Robustness of the global non-analytical fit to the analysis of peak-dip-hump lineshape in bilayer-split spectra of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$

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Abstract. The application of global non-analytical fit to the quantitative spectral analysis of the bilayer-split peak-dip-hump lineshape of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ at (\pi, 0) are revisited. The robustness of the results is verified by various fitting schemes confirming physically the correlation of the superconducting peak with the superfluid density.

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The most dramatic variation across the superconducting transition temperature ($T_c$) in spectral function is the development of \textit{peak-dip-hump} (PDH) structure near $(\pi, 0)$\cite{1}. This has been observed by angle-resolved photoemission spectroscopy (ARPES) in many high temperature superconductors (HTSC’s), and is thought to carry critical information about the superconducting transition\cite{2}. Particularly, on \textit{Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$} (Bi2212), we found the superconducting peak (SCP) intensity to be closely related to the condensate fraction of the system\cite{3}. This was achieved by a spectral analysis based on the SCP ratio (SPR) accounting for the phenomenologically-extracted coherent component in $(\pi, 0)$ ARPES lineshape. The phase-coherent like behavior of SPR (increases with doping increases) in the underdoped regime was later confirmed by H. Ding et al. based on a similar analysis of the lineshape by means of the so-called renormalized quasiparticle weight (RQW), a quantitative equivalent to SPR\cite{4}. However, as a contrast, the decrease of the SPR upon doping increase across the optimal doping was not reproduced. This led the authors to think it was necessary to combine the additional effect by the gap opening to yield, rather than simply taking the SPR as, the long-sought superconducting order parameter for the cuprates.

This controversy remains until later another important finding was made, the existence of bilayer band splitting (BBS) in heavily overdoped (OD) Bi2212\cite{5}. This gives birth to a sharp anti-bonding band remnant (AB hump) even in the normal state at the SCP binding energy position tending to invalidate the SPR (RQW)-based phenomenological background substraction: the SPR (RQW) obtained this way contains a substantial spectral weight contribution from the AB hump, which should not be counted in in order to obtain a true ratio reflecting the SCP only. The increasing overestimation of the true peak ratio prevents a similar analysis from applying to the more OD regime where the AB band becomes sharper. In Ref. \cite{6}, a lineshape modelling based on a physically sensible description of the two quasi-particle bands\cite{7} proved its eligibility to reproduce the complex PDH lineshape under a considerable BBS complication and yielded a reduced SPR strengthening its correlation with the superfluid density in the very OD regime.

In this paper, we revisit the investigation by presenting more results reflecting the robustness of the conclusion, which include the insensitiveness to a physical variation in the spectral function, to a different self-normalization scheme adopted.

For clarity, we recap below the fitting function used for the lineshape modelling in Refs. \cite{6, 8}. Note that only possible variations in some expressions are pointed out and the denominations of symbols completely follow those in Refs. \cite{6, 8} otherwise.

\begin{align*}
I(\omega, T, h\nu) & = I_0(T, h\nu) \cdot \left[ \left( \sum_{\alpha} J_\alpha(\omega, T, h\nu) \cdot f(\omega, T) \right) \otimes R(\omega, \Gamma(\nu)) + B(\omega, T) \right] + I_1(T, h\nu), \\
J_{ab}(\omega, T, h\nu) & = M_{ab}(h\nu) \cdot C_a(T) \cdot A_b(\omega, T, \alpha, \varepsilon_{ab}), \\
J_{bh}(\omega, T, h\nu) & = M_{bh}(h\nu) \cdot C_b(T) \cdot A_h(\omega, T, \alpha, \varepsilon_{bh}), \\
J_{ap}(\omega, T, h\nu) & = M_{ap}(h\nu) \cdot (1 - C_a(T)) \cdot A_p(\omega, \Gamma_a(T), \varepsilon_{ap}),
\end{align*}
Figure 1. (color) Results of Scheme II of the global convolve fit on the $T$-dependent (a) (see also [f] for an enlargement of the $T=30$ K curves) and $h\nu$-dependent ARPES spectra at $(\pi, 0)$ of (Ph)-OD65 in the superconducting state at $T=10$ K (b) and normal state at $T=80$ K (c). The AB hump lies lower in energy than the BB hump. The width difference of the SCP is due to resolution variations from 10 to 18 meV at different $h\nu$'s. The fitted $h\nu$-dependent matrix elements (d) and $T$-dependent energy positions of the maxima (e) of various spectral features are shown reminiscent of the similar results in Ref. [6]. Inset of (e) illustrates the constancy of the AB peak width upon $T$ variation in the superconducting state.
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\[ J_{bp}(\omega, T, h\nu) = M_{bp}(h\nu) \cdot (1 - C_b(T)) \cdot A_p(\omega, \Gamma_b(T), \varepsilon_{bp}), \]
\[ A_h(\omega, T, \alpha, \omega_0) = \frac{\xi |\Sigma''(\omega, T)|}{(\omega - \sqrt{\omega_0^2 + \Delta sc(T)^2})^2 + \Sigma''(\omega, T)^2}, \]
\[ A_p(\omega, \Gamma(T), \omega_0) = \frac{2\sqrt{\ln 2}}{\sqrt{\pi \Gamma(T)}} \exp[-(\omega - \omega_0)^2]. \]

