

Unadulterated spectral function of low-energy quasiparticles

Evtushinsky Daniil



Moscow Institute
of Physics and
Technology



Institute of Metal
Physics,
Kiev, Ukraine

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 $\omega \rightarrow 0$ and at $T \rightarrow 0$?
- Behavior near T_C ?
- Evolution with doping?

Problems

- How to remove **resolution effects** accurately?

R-?

- How to disentangle **impurity scattering** from **quasiparticle interaction**?

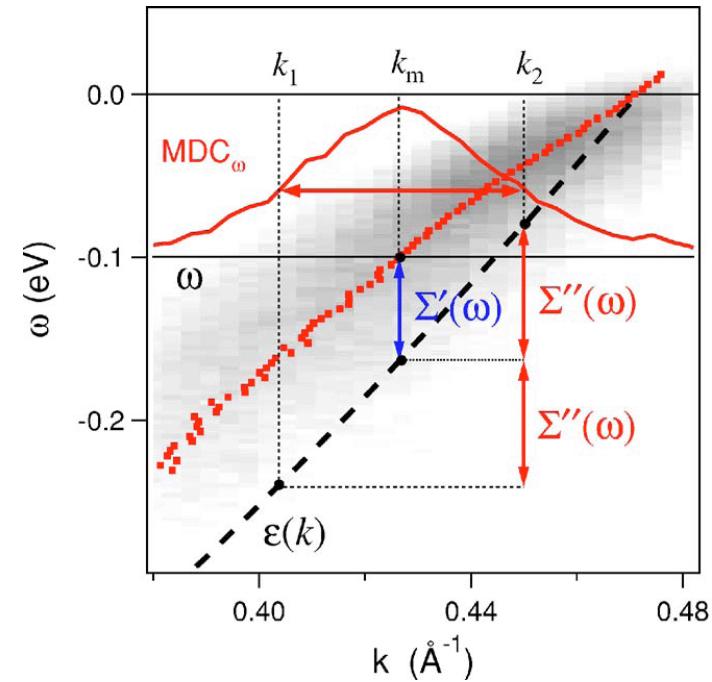
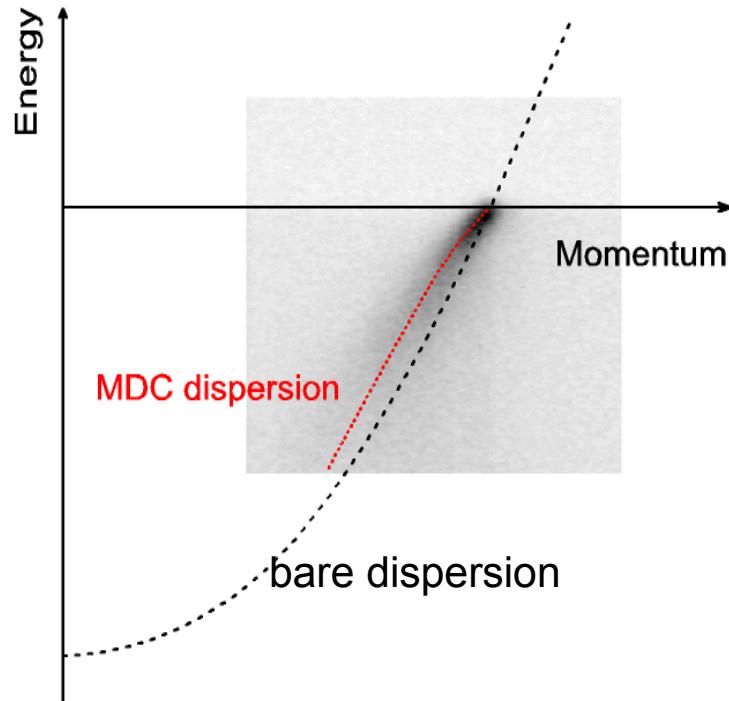
$$\Sigma''_{\text{int}} = \Sigma'' - \Sigma''_{\text{imp}}$$

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



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

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

$$\text{MDC}(k) = A(\omega, k), \omega = \text{const}$$

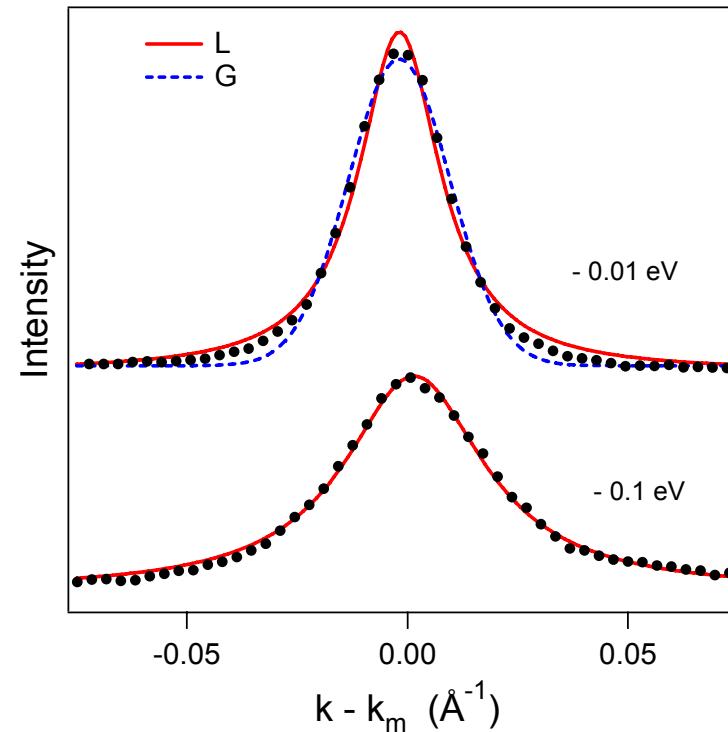
Spectral Function Extraction from ARPES Data

$$I(k, \omega) \propto A(k, \omega) \otimes R(k, \omega)$$

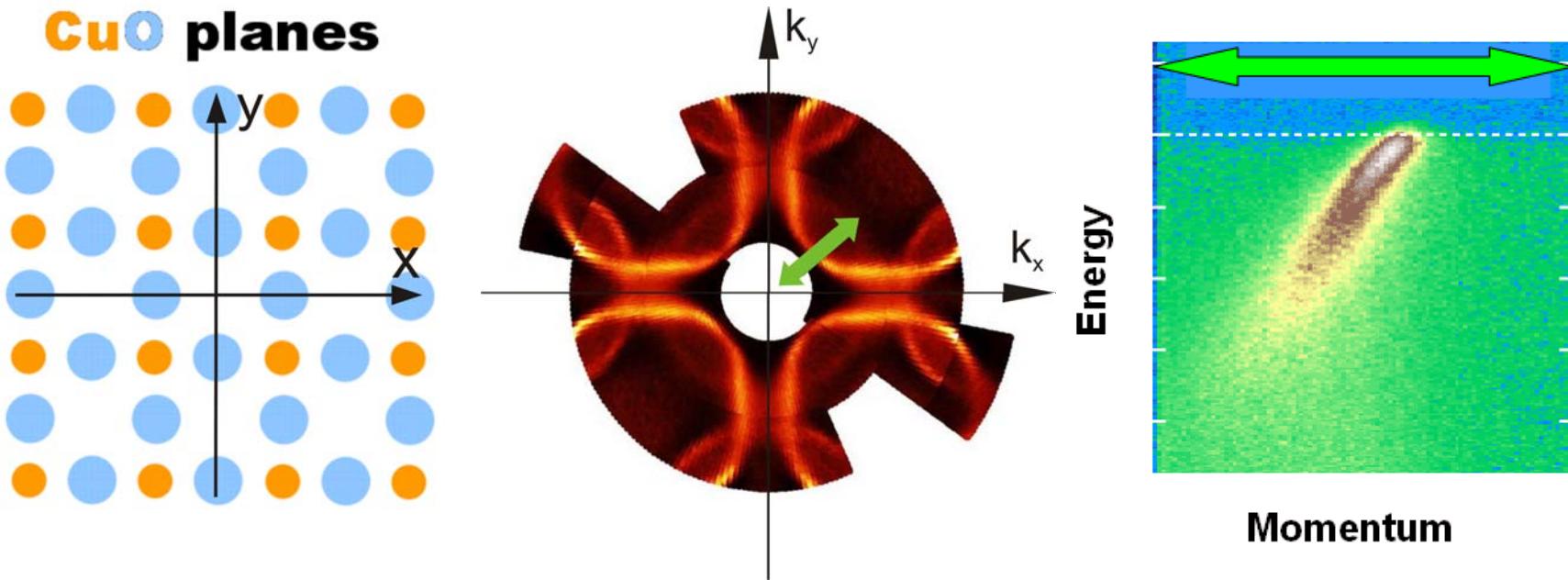
We measure $I(k, \omega)$

We are interested in $A(k, \omega)$

We need to remove $R(k, \omega)$



Nodal Direction



No gap

Momentum Resolution

$$\Sigma(k, \omega) = \Sigma(\omega) \quad M(k) = \text{const} \quad \varepsilon(k) \text{ linear}$$

Without resolution effects MDC is perfect **lorentzian**:

$$L(k) = A(k, \omega_0) = -\frac{1}{\pi} \cdot \frac{\Sigma''(\omega_0)}{(v \cdot (k - k_{\max}))^2 + (\Sigma''(\omega_0))^2}$$

Real MDC is a **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 **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 Resolution
(Lorentzian) (Gaussian)

Lorentzian \otimes Gaussian = 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 \mathbf{W}_L and \mathbf{W}_G

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

HWHM of Voigt profile, \mathbf{W}_V :

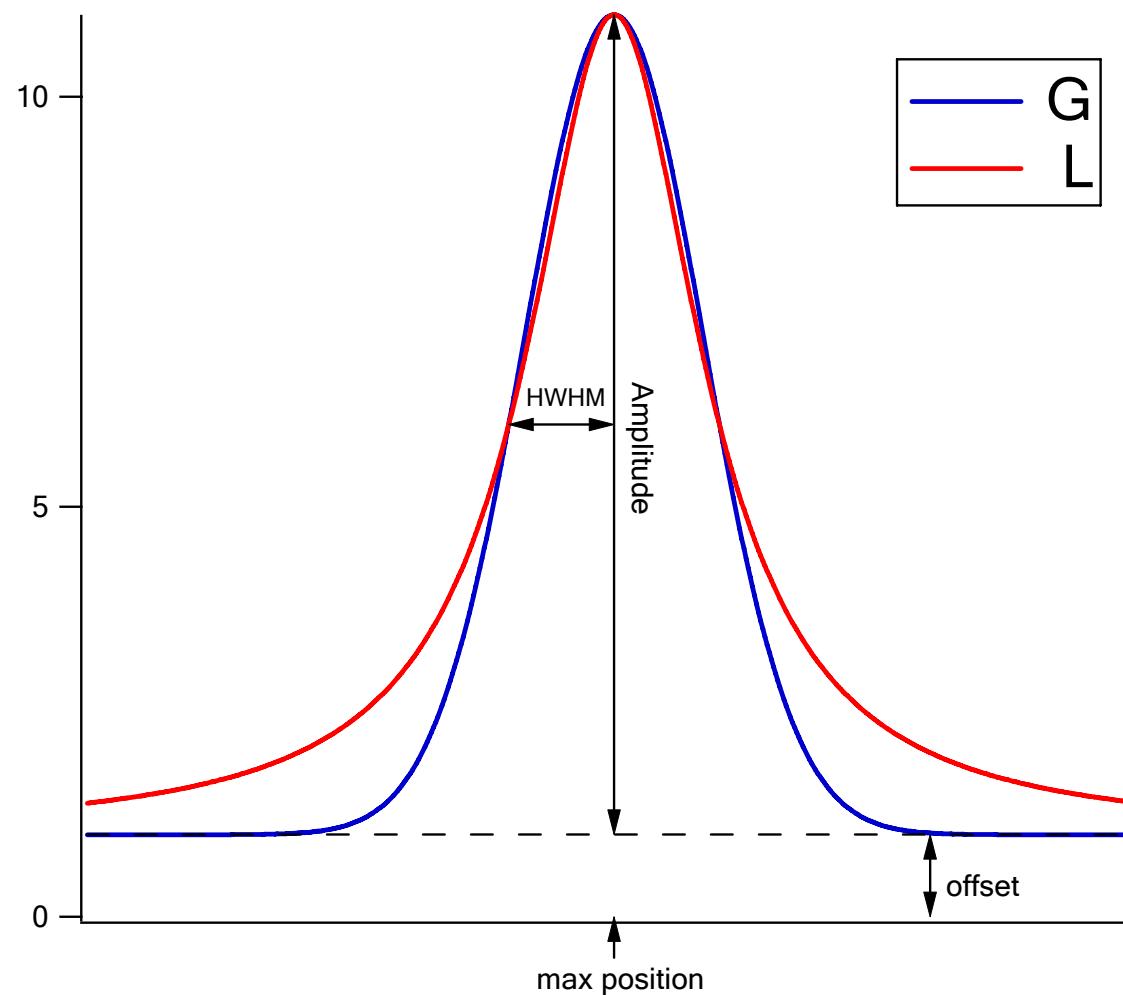
$$W_V \approx \frac{W_L}{2} + \sqrt{\frac{W_L^2}{4} + W_G^2} \quad \text{error < 1.2 \%}$$

$$W_L \ll W_G \Rightarrow W_V \approx \frac{W_L}{2} + W_G$$

Lorentz, Gauss

L, G:

1. Offset
2. Max position
3. Amplitude
4. Width



Lorentz, Gauss and Voigt

L, G:

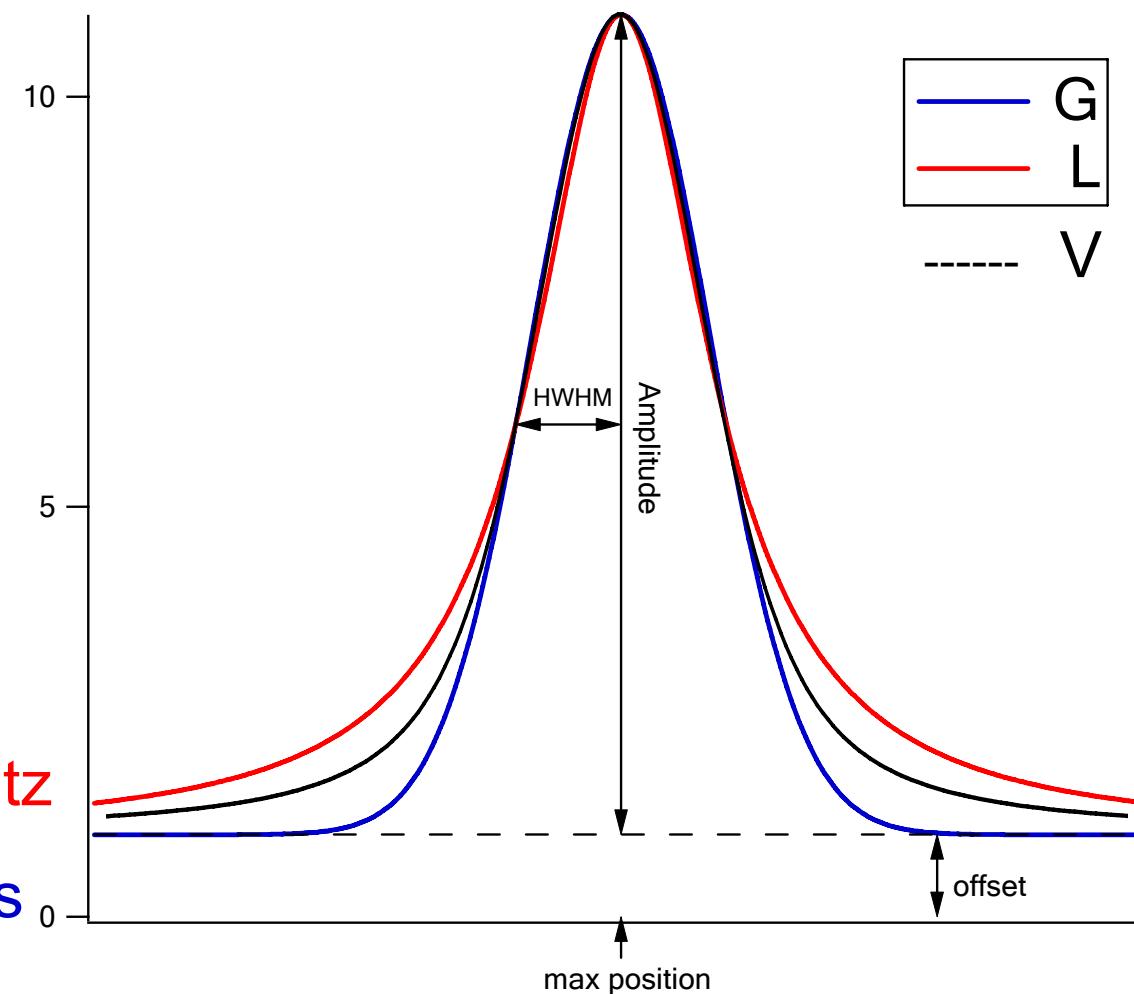
1. Offset
2. Max position
3. Amplitude
4. Width

One more parameter:

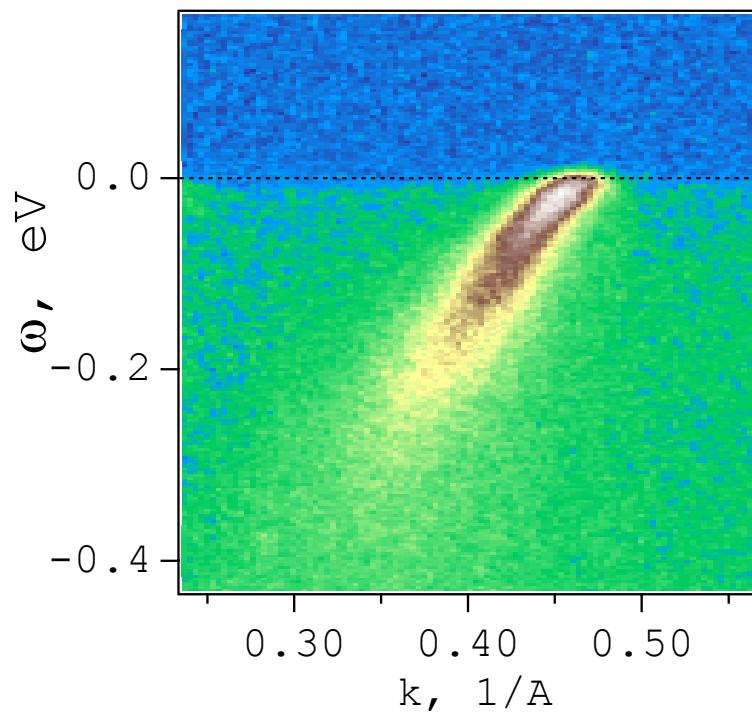
$$5. \eta = W_G / W_L$$

$\eta \rightarrow 0$ Voigt \rightarrow Lorentz

$\eta \rightarrow \infty$ Voigt \rightarrow Gauss



Old Procedure of Self Energy Extraction

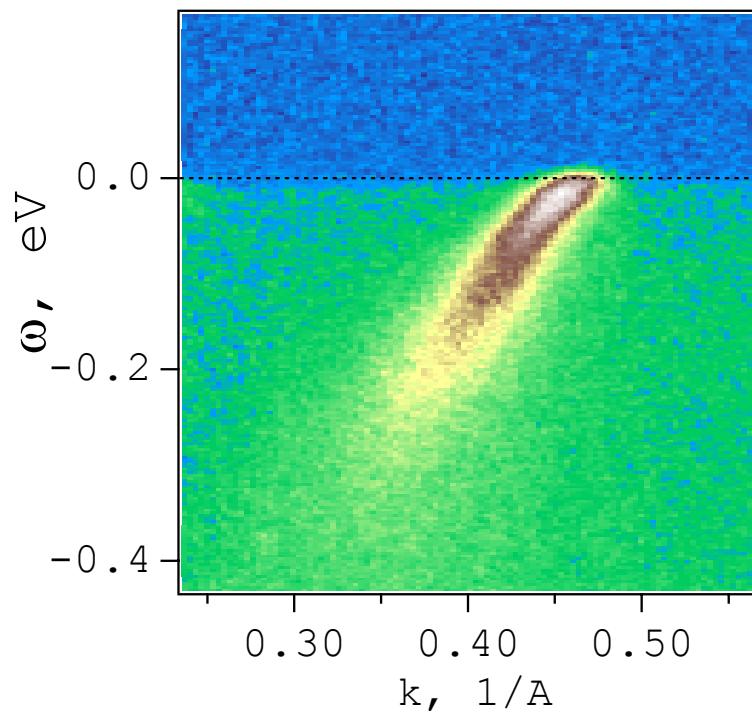


Lorentz-Fit



Overall
width

New Procedure of Self Energy Extraction



Lorentz-Fit



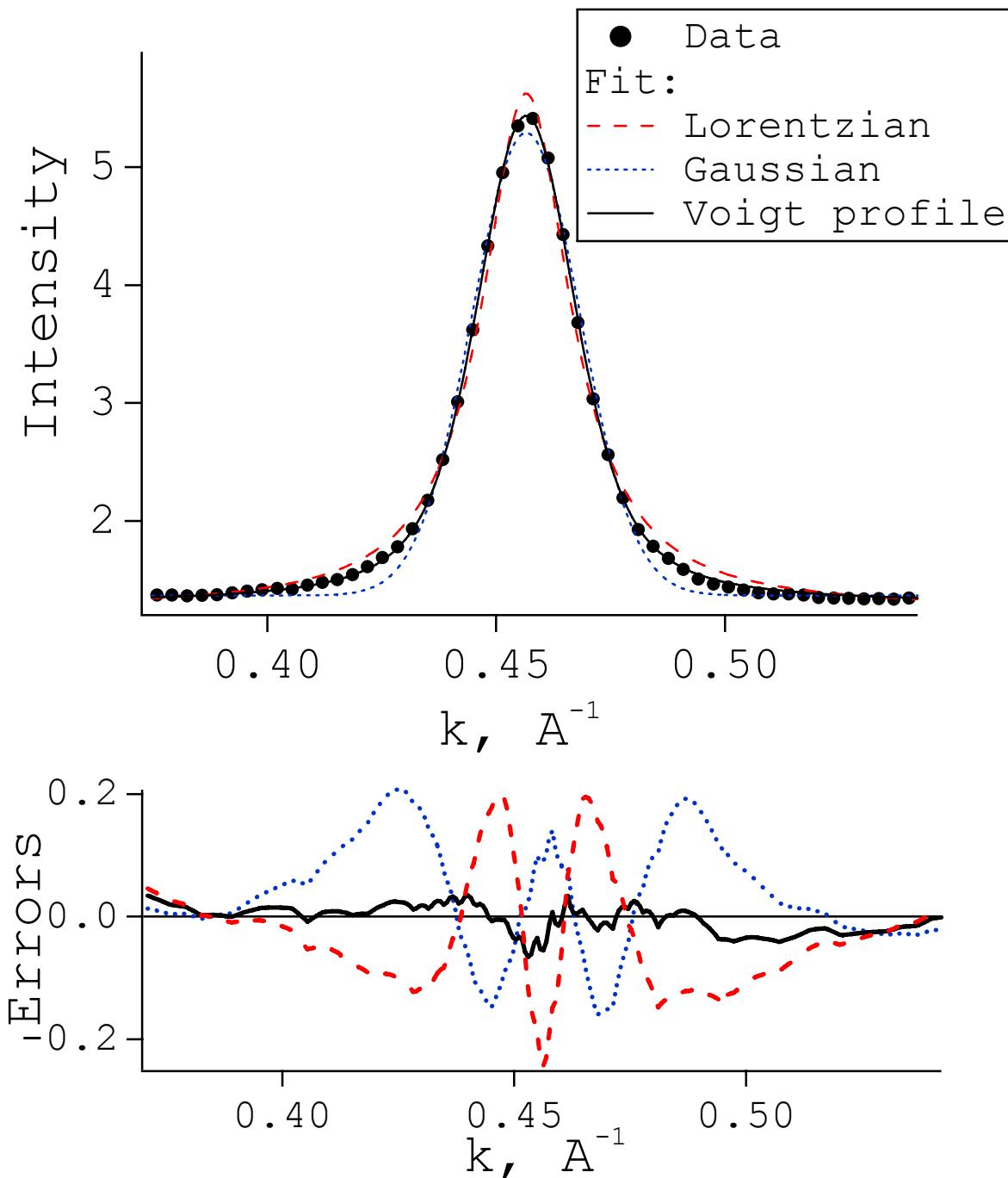
Overall width

Voigt-Fit

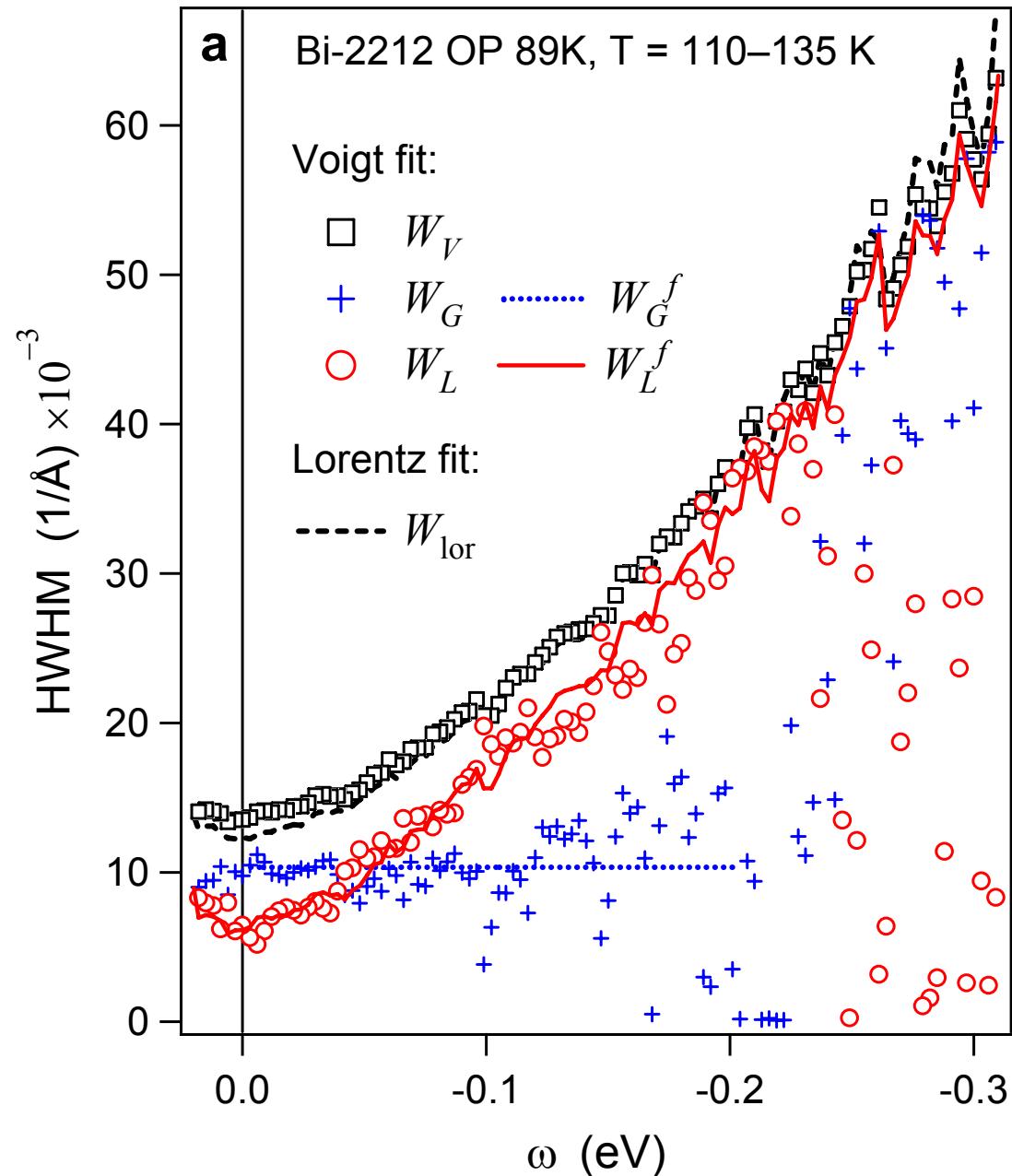


Intrinsic width
and
resolution

MDC Shape

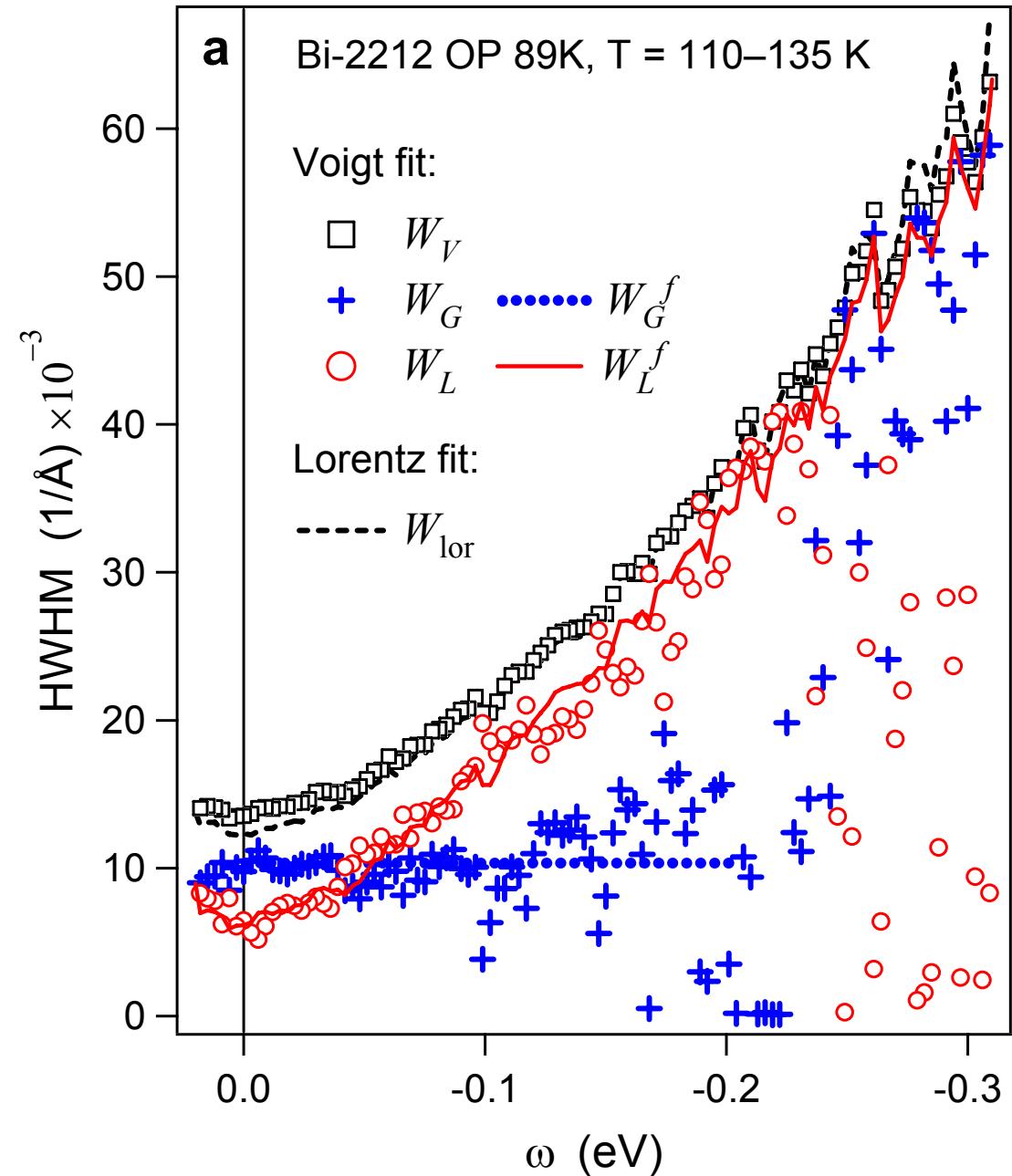


$\Sigma(\omega)$ from Voigt Fit



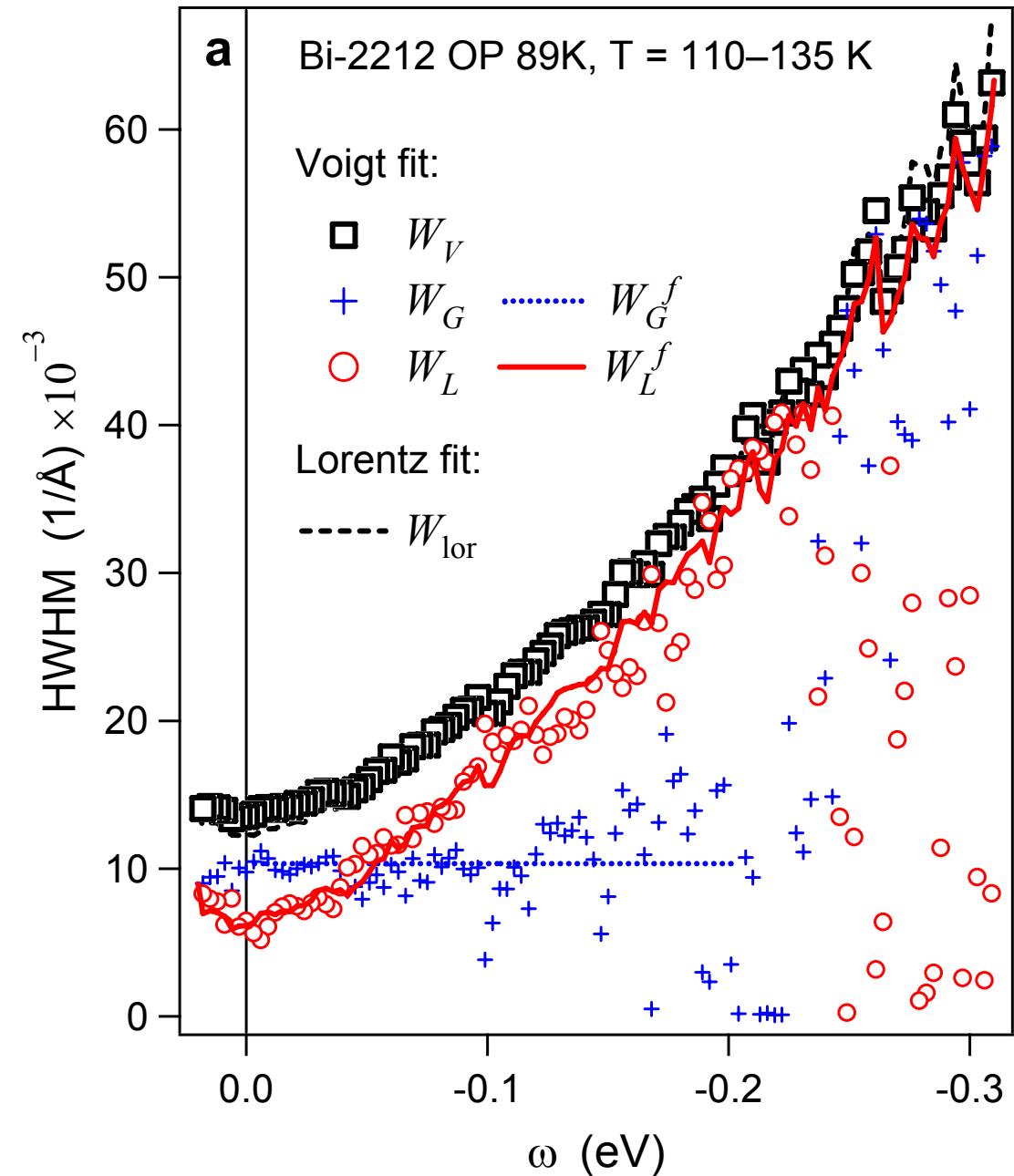
$\Sigma(\omega)$ from Voigt Fit

Resolution:
 $W_G = const$



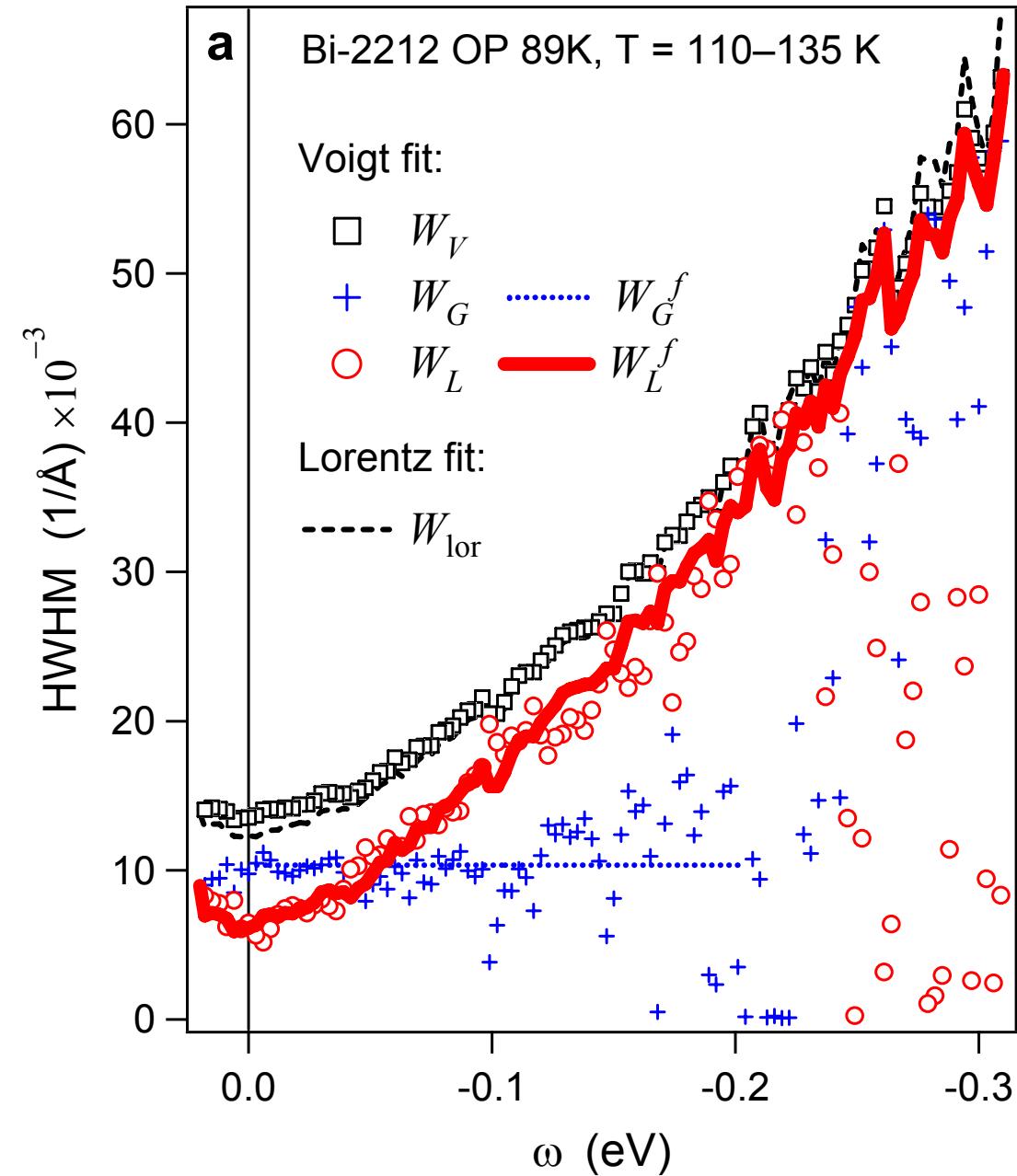
Overall width,
 W_V

$\Sigma(\omega)$ from Voigt Fit



$\Sigma(\omega)$ from Voigt Fit

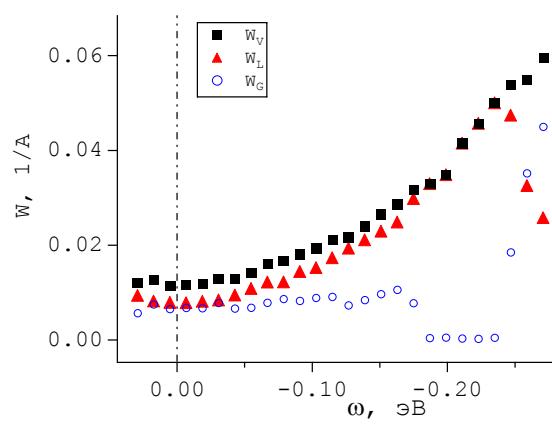
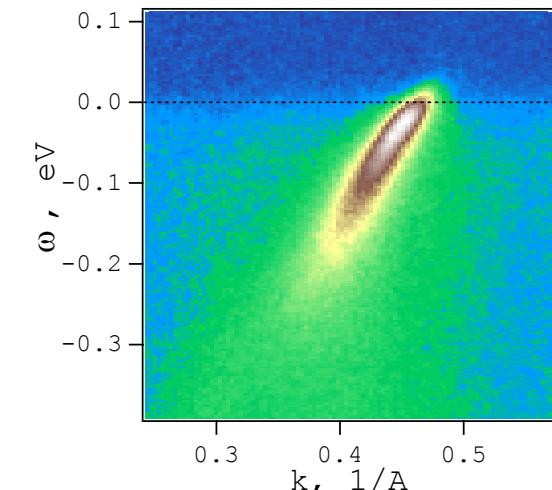
Intrinsic width,
 W_L



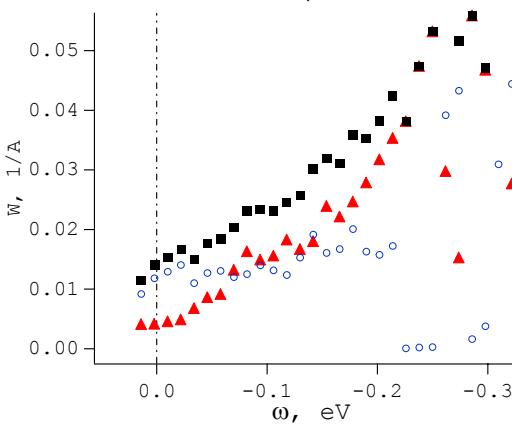
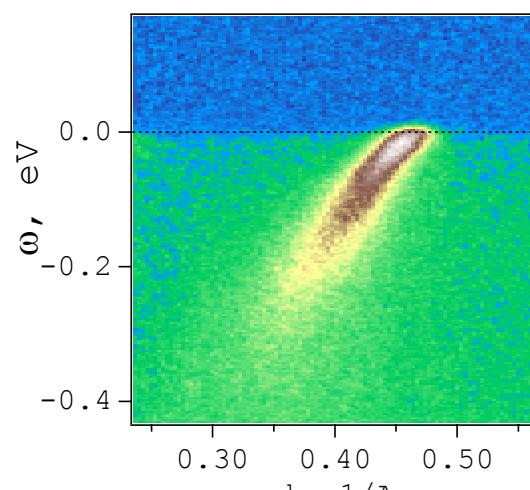
Examples of Voigt fit Application to ARPES Data

