Gap anisotropy in the angle-resolved photoemission spectroscopy of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$

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Abstract

The gap anisotropy in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ is revisited in the framework of a d-wave scenario in view of the recent angle-resolved photoemission experiment. Based on a tight-binding fit to the normal state dispersion, a detail analysis on the effects of the inclusion of the next harmonic in the d-wave has been presented. Significant effect has been observed in the superconducting $T_c$. The density of states is linear at the nodes with enhanced weight, caused by a marked increase in the low energy excitations which affect the thermodynamics considerably. The slope of the $\rho_s - T$ curve in the low temperature regime increases and the specific heat reflects the enhanced entropy at low temperatures. The leading edge of the ARPES energy distribution curves have been calculated and found to shift towards higher energy. The effect of scattering by non-magnetic impurities in this context are also outlined.

PACS Nos. 74.72-h, 74.20.Fg

Introduction

The nature of the superconducting gap anisotropy in the high temperature superconductors has attracted a lot of attention in the last few years[1, 2]. A considerable progress has been made in the recent past with the resolution and clarity of the angle-resolved photoemission spectroscopy (ARPES) having reached a very high level backed by careful and thorough analysis of the data[3]. A general consensus seems to have emerged that the symmetry of the order parameter (OP) in most of the high temperature superconductors is predominantly d-wave. In a very recent ARPES experiment on the underdoped Bi2212 system Mesot et. al.[4] have reported an observable departure from a simple interpretation in terms of the usual d-wave symmetry. Inclusion of the next higher harmonic in the superconducting pairing function seems to give a better fit to their data. We develop the idea in order to look for other observable effects of such a term, and calculate its effects on various physical quantities in the framework of the usual phenomenological theory[7] in the weak coupling limit and suggest further experiments. We have calculated the changes in superconducting transition temperature, nodal structure on the fermi surface (FS), the density of states (DOS) in the superconducting state and its effect on the specific heat. The energy distribution curves (EDC) (that are seen in the ARPES experiments) are also obtained. Fluctuations

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are included in one loop level and the superfluid density (and hence the penetration depth) is obtained as a function of temperature. We observe the differences in slopes of $\rho_s(T)$ in the low temperature regime with increasing level of mixing of the higher harmonic. We also calculate the effect of both doping and the mixing of higher order terms on the specific heat.

**Model and Calculations**

In the experiments of Mesot et al, ARPES results have been fitted to a d-wave gap function for several Bi2212 systems. The maximum gap values have been adjusted at each of the doping levels for the best fit, and the EDCs at different angles and the slope of the gap function close to the node have been carefully fitted. Clear deviation from the usual $d_{x^2-y^2}$ behaviour is observed and attempts were made to fit the data with an admixture of about 4-10% of the next harmonic $\cos(6\phi)$. A much improved fit was indeed obtained with the inclusion of this higher order term. As one underdopes the system, the normal state resistivity is known to increase and effective screening becomes weaker. Under such a situation it is reasonable to assume that the higher harmonics in the effective interactions have to be brought in, and highly sensitive experiments would reveal the effects due to the growing range of interaction. In the spin fluctuation models too the pairing interaction grows sharply in the momentum space with underdoping and long range effects in real space become increasingly relevant.

We undertake to examine the ramifications arising out of the addition of the higher harmonic with a model band structure that reproduces the observed FS and the location of the van-Hove singularity in Bi2212 accurately. The six parameters describing the hopping on the BiO plane used to obtain the fit were [0.131, -0.149, 0.041, -0.013, -0.014, 0.013] (in eV), corresponding to a doping of $\delta = 0.17$. The van-Hove singularity, due to the saddle points $k = (\pi, 0), (0, \pi)$ is 30meV below the FS, as observed in ARPES.

