

Temperature dependent gap anisotropy from interlayer
tunneling

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Abstract

A recent experiment by Ma and collaborators shows that the gap anisotropy in $\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_{8+x}$ is strongly temperature dependent. In particular, the superconducting gap along the $\Gamma - M$ direction shows a weaker temperature dependence than the gap along the $\Gamma - X$ direction which decreases rapidly with temperature. We explain this novel feature as a natural consequence of the interlayer tunneling mechanism of superconductivity.

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The nature of the order parameter in the cuprate superconductors is of central importance to the study of high temperature superconductivity. While several experiments such as IR reflectivity [1], Raman spectroscopy [2], NMR [3] and Josephson tunneling [4] imply that a conventional s-wave order parameter as in BCS theory is unlikely, Angle Resolved Photoemission Spectroscopy (ARPES) provides direct evidence that the gap in the cuprate superconductors is highly anisotropic [5]. The main results that can be inferred from low temperature ARPES [6] are : (i) the superconducting gap attains its maximal value along the $\Gamma - M$ direction (Cu-O bond direction in real space); (ii) the gap is smallest along the $\Gamma - X(Y)$ direction (diagonal to the Cu-O bond direction) and (iii) there is a monotonic increase in the magnitude of the gap from its smallest value along the $\Gamma - X$ line to the largest value along $\Gamma - M$, thereby indicating true anisotropy.

In a recent paper [7], Ma and co-workers have presented the first detailed analysis of photoemission spectra of superconducting Bi 2212 observed along $\Gamma - M$ and $\Gamma - X$ directions at different temperatures. Their results show that the gap anisotropy observed in this material is *strongly dependent on temperature*, contrary to what happens in conventional anisotropic superconductors such as Pb. In particular they show that the gaps observed along the two high symmetry directions obey different temperature dependences. The gap along the $\Gamma - M$ direction shows a very weak temperature dependence whereas the gap along $\Gamma - X$ decreases rapidly as temperature increases. Consequently, the gap anisotropy increases with temperature by about a factor of 8 before falling to zero at T_c . Since these results reflect the property of the superconducting condensate in the two different high symmetry directions, they impose constraints on possible mechanisms of high temperature superconductivity.

In this letter, we show that these results can be explained by the interlayer tunneling mechanism of high temperature superconductivity [8]. We show that the gap equation resulting from interlayer tunneling [9] readily distinguishes between the gaps along the $\Gamma - M$ and $\Gamma - X$ directions and the temperature dependences of the gaps along these two high symmetry directions are completely different. Therefore, a temperature dependent gap anisotropy

follows very naturally from the interlayer tunneling mechanism. Our analysis shows that the gap anisotropy increases rapidly with temperature and the results are consistent with those reported in ref. [7].

We begin by writing the gap equation from interlayer tunneling [9],

$$\Delta_k = T_J(k) \frac{\Delta_k}{2E_k} \tanh \frac{\beta E_k}{2} + V_{BCS} \sum_q' \frac{\Delta_q}{2E_q} \tanh \frac{\beta E_q}{2}. \quad (1)$$

This equation can be obtained by considering two close Cu-O layers as in Bi 2212 coupled by a Josephson tunneling term of the form,

$$H_J = -\frac{1}{t} \sum_k t_{\perp}^2(k) (c_{k_1}^\dagger c_{-k_1}^\dagger d_{-k_1} d_{k_1} + \text{h.c.}),$$

where t is a band structure parameter in the dispersion of electrons along the Cu-O plane and $t_{\perp}(k)$ is the bare single electron hopping term between the two coupled layers c and d . The quantity $T_J(k)$ in the right hand side of equation (1) is given by $T_J(k) = \frac{t_{\perp}^2(k)}{t}$. The dispersion of electrons along the Cu-O plane is chosen to be of the form

$$\epsilon(k) = -2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y,$$

with $t = 0.25$ eV and $\frac{t'}{t} = 0.45$. We also choose $\epsilon_F = -0.45$ eV corresponding to a Fermi surface which is closed around the Γ - point. These choices are inspired by band structure calculations [10]. Note that the Josephson coupling term in H_J conserves the individual momenta of the electrons that get paired by hopping across the coupled layers. This is as opposed to a BCS scattering term which would only conserve the center of mass momenta of the pairs. This is the origin of all features that are unique to the interlayer tunneling mechanism. The second term in the right hand side of equation (1) is obtained by postulating that the dominant *in-plane* pairing mechanism is the electron-phonon interaction. The primed sum in equation (1) is over a shell about the Fermi surface of width $\hbar\omega_D$, the Debye energy.

