Unusual Dispersion and Line Shape of the Superconducting State Spectra of $Bi_2Sr_2CaCu_2O_{8+\delta}$

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Photoemission spectra of $Bi_2Sr_2CaCu_2O_{8+\delta}$ below T_c show two features near the $(\pi, 0)$ point of the zone: a sharp peak at low energy and a higher binding energy hump. We find that the sharp peak persists at low energy even as one moves towards $(0, 0)$, while the broad hump shows significant dispersion which correlates well with the normal state dispersion. We argue that these features are naturally explained by the interaction of electrons with a sharp mode which appears only below T_c, and speculate that the latter may be related to the resonance seen in recent neutron data. [S0031-9007(97)04393-7]

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Angle-resolved photoemission data on the quasi-two-dimensional high temperature superconductors can be interpreted in terms of the one-electron spectral function [1]. This implies that important information about the self-energy Σ, and how it changes from the normal to the superconducting (SC) state, can be obtained by analysis of the angle-resolved photoemission spectroscopy (ARPES) line shape. This obviously has important ramifications in elucidating a microscopic theory of high temperature superconductors.

Perhaps the most dramatic effect in this regard is the temperature dependence of the line shape in Bi2212 (Fig. 1). A very broad normal state spectrum near the $(\pi, 0)$ point of the zone evolves quite rapidly for $T < T_c$ into a sharp, resolution limited, quasiparticle peak [1] followed at higher binding energies by a dip [2,3] then a hump, the latter corresponding to where the spectrum recovers to its normal state value. Similar effects are observed in tunneling spectra [4].

In this paper we focus on another remarkable difference between the normal state and SC state data which has not been noticed earlier. In Fig. 2, we show spectra for a $T_c = 87$ K Bi2212 sample along $\Gamma - \bar{M} - Z$, i.e., $(0, 0) - (\pi, 0) - (2\pi, 0)$, in (a) the normal state (105 K) and (b) the SC state (13 K), from which we note two striking features. First, we see that the low energy peak in the SC state persists over a surprisingly large range in **k** space, even when the normal state spectra have dispersed far from the Fermi energy. For example, the sharp peak is visible at about 40 meV even in curve 4 of Fig. 2(b), when the corresponding normal state spectrum is peaked 320 meV below E_F. Second, when the hump in the SC state disperses, it essentially follows that of the normal state spectrum. This is accompanied by a transfer of weight to the hump from the low frequency peak, which is fairly fixed in energy. The same phenomena are also seen along $\bar{M}$ to Y [Fig. 2(c)]. We will argue in this paper that the unusual dispersion seen in the SC state of Fig. 2 is closely tied to the line shape change observed in Fig. 1.

The data of Figs. 1 and 2 were obtained on high quality slightly overdoped Bi2212 single crystals ($T_c = 87$ K), with measurements carried out at the Synchrotron Radiation Center, Wisconsin, using a high resolution 4 m

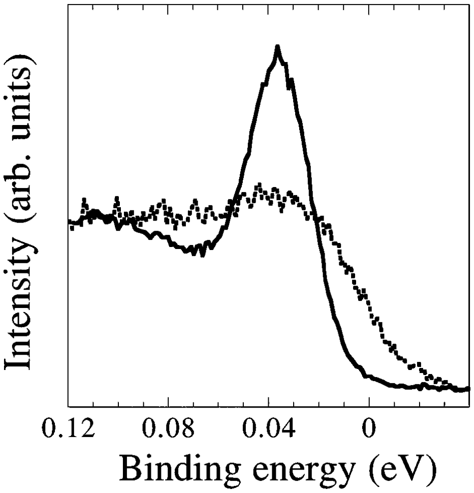

FIG. 1. Comparison of data at $\bar{M}$ in the normal state (105 K, dashed line) and the superconducting state (13 K, solid line) for a slightly overdoped ($T_c = 87$ K) Bi2212 sample with photon polarization $\Gamma - \bar{M}$.

