Direct extraction of the Eliashberg function from high-resolution angle-resolved photoemission

Junren Shi

Condensed Matter Sciences Division
Oak Ridge National Laboratory

Collaborators

University of Tennessee / ORNL:

E. W. Plummer and Zhenyu Zhang: Junren Shi (myself), S. J. Tang, Biao Wu

Stanford University / LBNL:

Z. X. Shen and collaborators: X. J. Zhou, W. L. Yang, V. Brouet, T. Yoshida, T. Cuk

Louisiana State University:

P. T. Sprunger

Outline

- Introduction
- Procedure: A case study of Be(1010)
- Application to other systems:
  - Be(0001)
  - High Tc cuprate: LSCO
- Summary

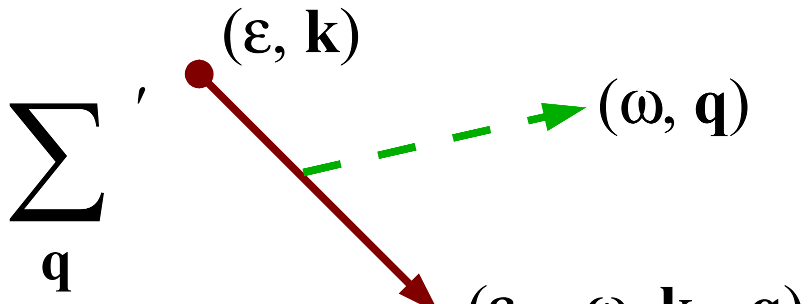
What is the Eliashberg function?

Eliashberg function characterizes the strength and spectrum of the electron-phonon (boson) coupling:

$$\alpha^2 F(\omega) = \alpha^2(\omega) \times F(\omega)$$

coupling strength phonon density of states

<u>More precise definition</u>: total transition probability from/to the electron state (ε, **k**) by coupling to the phonon modes with frequency ω.



$$\alpha^2 F(\omega) \rightarrow \alpha^2 F(\omega; \epsilon, \mathbf{k})$$

Application I: Strong coupling superconductivity

Theory of the strong coupling superconductivity:

$$T_c = \omega_{\log} \exp\left\{ -1.04 \frac{(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right\}$$

$$\lambda = 2 \int_0^\infty \frac{d\omega}{\omega} \alpha^2 F(\omega) \quad \longleftarrow$$

Mass enhancement factor

$$m^* = (1+\lambda) m$$

$$\omega_{\log} = \exp\left\{ \frac{2}{\lambda} \int_0^\infty \frac{d\omega}{\omega} \alpha^2 F(\omega) \ln \omega \right\}$$

Application II: Band distortion due to the electron-phonon coupling

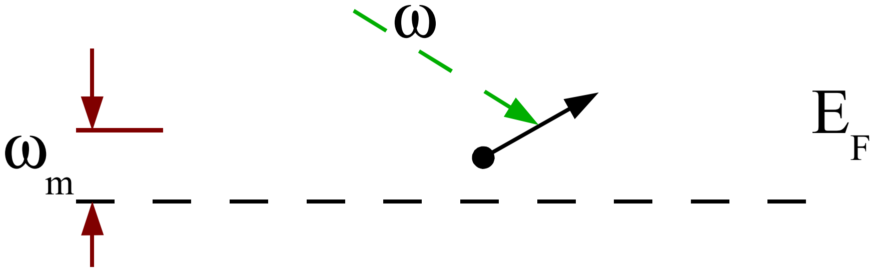
$$\epsilon(\mathbf{k})=\epsilon_0(\mathbf{k})+\mathrm{Re}\,\Sigma(\epsilon,\mathbf{k})$$

