Effects of a particle-hole asymmetric pseudogap on Bogoliubov quasiparticles

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We show that in the presence of a pseudogap, the spectral function in the superconducting state of the underdoped cuprates exhibits additional Bogoliubov quasiparticle peaks at both positive and negative energy which are revealed by the particle-hole asymmetry of the pseudogapped energy bands. This provides direct information on the unoccupied band via measurement of the occupied states. When sufficiently close, these Bogoliubov peaks will appear to merge with existing peaks leading to the anomalous observation, seen in experiment, that the carrier spectral density broadens with reduced temperature in the superconducting state. Using the resonating valence bond spin liquid model in conjunction with recent angle-resolved photoemission spectroscopy data allows for an empirical determination of the temperature dependence of the pseudogap, suggesting that it opens only very gradually below the pseudogap onset temperature T^*.

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Over the history of high-temperature superconductivity in the cuprates, many fundamental questions have been posed and some have been answered. It is now known that the charge carriers form in Cooper pairs,[1] with a pairing symmetry that is described as spin-singlet[2] $d_{x^2-y^2}$ wave[3] and the mechanism might be spin fluctuations,[4] although the latter issue is still a subject of considerable debate. Even the applicability of standard BCS theory has been questioned although experiments have been presented that give overwhelming evidence for a BCS description. One such experiment, which is both relevant to this paper and demonstrates the impact of the high-T_c field to encourage experimental innovation and improvements in technique, has been angle-resolved photoemission spectroscopy (ARPES). In ARPES, not only has the superconducting energy gap $\Delta_{\rm sc}(\boldsymbol{k})$ been determined as a function of momentum $\boldsymbol{k}$,[5] but also the predicted Bogoliubov quasiparticle (BQP) bands $\pm E_{\boldsymbol{k}} = \pm\sqrt{\epsilon_{\boldsymbol{k}}^2+\Delta_{\rm sc}^2(\boldsymbol{k})}$ and BQP amplitudes $u_{\boldsymbol{k}}^2$ and $v_{\boldsymbol{k}}^2$ have been observed and verified to agree with d-wave BCS theory.[6–8] While this has provided important advances to our understanding of the cuprates at optimal and overdoping, it was quickly noted that for underdoped cuprates, the picture was less clear. Indeed many properties of the superconducting state appear non-BCS-like and the normal state harbors a not-yet-understood energy-gap-like feature termed the "pseudogap."[9] The proximity to the antiferromagnetic Mott insulator suggests strong correlation effects with possibly some competing order and hence the major questions in the cuprates revolve around understanding the source of the pseudogap and its relation to superconductivity. Indeed, interest in these issues extend more broadly to the cold atom field of research where a pseudogap has been seen in a strongly interacting Fermi gas using a momentum resolved radio-frequency spectroscopy as an analog to ARPES.[10]

At present two general points of view exist. One is that the pseudogap is simply an image of the superconducting gap related to the existence of phase incoherent preformed pairs above T_c.[11] This is a one-gap scenario and argues for the pseudogap to open symmetrically about the Fermi surface. The second point of view treats the pseudogap as a manifestation of competing order with a second energy scale which, along with the superconducting gap, presents a two-gap scenario.[12,13] Key to this latter vision is that the pseudogap opens up on a surface in the Brillouin zone that is different from the Fermi surface. For instance, in the case of competing magnetic order, the pseudogap should be associated with the antiferromagnetic Brillouin-zone boundary. Regardless of the details of specific models, the two-gap scenario suggests that the pseudogap will be particle-hole asymmetric. Consequently, experimental evidence of symmetry or asymmetry would allow for the elimination of a number of models and provide a significant advancement to the field. In this paper, we discuss the effect that a particle-hole asymmetric pseudogap has on the observation of BQPs and propose that the anomalous broadening of the spectral function seen in ARPES[14] results from particle-hole asymmetry.

