



Self-consistency of quasiparticle description in high- T_c cuprates

Alexander Kordyuk

Institute of Metal Physics, Kiev, Ukraine

Institute for Solid State Research, Dresden, Germany

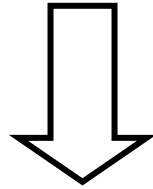
Complexity of HTSC

Complex physics?

Complex structure?

Complexity in ARPES?

HTSC are simple!



LDA + 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

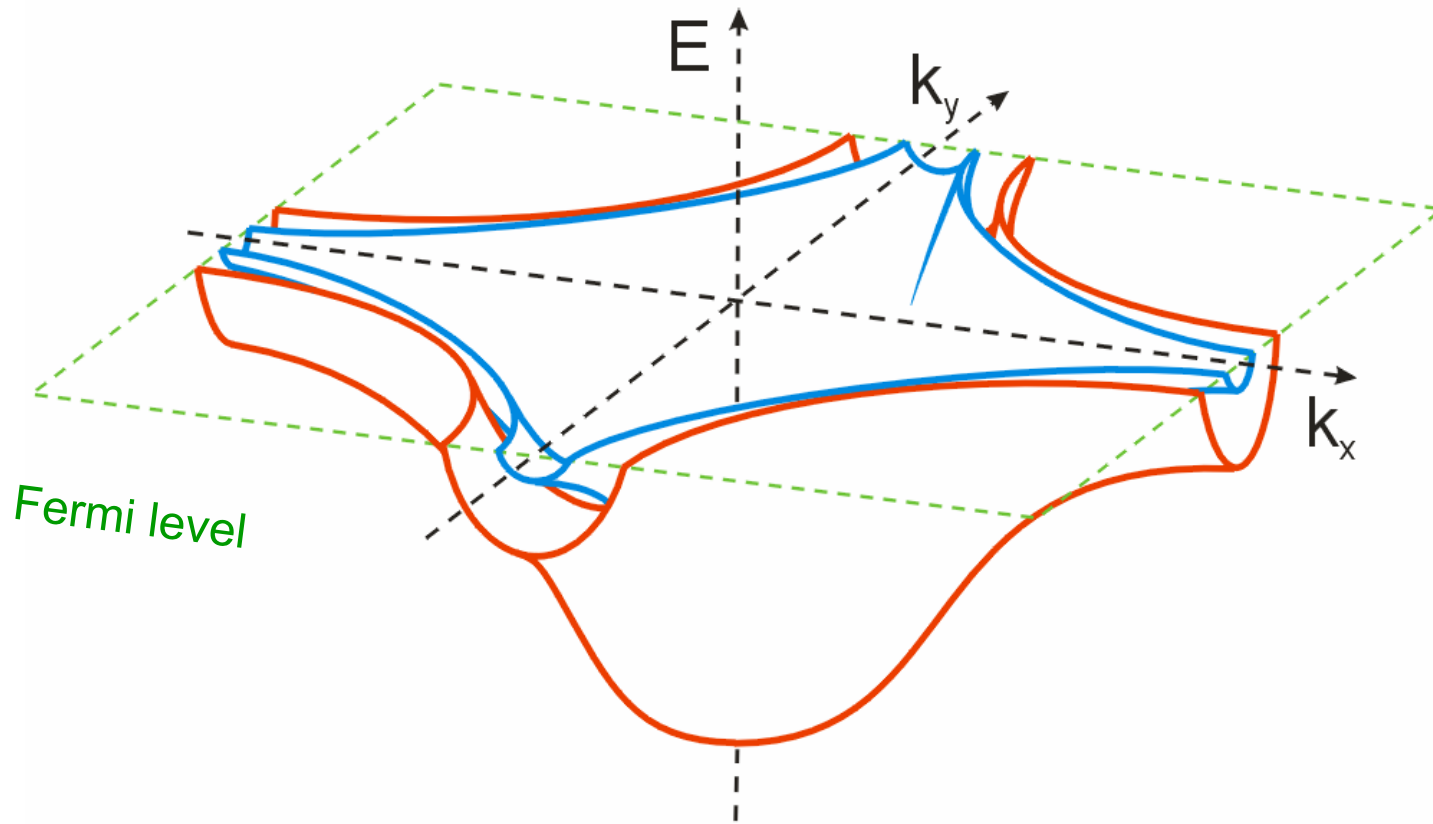
Quasiparticle spectrum in the whole Brillouin zone

k-dependent self-energy

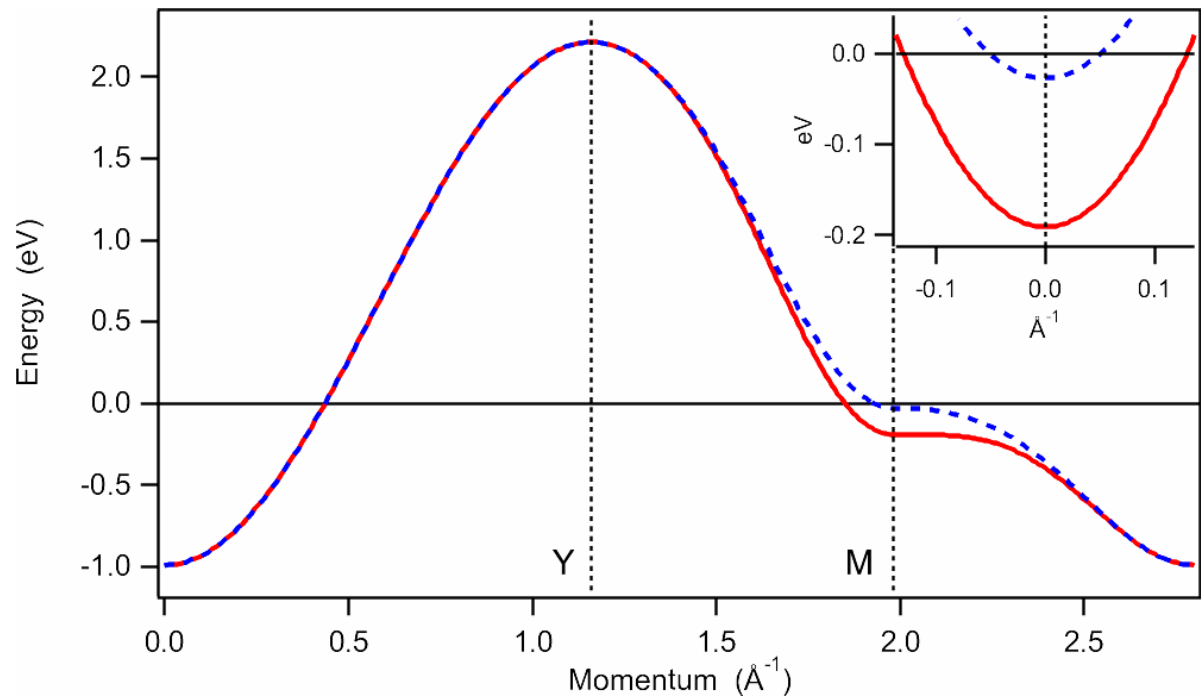
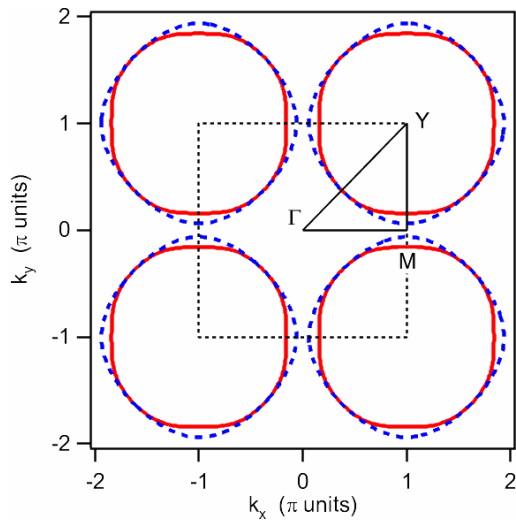
ARPES – INS

4. Pseudo-gap problem...

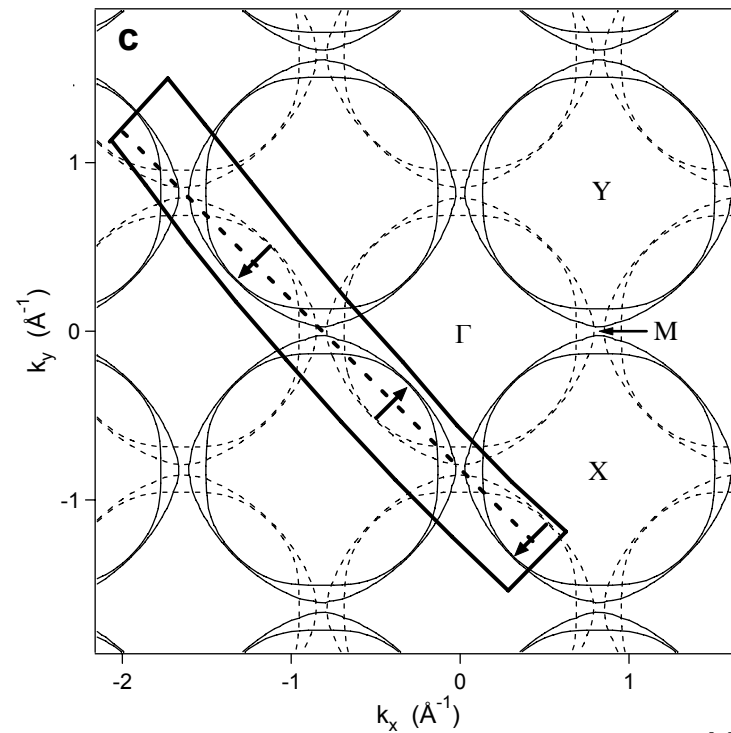
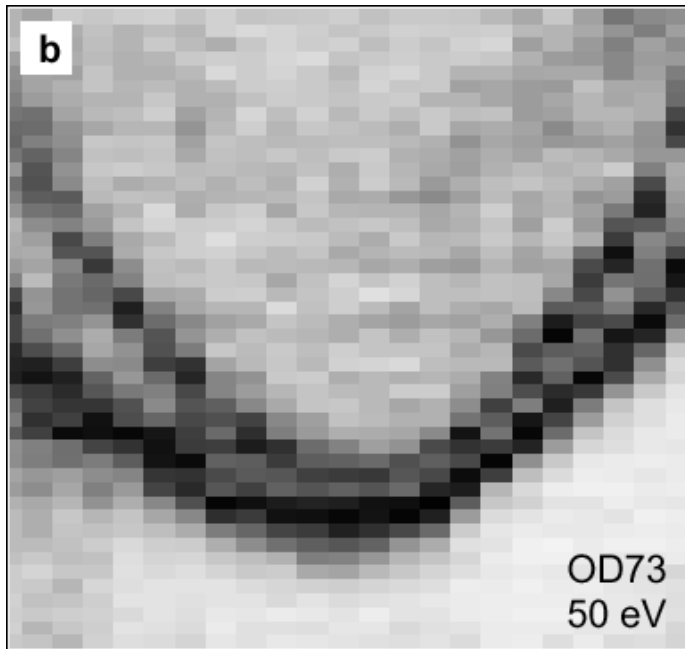
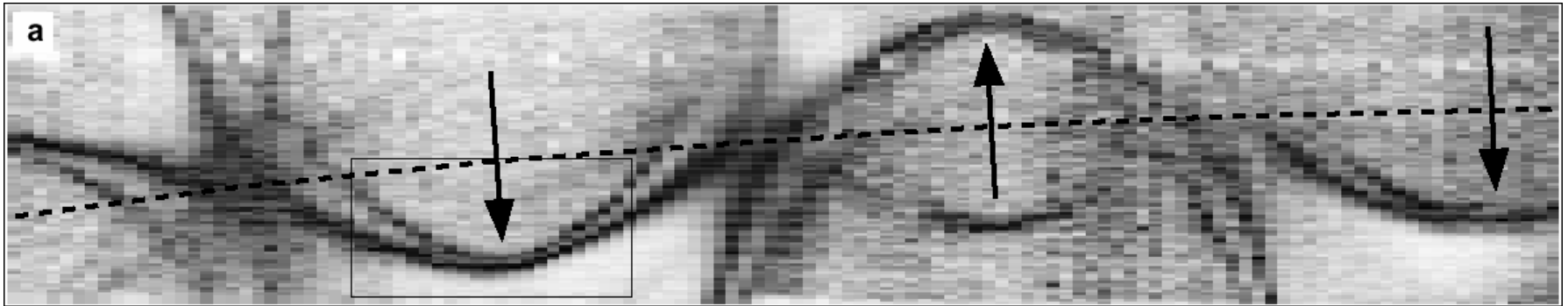
Complex electronic structure of CuO_2 bi-layer



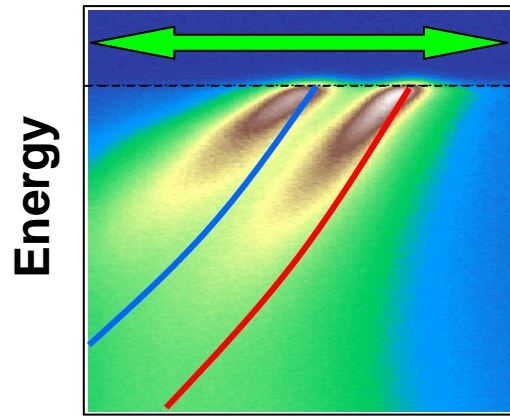
Complex electronic structure of CuO_2 bi-layer



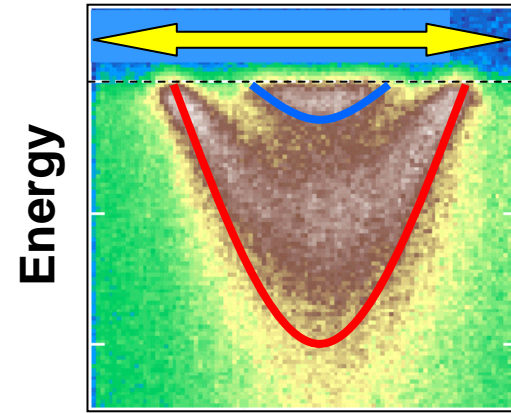
Bare band dispersion = LDA dispersion



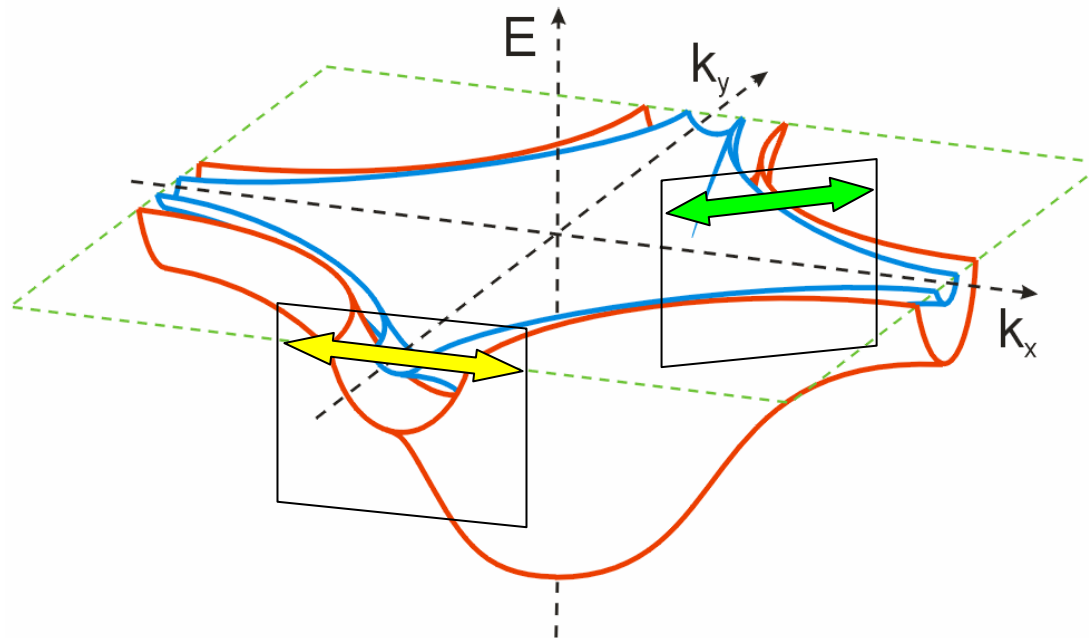
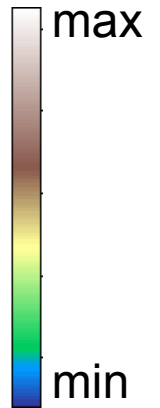
Electronic structure of HTSC is bare band dispersion + self-energy



