Angle resolved photoemission spectroscopy (ARPES) has emerged as a powerful tool for understanding the electronic structure of high temperature cuprate superconductors. This has occurred because of its unique energy and momentum resolved nature, and its interpretation in terms of the single particle spectral function.

Perhaps the most novel behavior which has been observed is the dramatic rearrangement of the ARPES lineshape at the \((\pi, 0)\) points of the Brillouin zone when cooling below \(T_c\). Above \(T_c\) one has a single broad spectrum, indicating incoherent states. Below, though, a gap opens up in this incoherent spectrum, and inside this gap, a sharp peak emerges, leading to the well-known peak-dip-hump structure which was first observed in tunneling spectra. This onset of coherence at \(T_c\) is quite dramatic, and has obvious implications for the microscopies of high temperature superconductors.

How the sharp peak appears below \(T_c\), though, has recently emerged as a controversial issue. Previous analysis pointed to a dramatic increase in the low-energy lifetime as the source of its appearance. This agrees with interpretations of microwave and thermal conductivity measurements. Recently, though, this picture has been challenged. Based primarily on new high resolution data, it has been asserted that the spectral peak width in energy remains fixed with temperature. Rather, its weight (the quasiparticle renormalization factor, \(z\)) tracks the temperature dependence of the superconducting order parameter, and thus vanishes as \(T_c\) is approached from below.

This new picture has a certain appeal to it, in that as Feng et al. show, one can draw a strong correlation between the temperature dependence of the spectral peak weight and other quantities, such as the superfluid density and the intensity of the magnetic resonance observed by inelastic neutron scattering. Similar conclusions have been reached by Ding et al., though their analysis has some aspects of the lifetime catastrophe scenario as well. Moreover, since the spectrum is completely incoherent above \(T_c\), it is natural to suppose that \(z\) does indeed monotonically decrease to zero as \(T_c\) is approached from below.

In this paper, we will argue that this new picture is misleading. Our analysis is based on a methodology we have developed where the electron self-energy is directly extracted from ARPES data. From this analysis, we find that the quasiparticle residue \(z\) is at best a marginally defined quantity at low temperatures, and becomes increasingly ill defined as \(T\) increases. Moreover, any reasonable attempt to define \(z\) leads to a quantity which actually increases with increasing \(T\) (more properly, the energy integrated spectral weight for binding energies less than the dip energy is temperature independent). This is due to a reduction in the mass renormalization as \(T\) increases, similar to what is obtained from a generalized Drude analysis of optical data. This, coupled with the increase of the low energy scattering rate (as also seen in optics), leads to a strong increase in the spectral peak width. That is, the spectral peak loses its integrity (rather than simply disappearing) due to a “lifetime catastrophe”.

The ARPES data were taken on an optimally doped \((T_c=90K)\) Bi2212 sample, with the \(\Gamma - M\) axis parallel to the photon polarization vector, and were previously reported in another connection. The measurements were carried out at the Synchrotron Radiation Center in Madison, WI, on the U1 undulator beamline, with a Scienta SES 200 electron analyzer having an energy resolution of 16 meV and a momentum resolution of 0.01 Å\(^{-1}\).

In Fig. 1, we show data taken at the \(M(\pi, 0)\) point of the Brillouin zone as a function of temperature. The leading edge of the spectral peak is determined by the superconducting gap, whose energy stays fairly fixed in temperature, and persists above \(T_c\) (the pseudogap). On the trailing edge, one sees a spectral dip, whose energy also remains fixed in temperature, and becomes filled in
above $T_c$. As these two energy scales define the two sides of the peak, this then gives the illusion that the peak width is independent of temperature. That such is not the case can be clearly seen by a closer inspection of the trailing edge of the peak. There is no question from Fig. 1 that the trailing edge is broadening with temperature, and this broadening is what is causing the spectral dip to fill in above $T_c$.

The earlier attempts to quantify this behavior involved separating the spectrum into a coherent ("peak") part and an incoherent ("hump") part. Although this a relatively straightforward procedure at low temperatures, where these two features are quite well defined, this becomes increasingly difficult as the temperature is raised and the spectral dip is filled in. The resulting ambiguity of what to call the coherent part, and what the incoherent part, has led to the differing conclusions in the literature.