In this work, we focus on ARPES and measurements of the spectral function $A(\boldsymbol{k},\omega)$. In an ordinary Fermi liquid, the spectral function is a simple peak or δ function that tracks the single-particle energy dispersion $\epsilon_{\boldsymbol{k}}$ as a function of energy ω and momentum $\boldsymbol{k}$ as shown schematically in Fig. 1(a). As ARPES only measures the occupied states at zero temperature due to a Fermi function cutoff at the Fermi level E_F, the peaks above E_F are not detected. At finite T, some information on the bands above E_F can be obtained via analysis of the thermal tails.[7] In the presence of superconductivity, the elementary excitations are the BQPs, which mix electron and hole states. This leads to a gap of $2\Delta_{\rm sc}$ in the dispersion and introduces two BQP bands $\pm E_{\boldsymbol{k}} = \pm\sqrt{\epsilon_{\boldsymbol{k}}^2+\Delta_{\rm sc}^2(\boldsymbol{k})}$, which show backbending from the Fermi energy and about the Fermi momentum k_F, which coincides with the position k_p of the peak in the backbending of the occupied states. The two BQP branches also acquire weighting of $u_{\boldsymbol{k}}^2 = (1+\epsilon_{\boldsymbol{k}}/E_{\boldsymbol{k}})/2$ and $v_{\boldsymbol{k}}^2 = (1-\epsilon_{\boldsymbol{k}}/E_{\boldsymbol{k}})/2$, as illustrated in Fig. 1(b). These pictures and their manifestation in experiment on an overdoped cuprate material were published by Matsui *et al.*[7] providing a confirmation of the applicability of d-wave BCS theory.

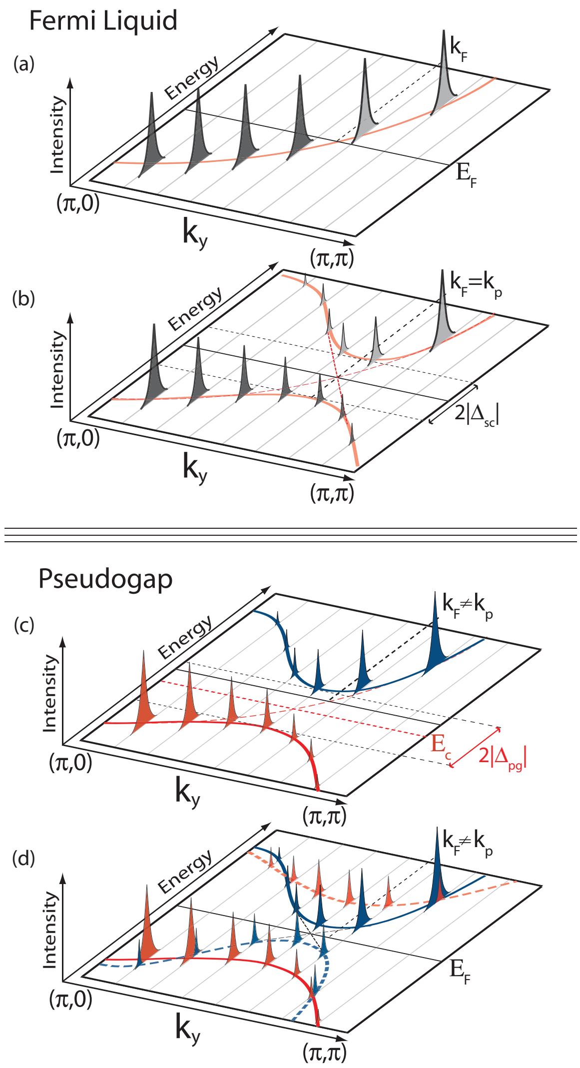

FIG. 1. (Color online) Schematic diagram of spectral function intensity, $A(\boldsymbol{k},\omega)$, as a function of energy and momentum for a single Fermi-liquid band, (a) and (b), and two asymmetric pseudogapped bands, (c) and (d), as described in the text. (b) and (d) show the formation of BQP bands in the superconducting state. In the presence of superconductivity, extra spectral peaks in the pseudogapped case at fixed $\boldsymbol{k}$ are revealed that would not be separately resolved for a pseudogap opening symmetrically about the Fermi level.

When a pseudogap exists in the normal state, the picture alters and the energy dispersion will be split into two bands, as shown in Fig. 1(c). Furthermore, in the presence of a particle-hole asymmetric pseudogap Δ_{pg}, the bands do not open about E_F but rather about some other energy E_c and the backbending peak position $k_p \neq k_F$, as shown. In the presence of superconductivity, each band now splits into two BQP bands positioned symmetrically about E_F [shown as the dashed blue (dark gray) curve and quasiparticle peaks for the upper band and dashed red (light gray) for the lower band in Fig. 1(d)]. This gives rise to four BQP peaks as a function of energy, at fixed $\boldsymbol{k}$, with two positioned at negative energy and two at positive energy for E_F taken as 0. Note that if the pseudogap opens in a particle-hole symmetric fashion, the two BQP peaks at negative energy would merge into one, as would the two above E_F. It is the combination of the particle-hole asymmetric pseudogap with the symmetric superconducting gap that allows the extra hidden BQP peaks to be revealed and displayed separately. Therefore information on the unoccupied band above E_F can now be obtained from analysis of its reflected BQP band on the occupied side, avoiding, in principle, the need for analysis of thermal tails above E_F.