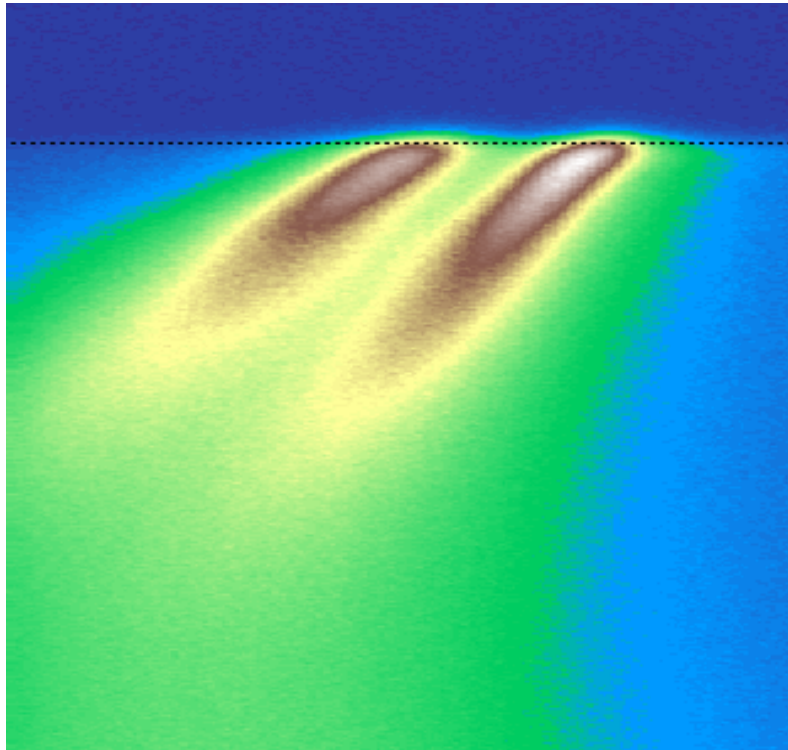
Momentum



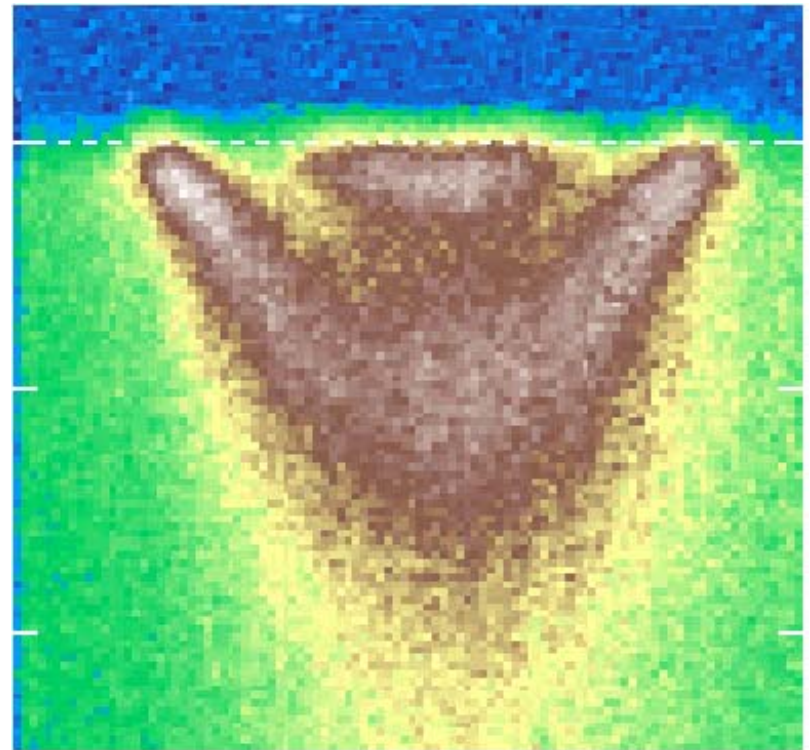
Momentum



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



2006

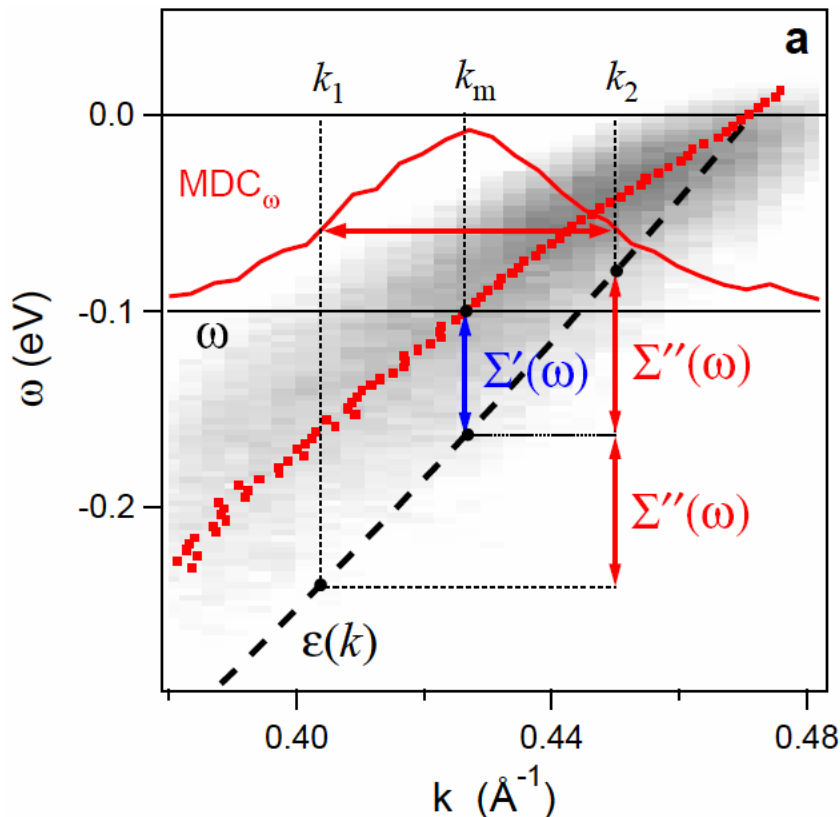


2002

Unadulterated spectral function

Introduction to the nodal spectra analysis

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

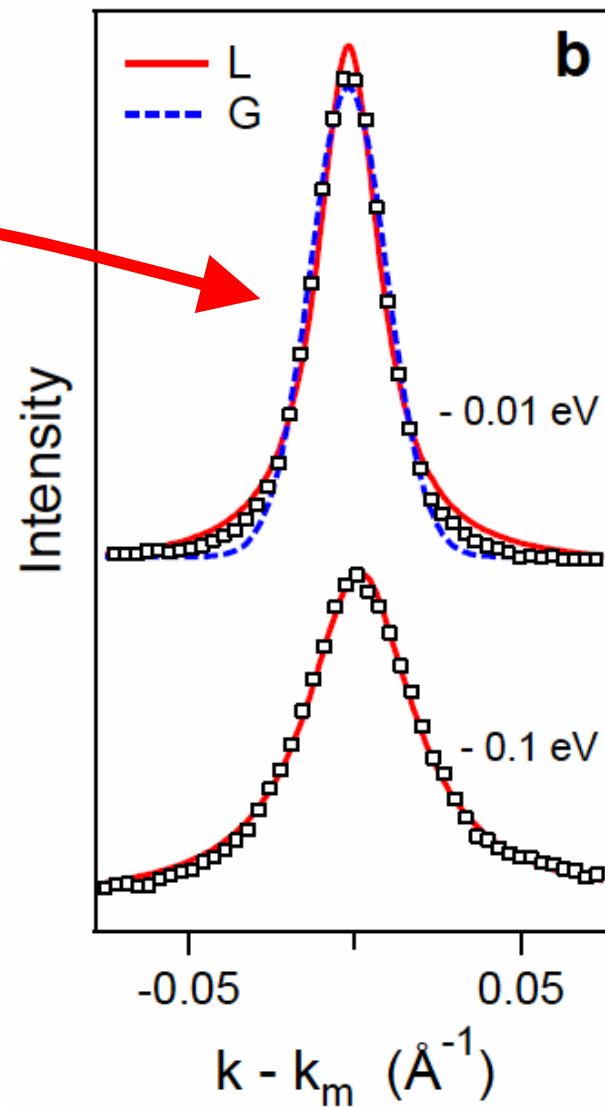
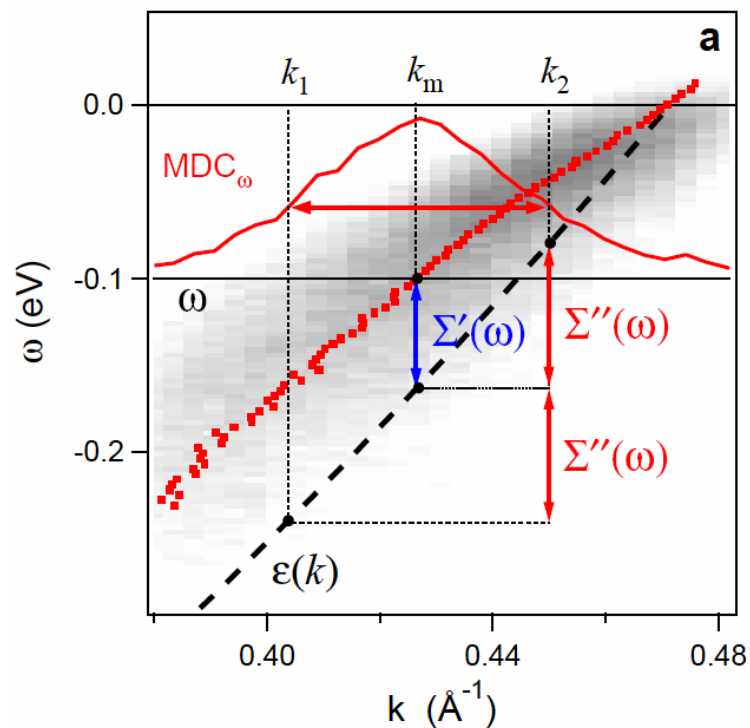


$$\Sigma'(\omega) = \omega - \varepsilon(k_m)$$

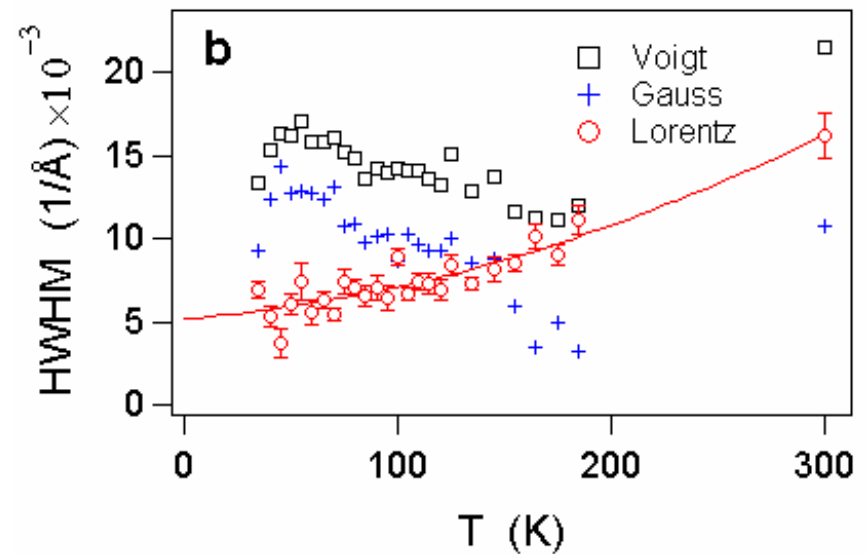
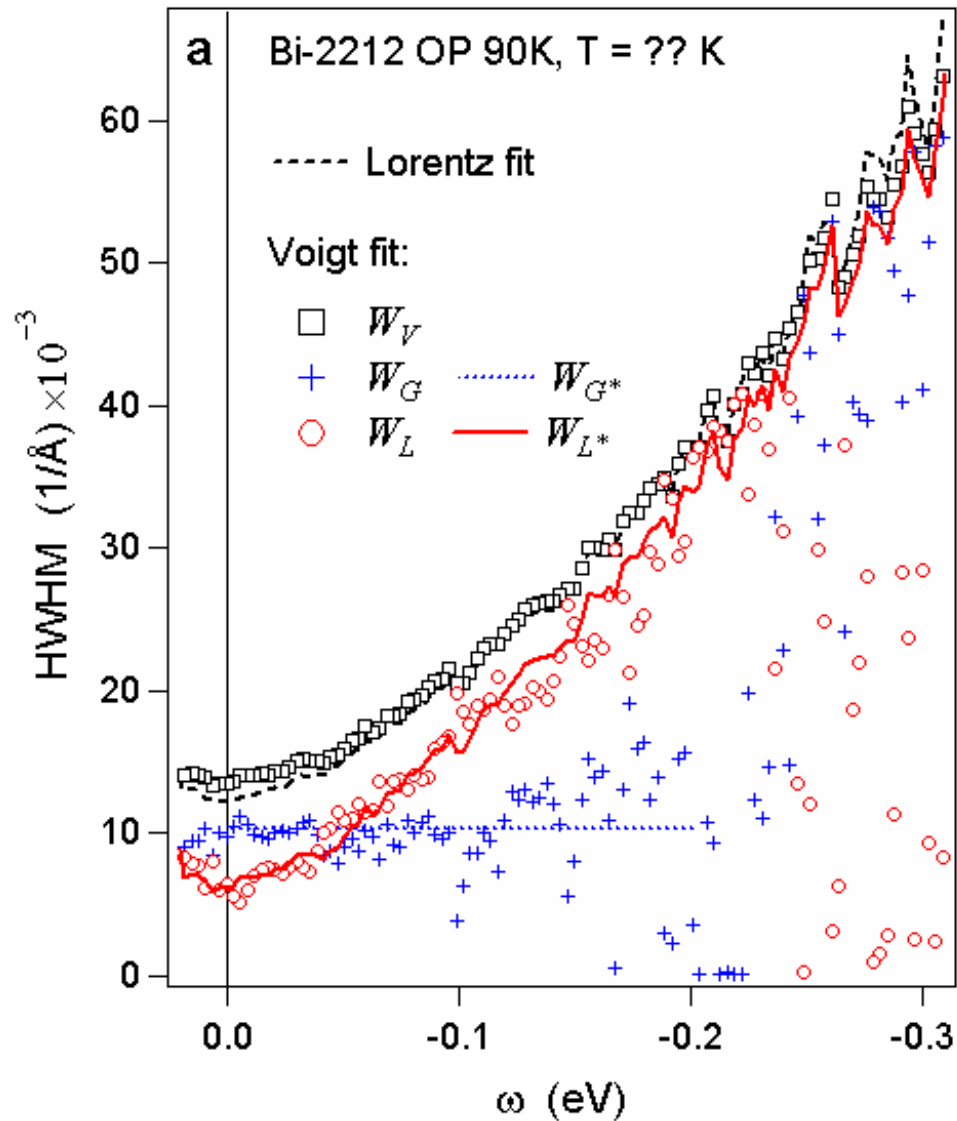
$$\Sigma''(\omega) = -v_F W(\omega)$$

Lorentzian to Gaussian

Voigt profile = Lor \otimes Gauss



Voigt fitting procedure



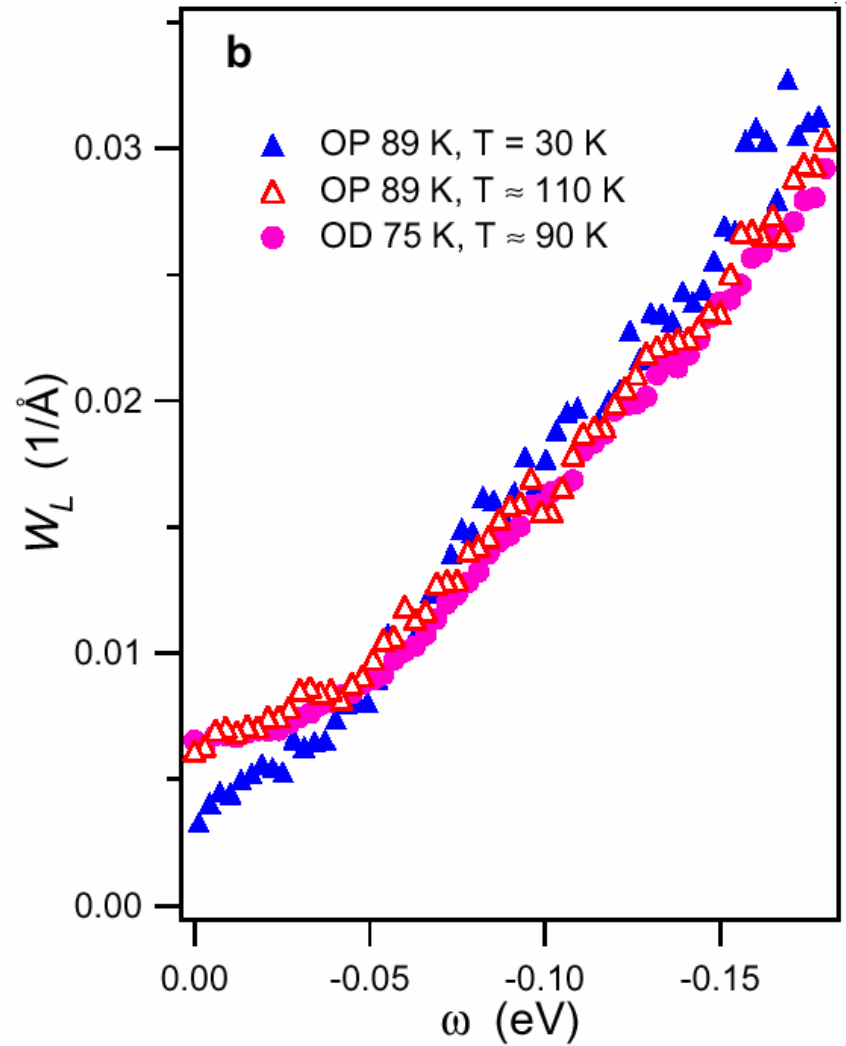
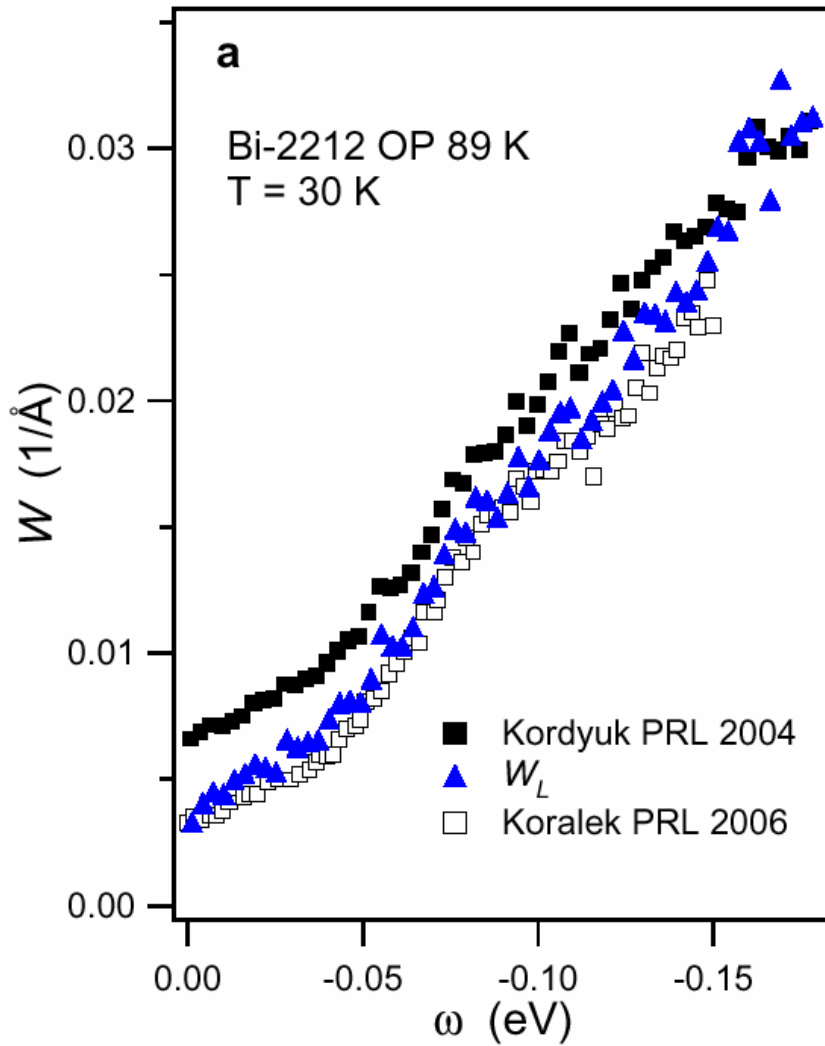
$$W_V = V(W_L, W_G)$$