Let us first consider equation (1) in the limit of zero temperature [9]. We then have

$$\Delta_k = \frac{T_J(k)}{2E_k} \Delta_k + \Delta', \quad (2)$$

where $\Delta' = V_{BCS} \sum_q' \frac{\Delta_q}{2E_q}$, is a finite s-wave component of the gap. Obviously, the anisotropy in the gap at zero temperatures is principally due to the momentum dependence of $T_J(k)$, viz., that of $t_{\perp}(k)$. This momentum dependence can be inferred from electronic structure calculations. As shown in ref. [9], it is adequate to choose $T_J(k) = \frac{T_I}{16} (\cos k_x - \cos k_y)^4$ to reproduce the results of such calculations. With this choice then, it is obvious from equation (2) that the gap is smallest when $T_J(k) = 0$ (as long as $T_J > V_{BCS}$). This happens when $k_x = k_y$. Therefore along the $\Gamma - X(Y)$ directions where $k_x = k_y$, the gap attains its smallest value Δ' . The largest value of the gap is obtained when the Fermi surface includes the points where $T_J(k)$ is maximum, viz., $(0, \pm\pi)$ and $(\pm\pi, 0)$. In this case, the value of the gap is given by $\frac{T_I}{2} + \Delta'$ as can be seen from equation (2). So, we see that the zero temperature gap from interlayer tunneling is highly anisotropic with maxima at $(0, \pm\pi)$ and $(\pm\pi, 0)$ and minima along the $k_x = k_y$ line. These results are in agreement with the ARPES data on gap anisotropy at low temperatures. We now show that this gap anisotropy increases as temperature increases.

To see this we go back to the gap equation at finite temperature, equation (1). We first consider the gap at $(0, \pi)$ on the $\Gamma - M$ line, $\Delta(\Gamma - M)$ which is given by

$$\Delta(\Gamma - M) = \frac{T_J}{2} \tanh \frac{\beta \Delta(\Gamma - M)}{2} + \Delta'(T), \quad (3)$$

where

$$\Delta'(T) = V_{BCS} \sum_q' \frac{\Delta_q}{2E_q} \tanh \frac{\beta E_q}{2}.$$

The temperature dependence of $\Delta(\Gamma - M)$ will be governed by the first term in the right hand side of equation (3) since we always choose to work in the limit of $\Delta'(T) \ll T_J$. This limit corresponds to the physical choice of T_J giving rise to high transition temperatures rather than the electron-phonon interaction V_{BCS} . Since the structure of the gap equation (3) is very different from that of the BCS gap equation, it is clear that the temperature dependence of $\Delta(\Gamma - M)$ will be unlike that of a BCS gap. For instance, $\Delta(\Gamma - M)$ will fall steeper near T_c than a BCS gap would. This is seen most simply in the limit $\Delta'(T) \rightarrow 0$ [11]. In this limit, the zero temperature gap $\Delta_0(\Gamma - M) = \frac{T_I}{2}$. It is readily seen that the temperature at

which $\Delta(\Gamma - M)$ falls to half its zero-temperature value is given by $\frac{T_J}{8 \tanh^{-1}(\frac{1}{2})}$. For typical values of t_1 and t , this temperature corresponds to $T \sim 0.95T_c$. Consequently, we expect $\Delta(\Gamma - M)$ to show a weak temperature dependence at low and intermediate temperatures. It should be emphasized that this temperature dependence (as given by the first term in the right hand side of equation (1)) is directly due to the "momentum-space locality" of the Josephson interaction H_J .