To facilitate our discussion, it is necessary to adopt a particular model. For this purpose we use a model proposed by Yang, Rice, and Zhang (YRZ),[15,16] who developed an ansatz for the electronic Green's function based on a resonating valence bond (RVB) spin liquid state. This model has a particle-hole asymmetric pseudogap and explains a large amount of anomalous data from the underdoped cuprates.[17–23] Indeed, we will show here that it is more effective at explaining recent ARPES data[14] than a prominent and extensively studied competing model, the d-density wave (DDW) model.[12,13,24–27] While the YRZ model is phenomenological, it has a base in the microscopic theory of arrays of two-leg Hubbard ladders in a doped spin liquid including long-range interladder hopping. Comparison with numerical results of Troyer *et al.*[28] for t-J ladders additionally support the YRZ choice of Green's function, which is initially based on considerations of the weak-coupling case. For a detailed discussion, see Ref. 15. A closely related model is the algebraic charge liquid described by Qi and Sachdev.[29] It is based on a fluctuating two-dimensional antiferromagnet and provides a Green's function that has a similar form to that of YRZ.

Within the ansatz for the RVB state proposed by Yang *et al.*, the coherent part of the spectral function is given as

$$A(\boldsymbol{k},\omega) = \sum_{\alpha=\pm} g_t W^{\alpha}\left[u_{\alpha}^2 \delta\left(\omega - E_{\mathrm{sc}}^{\alpha}\right) + v_{\alpha}^2 \delta\left(\omega + E_{\mathrm{sc}}^{\alpha}\right)\right], \quad (1)$$

where the energy of the gapped excitations in the superconducting state is $E_{\mathrm{sc}}^{\alpha} = \sqrt{(E^{\alpha})^2 + \Delta_{\mathrm{sc}}^2}$, with Bogoliubov amplitudes $u_{\alpha}^2 = (1 + E^{\alpha}/E_{\mathrm{sc}}^{\alpha})/2$ and $v_{\alpha}^2 = (1 - E^{\alpha}/E_{\mathrm{sc}}^{\alpha})/2$, which are applied to the pseudogapped bands indexed by $\alpha = \pm$ and given as $E^{\pm} = \epsilon_1 \pm \sqrt{\epsilon_2^2 + \Delta_{\mathrm{pg}}^2}$. Here, $\epsilon_1 = (\xi_{\boldsymbol{k}} - \xi_{\boldsymbol{k}}^0)/2$ and $\epsilon_2 = (\xi_{\boldsymbol{k}} + \xi_{\boldsymbol{k}}^0)/2$, where $\xi_{\boldsymbol{k}} = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a - 2t''(\cos 2k_x a + \cos 2k_y a) - \mu_p$, is a third nearest-neighbor tight-binding dispersion and $\xi_{\boldsymbol{k}}^0 = -2t(\cos k_x a + \cos k_y a)$ is that for first nearest neighbor, which for $\xi_{\boldsymbol{k}}^0 = 0$ defines the antiferromagnetic Brillouin-zone boundary. $W^{\pm} = (1 \pm \epsilon_2/\sqrt{\epsilon_2^2 + \Delta_{\mathrm{pg}}^2})/2$ are weighting factors for the pseudogapped bands in analogy with the u's and v's, and g_t is a Gutzwiller factor that reflects a reduction in the coherent part of the spectral function due to strong correlations.[21] These energy dispersions contain doping dependent coefficients: $t(x) = g_t(x)t_0 + 3g_s(x)J\chi/8$, $t'(x) = g_t(x)t_0'$, and $t''(x) = g_t(x)t_0''$, where $g_t(x) = \frac{2x}{1+x}$ and $g_s(x) = \frac{4}{(1+x)^2}$ are the energy renormalizing Gutzwiller factors for the kinetic and spin terms, respectively. These factors account for the narrowing of the bands with increased correlations. The pseudogap is taken to have the same d-wave symmetry as the superconducting gap and to be nonzero only for doping x below a quantum critical point at $x = x_c = 0.2$. A detailed statement of our parameters and the model's doping dependence is given in Ref. 20. Here, we will show generic results for that set of parameters with a doping $x = 0.16$. It is only in our final figure of this paper where we compare directly with experimental data and for that case we adjust the parameters to match the Fermi surface of the material under investigation. A finite pseudogap leads to Fermi-surface reconstruction from the large contours of Fermi-liquid theory to small holelike Luttinger pockets confined to the vicinity of the nodal direction. As the pseudogap first opens, there are, as well, electron pockets in the antinodal region but these progressively shrink to zero as the Mott transition is approached. The dispersion $\xi_{\boldsymbol{k}}$ uses μ_p as a chemical potential determined by the Luttinger sum rule in the form