$$= \frac{W_L}{2} + \sqrt{\frac{W_L^2}{4} + W_G^2}$$

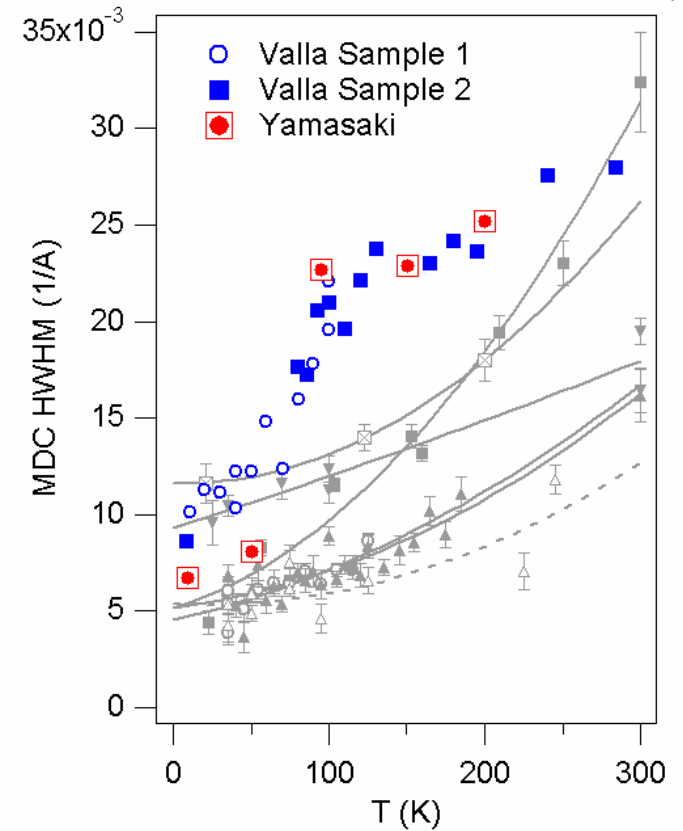
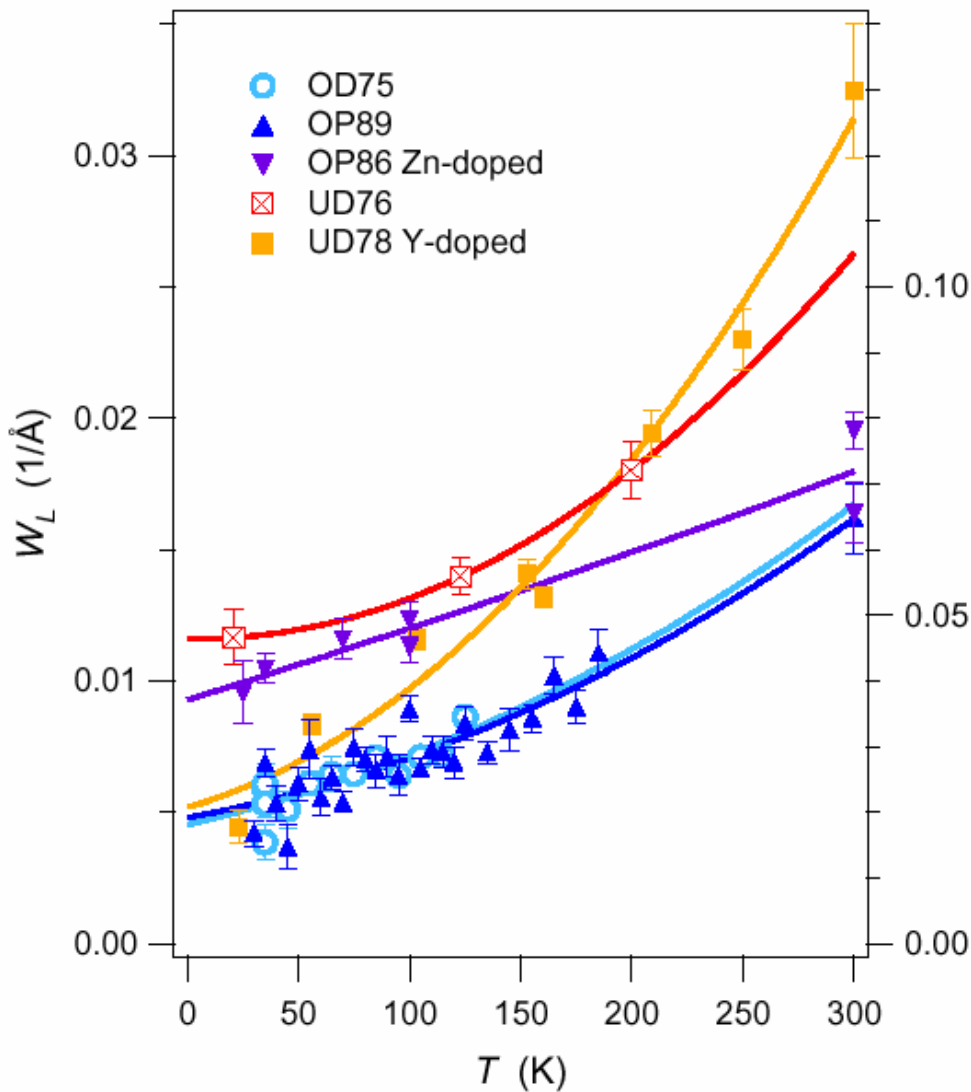
Now for the self-energy:

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

Energy dependence



Temperature dependence



pseudo-gap

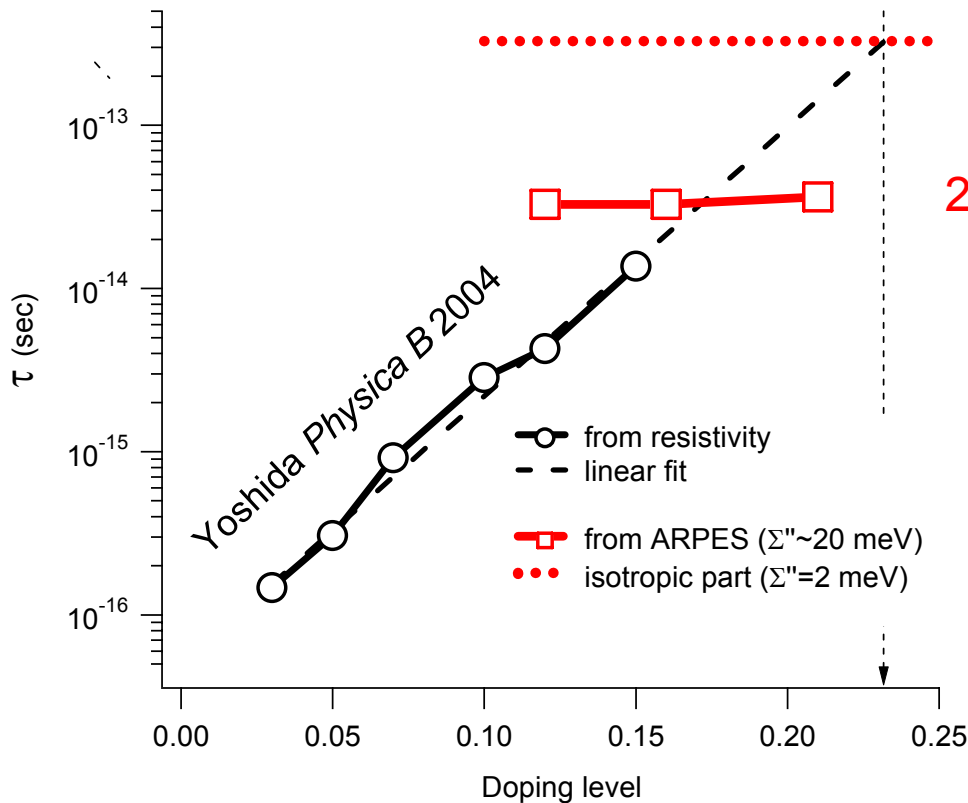
no "arcs" !

Impurity scattering

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

forward and isotropic (unitary)?

$$n \sim 1 - x$$



$n(x)$?

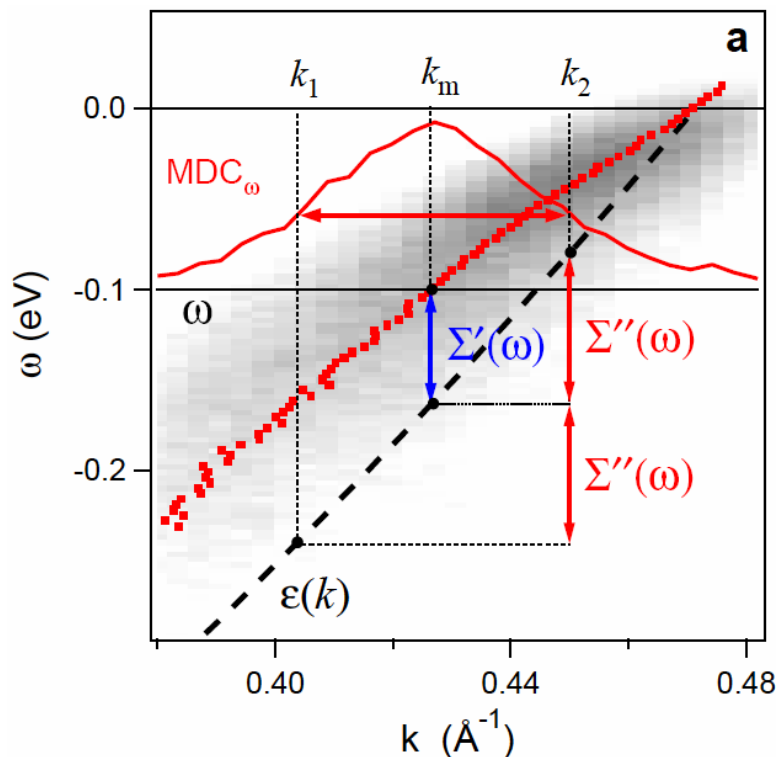
inhomogeneity

How Kramers-Kronig consistency works

Why we believe it is applicable

Bare Fermi velocity from the nodal spectrum

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

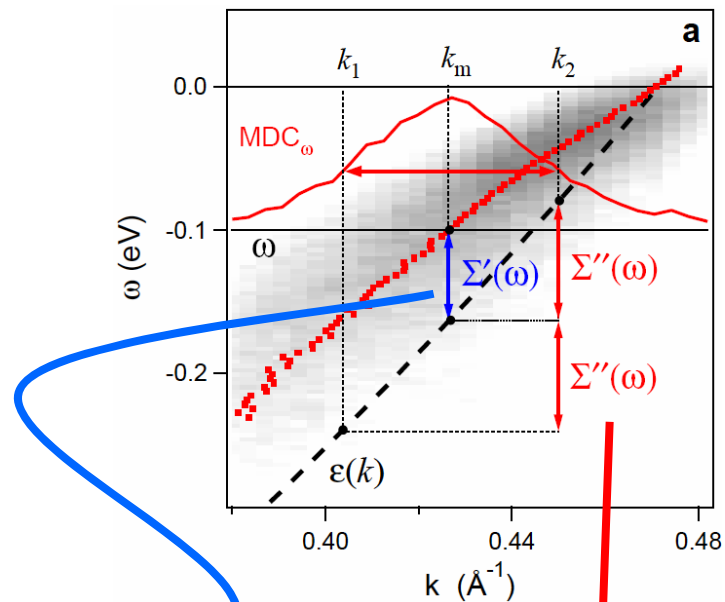
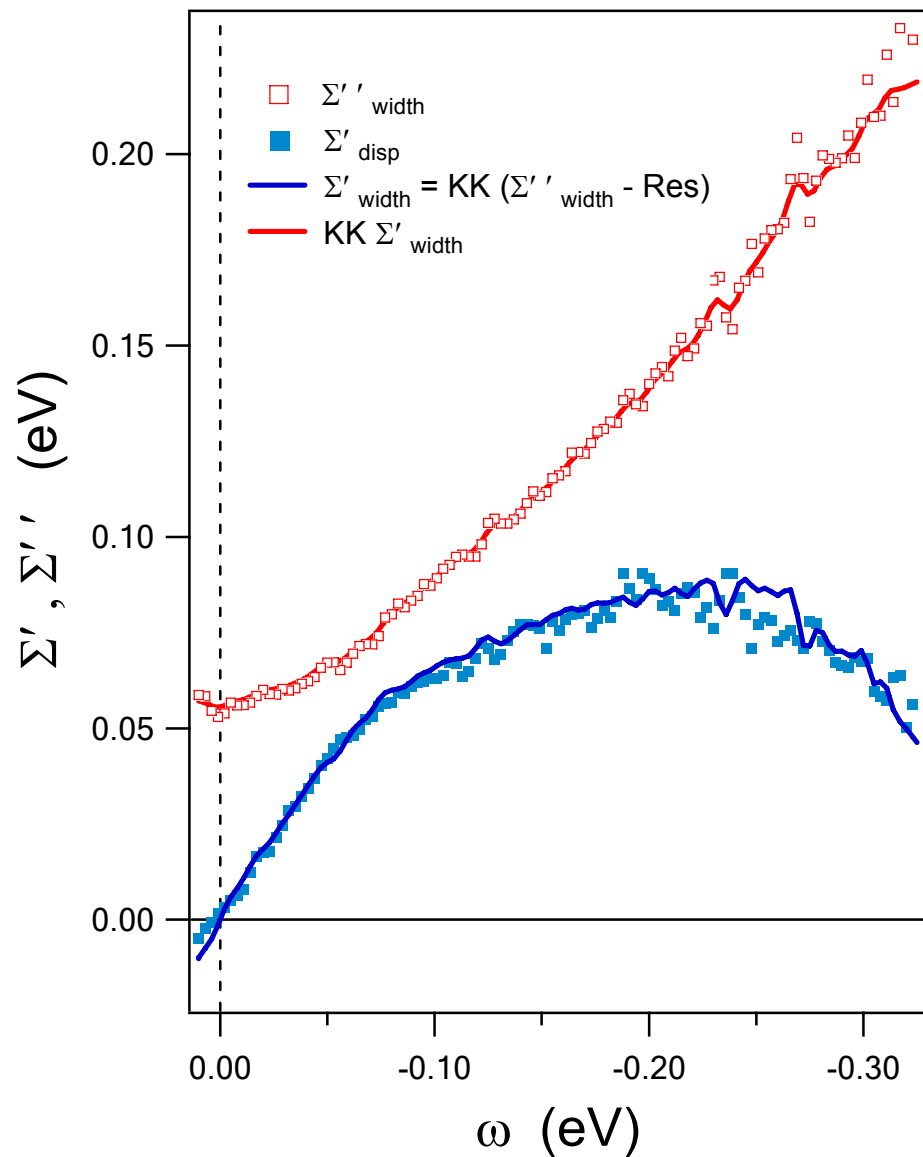


$$\Sigma'(\omega) = \omega - \varepsilon(k_m)$$

$$\Sigma''(\omega) = -v_F W(\omega)$$

$$\Sigma'(\omega) = \text{KK} \Sigma''(\omega)$$

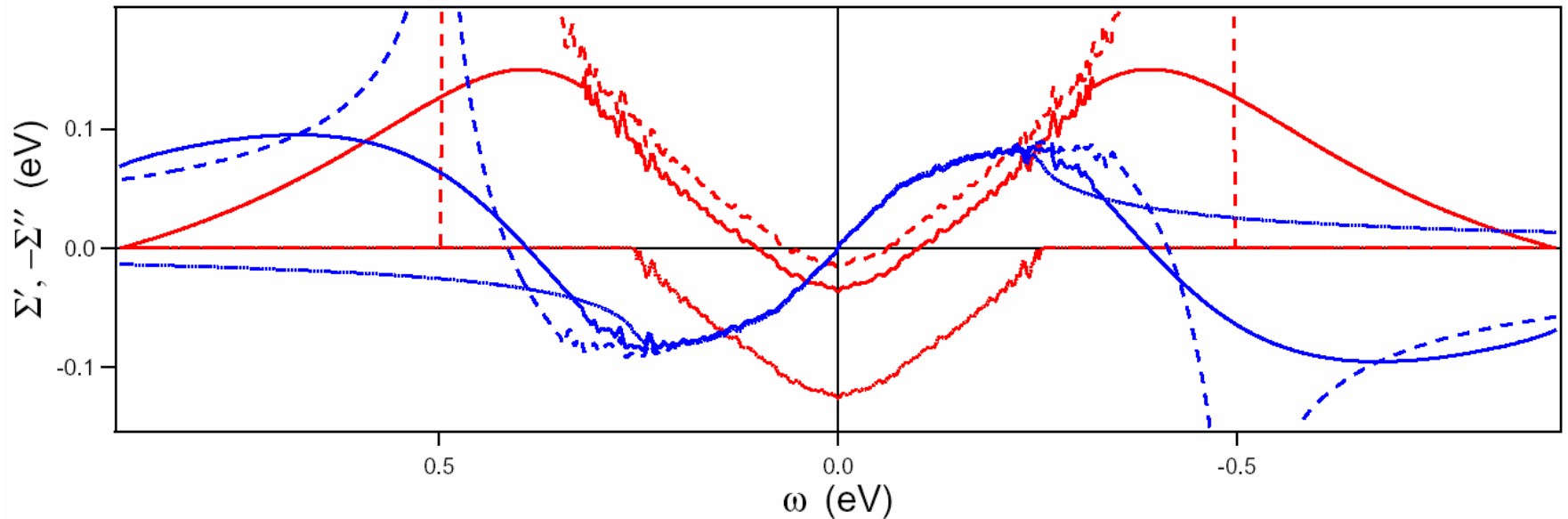
Kramers-Kronig transform



\blacksquare $\Sigma''(\omega)$
 — $\Sigma'(\omega) = \text{KK} \Sigma''(\omega)$

