Self-consistency of quasiparticle description in high-Tc cuprates

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Complexity of HTSC

Complex physics?

Complex structure?

Complexity in ARPES?
HTSC are **simple**!

\[ \text{LDA} + \text{Self-energy} + ? \]

complex but understandable

self-consistency as a tool
Self-consistency as a tool

1. How Kramers-Kronig (KK) consistency works
   Why we believe it is applicable.
   Fine details of quasiparticle spectral function.
   Room for complexity in photoemission process.

2. The waterfalls (Where the consistency stops).

3. Fingerprints of the bosonic spectrum
   Quasiparticle spectrum in the whole Brillouin zone
   k-dependent self-energy
   ARPES – INS

4. Pseudo-gap problem…
Complex electronic structure of $\text{CuO}_2$ bi-layer
Complex electronic structure of CuO$_2$ bi-layer
Bare band dispersion = LDA dispersion

Kordyuk PRB 2004
Electronic structure of HTSC is bare band dispersion + self-energy
Electronic structure of HTSC is bare band dispersion + self-energy

Borisenko *PRL* 2003
Unadulterated spectral function
Introduction to the nodal spectra analysis

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

\[ \Sigma'(\omega) = \omega - \varepsilon(k_m) \]

\[ \Sigma''(\omega) = -v_F W(\omega) \]
Lorentzian to Gaussian

Voigt profile = Lor $\otimes$ Gauss

Evtushinsky, PRB 2006
Voigt fitting procedure

(a) Bi-2212 OP 90K, T = ?? K

Voigt fit:

- \( W_V \)
- \( W_G \)
- \( W_G^* \)
- \( W_L \)
- \( W_L^* \)

(b) HWHM (1/Å) × 10^{-3}

HWHM vs. \( T \) (K)

\[
W_V = V(W_L, W_G) = \frac{W_L}{2} + \sqrt{\frac{W_L^2}{4} + W_G^2}
\]

Evtushinsky PRB 2006
Now for the self-energy:

1. Real impurity scattering
2. Careful energy dependence
3. Careful temperature dependence
Energy dependence

(a) Bi-2212 OP 89 K
T = 30 K

(b) OP 89 K, T = 30 K
OP 89 K, T ≈ 110 K
OD 75 K, T ≈ 90 K

Evtushinsky PRB 2006
Temperature dependence

pseudo-gap
no "arcs"!

Evtushinsky PRB 2006
Impurity scattering

$$\rho_0 = \frac{m^*}{ne^2 \tau} \approx \frac{k_F}{ne^2 \hbar} \frac{\Sigma''_{im}}{\nu_r}$$

forward and isotropic (unitary)?

$$n \sim 1 - x$$

$n(x)$ ?

inhomogeneity
How Kramers-Kronig consistency works

Why we believe it is applicable
Bare Fermi velocity from the nodal spectrum

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

\[ \Sigma'(\omega) = \omega - \varepsilon(k_m) \]

\[ \Sigma''(\omega) = -v_F W(\omega) \]

\[ \Sigma'(\omega) = KK \Sigma''(\omega) \]
Kramers-Kronig transform

\[ \Sigma''(\omega) = \text{KK} \left( \Sigma'_{\text{width}} - \text{Res} \right) \]

Kordyuk PRB 2005
Kramers-Kronig transform \( \Sigma'(\omega) = KK \Sigma''(\omega) \)

\[
\Sigma''(\omega) = \begin{cases} 
\Sigma''_{\text{width}}(\omega) & \text{for } |\omega| < \omega_m, \\
\Sigma''_{\text{mod}}(\omega) & \text{for } |\omega| > \omega_m,
\end{cases}
\]

\[
\Sigma''_{\text{mod}}(\omega) = -\frac{\alpha \omega^2 + C}{1 + \left|\frac{\omega}{\omega_c}\right|^n},
\]

Kordyuk PRB 2005
Evolution of the kink

Kordyuk *PRL* 2006
Evolution of the self-energy

Kordyuk *PRL* 2006
Parameters of the kink → 2 channels

\[ \lambda = -\left( \frac{d \Sigma'}{d \omega} \right)_{\omega=0} \]

Kordyuk PRL 2006
Intensity of the bosonic channel
Eliashberg function from YBCO

Averaged (over npnts) Eliashberg function from self energy
B_HIN366_sum89:

\[ \Sigma'' \quad \Sigma' \]

B_HIN366_sum99:

\[ \Sigma'' \quad \Sigma' \]

kink

Evtushinsky 2007
Two channels

1 "Fermionic"

- mainly $xT$-independent
- featureless: $\Sigma'' \sim \omega^2$, $\Sigma' \sim \omega$
- simple e-e interaction (Auger-like decay)
- FL

2 "Bosonic"

- critically depends on $(x, T)$
- energy structure:
  (i) kinky,
  - $\omega_k$ mainly $xT$-independent
  (ii) step-like,
  - does not confined at low $\omega$

\[ \text{phonons, gap} \rightarrow \text{SF} \]
The "waterfalls"

Where the consistency stops
"High-energy scale"
Extrinsic spectral weight
Waterfalls phenomenon
Waterfalls phenomenon
Waterfalls phenomenon

100 eV

90 eV

27 eV

18 eV

100 eV
Waterfalls phenomenon

Intensity vs. $|k|$, 1/Å

- Red: 18 eV
- Blue: 20 eV
- Cyan: 27 eV
- Purple: 100 eV

Inset: Binding energy (eV) vs. Momentum (Å⁻¹)
Waterfalls phenomenon

Diagram showing binding energy and momentum relationships with arrows indicating specific paths: (0, -\pi) - (0, 0) - (0, \pi) and (2\pi, -\pi) - (2\pi, 0) - (2\pi, \pi).
Waterfalls phenomenon

Inosov cond-mat/0703223
Room for complexity of the photoemission process
MDC asymmetry

\[ \Sigma_{\text{min}} = 16 \text{ meV} \]
MDC asymmetry
Fingerprints of the bosonic spectrum

Quasiparticle spectrum in the whole Brillouin zone
k-dependent self-energy
ARPES – INS
\( G_0 \star \chi_{\text{exp}} \sim \sum_i \)

\( G_i^{-1} = G_0^{-1} + \sum_i \)

FIG + Forschergruppe + Dahm & Scalapino 2006
Looking for "fingerprints"

of $\chi(k,\omega)$ in $\Delta(k,\omega)$

ARPES: $A(k,\omega) f(\omega) \rightarrow \Delta(k,\omega)$

$\Delta(k,\omega)$, $\Sigma(k,\omega)$, $\varepsilon_k$

(if)

$(\Delta, \Sigma) = EE(\Delta, \Sigma, \varepsilon, \chi)$

$\Sigma \sim G \star \chi$
Pseudogap and CDW in two dimensions

TaSe$_2$

Borisenko arXiv:0704.1544
Pseudogap and CDW in two dimensions

Borisenko arXiv:0704.1544
Pseudogap and CDW in two dimensions

Borisenko arXiv:0704.1544
Conclusions

- **Magnetic excitations** strongly couples to the conduction electrons—and are, thus, the most probable candidate for mediation of the electron pairing in HTSC.

- The unification of the momentum resolving techniques are required:
  1. to identify **ultimately** the "fingerprints" of the relevant bosonic spectrum in both \( \Sigma(k, \omega) \) and \( \Delta(k, \omega) \);
  2. to determine the origin of the bosonic spectrum (the degree of itinerancy, in case of spin-fluctuations);
  3. to understand the role of space inhomogeneity in pairing.

- The current rate of improvement of all of the momentum resolving techniques suggests that these problems will be solved very soon.
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