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

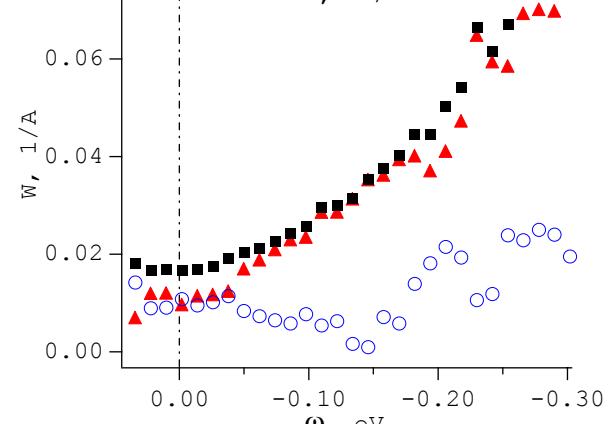
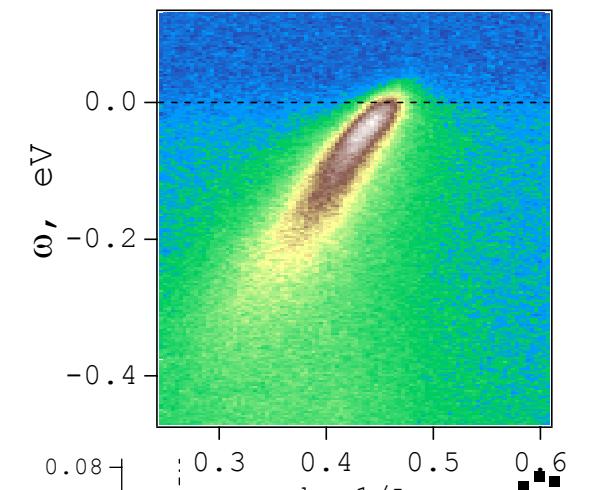
Examples on BSCCO



$x=0.21, T=100\text{ K}$



$x=0.16, T=40\text{ K}$



$x=0.12, \text{Low T}$

Voigt Fit in application to YBCO

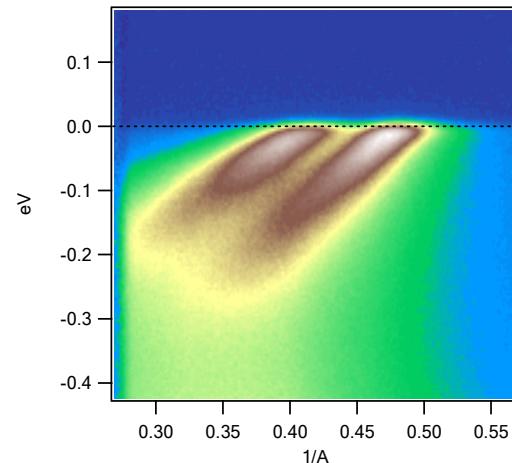


Image1, 24 K

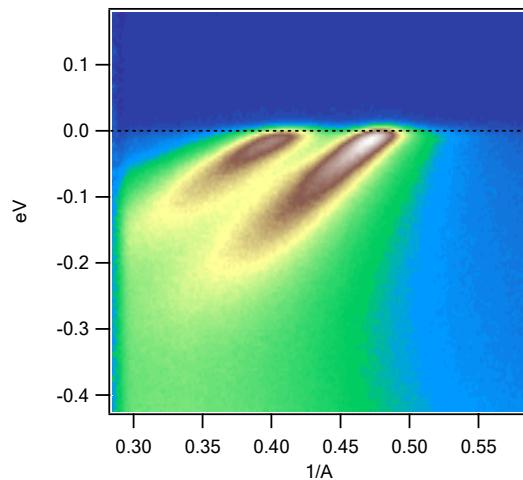
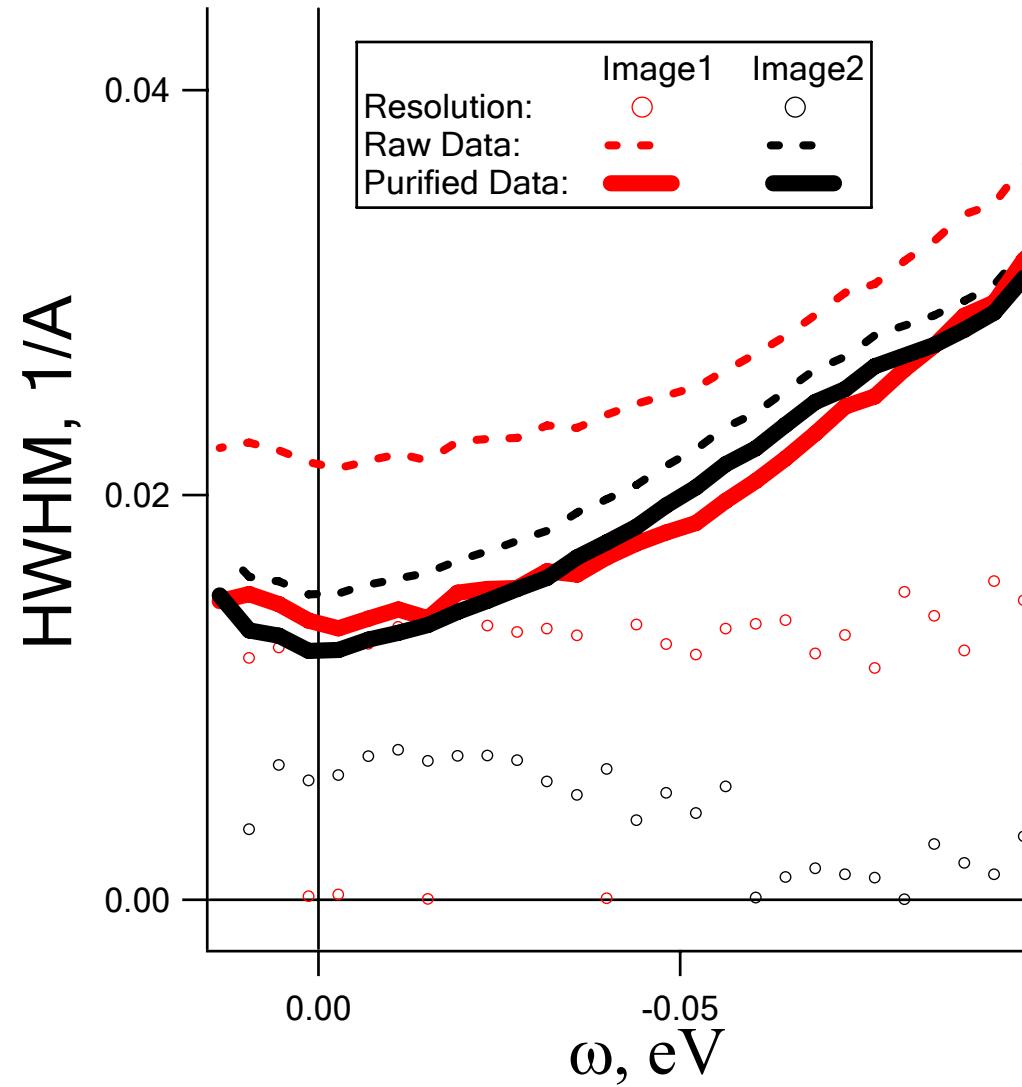
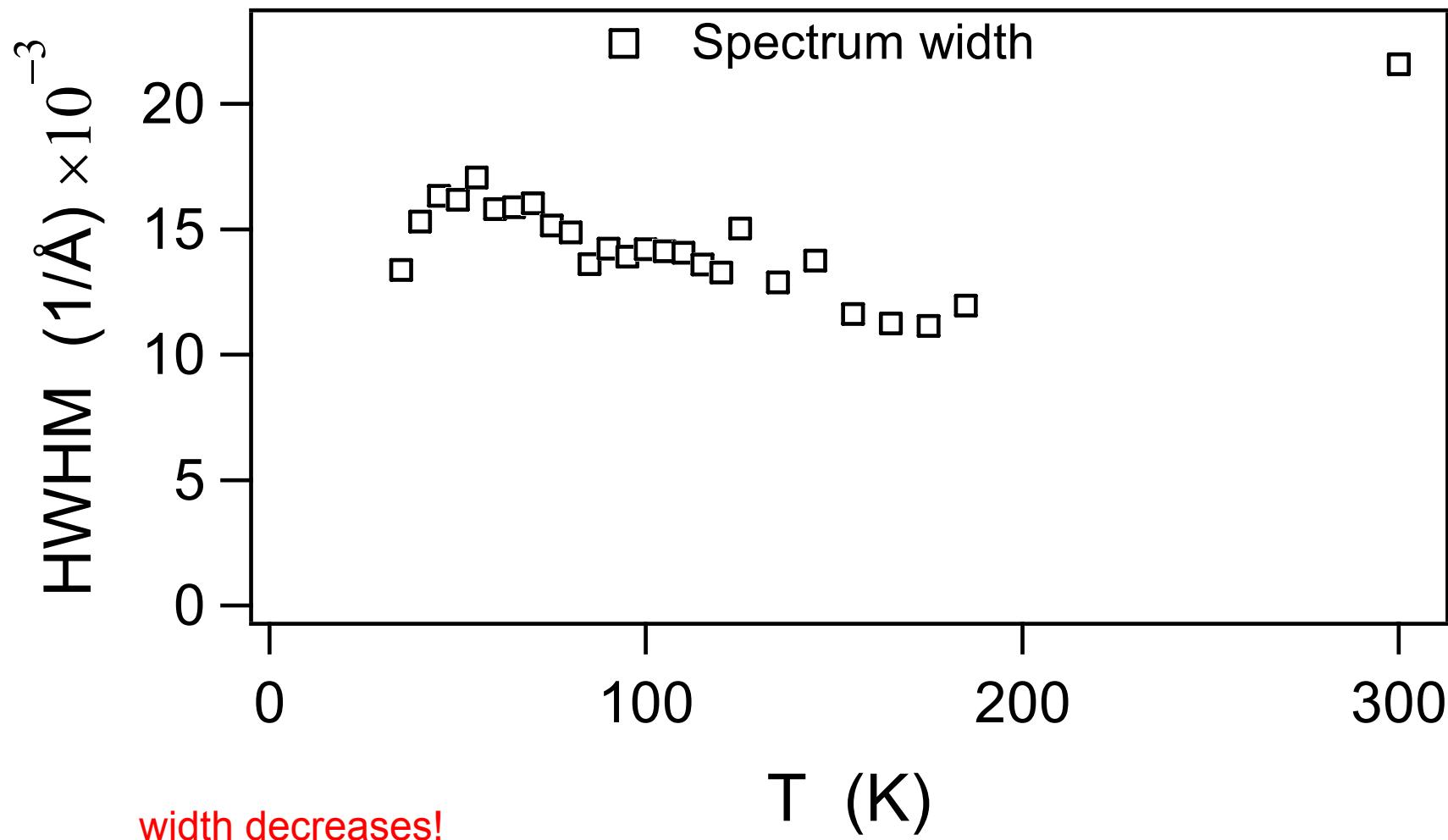


Image2, 24 K



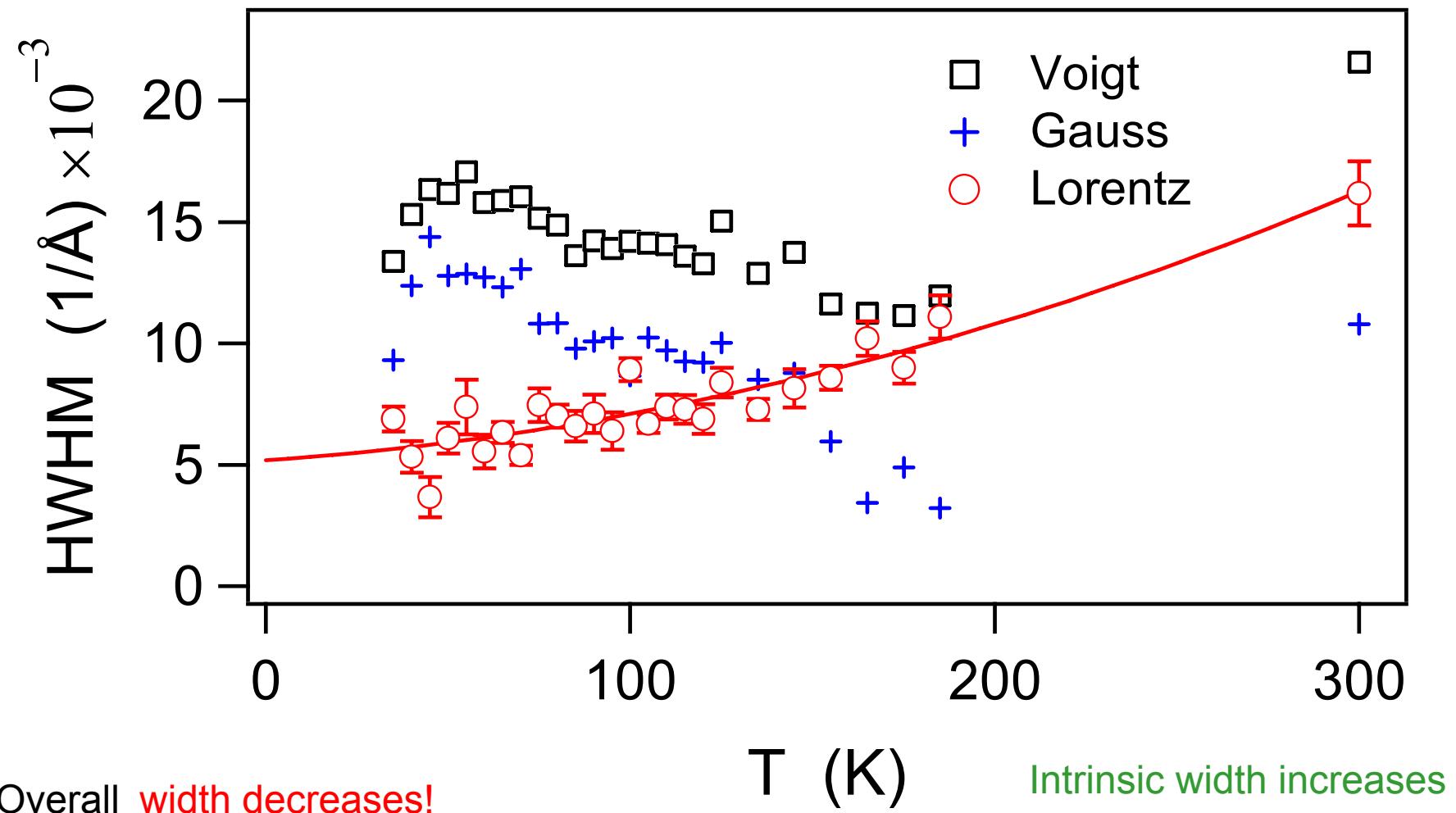
Temperature dependence of scattering rate

