Temperature Dependent Photoemission Studies of Optimally Doped $Bi_2Sr_2CaCu_2O_8$

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High resolution angle-resolved photoemission is used to study the electronic structure of optimally doped $Bi_2Sr_2CaCu_2O_8$. These studies, with an energy resolution of 8 meV, show that the sharp peak observed in the superconducting state has an intrinsic width of the order of 14 meV. Detailed temperature dependent studies reveal that this peak is fixed in binding energy at all temperatures at which it is observable and further that it exists at temperatures even above the superconducting transition temperature T_c. However, our analysis indicates that with the onset of long range phase coherence a gap emerges in the spectral response between the main incoherent peak and the Fermi level. [S0031-9007(99)08634-2]

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The mechanism responsible for the high T_c observed in the cuprate superconductors remains the subject of intense research activity. Among the many experimental probes, photoemission studies have provided a number of insights including the observation of an anisotropy in the superconducting gap of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) [1], the presence of a pseudogap in the normal state of the same material in the underdoped regime [2,3], and the possibility of extended Van Hove singularities in the $YBa_2Cu_4O_8$ superconductor [4]. Several studies have offered a description of the BSCCO photoemission spectra which, in the superconducting state, are characterized by a sharp feature immediately below the Fermi level near the $(\pi, 0)$ point in the Brillouin zone. Shen and Schrieffer [5] argue that in the case of underdoped samples, these spectra recorded near the $(\pi, 0)$ point show evidence that the photohole couples strongly to a collective mode whose spectral function peaks near $Q = (\pi, \pi)$ as observed in neutron scattering studies of the cuprates. In a model of Norman and Ding [6], the presence of the sharp peak in the superconducting state is thought to reflect a rapid change in the imaginary component, $\mathrm{Im}\Sigma$, of the self-energy at the transition temperature T_c. Above T_c a large $\mathrm{Im}\Sigma$ results in the broad spectrum characteristic of the normal state; below T_c a small $\mathrm{Im}\Sigma$ results in a sharp quasiparticle feature appearing in the spectrum.

One theoretical model of high temperature superconductivity proposes the separation of the electronic structure of the underlying material into distinct regions represented by the spin and charge degrees of freedom. The segregation of doped holes leads to a dynamical local charge inhomogeneity in which the mobile holes are confined to charged stripes which are domain walls for the spins in the intervening undoped antiferromagnetic regions [7]. Locally the electronic structure in such a system would be quasi-one-dimensional in character. Furthermore, in such a system, unlike the BCS theory, the pairing of electrons and the long range phase coherence would occur at different temperatures. Evidence for the presence of the stripe phases has been found in neutron scattering studies of the superconducting materials of the La_2CuO_4 family [8] and of $YBa_2Cu_3O_{6.6}$ [9]. Several photoemission studies have been interpreted in terms of such a model. In a study of optimally doped BSCCO in the normal state, Saini *et al.* claim the observation of a one-dimensional state dispersing along the $(\pi, 0)$ direction consistent with the presence of the 1D magnetic fluctuations [10]. In a more recent study of underdoped BSCCO, Shen *et al.* have proposed that detailed studies of line shape changes in the spectra above and below T_c are indicative of a momentum transfer of spectral weight possibly consistent with the presence of the stripes [11].

As we have noted, the development of a superconducting gap has been central to the discussion of photoemission spectra from these materials. The anisotropy or d-wave symmetry of the gap has been determined by the binding energy or leading edge of the sharp feature in the spectra [1]. The presence of the pseudogap, having the same d-wave symmetry, is taken as evidence of electron pairing well above the transition temperature T_c for the underdoped phase [2,3]. In the present paper we again focus on the development of a gap in the spectra. We present the results of a detailed temperature dependent high resolution photoemission study of optimally doped BSCCO, which indicates that the sharp feature characterizing the superconducting state is observed at the same binding energy for all temperatures, and, further, that it is still observable at temperatures ≥ 10 K above T_c. However, we show that there is considerable evidence for the emergence of a gap in the spectral response with the onset of long range phase coherence reflecting the superconducting transition.