where the imaginary part of the self-energy is defined either by
\[ \Sigma''(\omega, T) = (\alpha \omega)^2 + (\beta T)^2 \] (1)

\[ \text{or by} \]
\[ \Sigma''(\omega, T) = |(\alpha \omega)^2 + (\beta T)^2 + \zeta| \]

\[ \text{where lifetime broadening associated with the impurity level of samples is reflected by } \zeta \text{ and that with doping level of by } \alpha \text{ and } \beta, \text{ which are photon energy } (h\nu) \text{ and temperature } (T) \text{ independent. } \Gamma(T) \text{ is a } T-\text{dependent linewidth (FWHM) for the SCP.} \]

Note that, as a sum rule for an overall spectral weight conservation upon } T \text{ variation, we adopt either}
\[ \int_{-\infty}^{\infty} A_h(\omega)d\omega = 1 \] (3)

\[ \text{Refs. [6, 8] or} \]
\[ \int_{-\infty}^{\infty} f(\omega)A_h(\omega, T)d\omega = n(T) \] (4)

\[ \text{where } n(T) \text{ is the occupation number at } (\pi, 0), \text{ which is nearly independent of } T \text{ and thus assumed to be a constant here. As a result, spectral weight transfer (SWT) } (= 1 - C_{a(b)}, 0 \leq C_{a(b)}(T) \leq 1) \text{ is well defined for the description of the SCP formation disregarding the kind of dependence under investigation[6]. In any case, a realistic SCG or pseudogap opening extracted with the leading edge gap method on the same sample introduces an effective } T-\text{dependent energy shift to the bilayer-split bands in the superconducting state while the energy position of the SCP is subjected to the fit.} \]

In order to retrieve reliable quantitative information from a multi-dimensional fit to a set of interconnected EDC’s, we developed a powerful fitting routine under WaveMetrics Igor Pro 4.0[10], which has been applied in our previous work[6] and detailed in Ref. [8]. Physically, the goal is to achieve a systematic understanding of both the } h\nu- \text{ and the } T-\text{dependent behavior of the lineshape where many physical constraints are involved and strictly followed. For example, in the the } h\nu-\text{dependent set, all functions of } T \text{ are shared variants to all EDC’s at the same } T \text{ while the functions of } h\nu(\text{matrix elements}) \text{ are locally specified, and in the } T-\text{dependent set, vice versa. The renormalized band energy position } \varepsilon \text{ is always a global fitting parameter for the EDC’s of samples at the same doping level. Technically, reminiscent of the great contrast in the overall quality (or details) of the fit between the one shown in Fig. 2 of Ref. [7] and ours, in Refs. [6, 8], though on data sets generally twice larger in size, the inherently local fit scheme[7, 11] with manual adjustments on the globally defined fitting parameters is unlikely to give a reliable result in a truly global sense. In contrast, our fully-automatic}
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Figure 2. (color) Results of the three schemes of the global non-analytical fit. The fitted $h\nu$-dependent matrix element hump ratios, $\frac{M_{ah}}{M_{mh}}$ (filled markers), and peak-hump ratios, $\frac{M_{ap}}{(M_{ah}+M_{mh})/2}$ (empty markers) are shown in (a). (b) shows the fitted $T$-dependent energy positions of the AB peak (empty markers) and AB hump maxima (filled markers). (c) The $T$-dependent SWT’s and an interpolation on the averaged dependence according to the function $\text{SWT}=\text{SWT}_0[1-(T/T_c)^\zeta]$ (see Ref. [12]). The fitted value, $\zeta = 2.56$, agrees with the $T$-dependent $\mu$SR result on $Tl_2Ba_2CuO_{6+\delta}$ at the same doping level (OD66 TI2201)(not shown). The contrast between the phenomenological SPR and SWT-based SPR’s extracted from the same set of data (taken with He-I) is given in the inset. (d) The doping-dependence of SPR ($h\nu=22.7$ eV, $T = 10$ K) supplemented by the global fit results on Pb-OD65.

fitting routine can yield a robust, physically-constrained global fit for a large set of EDC’s regardless of the initial values input.