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



Temperature dependence of scattering rate

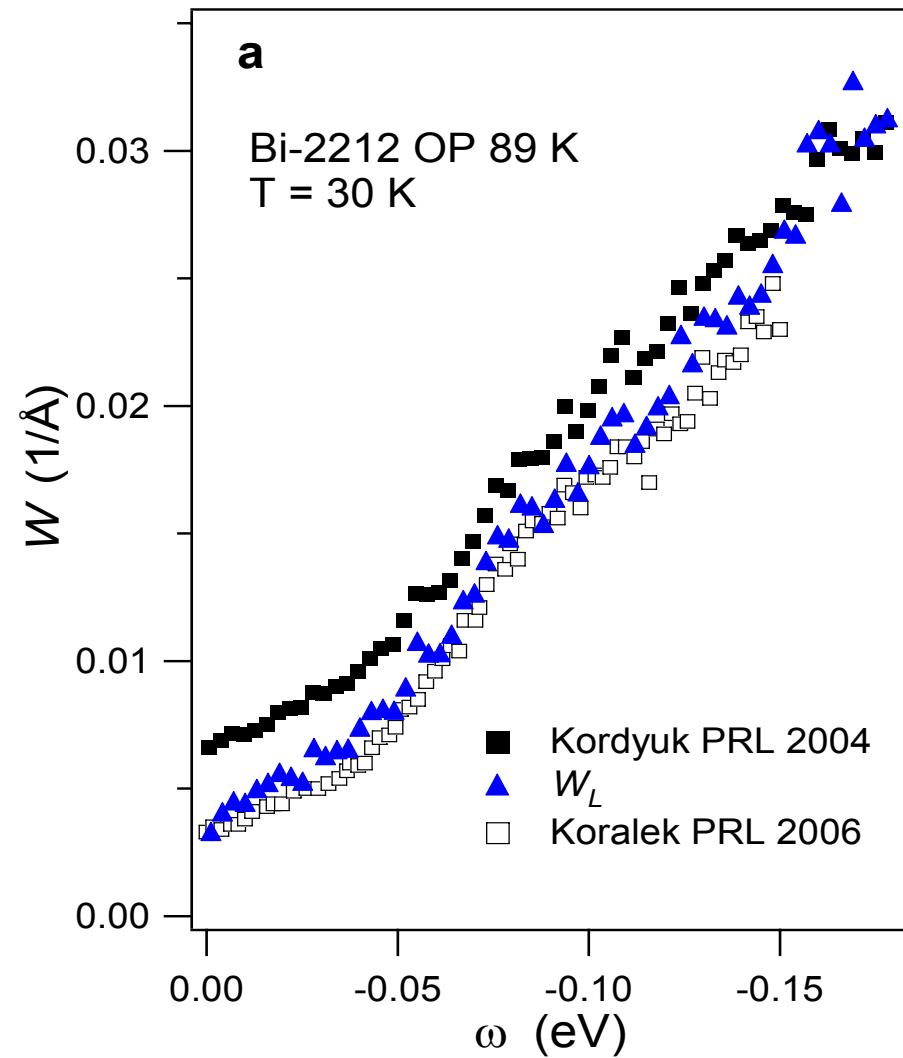
$\Sigma''(\omega=0, T)$



Comparison to the low-energy high-resolution data

$$R \sim (hv - \phi)^{-1/2}$$

$$R_{\text{6eV LASER}} / R_{\text{27eV synchrotron}} = 0.25$$



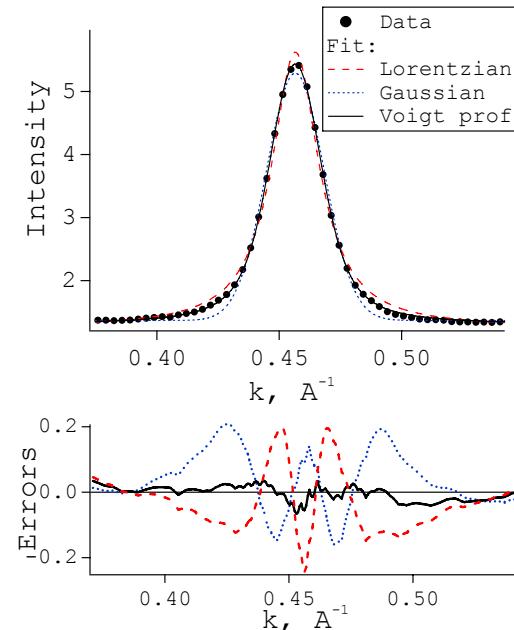
J. D. Koralek *et al.*, PRL 2006

Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)

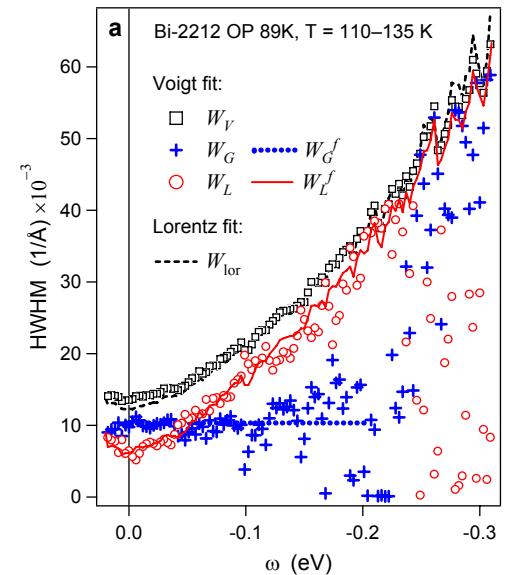
Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)



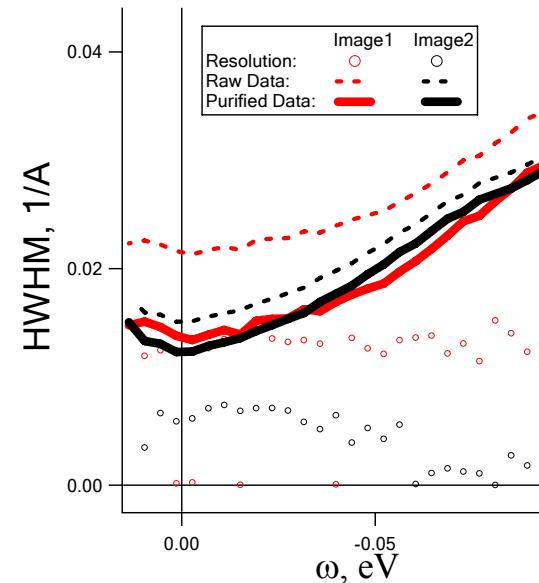
Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)



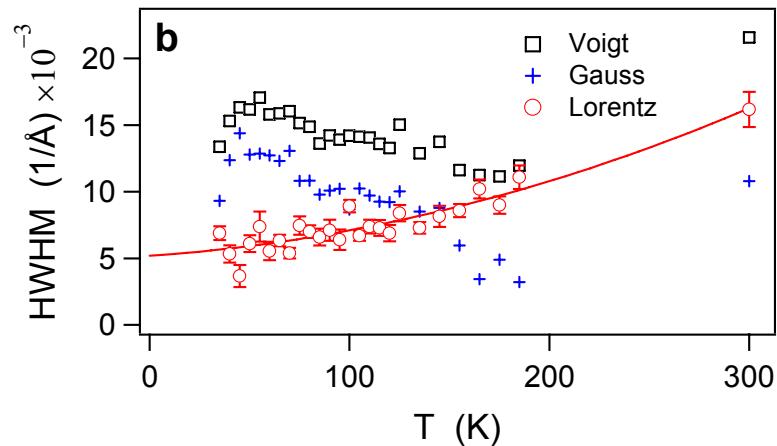
Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)



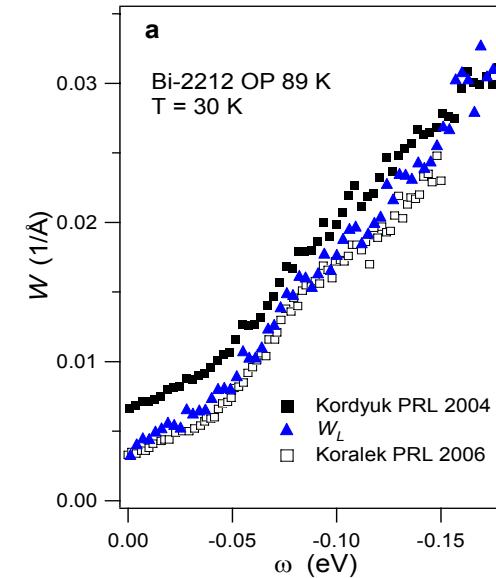
Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)



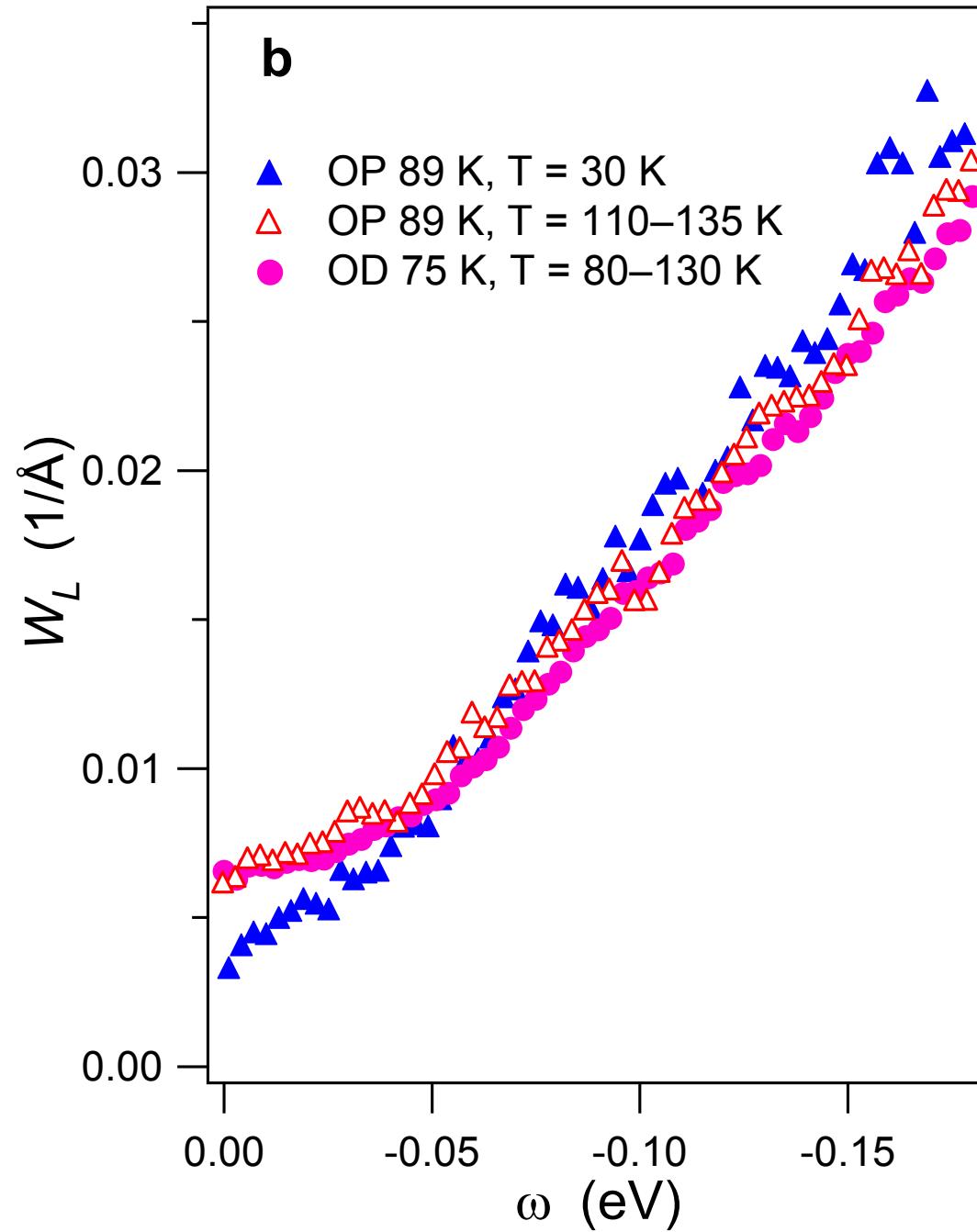
Justification of Voigt Fit procedure

- A. MDC Lineshape
- B. ω -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)