The experimental studies reported in this paper were carried out on an angle-resolved photoemission facility based on the use of a Scienta hemispherical analyzer. In this instrument the total spectral response may be measured as a function of angle and energy simultaneously. Operated in such a mode the instrument has an angular resolution of 0.3° or better and an energy resolution of the order of 8 meV. Experimentally the latter was determined by measuring the Fermi cutoff of an evaporated gold film. A commercially available resonance lamp was used to provide incident light at a photon energy of 21.2 eV. At this photon energy the angular resolution of the instrument results in a momentum resolution of 0.01 Å^{-1}.

Samples of optimally doped ($T_c = 91$ K) $Bi_2Sr_2CaCu_2O_{8+\delta}$, produced by the floating zone method [12], were mounted on a liquid He cryostat and cleaved *in situ* in the UHV chamber with a base pressure of 2×10^{-11} mbar. The ability of the analyzer to measure energy and angle in parallel considerably reduces the amount of time required to collect data after each cleave and allows for detailed temperature dependent studies of the type reported here. During the recording of each spectrum the temperature was measured using a diode mounted at the base of the cryostat in the vicinity of the sample. However, to more accurately determine the temperature scale, a separate experimental run was used to calibrate the latter diode against a second diode that was mounted directly in place of the sample.

In Fig. 1(a) we show the spectral intensity recorded with the sample held at 46 K in the region corresponding to approximately 0.75 Γ to M. From Fig. 1(a) it is clear that the intensity of the sharp peak associated with the superconducting state is spread out over a considerable region in momentum space, although the intensity falls off as one approaches M. This observation is also evident in data reported elsewhere [11,13].

Figure 1(b) shows a series of angle-integrated photoemission spectra recorded at different temperatures corresponding to the emission along the ΓM line. Each spectrum is obtained by integrating the temperature dependent plots similar to that shown in Fig. 1(a) over the range of angles between $(0.75-1.0)\Gamma M$. Below the superconducting transition temperature of 91 K, the spectra are characterized by a sharp peak at 40 meV binding energy followed by a well resolved dip and a broad peak at a higher binding energy. The spectra recorded above the transition temperature provide clear evidence that the

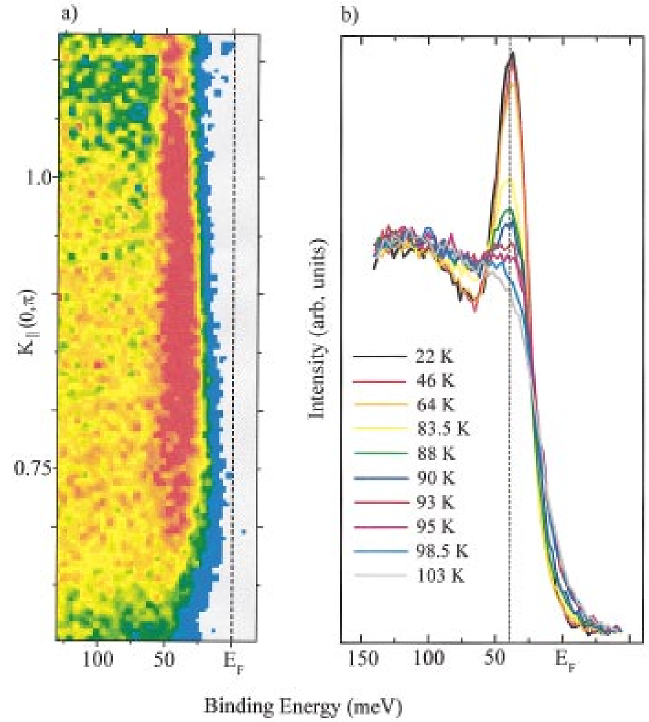

FIG. 1(color). (a) Spectral density plot recorded in the ΓM direction with the sample held at 46 K. The incident photon energy is 21.2 eV. The most intense emission is indicated in red. (b) Angle-integrated photoemission spectra recorded as a function of temperature and corresponding to the emission along the ΓM line. The different temperatures are indicated.

sharp peak still exists at the same binding energy but that the dip is considerably less well resolved. In the spectrum recorded with the sample held at the higher temperatures of 103 K the sharp peak has disappeared.