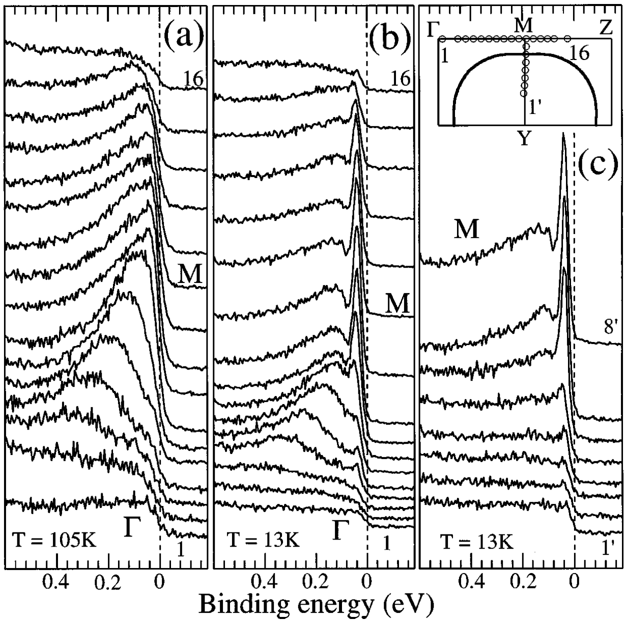

FIG. 2. EDCs in (a) the normal state (105 K) and (b) the superconducting state (13 K) along the line $\Gamma - \bar{M} - Z$, and (c) the superconducting state (13 K) along the line $\bar{M} - Y$, with the same sample and photon polarization as in Fig. 1. The zone is shown as an inset in (c) with the curved line representing the observed Fermi surface.

normal incidence monochromator [5]. The 22 eV photons polarized along $\Gamma - \bar{M}$ (the Cu-O bond direction) were used for both narrow energy scans (resolution FWHM = 18 meV) and wide energy scans (FWHM = 35 meV). Similar results were seen on a variety of samples with different doping levels, photon polarizations, and photon energies.

The simplest explanation of the SC state spectra would be the presence of two bands (e.g., due to bilayer splitting), one responsible for the peak and the other for the hump. However, this explanation is untenable. First, if the sharp peak were associated with a second band, then this band should also appear above T_c. But there is no evidence for it in the normal state data. Second, if the peak and hump were from two different bands, then their intensities must be governed by different matrix elements. However, we found [3] that the intensities of both features scaled together as the photon polarization was varied from in plane to out of plane, as if they were governed by a common matrix element. These arguments suggest that the unusual line shape and dispersion represent a single electronic state governed by nontrivial many-body effects.

Although the above arguments can also be used to eliminate a ghost image of the CuO band caused by the incommensurate superlattice [3,5] as the source of the unusual dispersive effects, it is still worthwhile to examine this in greater detail, particularly since one predicts a Fermi crossing of one of these images near curve 4 of Fig. 2. Our arguments against a superlattice interpretation are as follows. First, the ghost images are not visible in the normal state in this polarization geometry and therefore should not be visible in the SC state either. They do, however, become quite visible in the normal state if the photon polarization is rotated by 45°, as shown in Ref. [3]. Second, comparison of superconducting state spectra in these two polarizations indicate that the midpoint of the leading edge in the present polarization (20 meV) is near that of the $\bar{M}$ point, whereas in the 45° rotated polarization, the midpoint is 5 meV. The latter value would be consistent with the ghost image being measured at this **k** point, the former not. Third, the intensity of the peak monotonically rises from Γ with a maximum near $\bar{M}$, indicating only one spectral feature, unlike in the 45° polarization geometry where two strong maxima are found (one associated with the CuO band, the other with its superlattice image).