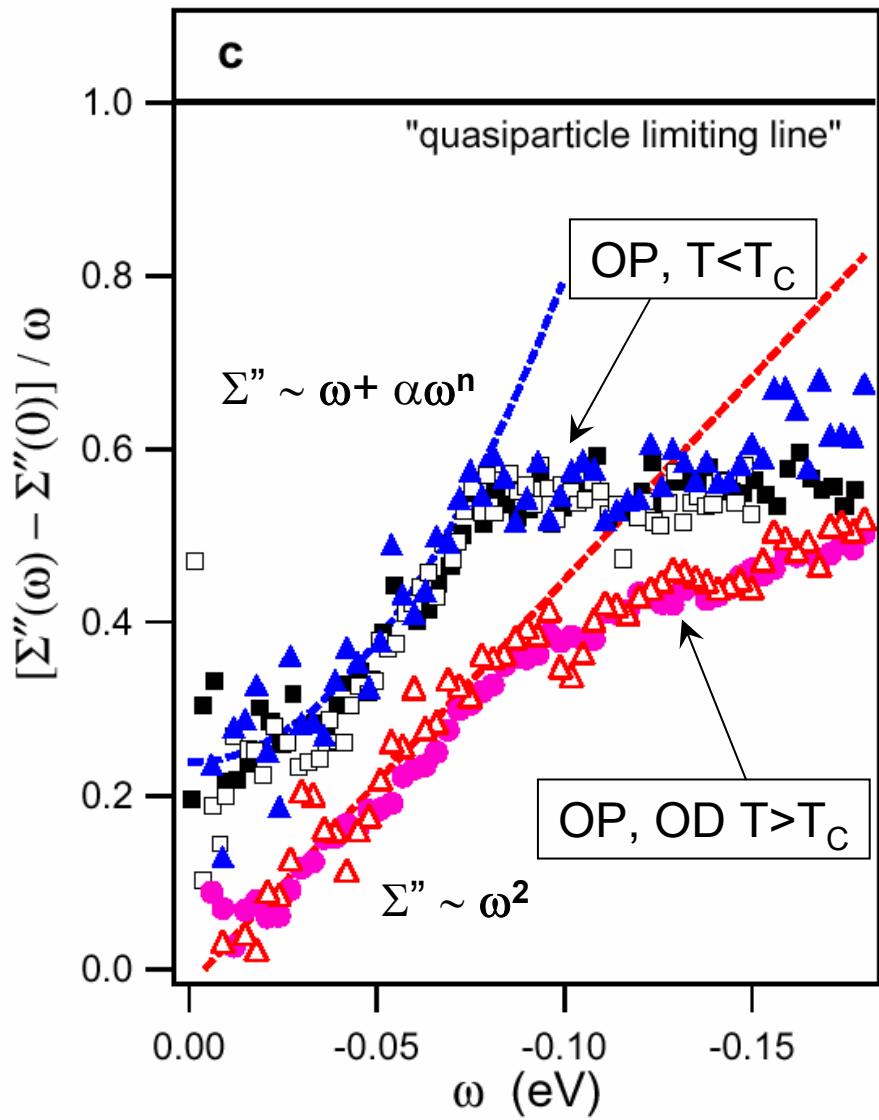


Most interesting part ☺

$\Sigma''(\omega)$
behavior in
vicinity of
Fermi-level



Reduced self-energy function



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

$$\Sigma'' = \text{const} \rightarrow \sigma = 0$$

$$\Sigma'' \propto \omega \rightarrow \sigma = \text{const}$$

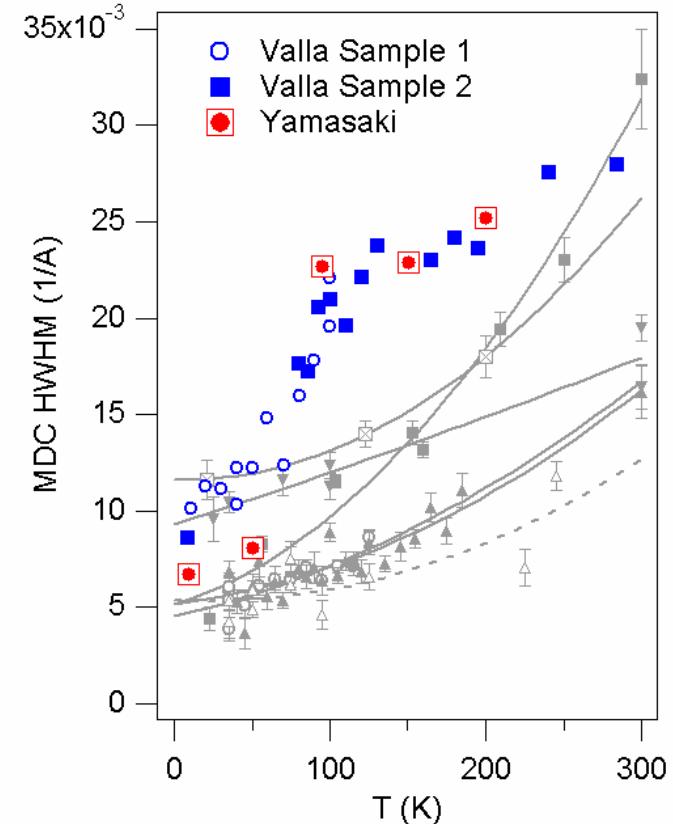
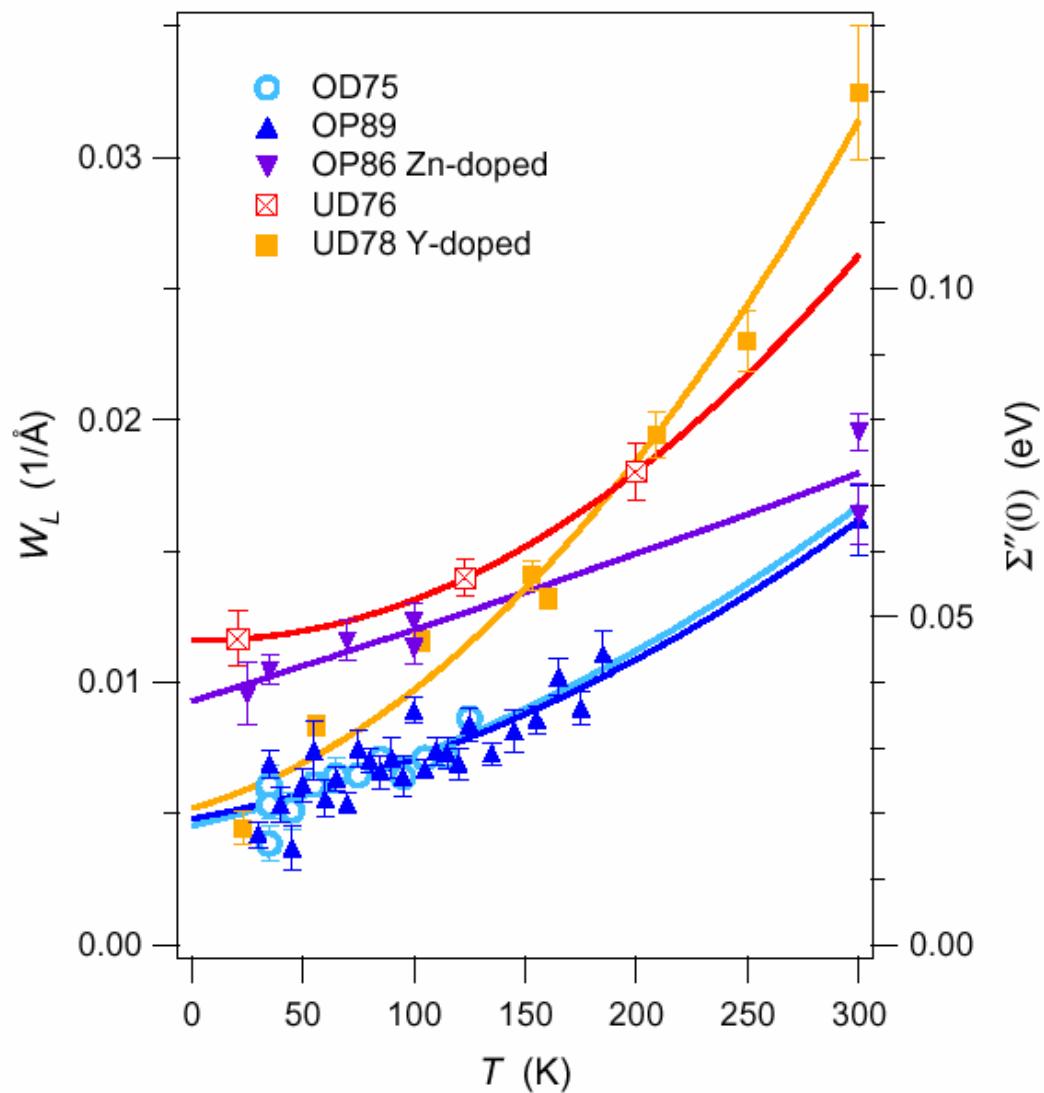
$$\Sigma'' \propto \omega^2 \rightarrow \sigma \propto \omega$$

$$\Sigma'' \propto \omega^3 \rightarrow \sigma \propto \omega^2$$

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

- Kordyuk PRL 2004
- ▲ OP 89 K, $T = 30 \text{ K}$
- Koralek PRL 2006
- △ OP 89 K, $T \approx 110 \text{ K}$
- OD 75 K, $T \approx 90 \text{ K}$

Temperature dependence of scattering rate

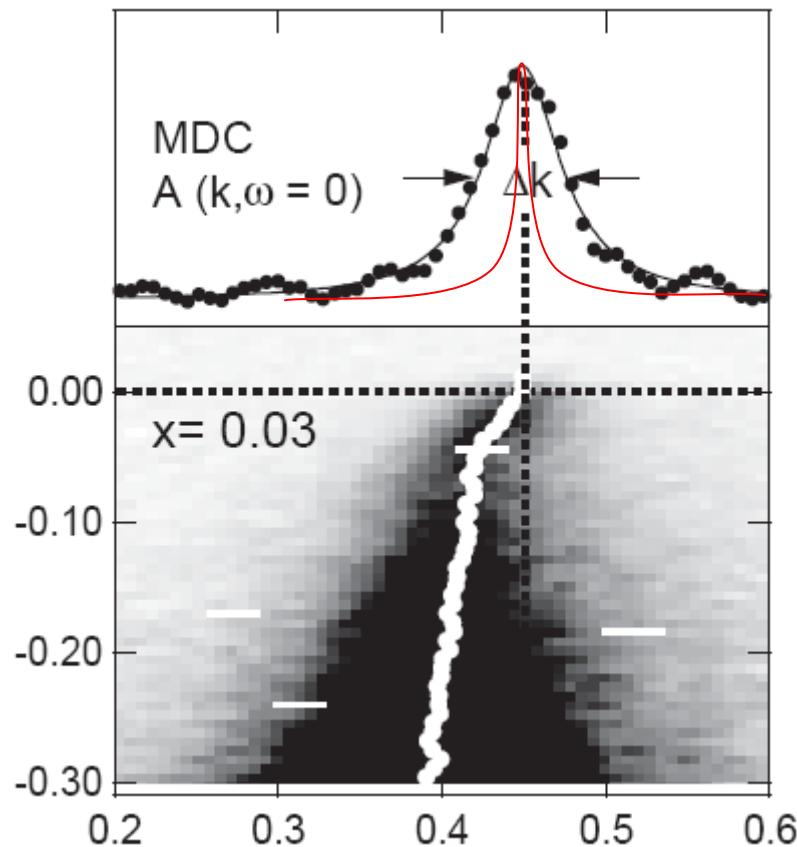


T.Valla *Physical Review B*, 2006

T. Yamasaki et al., cond-mat/0603006

ARPES
vs.
Transport

MDC Width: 0.030 vs **0.004** 1/Å

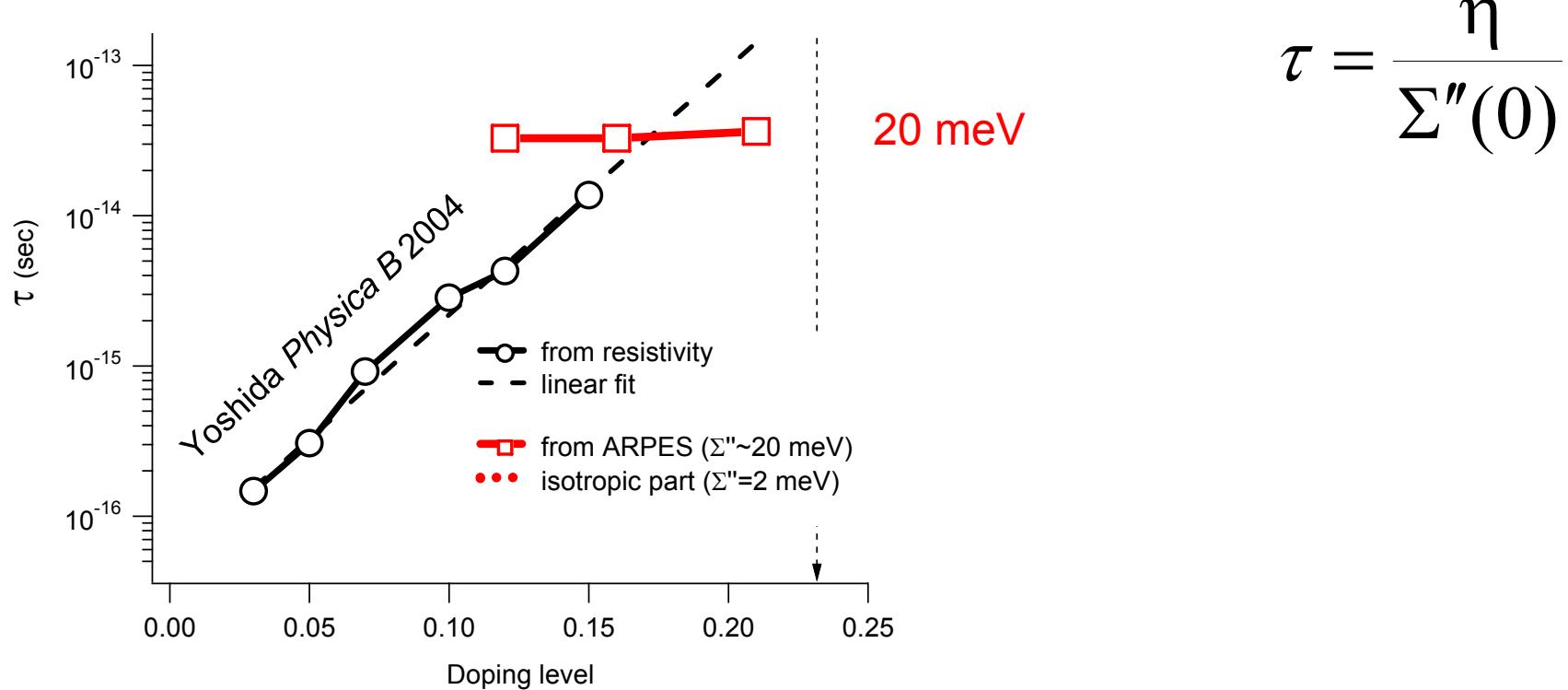


Yoshida's MDC used to calculate resistivity.
HWHM=**0.03** 1/Å
Compare to result, obtained by Voigt-fit procedure:
0.004 1/Å.