The presence of the sharp peak is clearly associated in some way with the superconducting state. However, if this peak represents the pairing of electrons, it is clear from Fig. 1(b) that its appearance in the spectra is not tied to the onset of long range coherence as defined by resistivity measurements. This raises the question "is there anything in the spectra that does characterize this transition"? In response we focus on the development of the dip. It is clear that as the temperature is lowered from temperatures above T_c, there is little change in the spectrum in the vicinity of the dip even though the sharp peak is increasing in intensity. Immediately below T_c the dip starts to rapidly develop. Furthermore we note that the intensity at E_F also undergoes a rapid decline at T_c.

To get more insight into the observations of Fig. 1, we fit the different angle-resolved spectra using a representative background and two functions, one to describe the broad peak at a high binding energy and the second to describe the sharp peak at the Fermi level. The fitting procedure is restricted to momentum resolved spectra representing 0.5° angle cuts in the region corresponding to $0.75\Gamma M$ of Fig. 1(a). This represents the region in the normal state at which the broad peak in the spectral response manifests itself most strongly in the spectra. The sharp peak observed in the spectra appears Lorentzian-like, and we use this form in our fitting procedure. As has been noted by several authors, the broad peak has a line shape that is uncharacteristic of the excitation of a well-defined quasiparticle but appears rather as the incoherent excitation of collective excitations of the system. In our fitting procedure we find that this broad peak is relatively well described by the function,

$$A(E) = \frac{(E - \Delta_0)}{C^2} \exp \frac{-(E - \Delta_0)^2}{C^2}, \qquad (1)$$

where C determines the energy scale and E is defined with respect to a gap parameter Δ_0. Initially Δ_0 is set to zero but allowed to assume any value to achieve the optimum fit to the spectra. Equation (1) is of a similar functional form to the spectral function developed in a description of quasi-one-dimensional systems [14].

Some representative form also has to be chosen to describe the background emission. It is important to remember that the background may reflect scattering from other points in the zone both within the copper-oxygen plane and outside of this plane. At points remote from the regions where the sharp and broad peaks exist the background is found to be almost steplike. Similar observations have been reported in spectra recorded elsewhere [3,13]. We therefore fit this experimentally measured background to obtain a functional form which is essentially linear with a Fermi function in the vicinity of the Fermi level.

In Fig. 2 we show the fits compared to the experimental data for a few select temperatures. Representative peaks used in the fitting are indicated in the inset. We also show in the figure the photoemission spectrum recorded from a gold film at 20 K. This provides a measure of the experimental resolution of the experiment. One immediate observation resulting from this fitting procedure is that the sharp feature remains at the same binding energy, 40 ± 5 meV with respect to the Fermi level throughout the entire temperature range. There is no indication of any shift in the binding energy, even in the vicinity of the transition temperature. Furthermore, the peak width is not instrument limited, but at temperatures well below T_c has an intrinsic width of approximately 14 meV. Interestingly we note that at this point in the Brillouin zone the sharp feature remains almost constant in width as a function of temperature. Farther out in the zone towards ΓM it gives the appearance of showing more broadening with temperature. This latter broadening is evident in the angle-integrated spectra of Fig. 1(b).

The experimentally measured width of a photoemission peak is a function of a number of different variables including the dispersion of the initial and final states [15]. However, in the present case the lack of any dispersion either in the perpendicular or parallel directions results in the measured width being solely dependent on the photohole lifetime or inverse scattering length. Thus if the width does reflect a lifetime, 14 meV, which is the same order of magnitude as the inverse scattering length observed in optical studies [16], it translates into a lifetime for the photohole or Bogoliubov quasiparticle of approximately 10^{-14} secs.