We now return to Fig. 1 which shows high resolution data at the $\bar{M}$ point. The data are consistent with a strong reduction of the imaginary part of the self-energy (ImΣ) at low frequencies in the SC state [6]. An important feature of this change in ImΣ has been addressed previously [7]. If the scattering is electron-electron–like in nature, then ImΣ at frequencies smaller than $\sim 3\Delta$ will be suppressed due to the opening of the superconducting gap. On closer inspection, though, Fig. 1 reveals a more interesting story than this simple picture. First, the SC and normal state data match beyond 90 meV (they continue to match for energies beyond those in the figure, as can be seen from the wider scan data of Fig. 2). This means that the self-energy of the electrons in the normal and superconducting states are equivalent beyond this energy. This simple observation has nontrivial consequences as shown below. From 90 meV, the dip is quickly reached at 70 meV, then one rises to the resolution limited peak. Notice that since the FWHM of the peak is around 20 meV, then the change in behavior of the spectra (from hump, to dip, to the trailing edge of the peak) is occurring on the scale of the energy resolution. That means that the intrinsic dip must be quite sharp. We have attempted to fit the SC state data with various assumed forms for ImΣ, taking into account the observed momentum and energy resolution [8]. The surprising conclusion is that the large ImΣ at high energies (equivalent to that in the normal state, as mentioned above) must drop to a small value over a narrow energy interval to be consistent with the data. For instance, if one assumes that ImΣ is of the form $\omega(\omega/\tilde{\omega})^n$ (where $\tilde{\omega}$ is near the energy of the dip), then n must be large to be consistent with the data; i.e., there is essentially a step in ImΣ. This is interesting, since the standard analysis based on a d-wave pairing state would give $n = 2$ [9], which does not give a dip at all. Moreover, the models mentioned above [7] predict ImΣ to decay smoothly to zero, rather than the abrupt change indicated by the data. In fact, the data are not only consistent with a step in ImΣ, but the depth of the dip is such that it is best fit by a peak in ImΣ at the dip energy, followed by a rapid drop to a small value.

What are the consequences of this behavior in ImΣ? If ImΣ has a sharp drop at $\tilde{\omega}$, then by Kramers-Kronig transformation, ReΣ will have a sharp peak at $\tilde{\omega}$. This peak can very simply explain the unusual SC state dispersion shown in Fig. 2, as it will cause a low energy quasiparticle pole to appear even if the normal state binding energy is large. The most transparent way to appreciate this result is to note that a sharp step in ImΣ is equivalent to the problem of an electron interacting with a sharp (dispersionless) mode, since in that case, the mode makes no contribution to ImΣ for energies below the mode energy, and then makes a constant contribution for energies above. This problem has been treated by Engelsberg and Schrieffer, and extended to the superconducting state by Scalapino and co-workers [10]. The difference in our case is that since the effect only occurs *below* T_c, it is a consequence of the opening of the superconducting gap in the electronic energy spectrum, and thus of a collective origin, rather than a phonon as in Ref. [10]. To facilitate comparison to this classic work, in Fig. 3 we plot the position of the low energy peak and higher binding energy hump as a function of the energy of the single broad peak in the normal state. This plot has a striking resemblance to that predicted for electrons interacting with a sharp mode in the superconducting state [11], and one clearly sees the low energy pole which we associate with the peak in ReΣ. Moreover, the predicted spectral functions of that work, when convolved with energy resolution, give a good representation of the data shown in Fig. 1 (with the probable peak in ImΣ discussed above due to the peak in the SC density of states) [8]. On general grounds, the flat dispersion of the low energy peak seen in Fig. 3 is a combination of two effects: (1) the peak in ReΣ, which provides an additional mass renormalization of the SC state relative to the normal state, and thus pushes spectral weight towards the Fermi energy, and (2) the superconducting gap, which pushes spectral weight away. This also explains the strong drop in intensity of the low energy peak as the higher binding energy hump disperses.

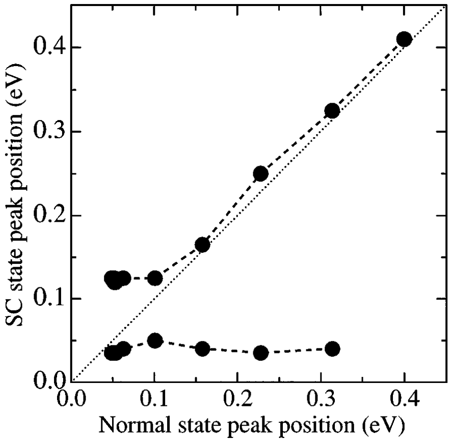

FIG. 3. Positions (eV) of the sharp peak and the broad hump in the SC state versus normal state peak position obtained from Figs. 2(a) and 2(b). Solid points connected by a dashed line are the data; the dotted line represents the normal state dispersion.