Kramers-Kronig transform

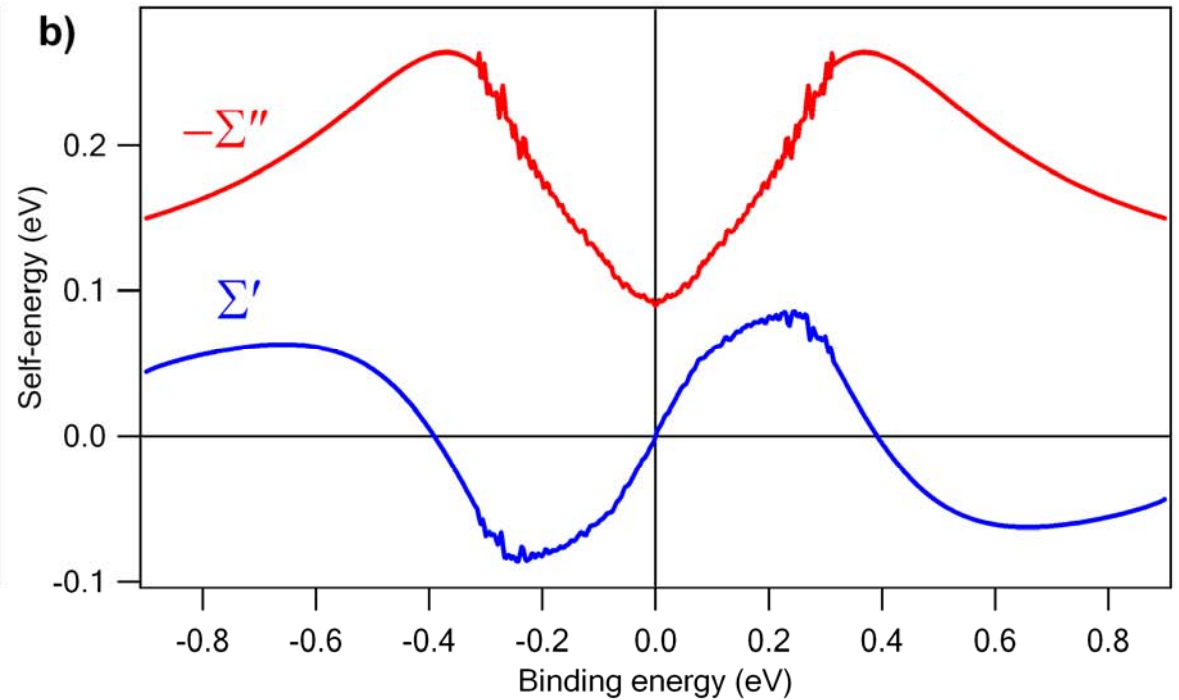
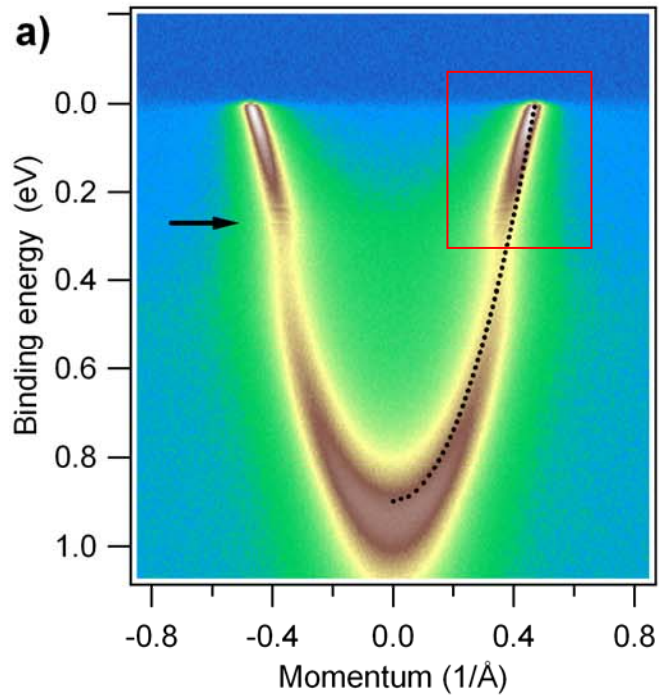
$$\Sigma'(\omega) = \text{KK} \Sigma''(\omega)$$



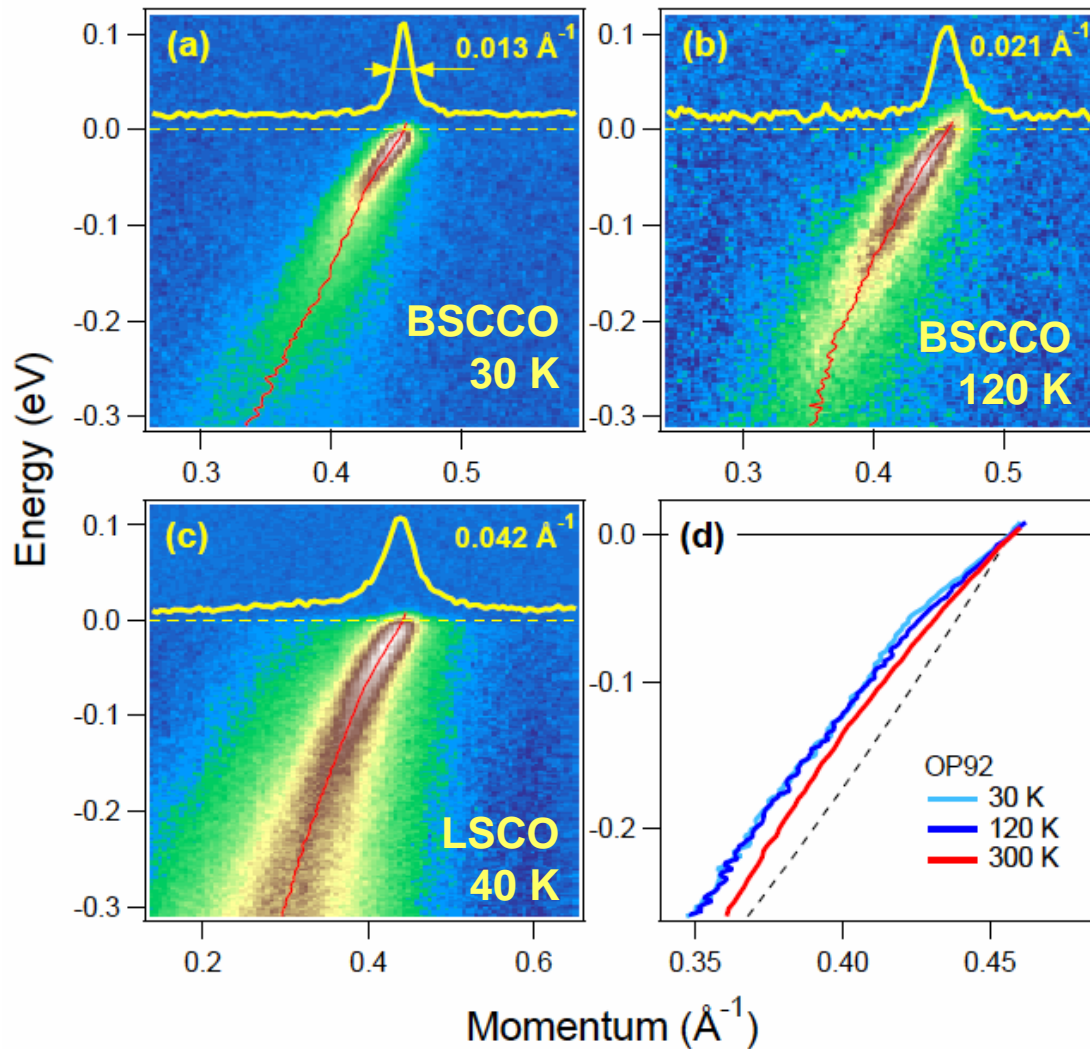
$$\Sigma''(\omega) = \begin{cases} \Sigma''_{width}(|\omega|) & \text{for } |\omega| < \omega_m, \\ \Sigma''_{mod}(\omega) & \text{for } |\omega| > \omega_m, \end{cases}$$

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

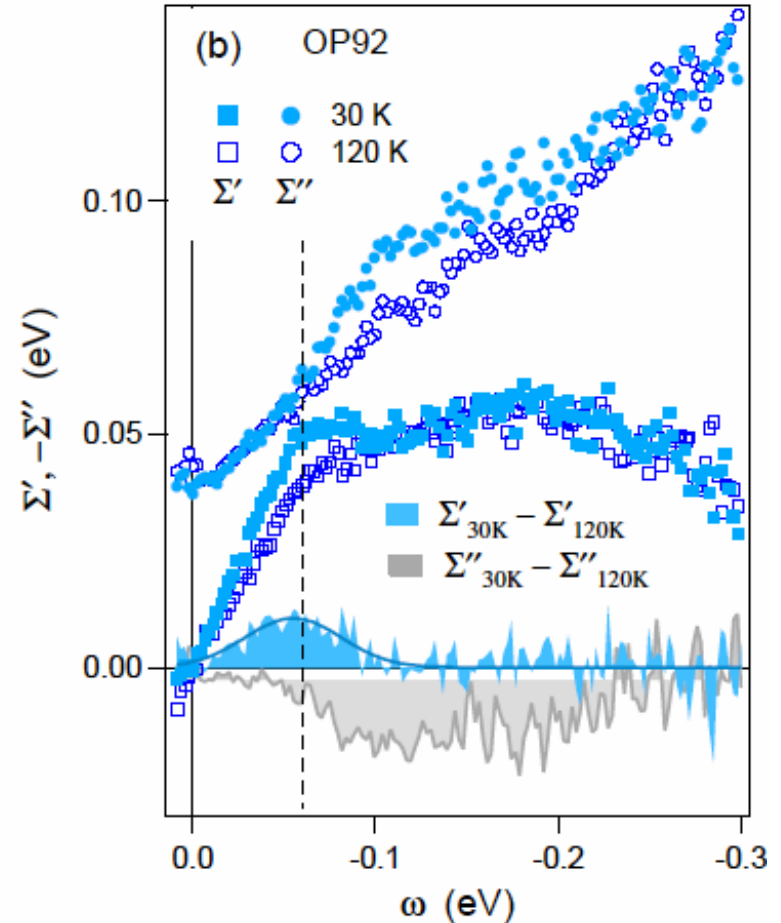
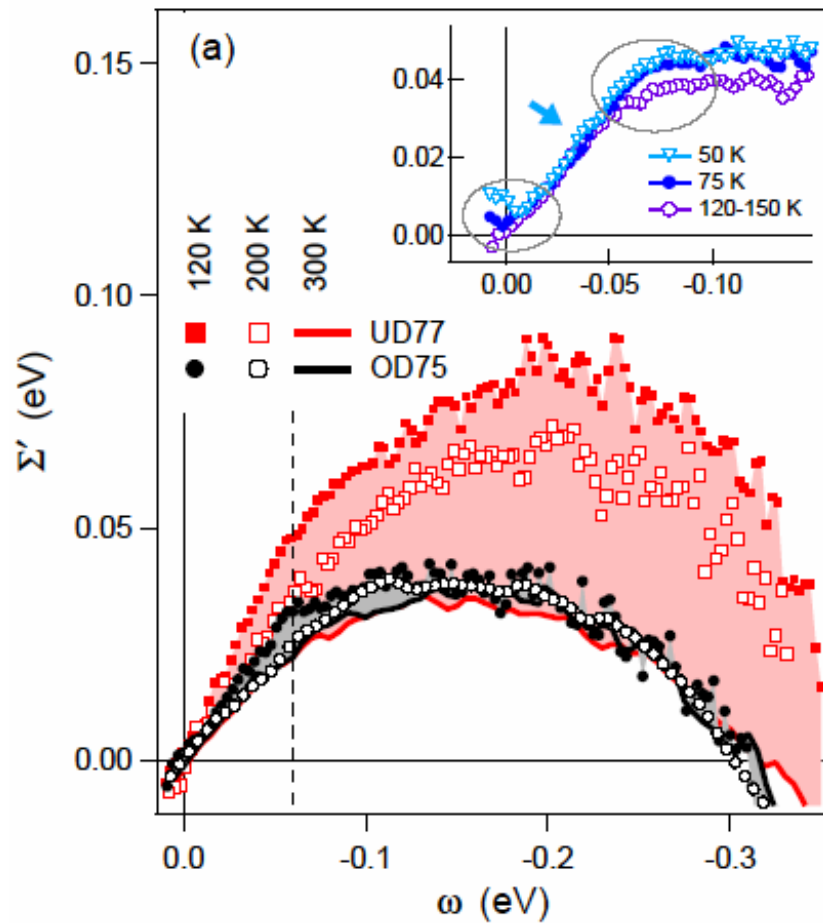
"High-energy scale"



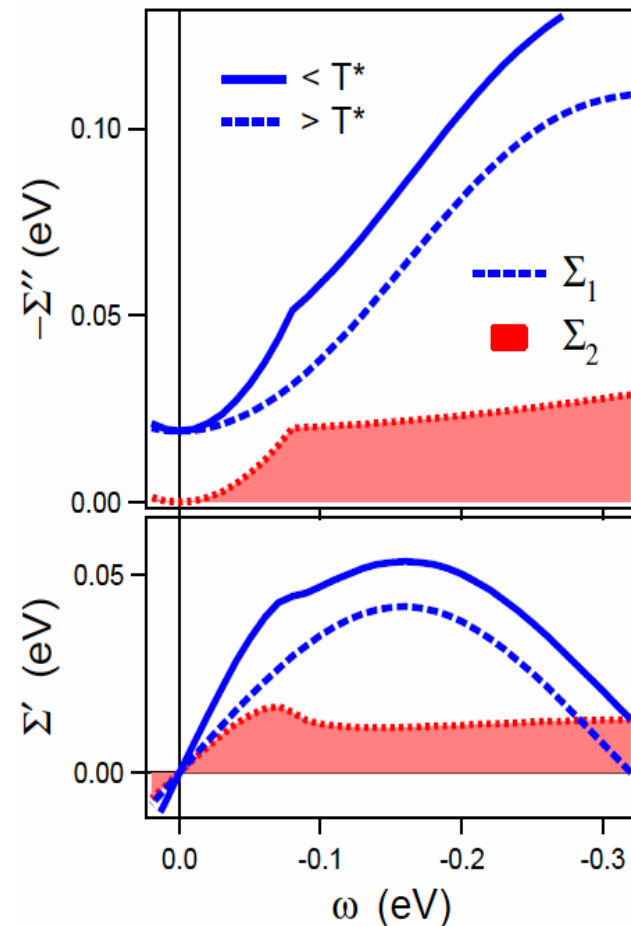
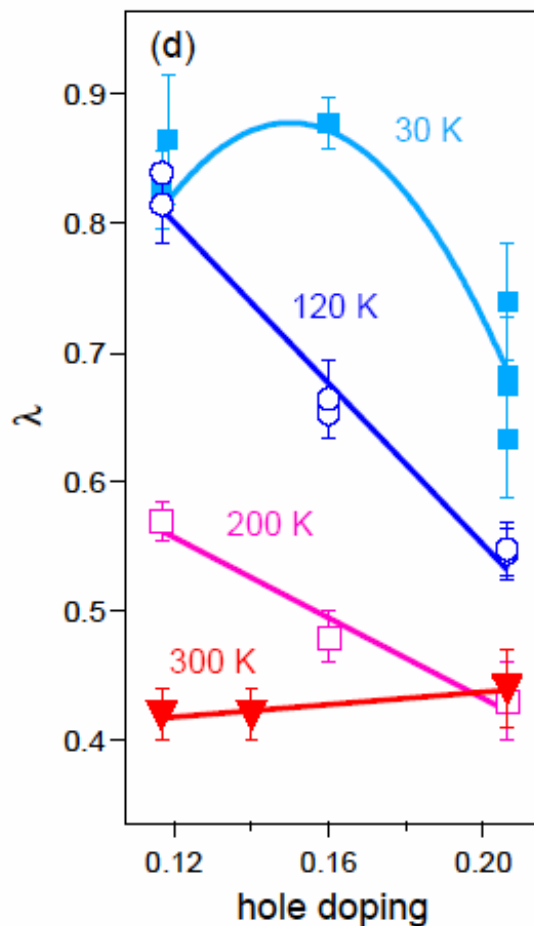
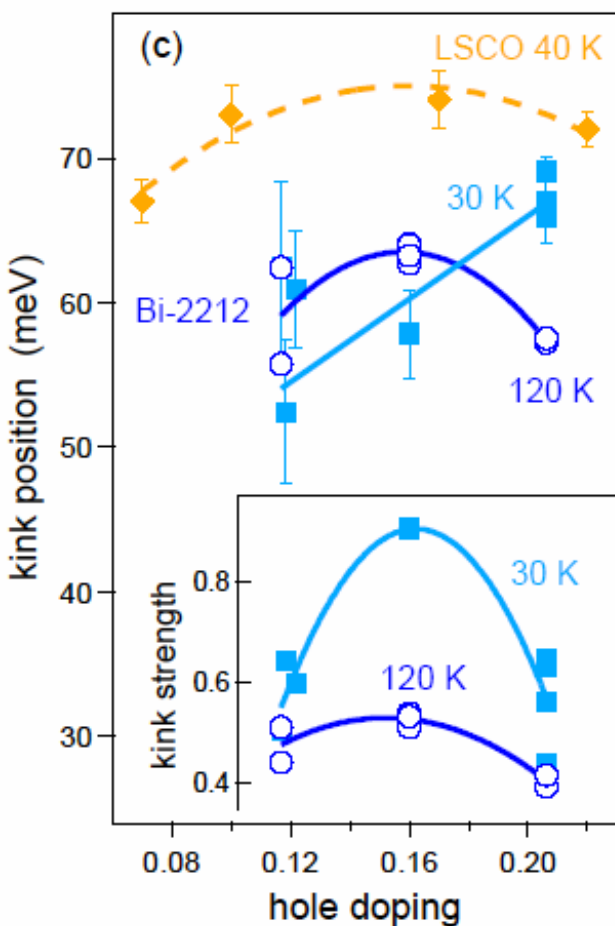
Evolution of the kink