Superconductivity occurs through attractive long range interactions of which we keep only the near-neighbour part. Combined with the fact that there is a reasonably strong on-site repulsion between the electrons in the cuprates, forcing the pairing function $\Psi(r = 0) = 0$, such an interaction is known to support d-wave pairing. The vanishing of the on-site part of the pairing function implies that the $\sum_q \Delta(q) = 0$, where the $q$-sum runs over the entire Brillouin zone (BZ), thereby contributing equal regions of positive and negative sign to the OP. The usual $d_{x^2-y^2}$ (or $\cos(2\phi)$) OP admits of such constraints. All the higher harmonics, $\cos[(2 + 4n)\phi]$ are also admissible under the symmetry restrictions of the d-wave. In the underdoped systems, it is likely that higher neighbour interactions contribute increasingly, but in the present analysis we kept only the first of such terms. We also include only the singlet component of the order parameter in our analysis, as there is no reason so far to include the triplet part in the parameter regions that one works with in these systems.

The superconducting gap equation that is numerically solved is the usual mean-field
factorized gap equation

\[ \Delta_k = \frac{1}{N} \sum_{k'} V(k - k') \frac{\Delta_{k'} \tanh(\beta E_{k'}/2)}{2E_{k'}} \]

where \( V(k - k') \) is written in the separable form

\[ V(k - k') = g \eta(k) \eta(k') \]

Here we have chosen the basis function \( \eta(k) \) to be the \( B_1 \) representation of the one dimensional irreducible representations of \( C_{4v} \), \( \eta(k) = \frac{1}{2} (\cos k_x - \cos k_y) \) (the usual \( d_{x^2-y^2} \) symmetry); \( g \) measures the strength of the attractive interaction. The triplet channels of pairing have not been considered in the foregoing. The value of \( g \) was chosen (320 meV) such that the transition temperature \( T_c \) at \( \delta = 0.17 \) remains close to 80K (without any admixture of \( \cos(6\phi) \) term). In the spirit of Mesot et al., we introduced the next order term \( \cos(6\phi) \) in \( \eta(k) \) as \( \eta(k) = \alpha \cos(2\phi) + (1 - \alpha) \cos(6\phi) \), where \( \alpha \) measures the relative contributions of the two terms.

The superconducting gap has been calculated for each filling \( \delta \) at different levels of mixing of the higher harmonic. As representative curves, we show in Fig.1 the ones with 0, 4, 10 and 20% of mixing for \( \delta = 0.17 \). The solutions of the gap function for different \( \alpha \) show typical square root behaviour as \( T \to T_c \). The transition temperature (and \( \Delta(0) \)) reduces considerably as \( \alpha \) deviates from one (the inset to Fig. 1). The gap function with the same set of values of \( \alpha \) are drawn in the Y-quadrant (Fig. 2) for a demonstration of how they change with the mixing of \( \cos(6\phi) \). Similar shifts have been seen by Mesot et al. as well.

Calculation of the density of states (DOS) in the superconducting state with and without the higher harmonic term is straightforward. For \( \alpha = 1 \), one gets the usual d-wave DOS with \( \rho(E) \propto |E| \) for \( E \to 0 \). Addition of the higher harmonic term makes the rise steeper as there are now more excitations available at lower energy though the low energy behaviour of the DOS remains the same (linear). In Fig. 3 the DOS is shown for the normal and the broken symmetry states (with only \( \alpha = 1 \), as the \( \alpha = 0.8 \) curve is indistinguishable in the scale of that figure). The typical d-wave V-shaped DOS is obtained with the shoulders at \( \pm \Delta \) around \( E = 0 \). The inset shows for a comparison, in an enhanced scale of energy, the effect of the addition of the higher harmonic term. The pile-up of states at lower energy is quite evident.

In order for an analysis of the ARPES spectra we take the point of view that the spectral function \( A(k, \omega) \), convoluted with the fermi function \( f(\omega) \) and the resolution of the detector, gives the EDC. The ARPES intensity (without the detector resolution) is given by \( I_0 f(\omega) A(k, \omega) \) where, \( I_0 \) is a prefactor weakly dependent on \( T \) and \( \omega \). It depends on the incident photon energy, momentum and the (electron-phonon) matrix element between the initial and final states. The momentum resolution of the detectors used in experiments considered is about one degree in the BZ and is assumed constant over a circular window of 1° radius. With the incident photon energy around 20eV, the energy resolution of the detector is taken to be a Gaussian of standard deviation 7meV, a value consistent with the present day experimental resolutions.
With all these taken into account, the ARPES intensity is given by

$$I(k, \omega) = I_0 \int_{k'} \int_{\nu} \tilde{G}(\omega - \nu) f(\nu) A(k', \nu).$$