An important feature of the data is the dispersionless nature of the sharp peak. The mode picture discussed above would imply a dispersion of the peak from Δ_k to $\tilde{\omega} = \omega_0 + \Delta_k$ as the normal state binding energy increases (where ω_0 is the mode energy). However, this dispersion turns out to be weak. From the data at $\bar{M}$, we infer an $\omega_0 = 1.3\Delta_{\bar{M}}$, ω_0 being essentially the energy separation of the peak and dip. Since Δ_k is known to be of the $d_{x^2-y^2}$ form from ours and others' ARPES data, then Δ_k should go to zero as we disperse towards the Γ point. Therefore, the predicted dispersion is only from $\Delta_{\bar{M}}$ to $1.3\Delta_{\bar{M}}$ (32 to 42 meV). In fits we have done, the comparison of the model to the data can be greatly improved by assuming $\omega_0 = 1.3\Delta_k$ [8]. This not only leads to an almost dispersionless low energy peak as indicated by the data, it gives a much better description of the observed intensity falloff of the peak as one moves towards Γ. In a proper theory, though, ω_0 would depend not on k, but on the transferred momentum, so the above description is incomplete. We note that although a collective mode is the most natural explanation of the data, it may not be unique. The fact that the low energy peak always has an energy near $\Delta_{\bar{M}}$ may indicate that the peak is directly associated with Δ itself, i.e., due to the off-diagonal, rather than the diagonal, part of the Nambu self-energy. In this connection, we should remark that the line shape in Fig. 1 was previously attributed [12] to the off-diagonal self-energy, but under the (incorrect) assumption that the data represented a density of states rather than a spectral function.

To proceed further would require a detailed knowledge of the k dependence of Σ. At this stage, we can make only qualitative observations. Since the dip-hump structure is most apparent at the $(\pi, 0)$ points, it is natural to assume that it has something to do with $Q = (\pi, \pi)$ scattering, as recently discussed by Shen and Schrieffer [13]. But here we find a new effect. If one compares the data of Figs. 2(b) and 2(c), one sees that a low energy peak also exists along $(\pi, 0) - (\pi, \pi)$ for approximately the same momentum range as the one from $(\pi, 0) - (0, 0)$. That is, if there is a peak for momentum p, one also exists for momentum $p + Q$. This can be understood, since the self-energy equations for p and $p + Q$ will be strongly coupled if Q scattering is dominant. In the mode picture discussed above and in the limit where we consider only $\omega_0(Q)$, the part of ImΣ_p due to the mode will be proportional to A_{p+Q}. Thus, peaks in A_{p+Q} will cause peaks in Σ_p, which in turn will cause peaks in A_p, which will cause peaks in Σ_{p+Q}, which will finally cause peaks in A_{p+Q}. Thus, in such a model, the peaks in A for p and $p + Q$ self-consistently generate one another if the coupling is strong enough.

We now connect our observations to previous theoretical work. The fact that the linewidth collapses at low energies has been recognized for some time now, as remarked earlier. The most natural explanation is based on a one loop approximation ($\Sigma \sim \int \chi G$ where χ is an electronic susceptibility and G is the electron Green's function). Superconductivity will cause gaps in both χ and G leading to a suppression of $\mathrm{Im}\Sigma$ below 3Δ [7]. The unusual effects we describe here are in addition to the 3Δ effect, and can be obtained from such models by having a resonant or collective mode inside the (2Δ) gap in $\mathrm{Im}\chi$ (with the weight of the mode equal to the gapped weight so as to obtain an equivalent $\mathrm{Im}\Sigma$ to that of the normal state for energies beyond 3Δ). Several such theories have been proposed [14] to explain a resonant mode seen in neutron scattering data in $YBa_2Cu_3O_{7-\delta}$ (YBCO) below T_c [15]. In one such microscopic model, the resonant mode is responsible for all the pairing at low temperatures [16]. It is interesting to speculate that the mode we infer from our ARPES data in Bi2212 is related to the one seen in neutron data in YBCO, especially since the mode energies were found to be similar. This suggests to us that neutron scattering experiments on Bi2212 would be of interest in this regard.

In conclusion, we have shown the presence of a persistent low energy peak in photoemission spectra in Bi2212 in the SC state which exists over a large momentum range near the $\bar{M}$ point. The dispersion of this feature and the higher binding energy hump as a function of momentum suggests that the electrons in the SC state are interacting with a mode of resonant character with a frequency near $1.3\Delta_{\bar{M}}$. Our results once again emphasize that the self-energy is dominated by electron-electron interactions, which is consistent with an electron-electron origin to the pairing.

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