Evolution of the self-energy

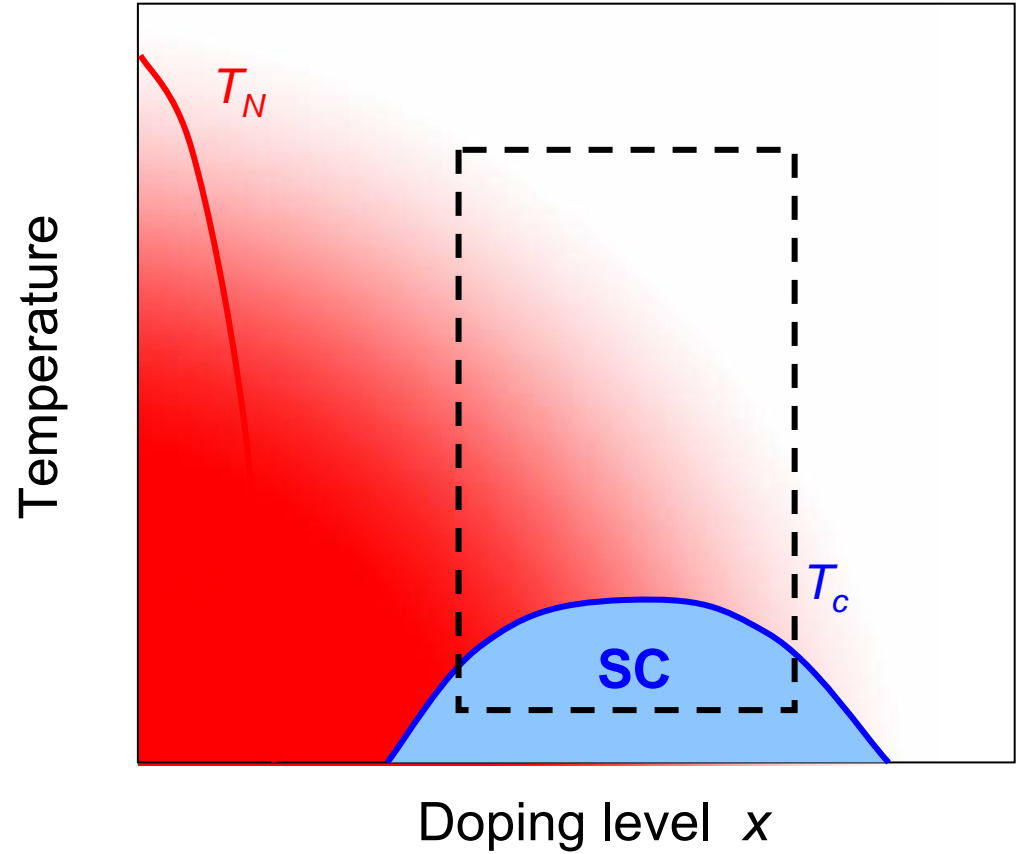
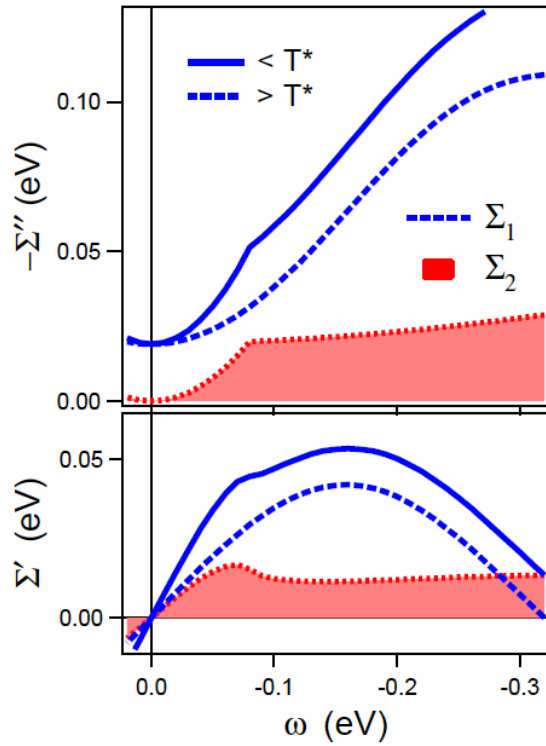


Parameters of the kink \longrightarrow 2 channels

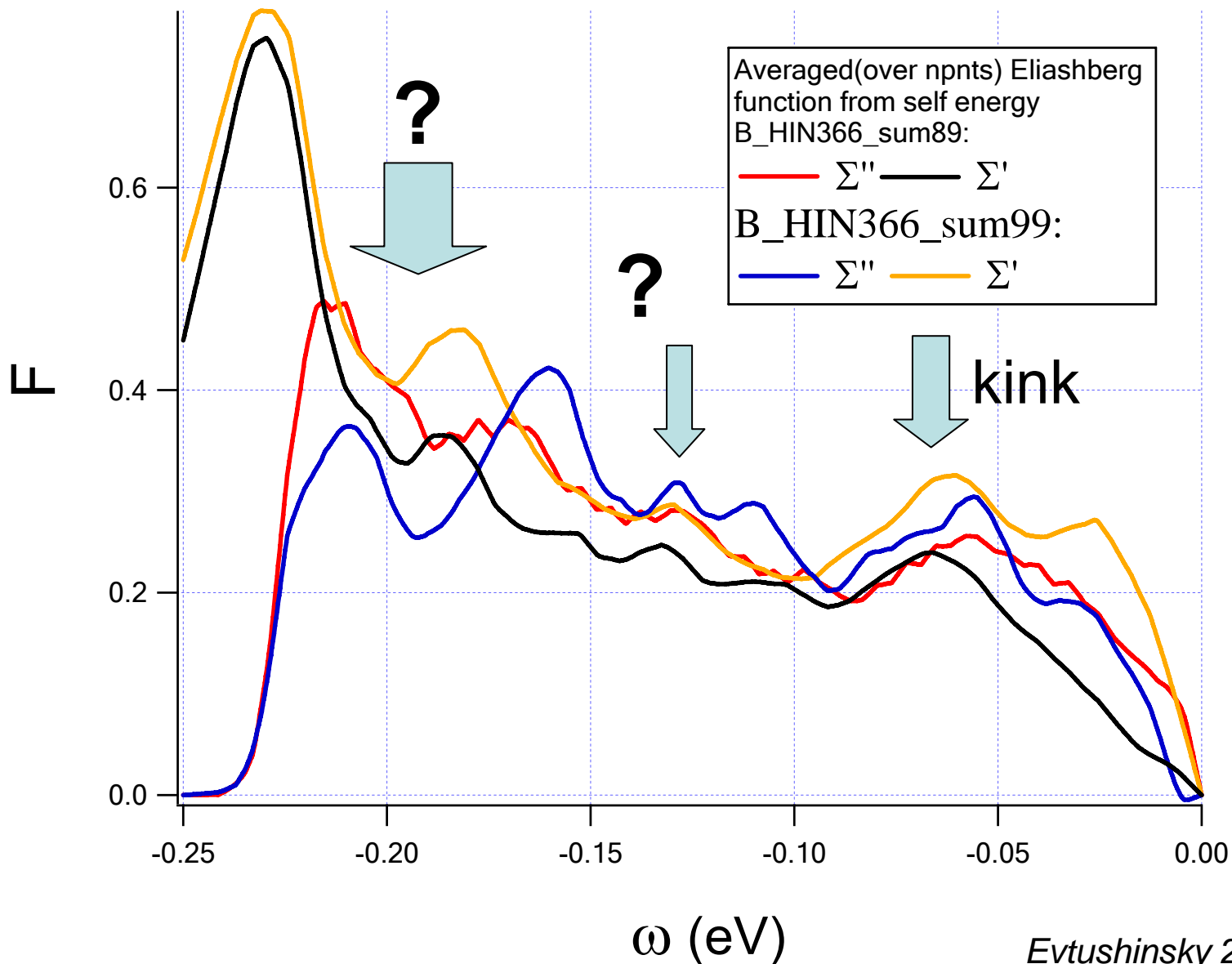
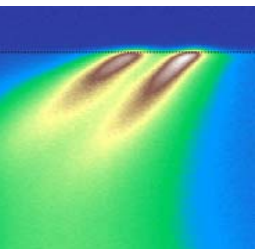


$$\lambda = - \left(\frac{d\Sigma'}{d\omega} \right)_{\omega=0}$$

Intensity of the bosonic channel



Eliashberg function from YBCO



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:

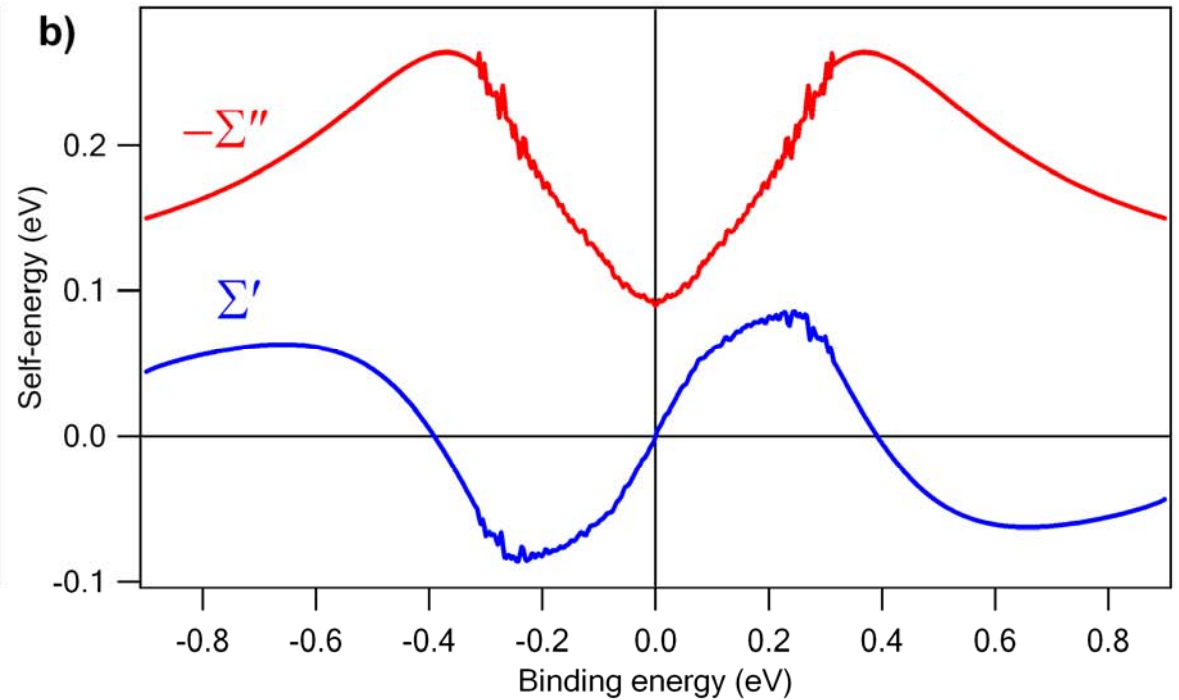
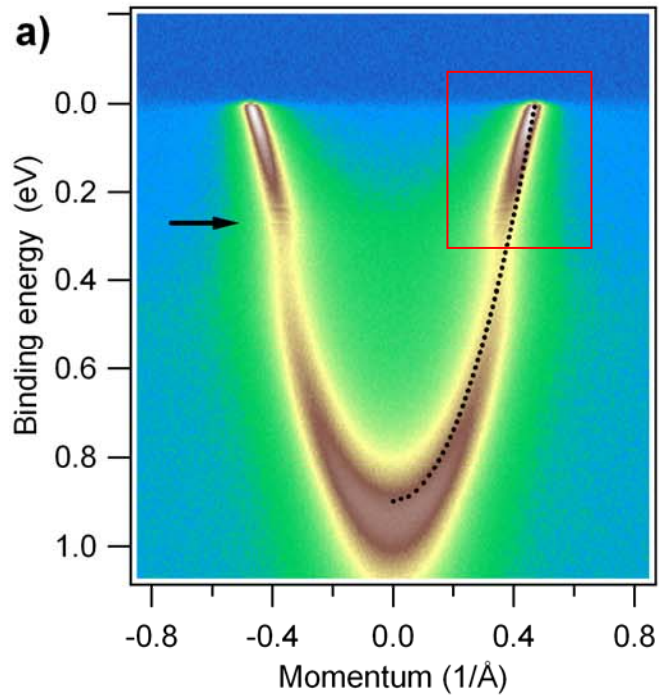
- (i) kinky,
 ω_k *mainly* xT -independent
- (ii) step-like,
does not confined at low ω

~~phonons, gap~~ \rightarrow SF

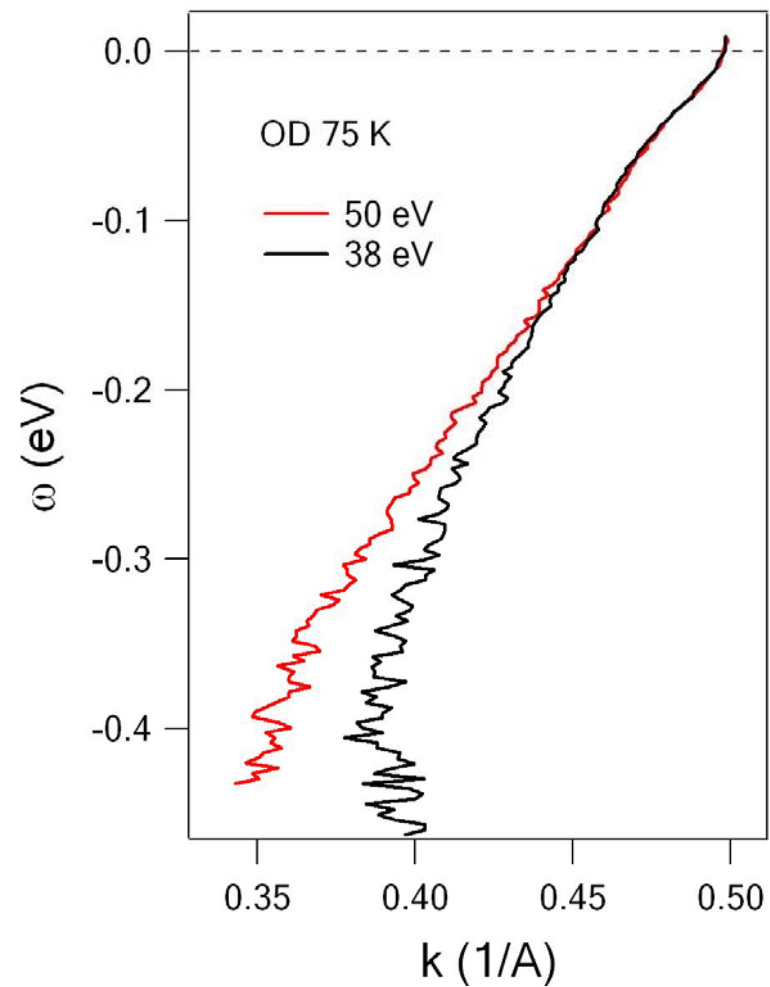
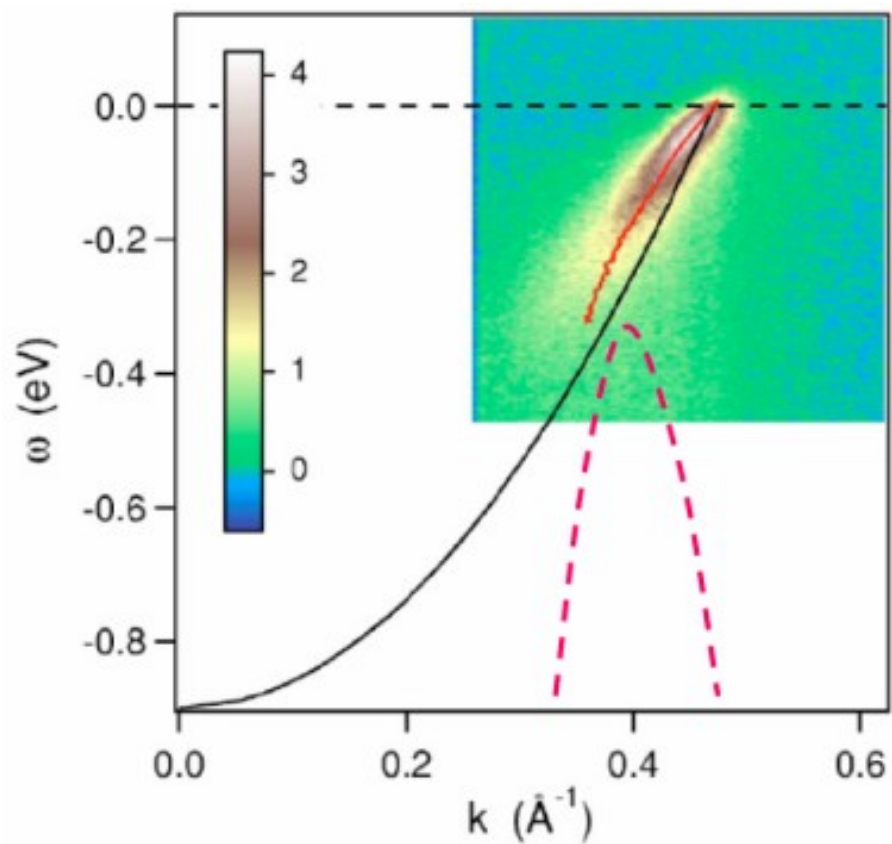
The "waterfalls"