The obvious way to overcome this difficulty is to treat the spectral function as a unified object. We note that the spectral function is defined as the imaginary part of the Greens function, that is

$$\text{Im} G(\omega) = \text{Im} \Sigma(\omega)$$

and

$$\text{Re} G(\omega) = \text{Re} \Sigma(\omega)$$

where $\omega$ is the energy and $\Sigma$ the Dyson self-energy. Therefore, the temperature evolution of the total spectral function is determined by the temperature evolution of the self-energy.

We now briefly review the work of Ref. 16 where the procedure for extracting $\Sigma$ from ARPES data was developed. To determine $\Sigma$ uniquely, we need to know both $\text{Re} G$ and $\text{Im} G$. Unfortunately, from ARPES, we only know the occupied part of $\text{Im} G$,

$$I(k, \omega) = C k \sum_{\delta k} \int d\omega' A(k', \omega') f(\omega') R(\omega - \omega') + B$$

where $I$ is the photocurrent, $C$ an intensity prefactor (proportional to the square of the dipole matrix element between initial and final states), $R$ the energy resolution function, and $B$ an extrinsic background, with the sum representing the momentum resolution. To make progress, certain assumptions have to be made. For instance, if we assume the spectrum is particle-hole symmetric, then the full $\text{Im} G$ (symmetrized data) can be obtained from the above equation by the identity,

$$A(\omega) f(\omega) + A(-\omega) f(-\omega) = A(\omega),$$

which holds even in the presence of resolution. Obviously, the particle-hole symmetry assumption is a reasonable approximation only on the Fermi surface. Since the spectral peak is dispersionless around $(\pi, 0)$, we will assume particle-hole symmetry for our purposes.

A more difficult problem is that the spectrum is a continuous function of energy, and contains an extrinsic background, $B$. Separating out what part of the spectrum is intrinsic, and what is due to the state near the Fermi energy, and what is due to the tail of the main valence band, is an unresolved issue. For our purposes here, we will make the minimal assumption that the entire spectrum is intrinsic, which we simply cut off at the lowest energy data were taken at $(\omega_c = -320 \text{ meV})$. As discussed extensively in Ref. 16 varying the cut-off and background assumptions make quantitative, rather than qualitative, differences in the results. This was verified in the present paper as well.

Therefore, our procedure is as follows. The photocurrent is symmetrized about zero energy (zero energy determined by measuring the chemical potential of a polycrystalline gold sample in electrical contact with the sample). The prefactor $C$ in Eq. 2 is eliminated by invoking the condition that the integral of $A$ is unity over the energy range considered $(\pm \omega_c)$, and $B$ is assumed zero. This then gives $\text{Im} G$. $\text{Re} G$ is determined by Kramers-Kronig transformation. From the full $G$, $\text{Re} \Sigma$ and $\text{Im} \Sigma$ is then uniquely determined ($\epsilon$ being taken as zero). Unlike Ref. 16, since the data were obtained from a high resolution detector, we elected to use raw data, i.e., the noise was not filtered out, nor the resolution deconvolved.

In Fig. 2a, $\text{Im} \Sigma$, as determined from Fig. 1, is plotted for various temperatures. At low temperatures and energies, it is characterized by a peak centered at zero energy due to the superconducting energy gap, and a “normal” part which can be treated as a constant plus an $\omega^2$ term. Besides the constant term, which is surprisingly large, this is the expected form for the self-energy for a superfluid Fermi liquid. A maximum in $\text{Im} \Sigma$ occurs near the energy of the spectral dip. Beyond this, $\text{Im} \Sigma$ has a large, nearly frequency independent, value (the slow decay at higher energies is due to the cut-off at -320 meV, and so should not be taken seriously). As the temperature is raised, the zero energy peak broadens, the constant term increases, and the $\omega^2$ term goes away.