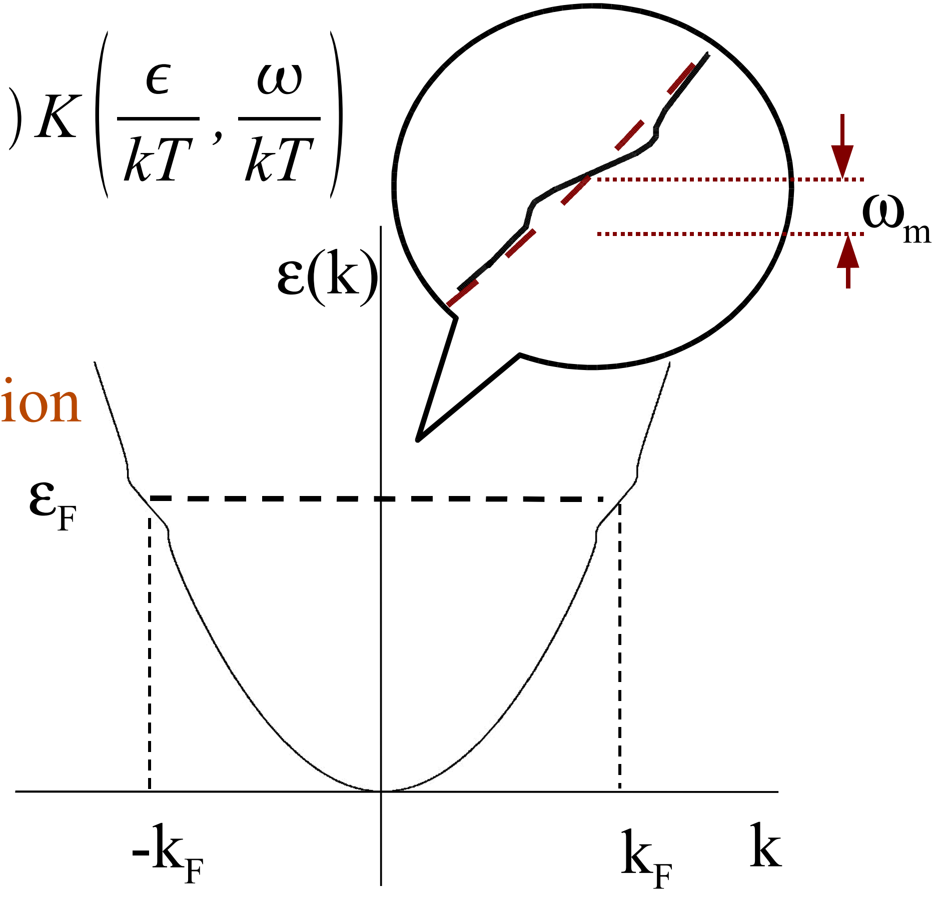
$$\mathrm{Re}\,\Sigma(\epsilon,\hat{\mathbf{k}};T)=\int_0^\infty d\omega\,\alpha^2F(\omega;\epsilon_F,\hat{\mathbf{k}})\,K\left(\frac{\epsilon}{kT},\frac{\omega}{kT}\right)$$