$$1 - x = \frac{2}{(2\pi)^2} \int_{G(\boldsymbol{k},\omega=0)>0} d^2k, \tag{2}$$

where the Green's function is in the normal state with finite pseudogap for $x < x_c$. Thus the chemical potential becomes dependent on both the value of the pseudogap and doping. It will also change at finite temperature.

In Fig. 2, we show how the bands change with temperature. As in the experiment that we compare to (Ref. 14) the dispersions are presented as a function of $\boldsymbol{k} = (\pi, k_y)$, with k_y varying about zero. This is a momentum cut in the antinodal region of the Brillouin zone where the pseudogap is maximal. In Fig. 2(a), the Fermi-liquid state at $T = T^*$ gives a single band which dips below the Fermi level as seen in the experiment. As the pseudogap develops in (b) and (c), the gap opens about a line below the Fermi level, breaking particle-hole symmetry. Initially, a double dip feature appears in the upper band positioned near the Fermi level [Fig. 2(b)] as is also seen in experiment[14] (we do not find such a feature in the DDW model). In the superconducting state shown in (d), the secondary BQP bands appear, shown with the dashed curves, which are mirror reflections about the Fermi energy of the original pseudogapped bands. An image of the original unoccupied band [solid blue (dark gray)] is now seen on the occupied side [dashed blue (dark gray)]. Figure 2(d) is shown again in (e) as a color map representing the intensity, $I = A(\boldsymbol{k},\omega) f(\omega)$, where the cutoff due to the Fermi function $f(\omega)$ is applied and the quasiparticle weights are included. One sees the two bands at negative energy clearly separated, but not far apart. To represent instrument resolution, in (f) we show the convolution of (e) with a Gaussian of standard deviation $\sigma = 0.04 t_0$, which would correspond to roughly 5–15 meV, depending on the value of t_0. The two bands now appear as one broadened band, particularly around the point of the backbending peak, near k_F, where the experiments reported anomalous broadening.[14] Indeed, as the temperature is lowered and Δ_{sc} increases, the extra BQP band gains weight and the net result appears as though there is an anomalous increase in broadening at low temperature. We are not including incoherent processes here. In reality, there will be a large incoherent background associated with the carrier spectral function, which will give tails that additionally fill in the region between the two peaks and consequently less broadening than we have used here will be needed to make them overlap and appear as a single line with a shoulder.