In Fig. 2b, the quantity $\omega - \text{Re} \Sigma$ is plotted. The low temperature, low energy behavior is again characteristic of a superfluid Fermi liquid. At low energies, there is a $1/\omega$ term due to the energy gap, and a “normal” part which is linear in $\omega$. As expected, the zero crossing is near the location of the spectral peak. Beyond this, there is a minimum near the spectral dip energy, then the data are approximately linear again, but with a smaller slope than near the zero crossing. As the temperature is raised, the gap ($1/\omega$) term broadens out and the low energy linear in $\omega$ term decreases, paralleling the behavior discussed above for $\text{Im} \Sigma$.

To further quantify this behavior, we have found that the following form for the self-energy gives a good description of data for low energies (smaller than the energy of the spectral dip)

$$\omega - \text{Re} \Sigma = Z \omega (1 - \frac{\Delta^2}{\omega^2 + \Gamma^2})$$

$$-\text{Im} \Sigma = c + c_{FL} \omega^2 + \frac{\Delta^2 \Gamma}{\omega^2 + \Gamma^2}$$

A discussion of this form is in order. The term involving
$\Delta$ is simply a broadened version of the BCS self-energy, with $\Gamma$ representing a combination of resolution and pair lifetime effects. Note that the quantity $\Delta_i/\sqrt{Z}$ in the expression for $\text{Im}\Sigma$ is approximately equivalent to $\Delta_i$, where $Z$ is the mass factor in the expression for $\text{Re}\Sigma$, and that $\Gamma_i$ and $\Gamma_\perp$ are essentially equivalent (these quantities would be identical by the Kramers-Kronig relations if the self-energy had this form for all energies). From this expression, one sees that the occupied quasiparticle weight is approximately

$$\text{Im}\Sigma \approx \frac{i}{\sqrt{Z}}.$$  

This is the mass factor in the expression for $\text{Im}\Sigma$, and $\Sigma$ is approximately equivalent to $\Delta$ (the other half of the quasiparticle weight lies above the Fermi energy). Also, if the gap term is neglected, one sees that the effective quasiparticle width is approximately $-\text{Im}\Sigma/Z$. Note that $Z$ is the inverse of the quasiparticle renormalization factor, $z$. The above assumes, of course, that quasiparticles exist, a matter which we will address below.

In Fig. 3, the temperature variation of these coefficients, obtained from fitting data over an energy range of $\pm 60$ meV, is shown. The most significant finding is that $Z$ decreases with temperature. This implies that quasiparticles exist, their weight increases with temperature. This is in contrast with earlier analyses, where $Z$ actually increases with temperature. This is in fact the strong variation of $Z$ with temperature, losing its integrity above $T_c$. Naturally, the quasiparticle weight $\Delta$ increases, and thus one would expect the spectral lineshape at $(\pi,0)$ to exhibit a magnetic resonance seen by neutron scattering. Since the intensity of this resonance decreases with temperature, then the coupling of the electrons to the magnetic resonance fills in, which we speculate is responsible for the “filling in” of $\text{Im}\Sigma$ seen in Fig. 2a. The combination of these two effects causes the spectral peak to broaden with temperature, losing its integrity above $T_c$.

In conclusion, we have studied the thermal evolution of the electron self-energy by direct analysis of ARPES data, and come to the conclusion that the spectral peak below $T_c$ broadens out above $T_c$ due to a “lifetime catastrophe”, rather than the quasiparticle weight $z$ monotonically decreasing to zero.

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FIG. 1. Temperature dependence of ARPES data at (π,0) for a Tc=90K Bi2212 sample. The vertical dotted lines mark the spectral dip energy and the chemical potential.

FIG. 2. Temperature dependence of (a) the imaginary and (b) real parts of the self-energy derived from the data of Fig. 1.

FIG. 3. Temperature dependence of the various coefficients of the self-energy from Eq. 3 obtained from fits of Fig. 2 over an energy range of ±60 meV.
FIG. 4. Temperature dependence of (a) the spectral peak weight (z and ratio) and (b) the width (FWHM) of the spectral peak (FW1 and FW2) as defined in the text. Also plotted is the low energy weight (low) and the peak energy (peak). For FW2, the low energy edge of the peak is either defined by the HWHM, or zero energy if A at zero energy is greater than half the maximum.