Here $\tilde{G}(\omega)$ is the Gaussian energy resolution function discussed above and the $k'$-integration is within a circular radius of $1^\circ$. The spectral function is the usual mean-field one

$$A(k, \omega) = u_k^2 \delta(\omega - E_k) + v_k^2 \delta(\omega + E_k)$$

where, $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$, and the coherence factors $u_k^2 = \frac{1}{2} (1 + \epsilon_k/E_k)$, $v_k^2 = \frac{1}{2} (1 - \epsilon_k/E_k)$.

Taking the normal state dispersion $\epsilon_k$ discussed above, $A(k, \omega)$ at five representative angles (on the FS) $\phi = 0, 10, 23, 35, 45$ have been calculated and their frequency and momentum-resolved behaviour (Fig. 4) obtained. The angles are measured with respect to the line $(\pi, \pi) - (\pi, 0)$ as is the practice[7]. We have restricted ourselves to the Y-quadrant of the Brillouin zone in order to avoid the complications with the shadow bands that appear in the X-quadrant due to the presence of an incommensurate superlattice (along $\Gamma - Y$ direction) in the BiO planes[4, 7]. We choose a point on the FS (at the above angles), and perform the resolution averaging around that point in momentum and frequency. Extreme care is required in evaluating the averages on the FS where the band is most dispersive, i.e., around $45^\circ$. Panel 1 in Fig. 4 shows frequency averaged $A(k, \omega)$ and panel 2, the momentum-averaged one. The procedure has been repeated for $\alpha = 1.0$ and 0.90 to show the effects of the higher harmonic on the gap function as one moves along the FS.

With the momentum and frequency averaged $A(k, \omega)$ obtained, it is easy to calculate the ARPES intensity around different points on the FS. The curves at different angles are shown in panel 3 of Fig. 4. The maximum gap is taken to be 30 meV, the same as used by Mesot et al, for demonstration. The temperature used is 10K, a typical value used in experiments at low temperatures.

It easily follows from the above discussions that the thermodynamic properties will be affected by the addition of the higher harmonics. We calculate the specific heat as a function of temperature (Fig. 5) in the superconducting state by taking a derivative of the entropy with temperature. Figs. 5 (a), (b) and (c) show the specific heat for different values of $\alpha$ at several levels of doping. It is clear from the graphs (a) - (c) that in order to account for the extra entropy, the curves move up as higher harmonics are brought in and then the area is conserved with reduced transition temperatures. As the doping increases, the curvatures of the Fermi surface affect the specific heat as seen in the normal state specific heat curve in (c). At $T_c$ the specific heat jumps to its normal state value as is typical of a second order transition.

The calculation of superfluid density $\rho_s$ has been performed using the standard techniques of many body theory[6, 11]. The diamagnetic and paramagnetic contributions to the current (and hence the phase stiffness) are calculated in the linear response by first making a Peierls substitution $t_{ij} = t_{ij} \exp(i e / \hbar) \int_{l_j} A \cdot d l$ in the hopping matrix element. The paramagnetic contribution at long wavelengths (via excitations above the condensate) in the linear response
theory is obtained in terms of the correlation function

\[ j^x_{\text{para}}(q) = \frac{i}{c} \lim_{\tau \to 0} \lim_{\omega \to 0} \int d\tau \theta(\tau) e^{i\omega\tau} \langle [j^x_{\text{para}}(q, \tau), j^x_{\text{para}}(-q, 0)] \rangle A_x(q). \]

The correlation function on the RHS is calculated at the one-loop level. Calculation of the diamagnetic contribution (from the Meissner condensate) is straightforward:

\[ j^x_{\text{dia}}(q) = -\frac{e^2}{N\hbar^2 c} \sum_{k, \sigma} \langle c_{k, \sigma}^\dagger c_{k, \sigma} \rangle A_x(q). \]