The global non-analytical fit implemented in Ref. [6] is based on Eq. 1 and 3 (Scheme I). In the following, we conducted another two schemes, the one with Eq. 2 and 3 (Scheme II) and the other with Eq. 2 and 4 to complement the results of analysis based on the global non-analytical fit. Our argument about the qualification of the SPR as the order parameter for the HTSC’s is invulnerable to the physical variation of the fitting scheme we choose. This checkup is hardly practical without a fully-automatic multi-level global non-analytical fit routine which can be easily oriented for any non-analytical global fitting task given.

In Fig. 1 we present the results of Scheme II, reminiscent of Fig. 2-3 in Ref. [6].
The fitting quality is exemplified in Fig. 1(f). Keep in mind that this quality is common to the fits of the 35 EDC’s in contrast to a local best fit on a few selected curves at the expense of a global agreement on a much larger assembly within the usual manual fitting framework[7]. In Scheme II, when we further release the constrain on Γa to let it fittable, we find its T-dependence is negligible as obtained by our phenomenological fitting. This argues against the Fermi liquid approach that attributes the disappearance of the sharp peak above $T_c$ to broadening caused by phase fluctuations[13, 14].

Note that the addition of an impurity term (whose fitted value is $-0.0058 \pm 0.0004$ for Pb-OD65 and $-0.0067 \pm 0.0004$ for OD65) in the imaginary self-energy doesn’t result in any qualitative change in the $h\nu$-dependence of matrix elements as well as the $T$-dependence of the energy positions of spectral features [Fig. 1(d)(e)]. However, quantitative changes is discernible when we plot the results of the three schemes together as in Fig. 2. Though the modification of the normalization equation is not expected to alter much the energy positions of features whose maximums are more or less self-pinned [Fig. 2(b)] and the anti-phase-like $h\nu$-dependence of the hump matrix elements as predicted by theory[15, 16], the matrix element ratio of the two hump bands $(M_{bh}/M_{ah})$ is, in principle, a touchstone for the justification of the physical normalization method. The average of matrix element hump ratio over a large $h\nu$ window is supposed to approach unity as expected from a pair of bands of the same atomic character split by the c-axis bilayer coupling. Though the $h\nu$ window concerned here is not large enough, Scheme I and II give a ratio of 0.91 ± 0.01 and 1.21 ± 0.04, respectively, quite approaching unity, while Scheme III yields 1.55 ± 0.02.

Interestingly, compared with the hump ratio, the matrix element ratio between the peak and the hump, defined by $M_{ap}/(M_{ah}+M_{bh})/2$, exhibits a constancy over $h\nu$. Reminiscent of the absence of SCP finding report in spectra of mono-layer cuprate Bi$_2$Sr$_2$CuO$_{6+\delta}$, this probably imply the AB peak has a hybrid origin of AB and BB humps at the same time. It is argued by the magnetic resonance ($\pi, \pi, \pi$) mode scenario that the c-axis momentum transfer by the mode scattering occurs between AB and BB which leads to the formation of the PDH lineshape[17]. However, in our picture the SCP is a new quasi-particle developed from its normal state counterpart of hump, just the opposite to the magnetic mode scenario where the dip(hump) is argued to contain the incoherent spectral weight subjected to the scattering of the quasi-particle peak. This critical question concerning the SC origin is still unaddressed.

As told by Fig. 2(c), the SWT saturates at low temperature to be (0.26 ± 0.03), a value far below 1, which is required by the magnetic mode scenario in which the collective mode induces an on/off damping mechanism at the dip position driving the whole lower-lying AB component coherent with no AB hump remanence[18]. As mentioned before, the large remanence of AB hump proportion at the experimentally observed SCP energy position in the superconducting state also questions the validation of the SPR (RQW)-based phenomenological background substraction[3, 4] in the very OD regime. This can be illustrated by the contrast in the inset of Fig. 2(c) with the phenomenological SPR featured by an overall overestimation in value and a non-zero normal state baseline.
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followed by a rounded onset spreading over a large $T$ region across $T_c$.

The collapses of the $T$-dependent SWT (SPR) onto the superfluid density curve [Fig. 2(c)] and of the SWT-based SPR’s by the three schemes onto the $T_c$ guideline strength [Fig. 2(d)] strengthen again the qualification of SPR (SWT) as a superconducting order parameter for Bi2212. However, the component-resolved matrix-element-free merit of SWT makes it an ideal quantity for the quantitative spectral analysis of the complex lineshape at $(\pi,0)$. A systematic investigation of both the doping and $T$ dependence of SWT based on an indispensable global fit facility is needed for a comprehensive understanding of its relation to the possible mechanism for high-temperature superconductivity.

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