We have solved equation (3) for temperatures ranging from 0 to T_c . Our choice of parameters are : $t = 0.25$ eV, $t' = 0.1125$ eV and $\epsilon_F = -0.45$ eV as mentioned earlier, $t_1 = 0.091$ eV, $V_{BCS} = 0.06$ eV and $\hbar\omega_D = 0.02$ eV. This choice of parameters leads to a purely *in-plane* T_c of ~ 5 K and a bulk T_c of 83K. The zero temperature gap at $(0, \pi)$, $\Delta_0(\Gamma - M)$ is found to be 18.09 meV. In fig.(1), we have shown our results for the temperature dependence of $\Delta(\Gamma - M)$ and compared them with the experimental results of Ma et al [7]. For completeness, we have also calculated the temperature dependence of an order parameter having mixed s and d - symmetries. Note in particular that the measured gap (a) is very weakly temperature dependent at low and intermediate temperatures and (b) falls very steeply near T_c . As we mentioned earlier, both these features follow directly from equation (3) as consequences of the Josephson interaction H_J . In view of this, we suggest that PES along the $\Gamma - M$ direction actually probes the gap resulting from interlayer tunneling.

We now consider the gap along the $\Gamma - X(Y)$ directions where $k_x = k_y$. In this case, the first term in the right hand side of equation (1) drops out and the gap $\Delta(\Gamma - X)$ is given by

$$\Delta(\Gamma - X) = \Delta'(T) = V_{BCS} \sum_q \frac{\Delta_q}{2E_q} \tanh \frac{\beta E_q}{2}. \quad (4)$$

It is obvious that the temperature dependence of $\Delta(\Gamma - X)$ will be different from that of $\Delta(\Gamma - M)$. Note that equation (4) looks very much like the BCS gap equation. However it should be emphasized that $\Delta(\Gamma - X)$ is *not* a BCS gap since the sum in equation (4) also contains the T_c enhancement effects of the Josephson interaction. In fact our results show that the gap $\Delta(\Gamma - X)$ falls much faster from its zero temperature value than a BCS gap does. Therefore we get a non BCS-like temperature dependence for $\Delta(\Gamma - X)$

as well. It is not necessary to solve equation (4) to obtain the temperature dependence of $\Delta(\Gamma - X)$ since $\Delta(\Gamma - X) = \Delta'$ and we have already solved for $\Delta'(T)$ when we obtained the temperature dependence of $\Delta(\Gamma - M)$. From our results for $\Delta(\Gamma - M)$, it is easy to see why $\Delta(\Gamma - X)$ decreases rapidly with temperature. For instance, as T increases from $0.1T_c$ to $0.8T_c$, $\Delta(\Gamma - M)$ decreases from 18 meV to 13 meV, we find that Δ' has to decrease by a factor of 3 for equation (3) to be self consistent. This is because of the first term in the right hand side of equation (3) which depends weakly on temperature. Therefore, the rapid decrease of $\Delta(\Gamma - X)$ with temperature is actually a consequence of the weak temperature dependence of $\Delta(\Gamma - M)$. We have obtained $\Delta(\Gamma - X)$ for various temperatures with the same set of parameters as before. We find that there is a quantitative discrepancy between our results and those of Ma et al. With our choice of parameters, we find the zero temperature value of the gap along $\Gamma - X(Y)$, $\Delta_0(\Gamma - X) \sim 2$ meV. This value is closer to the values reported in earlier ARPES experiments [6]. On the other hand, the low temperature value quoted by Ma et al is $\Delta(\Gamma - X) = 10 \pm 2$ meV at $T = 0.48 T_c$. While it is possible for us to tune V_{BCS} and obtain larger values of $\Delta(\Gamma - X)$ without altering T_J and T_c substantially, we have not done so for the following reasons. The first is that the observed values of the gaps along $\Gamma - X$ are very sensitive to sample quality and the time elapsed between cleaving and observation of the spectrum [6]. Secondly, we feel that given the level of approximation involved in this modelling, such a fine-tuning of parameters is unwarranted. Instead, to see how the gap anisotropy increases with temperature, we only consider the temperature dependence of $\Delta(\Gamma - X)$ normalized to its zero temperature value. This is still meaningful as we are only interested in seeing how the gap anisotropy grows from its low temperature value and not in the absolute values of the gaps themselves. On comparing our results for the temperature dependence of $\Delta(\Gamma - X)$, with those of Ma et al, we find that at low and intermediate temperatures there is a discrepancy of 5-10%. At temperatures close to T_c , the discrepancy is slightly more. This is because the experimental results indicate that the gap becomes vanishingly small at $0.84 T_c$ whereas a mean field theory such as ours would always produce gaps $\Delta(\Gamma - M)$ and $\Delta(\Gamma - X)$ that vanish self consistently at identical

temperatures.