In the resulting expression, the OP values were taken as their mean-field unrenormalized (by the fluctuations) ones, a procedure that is known to work except very close to \( T_c \). The resulting \( \rho_s - T \) curves are shown in Figs. 6 for \( \alpha = 1, 0.9 \) and 0.8 at different doping levels. Note that the calculations were done in the gauge \( A_y = 0 \) and the gauge invariance is restored if vertex corrections are included. Such an approximation entails neglecting the vortex-like fluctuations in the 2D model. The above expression for \( \rho_s \) is derived for an isotropic order parameter but is expected to work quite well even in the anisotropic case at hand as the asymptotic form of the vortex-vortex interaction (at high vortex density) is logarithmic and corrections to the expression above due to these fluctuations are indeed small.

**Results and Discussion**

The nature of the OP gleaned from Fig. 1 shows a sensitive dependence on \( \alpha \), going down as mixing increases. The \( \cos(6\phi) \) term changes sign four times now in each quadrant and such rapid changes average out to a smaller value. This is more pronounced if the next higher harmonic (\( \cos(10\phi) \)) is introduced. As \( \alpha \) decreases, the \( \Delta \) versus \( \phi \) curve becomes flatter around the node (Fig.2) enhancing the quasiparticle excitations above the condensate. Such excitations will reflect in a reduced \( T_c \) (and \( \Delta(0) \)) and pile up of states in the DOS at low energies (Fig. 3). This will, of course, affect the thermodynamics considerably. For example, though the specific heat follows the typical (mean-field) \( T^2 \) behaviour of a d-wave superconductor at low temperature, the increased entropy at lower energy (for \( \alpha \) deviating from one) manifests itself in the specific heat curves (Fig. 5).

The ARPES line shapes are shown in Fig. 4. The frequency and momentum-averaged spectral function is plotted in panel 1 and panel 2 at different angles relative to \( (\pi, \pi) \) on the FS. \( A(k, \omega) \) (not shown) has the usual delta function behaviour, two sharp peaks separated by \( 2\Delta \) at \( \phi = 0 \) and closing in as \( \phi \) increases and finally merging at \( \phi \to 45^\circ \). The frequency broadening (panel 1) is a mere consequence of the Gaussian averaging procedure on the \( A(k_F, \omega) \). Strong angle dependence is observed in panel 2 where momentum averaged \( A(k_F, \omega) \) is plotted for different \( \phi \). The OP does not change within the \( k \)-window for small angles, while for large angles, the effects are very strong. At large angles the band is highly dispersive and large changes in energy occur within the \( k \)-window. The \( k \)-dependence of the OP further enhances this angle dependence since close to the node \( \Delta_k \) varies linearly with \( k \) while at the gap-maximum the variation is a weaker quadratic one. The \( k \)-averaged spectral weight for \( \alpha = 0.9 \) shows perceptibly smaller gap as \( \phi \) increases. Such a reduction of the gap has been observed by Mesot et al. The effect of \( \alpha \) is clearly visible in the EDCs in panel 3.
The leading edges for the curves corresponding to $\alpha = 1$ and 0.90 move continuously away from the fermi energy as $\phi$ decreases, the curve for $\alpha = 1$ moving more rapidly. This is the scenario depicted in Mesot et al. for seven different angles, where the best fit is obtained with $0.89 \leq \alpha \leq 0.96$ for different samples. The peaks observed in our EDCs are due to the mean-field pile-up of states, and not due to electronic correlations\[14].

The superfluid density $\rho_s$ is proportional to $\lambda^{-2}$ ($\lambda$ is the penetration depth) and has a power law dependence on temperature\[15\] at low temperatures. Figs. 6 (a)-(c) show $\rho_s$ for three representative $\alpha$ (1.0, 0.90 and 0.80) and is seen to fall off faster with the inclusion of the higher harmonics. As observed earlier\[15, 16\], the curves are linear to a high degree close to zero temperature. We observe that the slope of $\rho_s(T \to 0)$ decreases monotonically with increasing $\alpha$ (i.e., increasing $T_c$). As temperature rises, excitations from the condensate tend to decrease $\rho_s$ at the expense of normal quasiparticles above the condensate. The gradual flattening of the $\Delta - \phi$ curve with decreasing $\alpha$ around the node makes quasiparticle excitations more accessible at lower temperatures, causing a faster descent of $\rho_s$ with temperature. We have also calculated $\rho_s$ at different doping levels and find that the slope increases as one underdopes, consistent with the observations of Mesot et al.

