(\Gamma - X)/\Delta(\Gamma - M)$ for the value of $\nu = 3.00$.

FIG. 4. The specific heat as predicted by the model. Near $0.7T_c$ there is a local maximum.