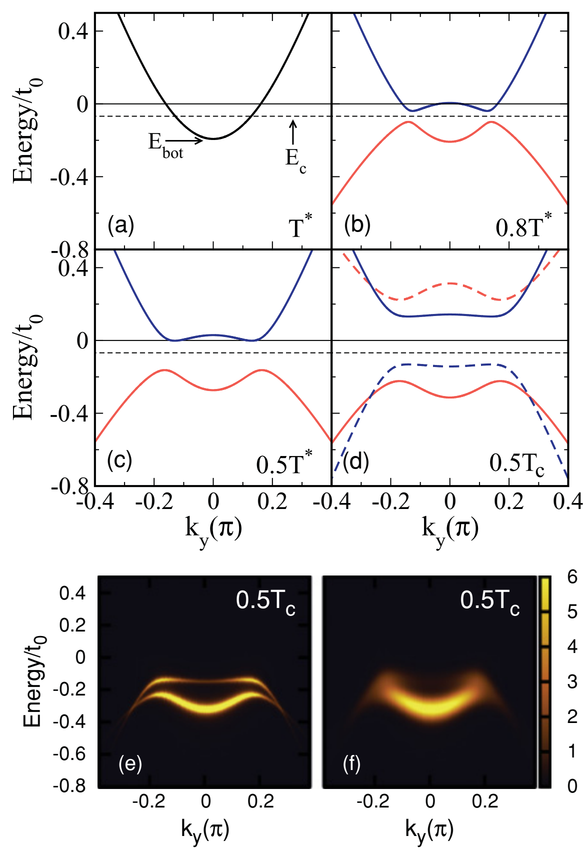

FIG. 2. (Color online) The band dispersions about the point $\boldsymbol{k} = (\pi, 0)$ for a momentum cut along k_y. (a) Fermi-liquid state at $T = T^*$. The pseudogap state for (b) $T = 0.8T^*$ where the upper band still shows below the Fermi level and (c) $T = 0.5T^*$. (d) The superconducting state shows four BQP bands that arise from the two particle-hole asymmetric pseudogap bands. (e) gives the case of (d) now presented as a color map of $I = A(k,\omega) f(\omega)$. (f) Same as (e) except I is now convoluted with a Gaussian of $\sigma = 0.04 t_0$.

This is further brought out in Fig. 3 where the intensity is shown for several temperatures below T_c at fixed $k_y = k_F$ and for varying ω/t_0. At T_c, the intensity contains two peaks that are not symmetric about E_F. Recent experiments indicate that a minimum in the spectral intensity occurs at the Fermi level.[14,30] One suggestion for this effect might be the existence of regions of spatially inhomogeneous superconductivity which persist above T_c.[31] While our pseudogap model is intrinsically asymmetric, superconductivity, which opens on the Fermi surface, restores particle-hole symmetry on an energy scale of the order of the superconducting gap. In the superconducting state there is a second weaker BQP peak at negative energy which, due to the convolution, appears as a shoulder on the main peak. This shoulder-type feature (which is traced by the arrows) exists in the experimental data of Hashimoto *et al.*[14] and disappears above T_c and, while unexplained in the experimental work, it acquires a natural explanation here as the BQP band arising from the second pseudogap band at positive energy.

Much of our discussion to this point has been generic to any model displaying particle-hole symmetry breaking. Now we address more specifically the issue of the temperature dependence of the pseudogap, which can be inferred from experiment, and demonstrate that the model used here is able to explain the distinct qualitative features of the data that a competing model, the DDW, cannot.

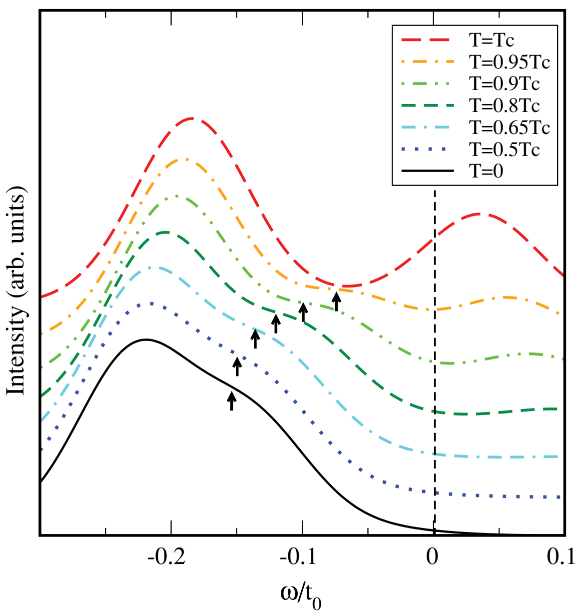

FIG. 3. (Color online) Intensity I versus energy at k_F [convoluted as in Fig. 2(f)] for various temperatures. Each subsequent curve is offset for clarity. Arrows track the extra BQP peak emerging at negative energy for $T < T_c$.

In Fig. 4(a) we plot the energy of the lower band at $(\pi,0)$ and at (π,k_p) (the position of the peak in the backbending) as a function of temperature. The curve for (π,k_F) is similar to (π,k_p). To obtain a good fit to the data of Hashimoto *et al.*,[14] we have adjusted the band-structure parameters to fit the antinodal region of the normal-state Fermi surface and have used a pseudogap value of 84 meV and a superconducting gap on the Fermi surface of 24 meV. Along with $t_0 = 300$ meV, these values are close to those obtained by Yang *et al.*[18] in their consideration of Andreev reflection in an underdoped Bi-based sample of similar T_c, which provides support to both of our fits.