It is known that non-magnetic impurities act as pair breaking scatterers for a $d$-wave superconductor\[18\]. Repeated scattering even with small momentum transfer on the fermi surface between lobes of opposite sign in the Brillouin zone effectively reduces the average gap value\[19\] thereby reducing the $T_c$. Owing to the presence of the $\cos(6\phi)$ term, such pair-breaking processes are clearly going to be more efficient and will reduce the transition temperature as the higher harmonic components increase\[12\]. The pair breaking effect of momentum dependent impurity potential and anisotropic gap including the higher harmonics have been studied recently\[20\] by solving the Abrikosov-Gorkov equations in the T-matrix representation where it has been found that states begin to appear in the gap as the impurity potential as well as the higher harmonic component is increased thereby reducing both the superconducting gap and the transition temperature.

In conclusion, we have worked out the effects due to the increasing presence of higher harmonics observed recently in a $d$-wave superconductor on underdoping. Based on the standard phenomenological theory for $d$-wave superconductors\[7, 9\], we observe that the transition temperature, density of states, specific heat, superfluid density, ARPES intensity and the slope of the OP at the node bear clear and detectable signature of this higher order term. Although the interaction between quasiparticles have not been included in the above, the conclusions drawn remain valid qualitatively on strong physical grounds as has been shown in a number of occasions earlier\[7, 6\]. The predictions made here are easily verifiable experimentally and will shed light on the nature and strength of the higher order term claimed to be present in these superconductors. More experiments are also required to fully understand the origin and the physics behind such additional terms.
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Figure captions

Fig. 1. Normalized (by $\Delta(0)$ at $\alpha = 1$) gap versus temperature for four different values of $\alpha$. The inset shows variation of the transition temperature with $\alpha$.

Fig. 2. The order parameter as a function of angle (measured with respect to the line $(\pi, \pi) - (\pi, 0)$ in the first BZ as in refs.[4, 7]) with increasing mixture of the higher harmonic.

Fig. 3 The Density of States in the superconducting state (dotted line) with $\alpha = 1$ and in the normal state (solid line) at $\delta = 0.17$. The inset shows the difference in the DOS for $\alpha = 1$ and $\alpha = 0.8$ in the superconducting state close to the node at very low temperature (the gaps were 15 meV and 11.8 meV as in Fig. 1).

Fig. 4. The frequency- and momentum-averaged $A(k, \omega)$ (panel 1 & 2) and the corresponding EDCs (panel 3, see text) at various angles (measured from $Y - \bar{M}$ direction) on the FS (shown outside the panel in the Y-quadrant). Figures (a)-(e) are for angles 45, 35, 23, 10 and 0 degree. The solid and dotted lines correspond to $\alpha = 1.0$ and 0.9.

Fig. 5 The specific heat curves at three different levels of mixing of the higher harmonic ((a), (b) and (c) correspond to $\delta = 0.10, 0.17$ and 0.28). The figures clearly reveal the enhanced quasiparticle excitations as $\alpha$ deviates from one.

Fig. 6. The superfluid density is shown against temperature for three different values of $\delta = 0.10, 0.17$ and 0.28 (Figs. (a)-(c)). The change in slope at low temperatures is clearly visible.
\[ \Delta(T) \]

\[ T(K) \]

- \( \alpha = 1.00 \)
- \( \alpha = 0.96 \)
- \( \alpha = 0.90 \)
- \( \alpha = 0.80 \)
\[ \alpha = 1.0 \]
\[ \alpha = 0.8 \]

DOS energy (eV)

energy (eV)
(a) $\alpha = 1.0$
(b) $\alpha = 0.9$
(c) $\alpha = 0.8$

$C$ (mJ/mol-K) vs $T$ (K)