τ from ARPES and Resistivity

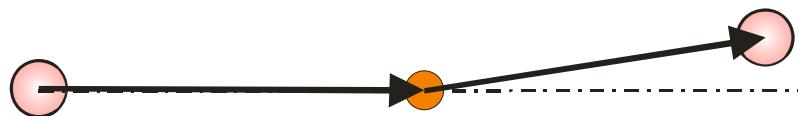
$$\rho_0 = \frac{m^*}{ne^2\tau} \approx \frac{k_F}{ne^2\eta} \frac{\Sigma''_{im}}{\nu_r}$$

$$n \sim 1 - x$$

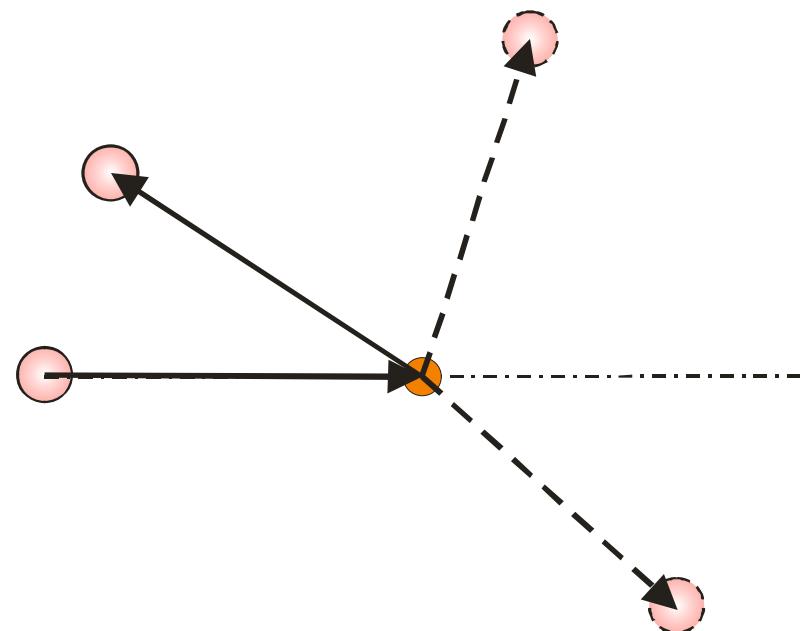


Forward and Isotropic Scattering

Forward, τ_f



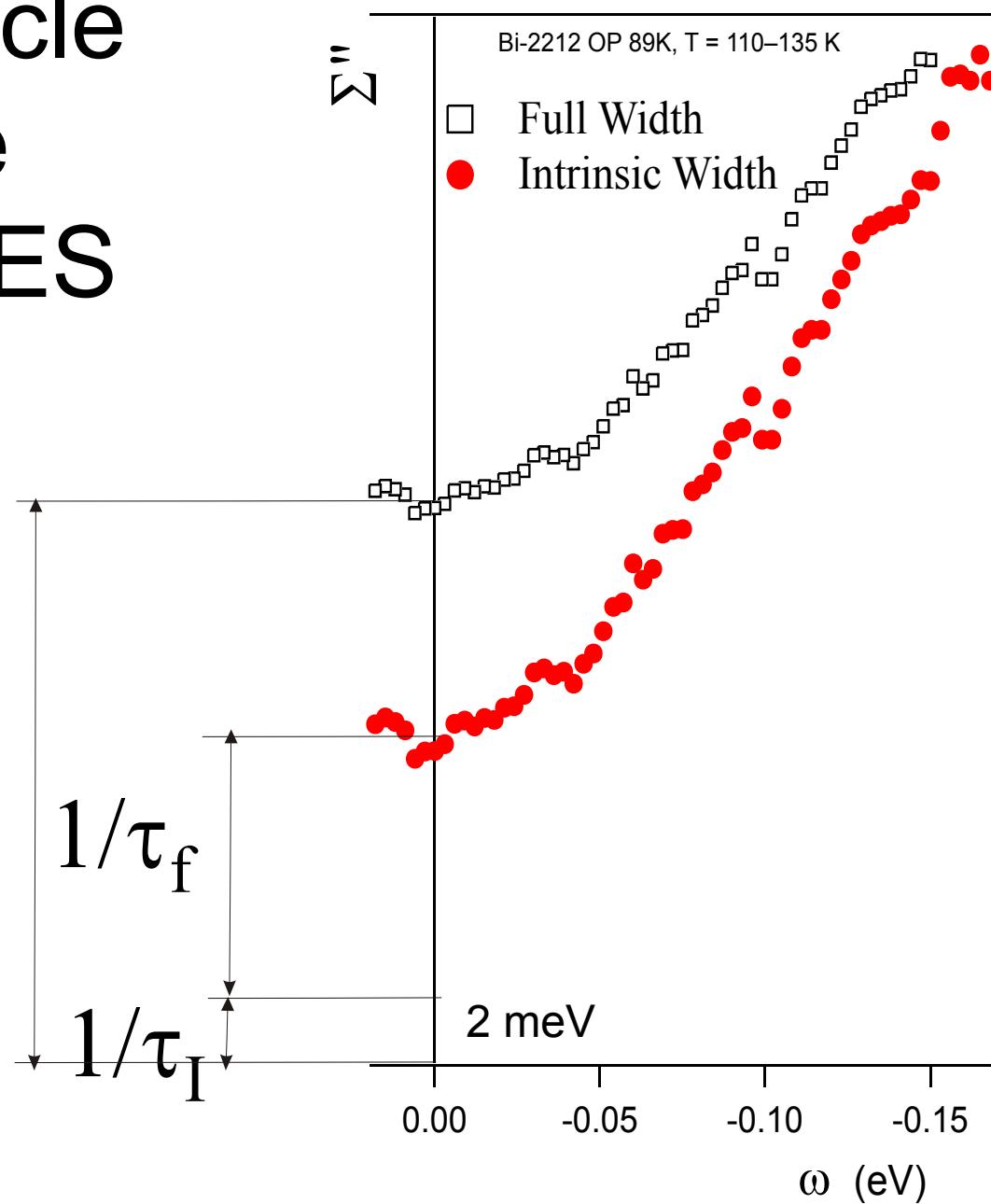
Isotropic, τ_I



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

$$\text{Transport: } \tau^l = \tau_I^{-1} + \alpha \cdot \tau_f^{-1}, \quad \alpha \ll 1$$

Quasiparticle Lifetime from ARPES

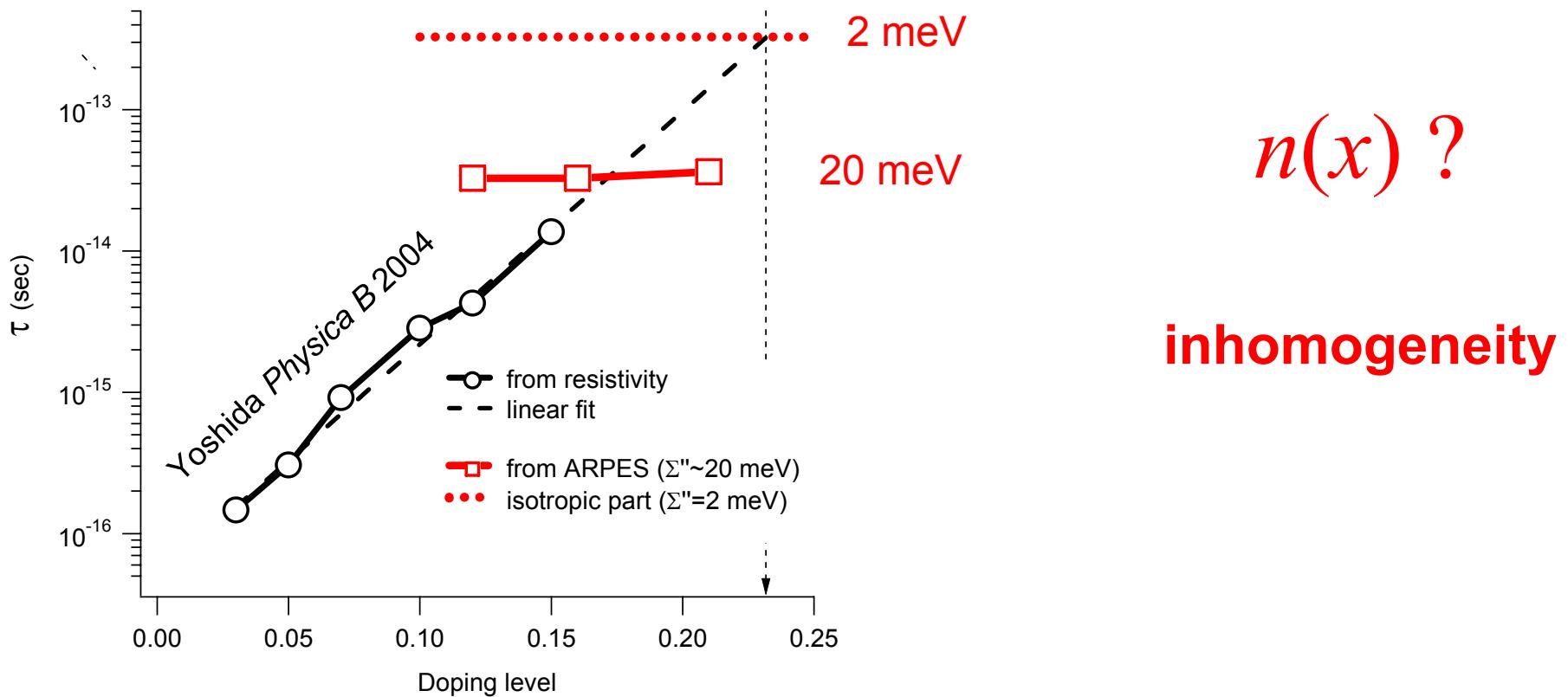


Impurity scattering

forward and isotropic (unitary)?

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

$$n \sim 1 - x$$



Resistivity from ARPES

Simple Drude formula: $\sigma = \frac{ne^2\tau}{m^*}$

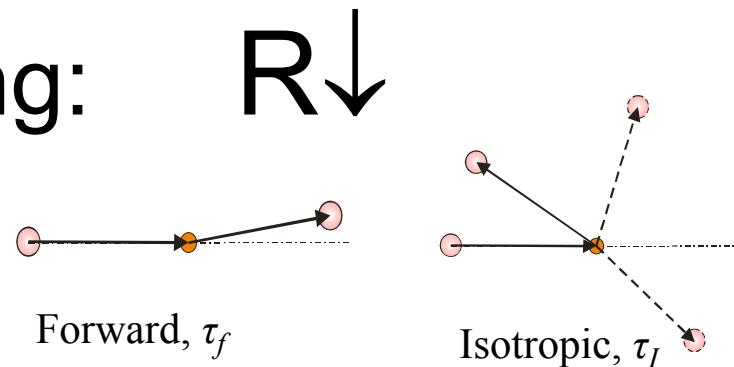
Note that m^* is calculated from renormalized dispersion.
 $n=(1-x)$

How resistivity changes if we take in to account some extra features?

Two kinds of scattering:

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

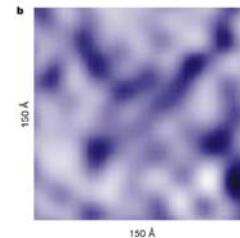
Transport: $\tau^I = \tau_I^{-1} + \alpha \cdot \tau_f^{-1}$, $\alpha \ll 1$



Inhomogeneity:

$$n \sim (1 - V_m) n_d + V_m n_m$$

V_m – metallic phase volume



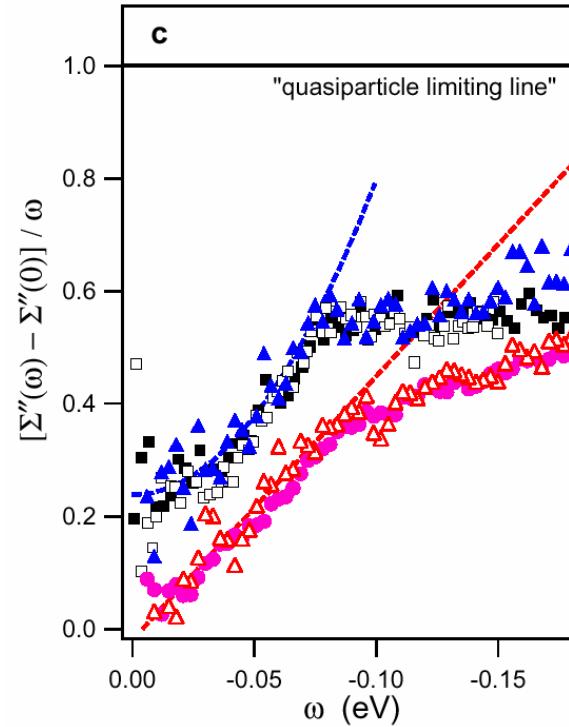
$R \uparrow$

Conclusions

- Quasiparticles are well-defined
- Non-zero $\Sigma''(T=0) \approx 16 \text{ meV}$
- No drop at T_C
- Σ'' depends rather on dopants than on x
- To compare to transport we need to disentangle isotropic and forward contributions

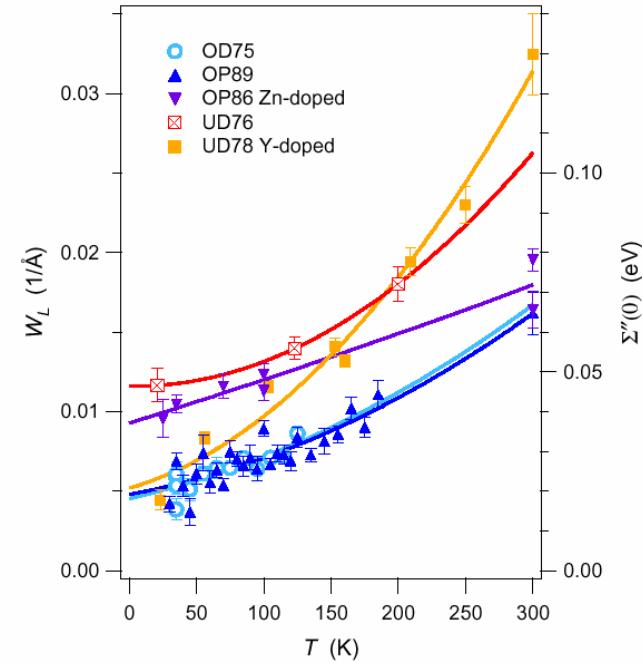
Conclusions

- Quasiparticles are well-defined
- Non-zero $\Sigma''(T=0) \approx 16$ meV
- No drop at T_C
- Σ'' depends rather on dopants than on x
- To compare to transport we need to disentangle isotropic and forward contributions