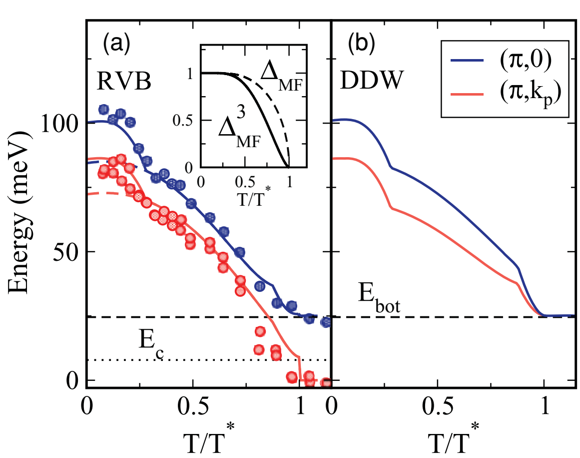

FIG. 4. (Color online) (a) Temperature-dependent energy of lower band at $(\pi,0)$ and (π,k_p), with and without superconductivity (solid and dashed lines, respectively). Data from Ref. 14, scaled by T^* in the x axis, are shown as dots. Using $\Delta^3_{\rm MF}(T)$ (see inset) for the temperature dependence of the pseudogap gives a good fit to the data with the RVB model, whereas $\Delta_{\rm MF}(T)$ does not. (b) The DDW model differs from the RVB model and cannot explain the data at T^*.

Additional fits with smaller gap values, for example 12 meV, give no significant changes to the results of Fig. 4(a) except in the superconducting state where the additional increase (hatlike structure) is considerably reduced. In our prior figures, we used a mean-field temperature dependence, $\Delta_{MF}(T)$, for both $\Delta_{\rm sc}$ and $\Delta_{\rm pg}$. The actual temperature dependence of $\Delta_{\rm pg}$ is still open to debate. Some argue for the pseudogap feature in the density of states to fill but not close,[9,32] suggesting a flat T dependence with a sudden drop at T^*. With a mean-field temperature dependence for the two gaps (dashed line in the inset) we were not able to agree with the nearly linear temperature dependence observed in the data between T_c and T^*. However, choosing $\Delta_{\rm pg}(T)$ to have a $\Delta^3_{MF}(T)$ behavior we find good agreement with experiment, suggesting that the pseudogap may open more gradually in temperature than previously thought.

In Fig. 4(b) we compare this RVB model and a DDW model. These two models differ in that the pseudogap opens on the antiferromagnetic Brillouin-zone boundary, $\xi^0_{\boldsymbol{k}} = 0$, and hence at $(\pi,0)$ for the DDW and on a surface $\xi_{\boldsymbol{k}} + \xi^0_{\boldsymbol{k}} = 0$ for the RVB model, which is offset from the region of $(\pi,0)$. Keeping the band-structure parameters the same, along with the temperature dependence of the gaps, we find a qualitative difference between the two models. The two curves for the DDW model merge to the same point at T^* as k_p goes continuously to zero, i.e., the backbending peak closes to an energy that is the bottom of the Fermi-liquid band, $E_{\rm bot}$, shown in Fig. 2(a) and located at $k_y = 0$. The $(\pi,0)$ curve of the RVB model also merges to this point but the k_p curve does not as the backbending peak in RVB closes at E_c, as can be seen in Fig. 2(b). The lack of separation of the two curves for $T = T^*$ in the DDW model excludes it as a candidate for the pseudogap in comparison with the RVB model.

In summary, the anomalous broadening and shoulder feature seen in ARPES measurements has a natural explanation in a second peak due to a BQP band in the superconducting state, which can only appear in the case of particle-hole asymmetry in the pseudogap state. Further, we find that the pseudogap closes rather gradually with increasing temperature toward T^*. We have also ruled out the DDW model as an alternative competing order, as it cannot explain the present ARPES data. As a general final comment, the existence of BQPs is fundamental to our understanding of the nature of the many-body coherence in the superconducting state. The observation and measurement of their spectral weight in ARPES was a significant milestone. In the underdoped cuprates, the BQP peaks may be further split by a particle-hole asymmetric pseudogap leading to a richness in BQP structure, which has only been hinted at in recent experiments. This effect also allows for the unoccupied bands to be studied in the occupied region of the spectral intensity. It would be important to find other systems where this phenomenon would reveal itself more clearly.

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