Unadulterated spectral function of low-energy quasiparticles

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Low-Energy QuasiParticle spectrum $\Sigma=\Sigma'+i\Sigma''$

- Is quasiparticle approach valid?
- ARPES vs. Transport?
- Nature of interactions in HTSCs?
Questions to behavior of $\Sigma'' \sim 1/\tau$

- Offset at $\omega \to 0$ and at $T \to 0$?

- Behavior near $T_C$?

- Evolution with doping?
Problems

• How to remove resolution effects accurately?

\[ R^-? \]

• How to disentangle impurity scattering from quasiparticle interaction?

\[ \Sigma''_{\text{int}} = \Sigma'' - \Sigma''_{\text{imp}} \]
Total response function

\[ R = R_A \otimes R_S \]

- **\( R_A \) – Analyzer**
  - Remains constant
  - Easy to measure

- **\( R_S \) – Sample Surface**
  - Varies with space and time
  - Difficult to measure
Processing of ARPES Image

\[ A(\omega, k) \sim \text{Im}(G(\omega, k)) \]

\[ A(\omega, k) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(k) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2} \]

\[ \text{MDC}(k) = A(\omega, k), \quad \omega = \text{const} \]
Spectral Function Extraction from ARPES Data

\[ I(k, \omega) \propto A(k, \omega) \otimes R(k, \omega) \]

We measure \( I(k, \omega) \)
We are interested in \( A(k, \omega) \)
We need to remove \( R(k, \omega) \)
Nodal Direction

CuO planes

No gap
Momentum Resolution

\[ \Sigma(k, \omega) = \Sigma(\omega) \quad M(k) = \text{const} \quad \epsilon(k) \text{ linear} \]

Without resolution effects MDC is perfect \textbf{lorentzian}:

\[
L(k) = A(k, \omega_0) = -\frac{1}{\pi} \cdot \frac{\Sigma''(\omega_0)}{\left(\nu \cdot (k - k_{\text{max}})\right)^2 + (\Sigma''(\omega_0))^2}
\]

Real MDC is a \textbf{convolution} between pure signal and resolution:

\[
MDC(k) = L \otimes R = \int L(k - \kappa) \cdot R(\kappa) \cdot d\kappa
\]

Where resolution is a \textbf{gaussian}:

\[
R(k) = \frac{1}{\sigma \sqrt{\pi}} e^{-\frac{k^2}{\sigma^2}}
\]
Real MDC = Pure MDC (Lorentzian)
Real MDC = Pure MDC $\otimes$ Resolution
            (Lorentzian)    (Gaussian)
Real MDC = Pure MDC \otimes \text{Resolution (Lorentzian)} \, \, \text{Pure MDC \otimes Resolution (Gaussian)}$

Lorentzian \otimes \text{Gaussian} = \text{Voigt profile}
Real MDC = Pure MDC \otimes Resolution
(Lorentzian) (Gaussian)

Lorentzian \otimes Gaussian = Voigt profile

What is Voigt Profile?
Voigt Profile

\[ V(k) = L \otimes G = \int L(k - \kappa) \cdot G(\kappa) \cdot d\kappa \]

Where L is a lorentzian, and G is gaussian. HWHM \( W_L \) and \( W_G \)

\[ L(x) = \frac{1}{1 + x^2 / W_L^2}, \quad G(x) = \frac{\ln(2)}{W_G\sqrt{\pi}} \exp(-\ln(2) \cdot x^2 / W_G^2) \]

HWHM of Voigt profile, \( W_V \):

\[ W_V \approx \frac{W_L}{2} + \sqrt{\frac{W_L^2}{4} + W_G^2} \]

error < 1.2%

\[ W_L \ll W_G \Rightarrow W_V \approx \frac{W_L}{2} + W_G \]
Lorentz, Gauss

L, G:
1. Offset
2. Max position
3. Amplitude
4. Width

Diagram showing the difference between Lorentzian (L) and Gaussian (G) functions with key parameters labeled.
Lorentz, Gauss and Voigt

L, G:
1. Offset
2. Max position
3. Amplitude
4. Width

One more parameter:

5. $\eta = \frac{W_G}{W_L}$

$\eta \rightarrow 0$ Voigt $\rightarrow$ Lorentz

$\eta \rightarrow \infty$ Voigt $\rightarrow$ Gauss
Old Procedure of Self Energy Extraction

Lorentz-Fit

Overall width
New Procedure of Self Energy Extraction

Voigt-Fit

Lorentz-Fit

Overall width

Intrinsic width and resolution
MDC Shape

Data Fit:
- Lorentzian
- Gaussian
- Voigt profile
$\Sigma(\omega)$ from Voigt Fit

**Bi-2212 OP 89K, T = 110–135 K**

Voigt fit:
- $W_V$
- $W_G$
- $W_L$

Lorentz fit:
- $W_{lor}$

$\omega$ (eV) vs. HWHM (1/Å) $\times 10^{-3}$
$\Sigma(\omega)$ from Voigt Fit

Resolution: $W_G = const$
\[ \Sigma(\omega) \text{ from Voigt Fit} \]

Overall width, \( W_V \)
Σ(ω) from Voigt Fit

Intrinsic width, $W_L$
Examples of Voigt fit Application to ARPES Data

- BSCCO
  - $x=0.21$
  - $x=0.16$
  - $x=0.12$
- YBCO
- Temperature dependence
- Comparison to high-resolution data
Examples on BSCCO

$x=0.21, \ T=100 \ K$

$x=0.16, \ T=40 \ K$

$x=0.12, \ Low \ T$
Voigt Fit in application to YBCO

Image1, 24 K

Image2, 24 K

Resolution:
Raw Data:
Purified Data:
Temperature dependence of scattering rate

$\Sigma''(\omega=0,T)$

width decreases!
Temperature dependence of scattering rate

\[ \Sigma''(\omega=0,T) \]

Overall width decreases!

Intrinsic width increases
Comparison to the low-energy high-resolution data

\[ R \sim (h\nu - \phi)^{-1/2} \]

\[ \frac{R_{6\text{eV \ LASER}}}{R_{27\text{eV \ synchrotron}}} = 0.25 \]

J. D. Koralek et al., PRL 2006
Justification of Voigt Fit procedure

A. MDC Lineshape

B. $\omega$-dependence: $WG(\omega)=\text{const}$

C. YBCO: different images give same result while exposed to Voigt Fit procedure

D. T-dependence: while WG exhibits almost random and strange behavior, WL(T) always increases with temperature

E. Purified by Voigt Fit data coincides with high-resolution data (Koralek PRL 2006)
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Most interesting part 😊
$\Sigma''(\omega)$ behavior in vicinity of Fermi-level
Reduced self-energy function

$$\sigma(\omega) = \frac{\Sigma''(\omega) - \Sigma''(0)}{\omega}$$

- $\Sigma'' = \text{const} \rightarrow \sigma = 0$
- $\Sigma'' \propto \omega \rightarrow \sigma = \text{const}$
- $\Sigma'' \propto \omega^2 \rightarrow \sigma \propto \omega$
- $\Sigma'' \propto \omega^3 \rightarrow \sigma \propto \omega^2$

Quasiparticle limit:
$$\Sigma''(\omega)/\omega \ll 1$$

- OP 89 K, $T = 30$ K
- OP 89 K, $T \approx 110$ K
- Koralek PRL 2006
- OD 75 K, $T = 90$ K

Evtushinsky Physical Review B 2006
Temperature dependence of scattering rate

T. Valla
Physical Review B, 2006
T. Yamasaki et al., cond-mat/0603006
ARPES vs. Transport
MDC Width: 0.030 vs 0.004 1/Å

Yoshida’s MDC used to calculate resistivity. HWHM=0.03 1/Å
Compare to result, obtained by Voigt-fit procedure: 0.004 1/Å.