In fig.(2), we have shown the temperature dependences of both $\Delta(\Gamma - M)$ and $\Delta(\Gamma - X)$ as obtained from equation (3). The solid line shows the temperature dependence of the former and the dashed line shows that of the latter. We find that $\Delta(\Gamma - X)$ falls to half its zero-temperature value at temperatures as low as $0.6T_c$! The observed experimental value of this temperature is $0.64T_c$ [7]. Recall that a conventional BCS gap falls to half its zero-temperature value at $T \sim 0.9T_c$. As $T \rightarrow T_c$, we find that $\Delta(\Gamma - X)$ decreases by an order of magnitude at $T \sim 0.9T_c$ while at this temperature, $\Delta(\Gamma - M)$ has only decreased by a factor of 2. Thus, the gap anisotropy increases from its low temperature value by a factor of 5.

For completeness, we have also investigated the temperature dependence of the gap anisotropy when the order parameter has mixed s- and d- wave symmetries. We have done this because the low temperature ARPES results [6] can also be explained by any model exhibiting d-wave superconductivity [12]. However the results of ref. [7], particularly the temperature dependent gap anisotropy cannot be obtained from an order parameter having pure d-wave symmetry. This is because the anisotropy ratio of the gap for any two k vectors is temperature independent if the gap function has a purely d-wave character. One possibility is an order parameter with mixed s- and d- symmetries. The pairing potential leading to such an order parameter will be of the form

$$V_{kk'} = V_0 + V_1(\cos k_x - \cos k_y)(\cos k_{x'} - \cos k_{y'}) .$$

We have solved the gap equation resulting from this interaction for various choices of V_0 and V_1 without including the interlayer Josephson interaction. We find that at low temperatures, the gap anisotropy always decreases irrespective of the relative strengths of V_0 and V_1 . At intermediate temperatures, it is possible to obtain an increase in the gap anisotropy by fine-tuning the parameters but this increase is only marginal. These results underscore the importance of the Josephson interaction H_J in establishing and enhancing the gap anisotropy.

Finally, we address the question of the sensitivity of our results *vis a vis* our choice of parameters. We have solved equation (1) for various choices of t_{\perp} and V_{BCS} keeping the other parameters fixed. We find that as long as the value of the s-wave component of the gap is much smaller than T_J , i.e., in the limit of interlayer tunneling being stronger than any intralayer interaction, the gap anisotropy always increases with temperature and differences in results are only quantitative.

To conclude, we have shown that the interlayer tunneling mechanism produces a gap anisotropy that grows with temperature. This is because the gap equation from interlayer tunneling leads to different temperature dependences for the gaps along the two high symmetry directions in Bi 2212. The gap along the $\Gamma - M$ direction shows a much weaker temperature dependence than the gap along the $\Gamma - X$ direction which decreases rapidly as temperature increases. Consequently, the gap anisotropy increases with temperature by a factor of ~ 5 . This is in good agreement with experimental results that show an increase by a factor of ~ 8 . Our results and those of Chakravarty et al. [9] show that the interlayer tunneling mechanism of high temperature superconductivity can account satisfactorily for the ARPES experiments in superconducting Bi 2212.

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Figure Captions

All the results were obtained with the following choice of parameters : $t = 0.25$ eV, $t' = 0.1125$ eV, $\epsilon_F = -0.45$ eV, $t_{\perp} = 0.091$ eV, $V_{BCS} = 0.06$ eV and $\hbar\omega_D = 0.02$ eV.

1. $\Delta(\Gamma - M)$ as a function of the reduced temperature $\frac{T}{T_c}$. Solid line is as calculated from equation (3) in text. The experimental data is from ref. [7].
2. Temperature dependence of the gaps (normalized to zero temperature values) along $\Gamma - M$ (solid line) and $\Gamma - X$ (dashed line) as a function of reduced temperature obtained from equation (3).