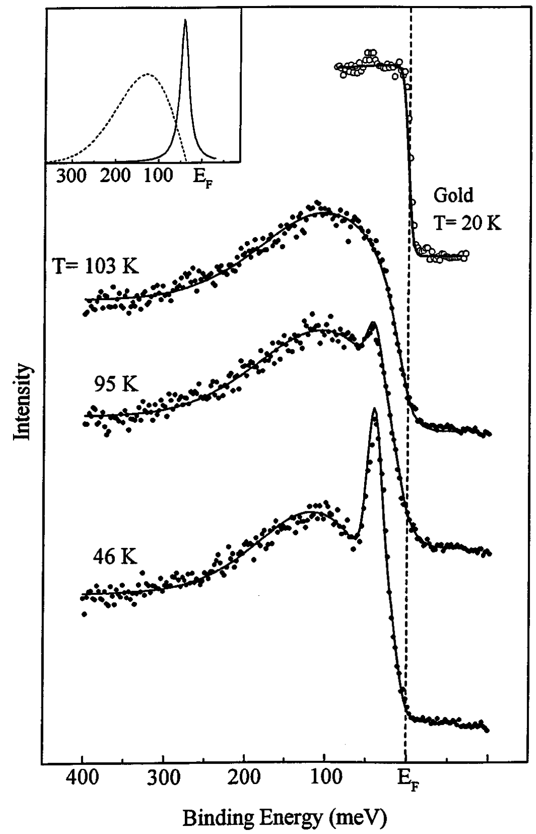

FIG. 2. Sample spectra at different temperatures showing the fit obtained using the two functions and background described in the text. The inset shows the two functions used in the fitting procedure. The parameter Δ_0 used in the latter fitting represents the separation of the leading edge of the broad peak from E_F, the Fermi level. The upper spectrum represents the Fermi edge obtained from an evaporated gold film.

The intensity of the sharp peak as obtained from the fitting procedure is shown in Fig. 3(a). We note that the sum of the fitted intensities of the broad and sharp peaks is approximately constant throughout the temperature range. Thus with the development of the superconducting phase, the intensity is transferred from one component to the other. The observation of the sharp quasiparticle peak in the spectra at temperatures above T_c, as indicated in Fig. 3(a), is not expected within mean field theories but will reflect the presence of critical fluctuations in the vicinity of the transition temperature. The observation that the sharp peak appears in the spectra even above T_c has also recently been made in a photoemission study of an overdoped BSCCO sample [17].

Our fitting procedure reveals yet another important observation. As the temperature is lowered through T_c,

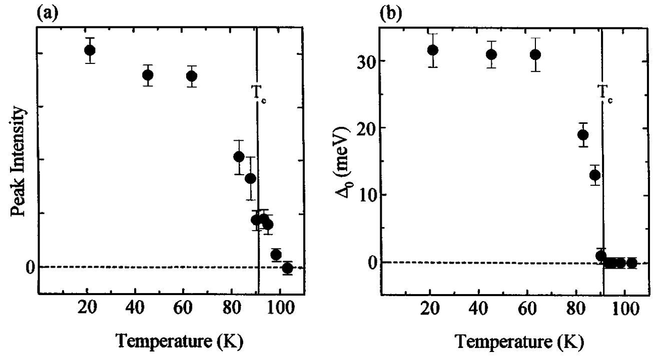

FIG. 3. (a) Intensity of the sharp peak as a function of the sample temperature. The transition temperature T_c is indicated. (b) The gap, Δ_0, between the leading edge of the broad peak and the Fermi level as obtained from the fitting procedure.

the leading edge of the broad peak moves away from the Fermi level and a gap Δ_0 opens up between the threshold for this peak and the Fermi level. The magnitude of this gap as a function of temperature is shown in Fig. 3(b). Interestingly the ultimate magnitude of this gap, 32 meV, is of approximately the same order as the displacement of the sharp peak from the Fermi level. In the raw data the opening of the gap is manifested in the development of the dip as seen in Fig. 1(b). We note that in order to account for the change in shape of the broad peak with the development of the dip at T_c, it is necessary to adjust the parameter C in our fitting procedure by approximately 7%. The temperature dependence of the gap as presented in Fig. 3(b) has the appearance in shape of being mean fieldlike. However, within the limits of the current fitting procedure, it is not possible to distinguish such behavior from other models in which the opening of the gap in the vicinity of T_c is much more rapid. This requires a more detailed study immediately below the transition temperature.

In summary, our analysis suggests that the electrons begin to locally form pairs above the transition temperature T_c as reflected in the appearance of the sharp peak. At the transition temperature T_c, *long range phase coherence leads to the onset of superconductivity and the opening of a full gap in the main spectral response between the incoherent broad peak and the Fermi level.* This latter development represents the extension of the pseudogap, which in the optimally doped materials is reported to exist above T_c, up to 130 K [18], to all states in the system. Finally we note that our high resolution studies indicate that the width of the sharp peak observed in the spectra in the superconducting state does not have a resolution limited width but rather an intrinsic width of the order of 14 meV.

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