Yoshida Physica B 2004
\[ \tau \text{ from ARPES and Resistivity} \]

\[ \rho_0 = \frac{m^*}{ne^2 \tau} \approx \frac{k_F}{ne^2 \eta} \frac{\Sigma''}{v_r} \]

\[ n \sim 1 - x \]

\[ \tau = \frac{\eta}{\Sigma''(0)} \]
Forward and Isotropic Scattering

Forward, $\tau_f$

Isotropic, $\tau_I$

ARPES: $\tau^{-1} = \tau_I^{-1} + \tau_f^{-1}$

Transport: $\tau^{-1} = \tau_I^{-1} + \alpha \cdot \tau_f^{-1}$, $\alpha \ll 1$
Quasiparticle Lifetime from ARPES
Impurity scattering

\[ \rho_0 = \frac{m^*}{ne^2 \tau} \approx \frac{k_F}{ne^2 \eta} \sum_{im}'' \]

forward and isotropic (unitary)?

\[ n \sim 1 - x \]

\[ n(x) \text{ ?} \]

inhomogeneity
Resistivity from ARPES

Simple Drude formula: \[ \sigma = \frac{n e^2 \tau}{m^*} \]

Note that \( m^* \) is calculated from renormalized dispersion.
\[ n=(1-x) \]

How resistivity changes if we take into account some extra features?

Two kinds of scattering:

ARPES: \[ \tau^{-1} = \tau_I^{-1} + \tau_f^{-1} \]
Transport: \[ \tau^{-1} = \tau_I^{-1} + \alpha \cdot \tau_f^{-1}, \quad \alpha \ll 1 \]

Inhomogeneity:

\[ n \sim (1-V_m) n_d + V_m n_m \]
\[ V_m \] – metallic phase volume
Conclusions

• Quasiparticles are well-defined

• Non-zero $\Sigma''(T=0) \approx 16 \text{ meV}$

• No drop at $T_C$

• $\Sigma''$ depends rather on dopants than on $x$

• To compare to transport we need to disentangle isotropic and forward contributions
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\( \Sigma''(\omega,T) \) asymmetry

\[ \Sigma''(\omega,T) = S(\omega) + S(\pi T) \]

\[ \Sigma''(\omega=0,T) = S(\pi T) \]

\[ \Sigma''(\omega,T=\text{const}) = S(\omega) + \text{const} \]

- \( \Sigma''(\omega,T=\text{95..125 K}) \)
- \( \Sigma''(\omega,T=\text{299 K}) \)

\( \Omega \)-doped (YDLY)
\[ w[0] + w[1]*T + w[2]*T^2 \]

- 0.21 \{0.0045, 1.90e-05, 7.2e-08\}
- 0.16 \{0.0052, 1.02e-05, 8.9e-08\}
- 0.16 (Ni) \{0.0054, -3.84e-06, 9.4e-08\}
- 0.16 (Zn) \{0.0093, 2.64e-05, 8.7e-09\}
- 0.11 \{0.0116, -1.44e-06, 1.7e-07\}
- 0.12 (Y) \{0.0052, 2.41e-05, 2.1e-07\}
Energy resolution in Voigt fit

\[ I(k, \omega) \propto A(k, \omega) \otimes R(k, \omega) \]

\[ R(k, \omega) = R_k \otimes R_\omega \]

Energy resolution has almost the same effect on the MDC shape as momentum resolution, so both \( R_\omega \) and \( R_k \) are taken into account by Voigt-fit procedure.
Pure MDC – Lorentzian
Real MDC = pure MDC \otimes \text{Resolution} - \text{Voigt}
Scattering mechanisms

Gap $\rightarrow$ DOS $\rightarrow$ $\Sigma''$
	onopening
change
change

Inelastic e - e scattering:

$$\Sigma''_{in}(\omega) \propto \int\int d\omega_1 d\omega_2 \text{DOS}(\omega_1) \text{DOS}(\omega_2) \text{DOS}(\omega - \omega_1 - \omega_2)$$

$$\Sigma''_{in}(\omega) \sim \omega^2, \quad T > T_C$$
$$\Sigma''_{in}(\omega) \sim \omega^n, \quad n \geq 3, \quad T < T_C$$

Scattering on impurities:

$$\Sigma''_{imp}(\omega) \propto \int \text{DOS}(\omega - \Omega) \cdot N_{imp}(\Omega) \cdot d\Omega$$

- $\Sigma''_{imp}(\omega) \sim \text{DOS}(\omega) \sim \text{const}, \quad T > T_C$
- $\Sigma''_{imp}(\omega) \sim \omega, \quad T < T_C$