Where the consistency stops

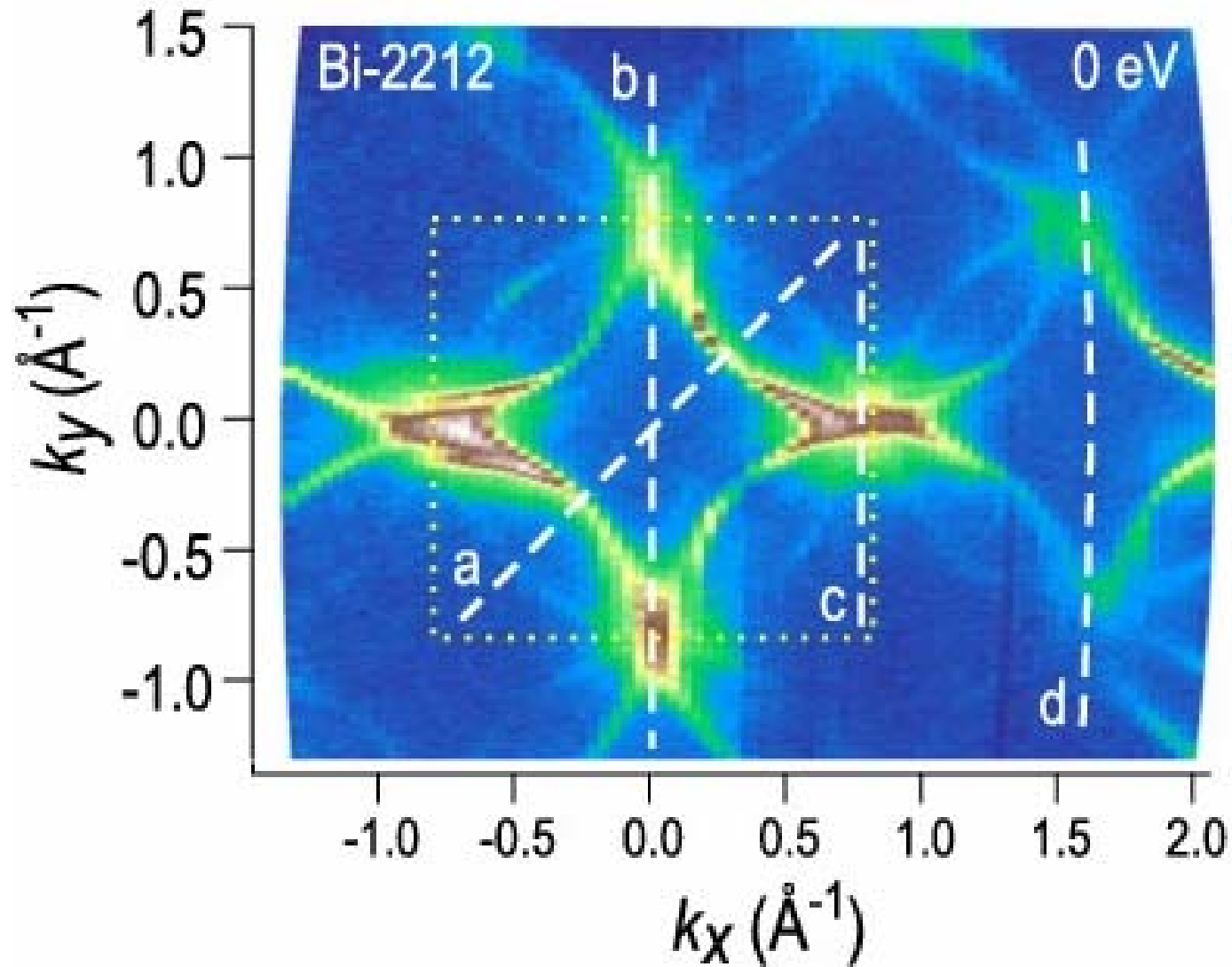
"High-energy scale"



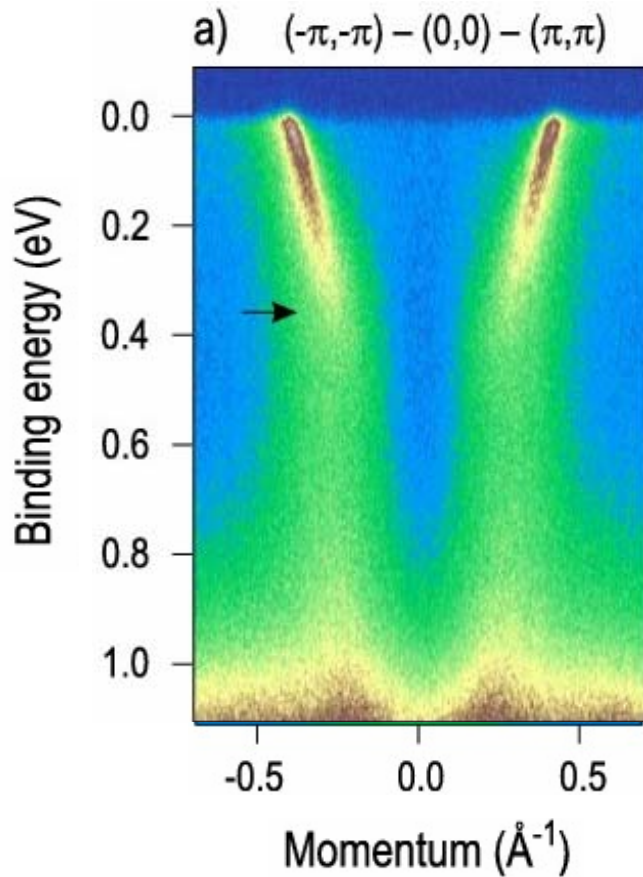
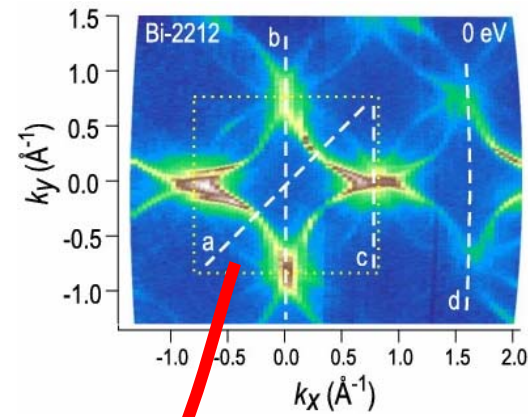
Extrinsic spectral weight



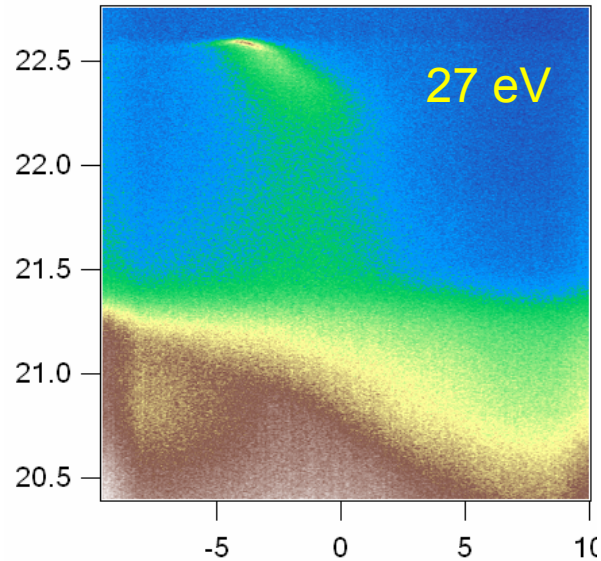
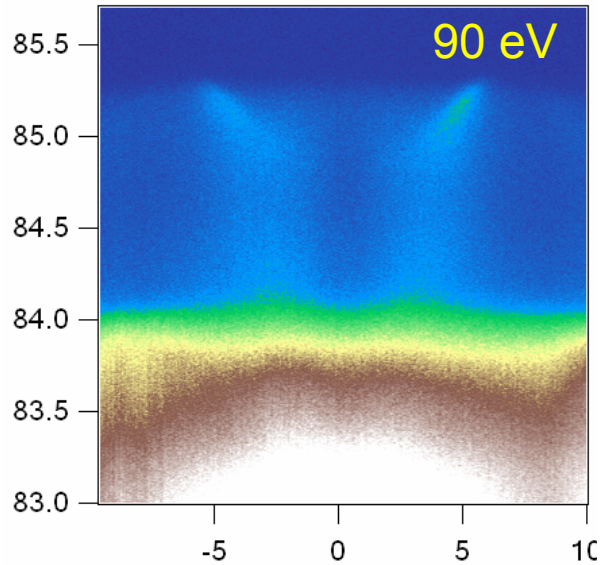
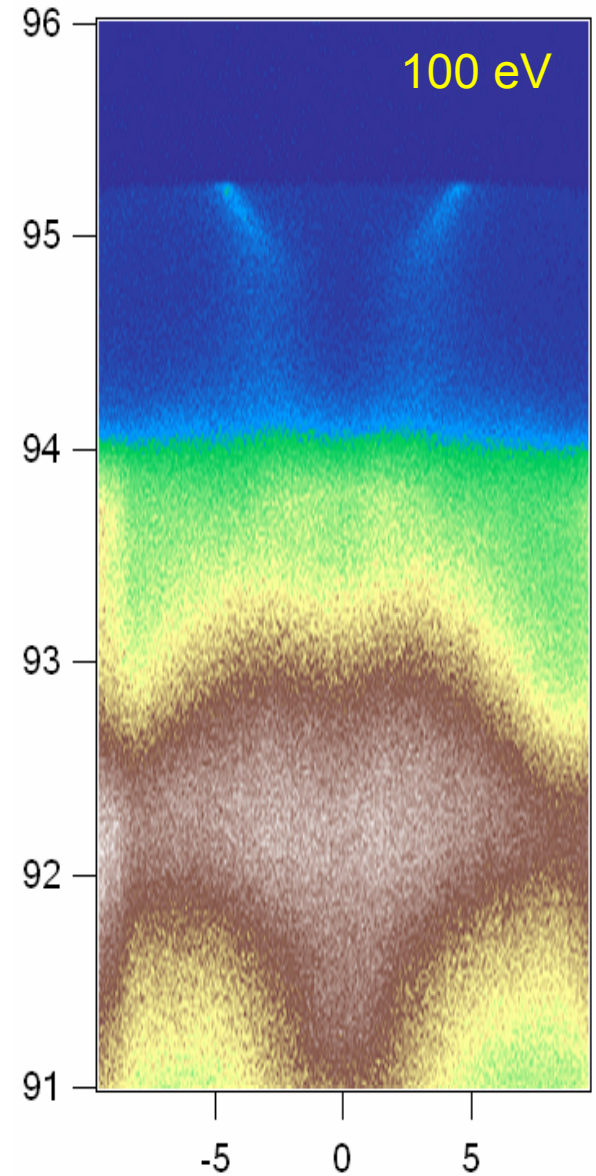
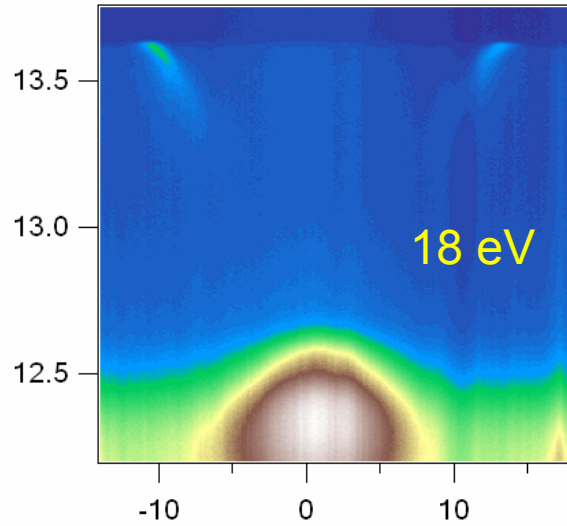
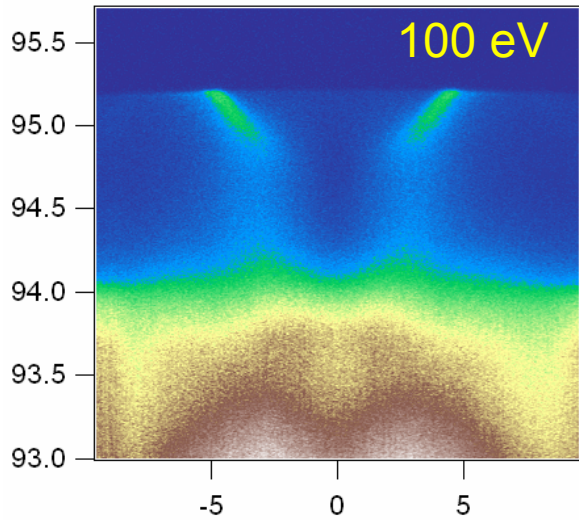
Waterfalls phenomenon



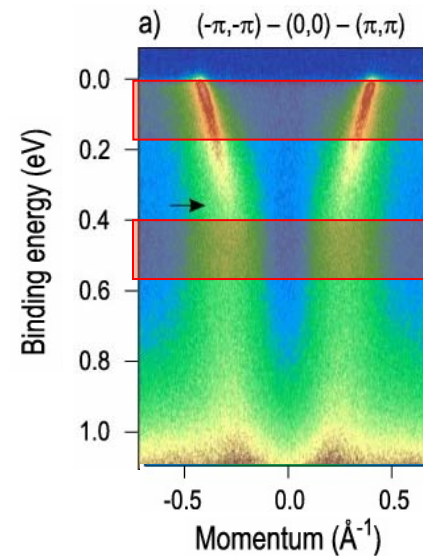
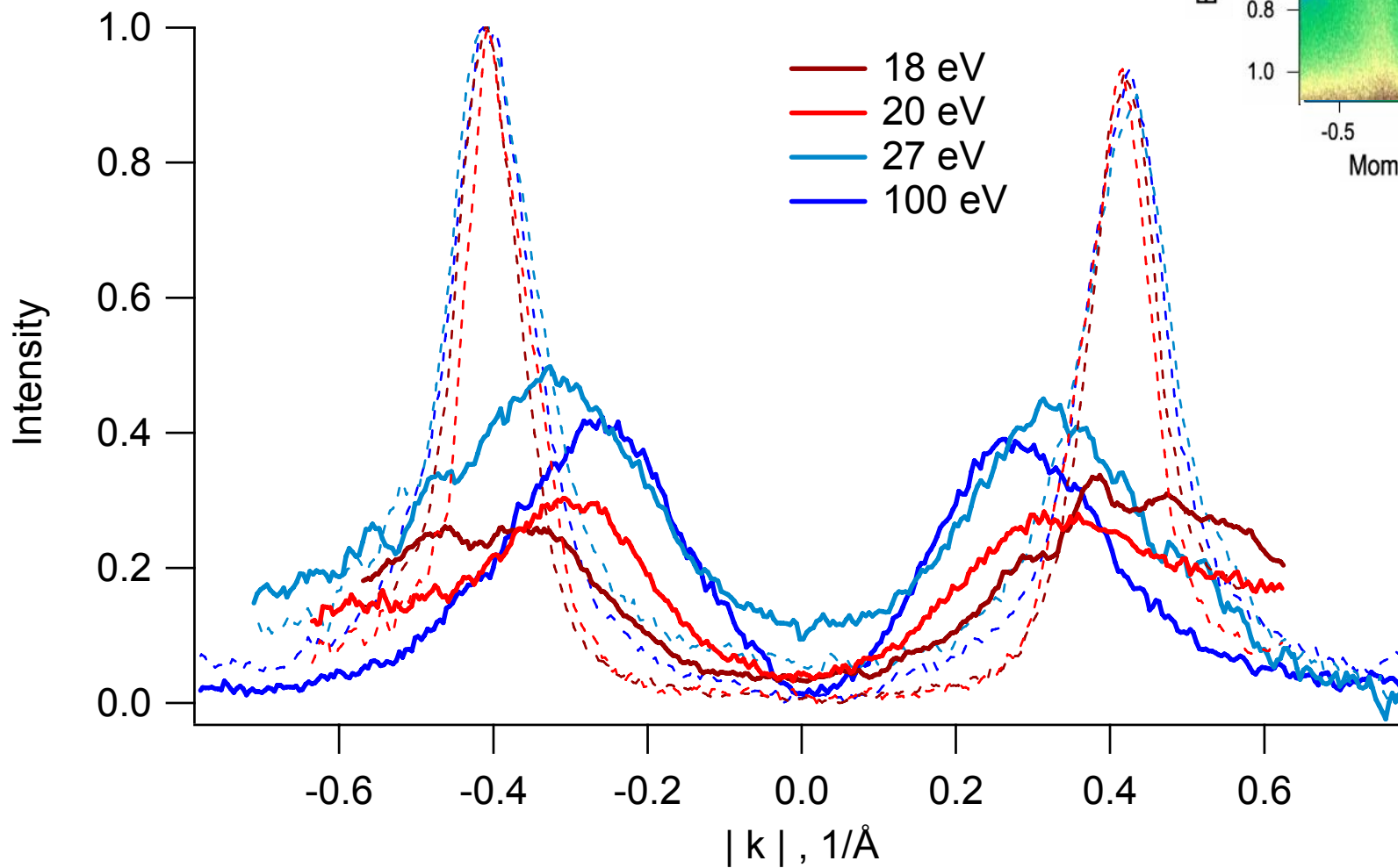
Waterfalls phenomenon