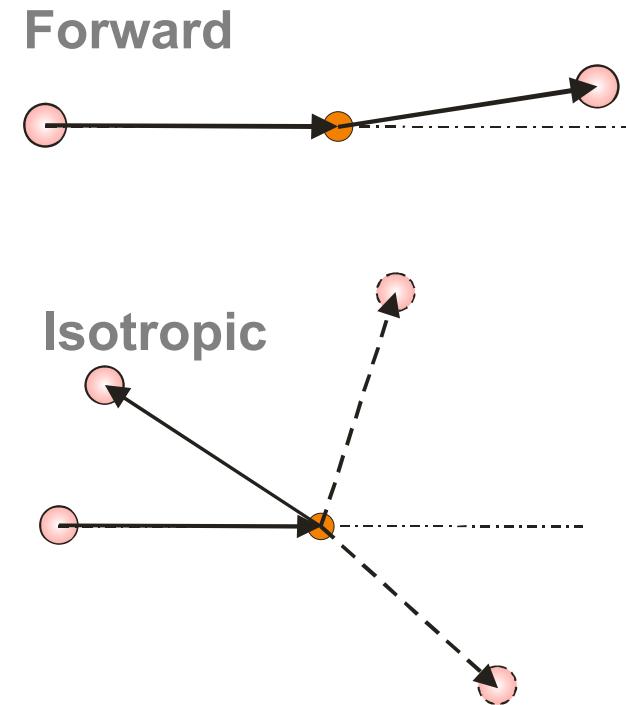
Conclusions

- Quasiparticles are well-defined
- Non-zero $\Sigma''(T=0) \approx 16$ meV
- No drop at T_C
- Σ'' depends rather on dopants than on x
- To compare to transport we need to disentangle isotropic and forward contributions



Conclusions

- Quasiparticles are well-defined
- Non-zero $\Sigma''(T=0) \approx 16 \text{ meV}$
- No drop at T_C
- Σ'' depends rather on dopants than on x
- To compare to transport we need to disentangle isotropic and forward contributions

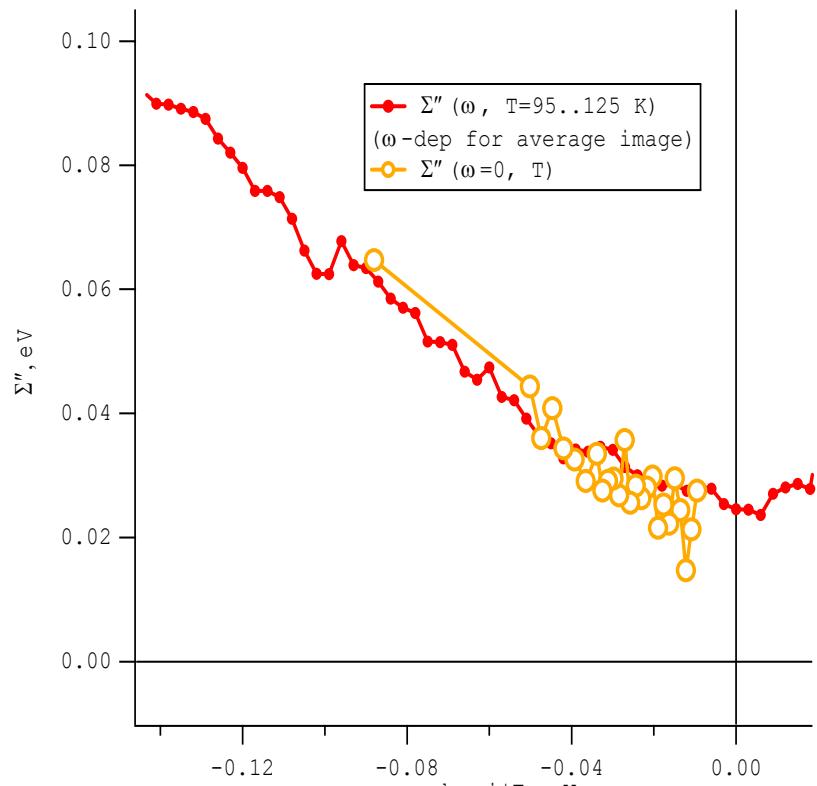


$\Sigma''(\omega, T)$ asymmetry

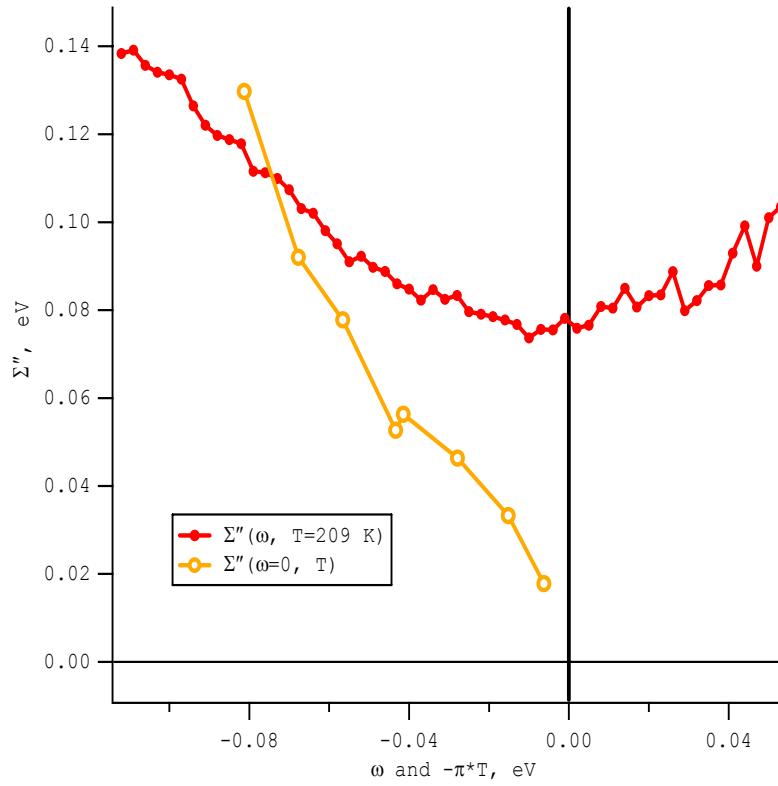
$$\Sigma''(\omega, T) = S(\omega) + S(\pi T) \longrightarrow$$

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

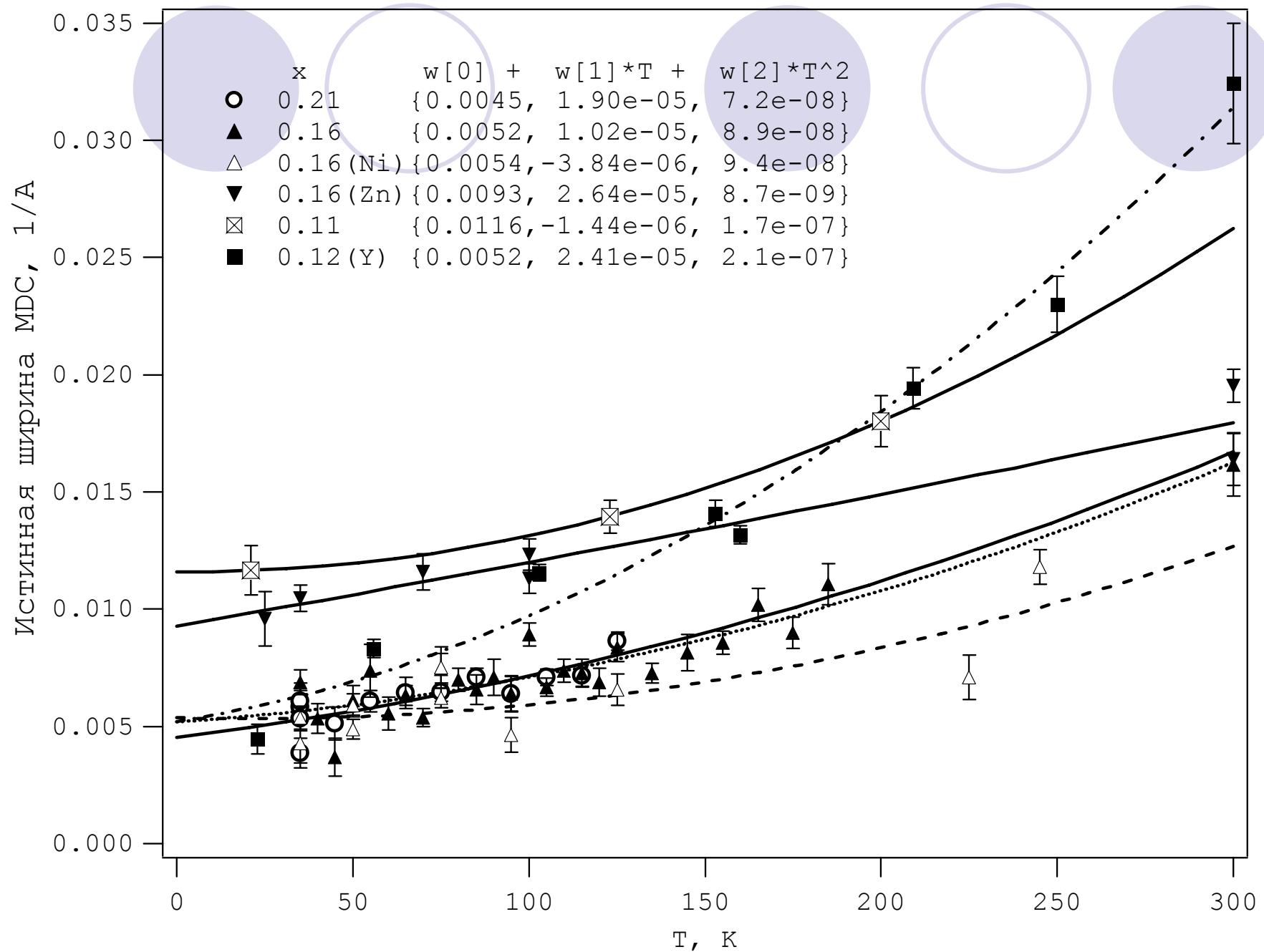
$$\Sigma''(\omega, T = \text{const}) = S(\omega) + \text{const}$$



OP (KEI)



Y-doped (YDLY)



Energy resolution in Foigt fit

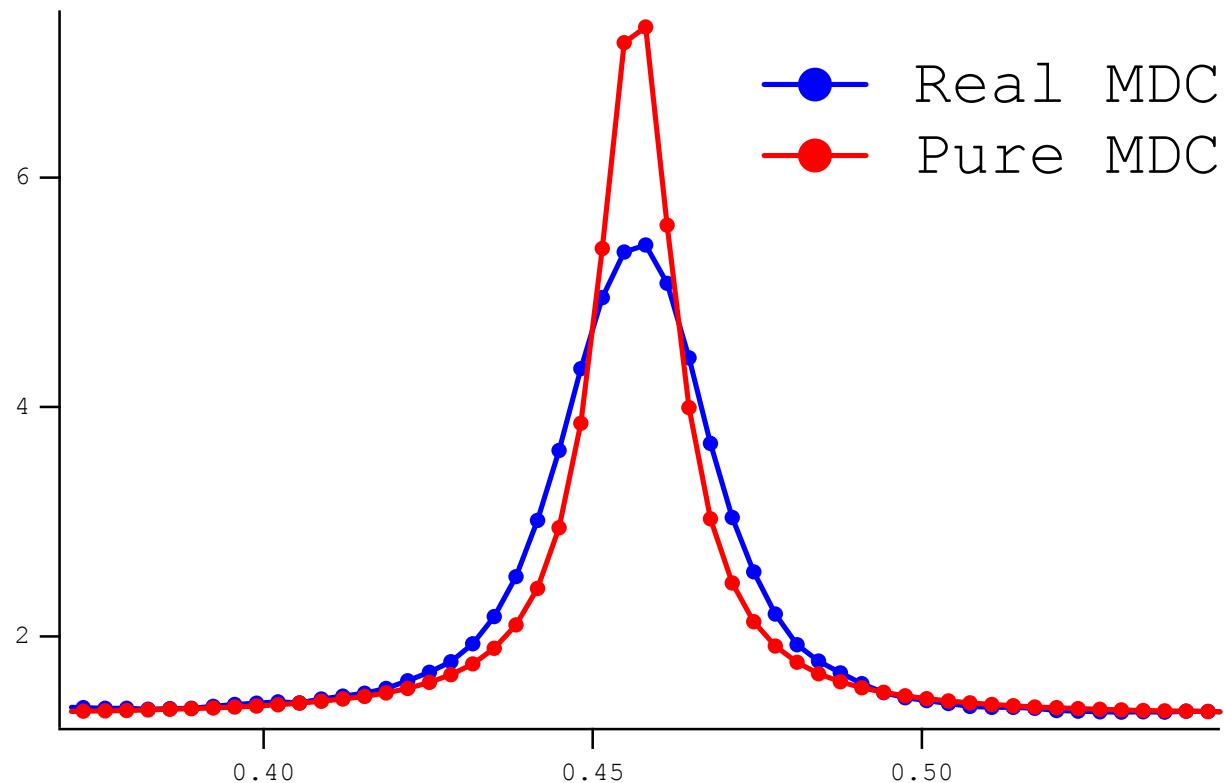
$$I(k, \omega) \propto A(k, \omega) \otimes R(k, \omega)$$

$$R(k, \omega) = R_k \otimes R_\omega$$

Energy resolution has almost the same effect on the MDC shape as momentum resolution, so both R_ω and R_k are taken into account by Voigt-fit procedure.

Pure MDC – Lorentzian

Real MDC = pure MDC \otimes Resolution - Voigt



Scattering mechanisms



Inelastic e - e scattering :

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

$$\Sigma''_{in}(\omega) \sim \omega^2, T > T_C$$

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

Scattering on impurities :

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

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