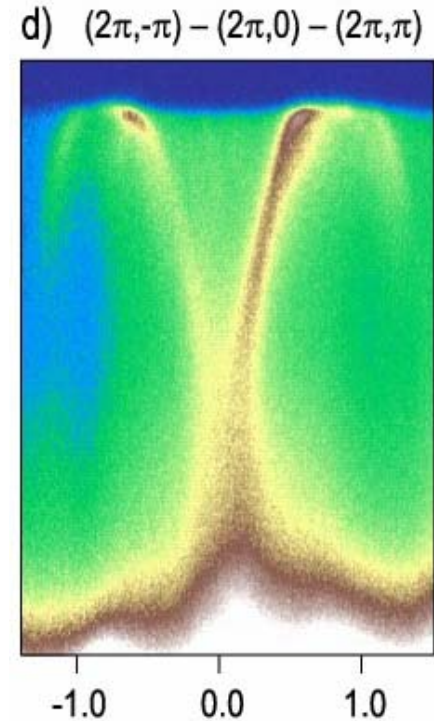
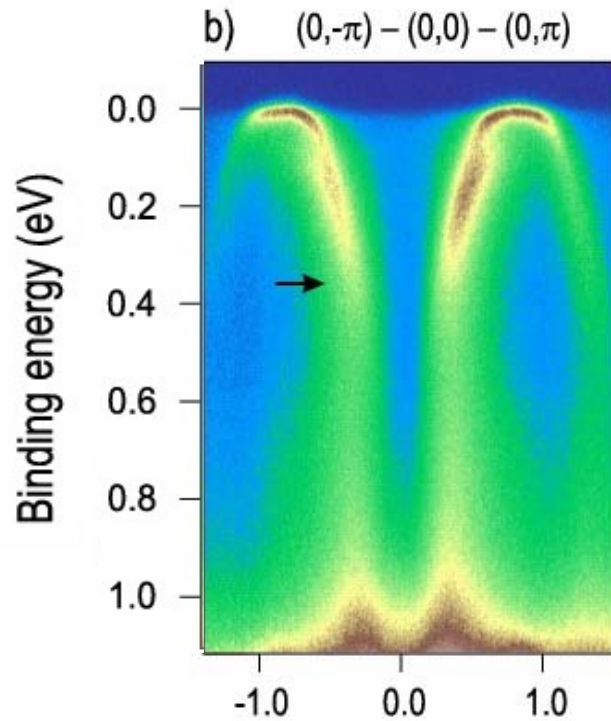
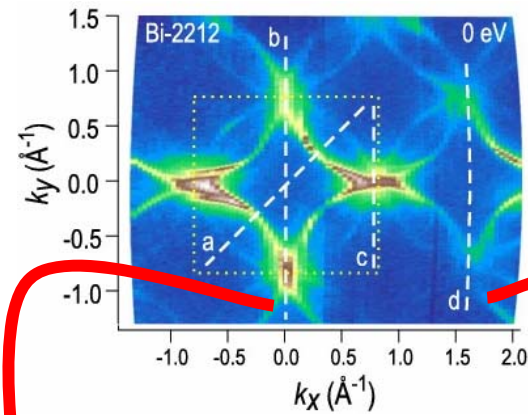
Waterfalls phenomenon



Waterfalls phenomenon

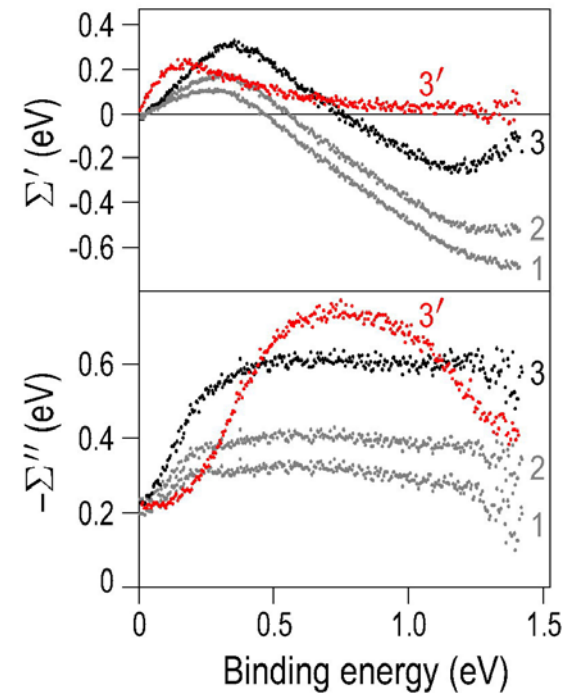
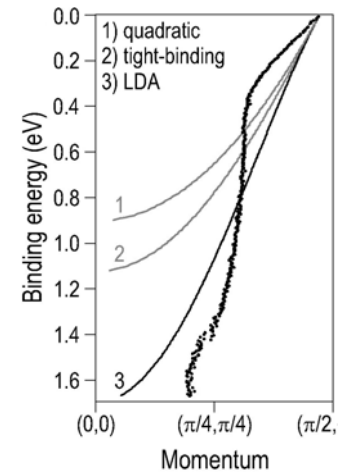
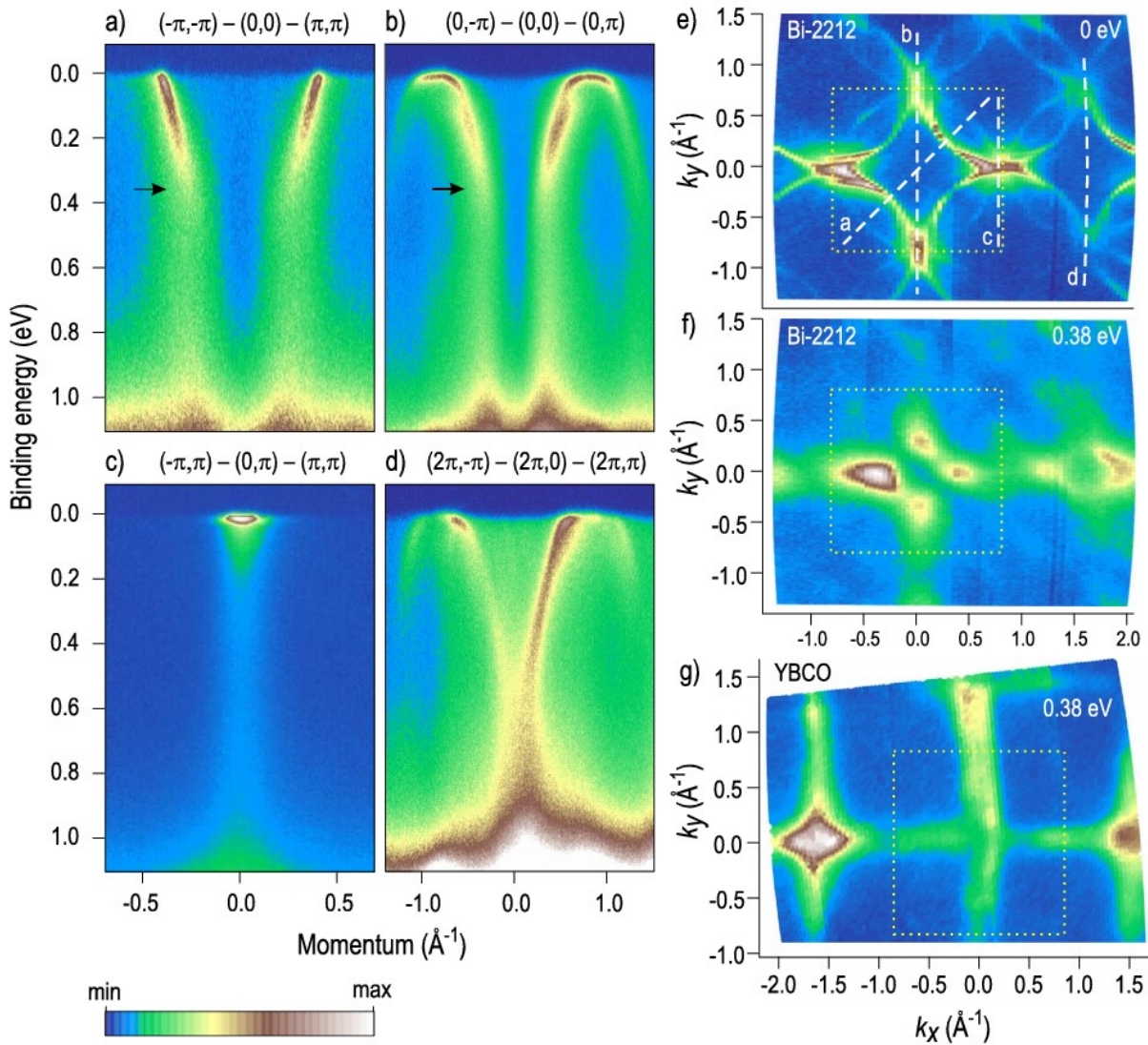


Waterfalls phenomenon



Momentum (\AA^{-1})

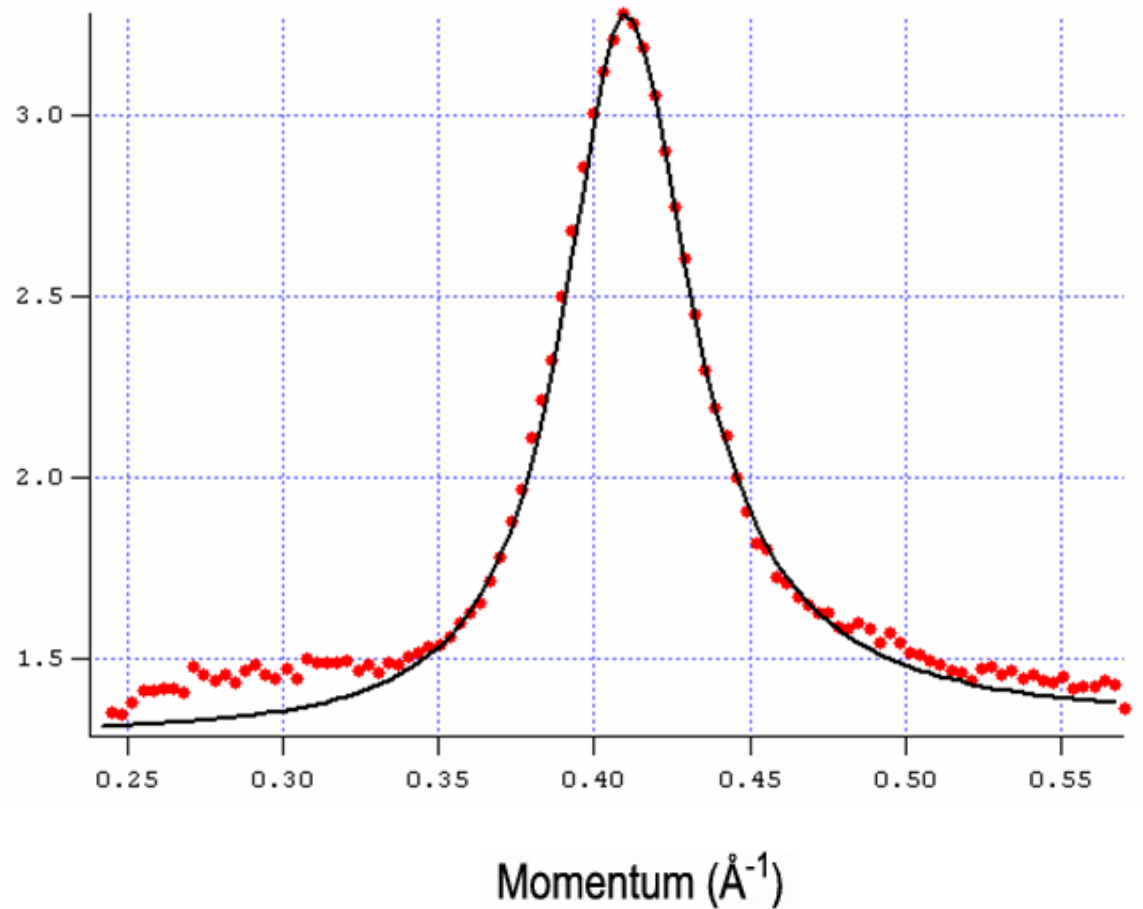
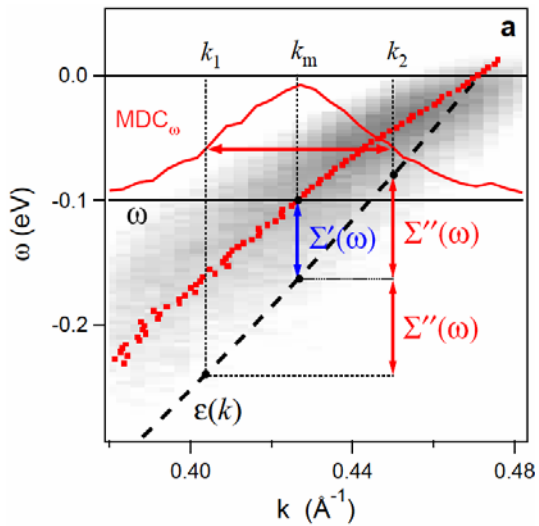
Waterfalls phenomenon



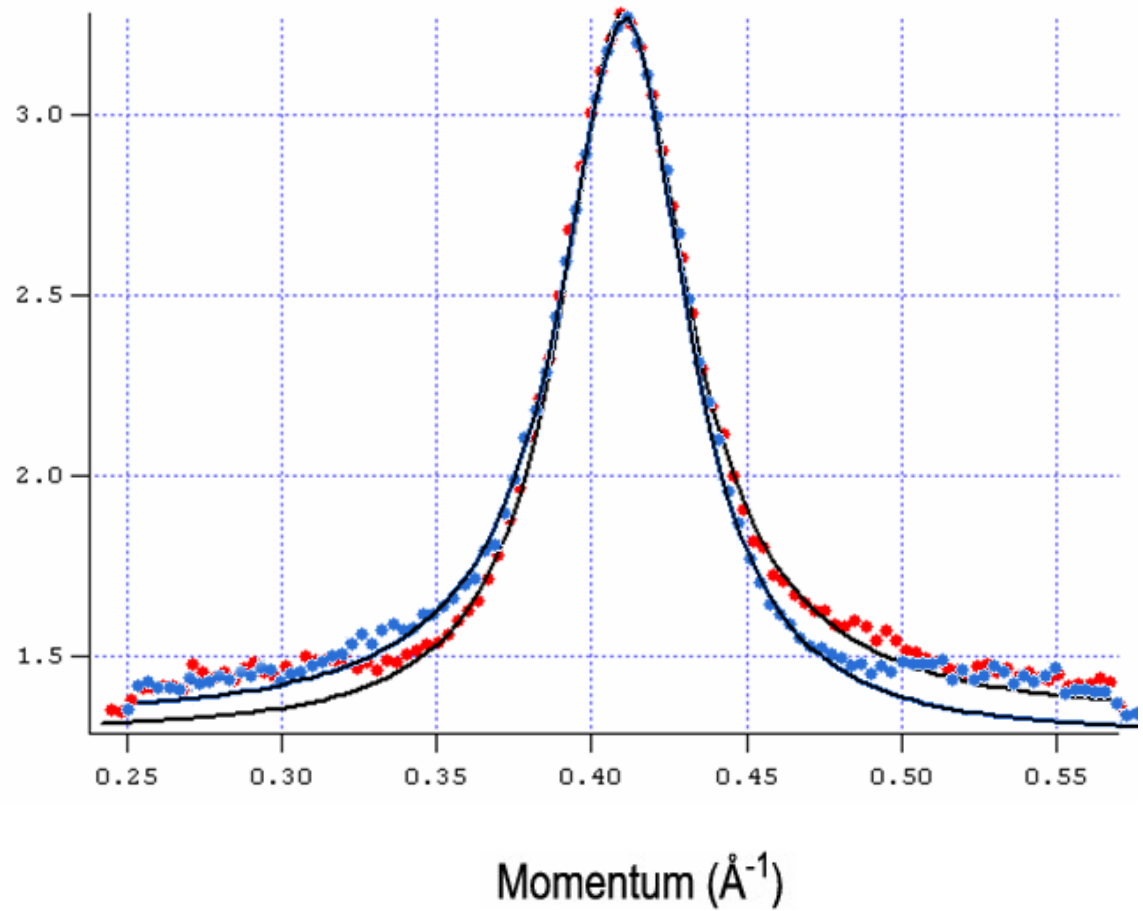
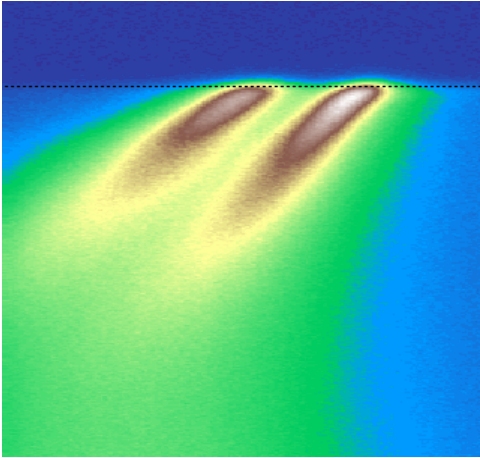
Room for complexity of
the photoemission process

MDC asymmetry

$$\Sigma_{\min} = 16 \text{ meV}$$



MDC asymmetry



Fingerprints of the bosonic spectrum

Quasiparticle spectrum in the whole Brillouin zone
k-dependent self-energy
ARPES – INS

①

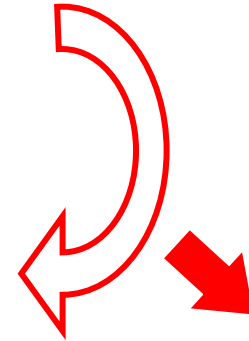
LDA or
ARPES

$$G_0 \star X_{\text{exp}} \sim \Sigma_i$$

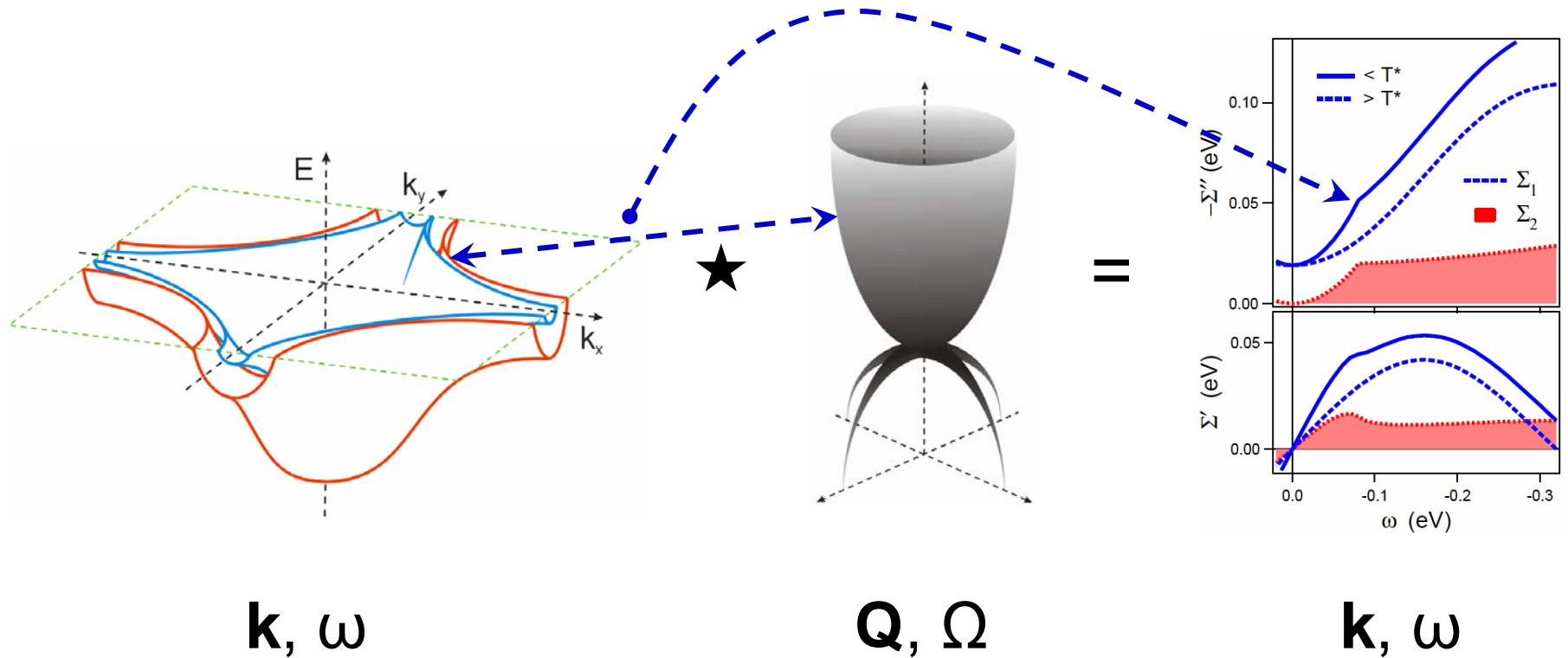


INS

$$G_i^{-1} = G_0^{-1} + \Sigma_i$$



ARPES



Looking for "fingerprints"

of $\chi(\mathbf{k},\omega)$ in $\Delta(\mathbf{k},\omega)$

ARPES: $A(\mathbf{k},\omega) f(\omega) \xrightarrow{?} \Delta(\mathbf{k},\omega)$

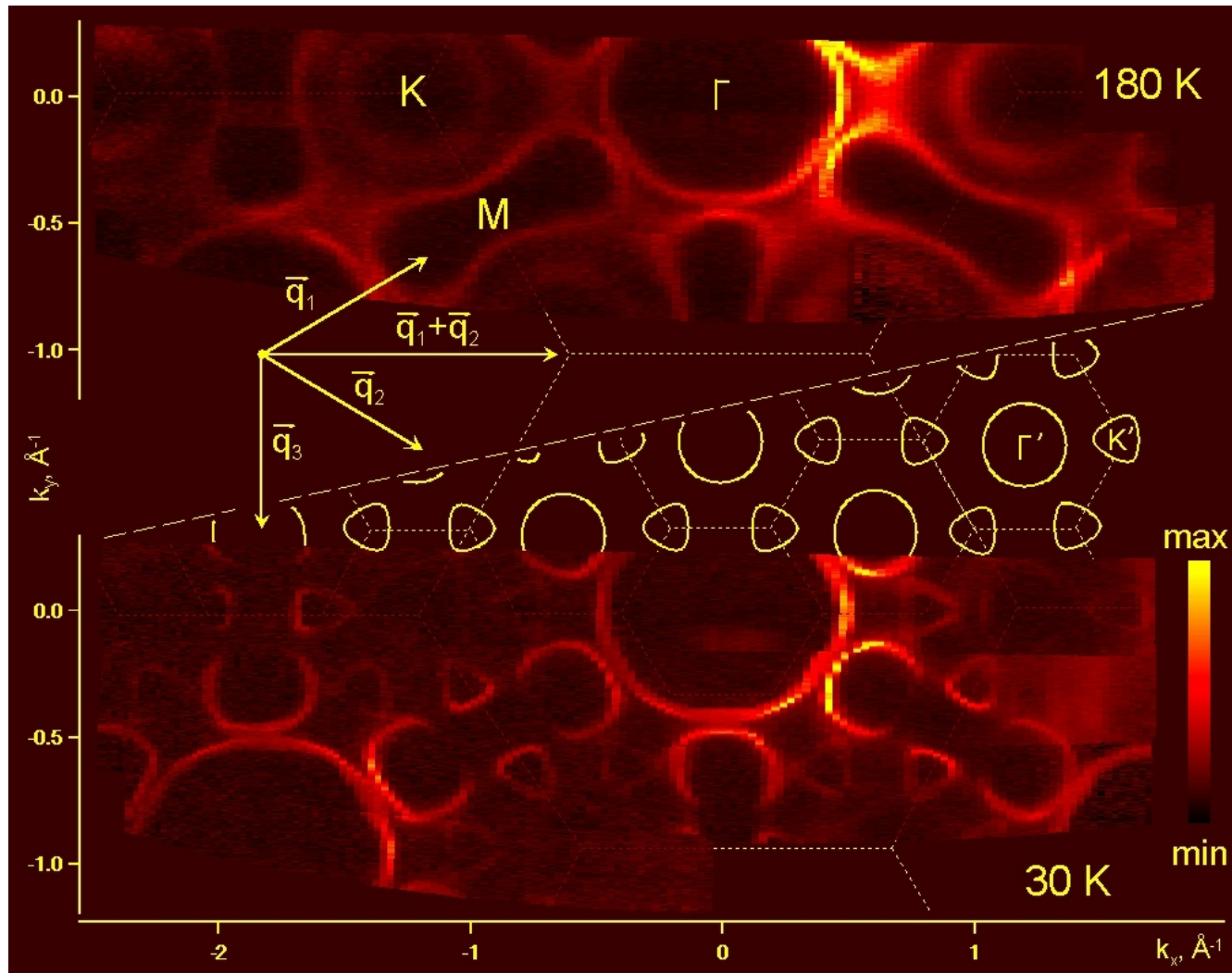
$\Delta(\mathbf{k},\omega), \Sigma(\mathbf{k},\omega), \epsilon_{\mathbf{k}}$

$$(\Delta, \Sigma) \stackrel{\text{(if)}}{=} \text{EE}(\Delta, \Sigma, \epsilon, \chi) \quad \text{SC}$$

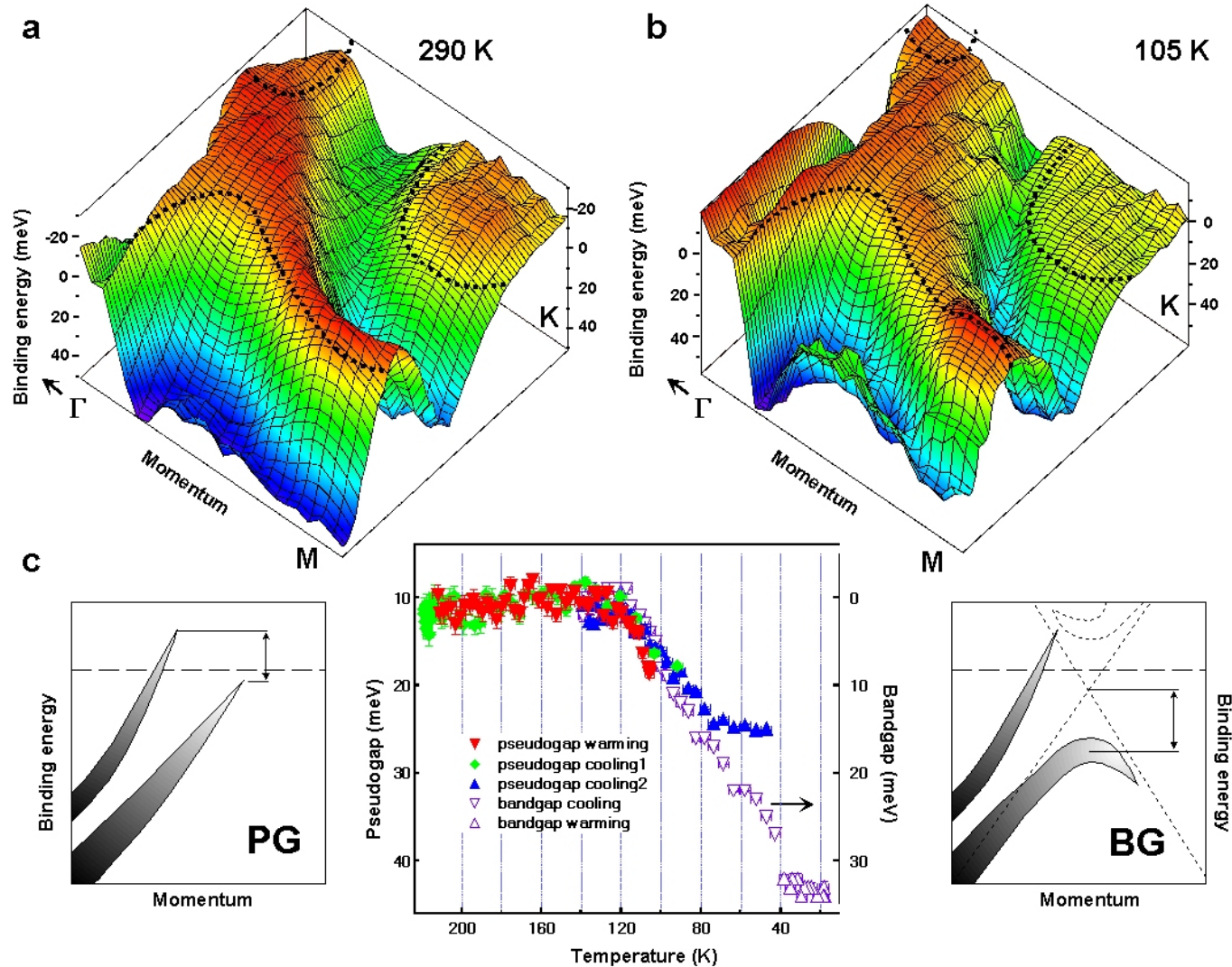
$$\Sigma \sim G \star \chi \quad \text{N}$$

Pseudogap and CDW in two dimensions

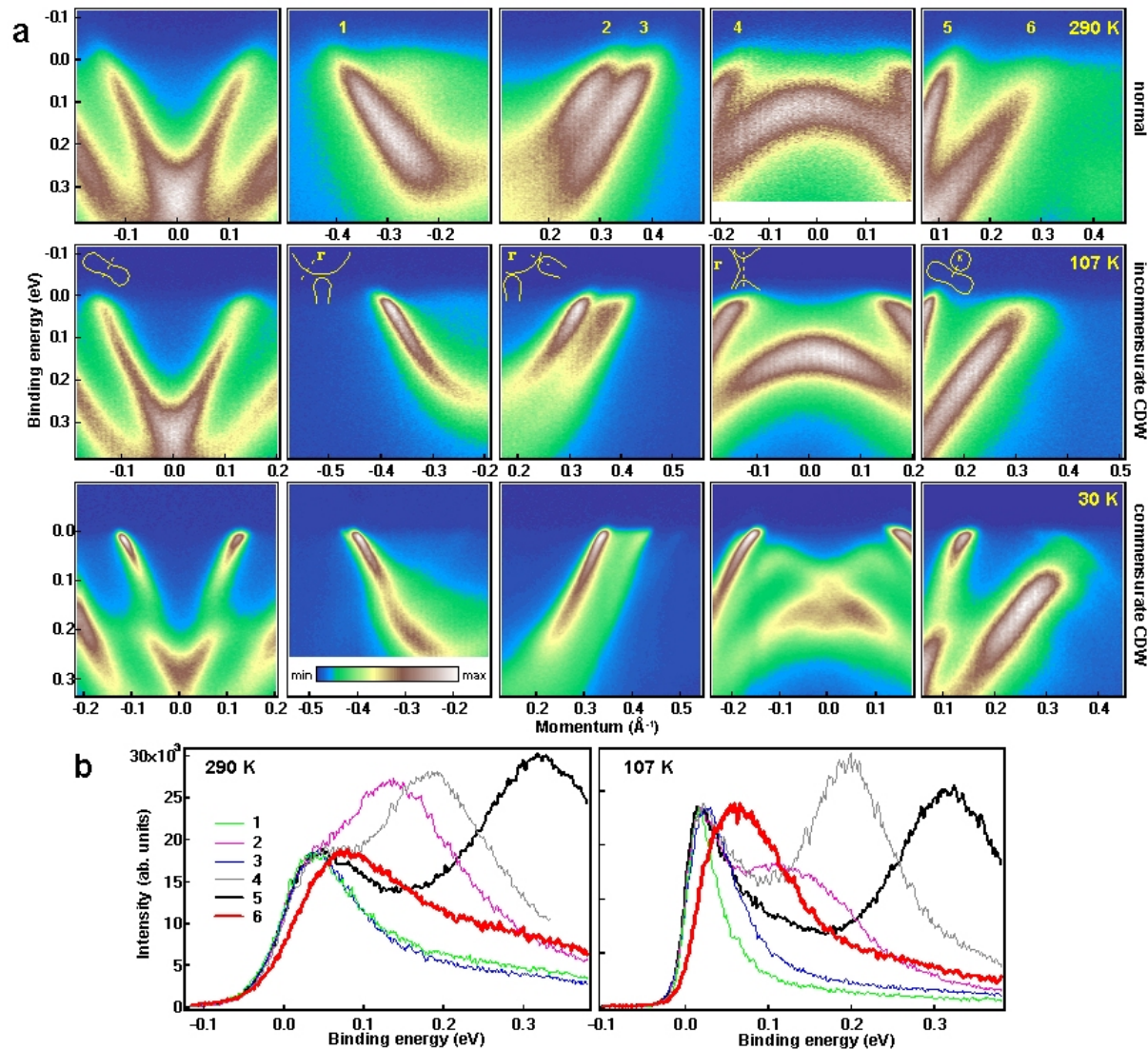
TaSe₂



Pseudogap and CDW in two dimensions



Pseudogap and CDW in two dimensions



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 $\Sigma(\mathbf{k}, \omega)$ and $\Delta(\mathbf{k}, \omega)$;
 - (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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Iliya Eremin, Alexander Yaresko

IMP Kiev

Daniil Evtushinskii





Single Crystals

Helmut Berger
Chengtian Lin, Bernhard Keimer
S. Ono, Yoichi Ando

EPFL Lausanne
MPI Stuttgart
CRIEPI Tokyo

Synchrotron Light

Rolf Follath

Ming Shi, Luc Patthey

BESSY Berlin

SLS Villigen