$$K(y,y')=\int_{-\infty}^{\infty}\frac{2y'}{x^2-y'^2}f(x+y)$$

Fermi function

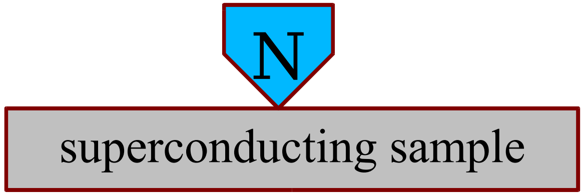
$$m^*=(1+\lambda)m$$

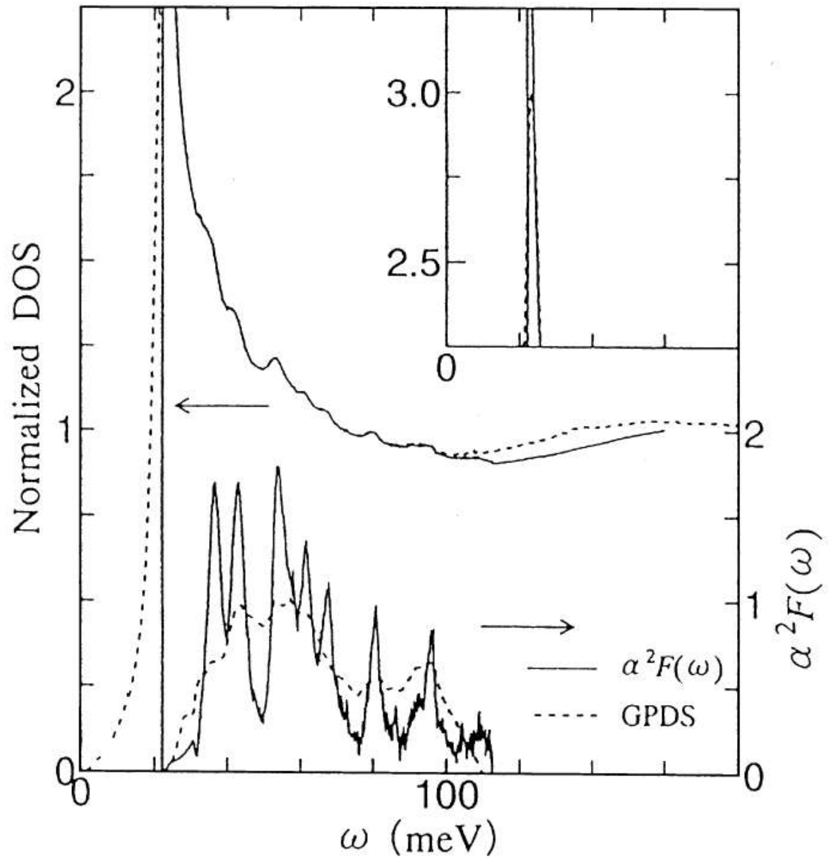




Traditional technique

McMillan-Rowell inversion on the tunneling characteristics





Limitations:

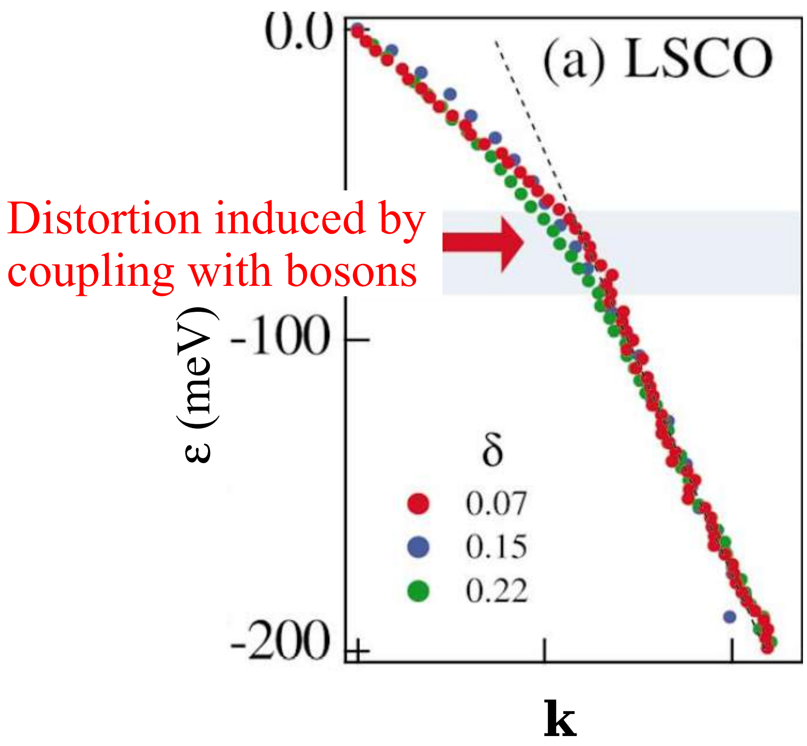
- Destructive technique – creation of a tunneling junction required
- Applicability
- No momentum resolution

For High Tc cuprates:

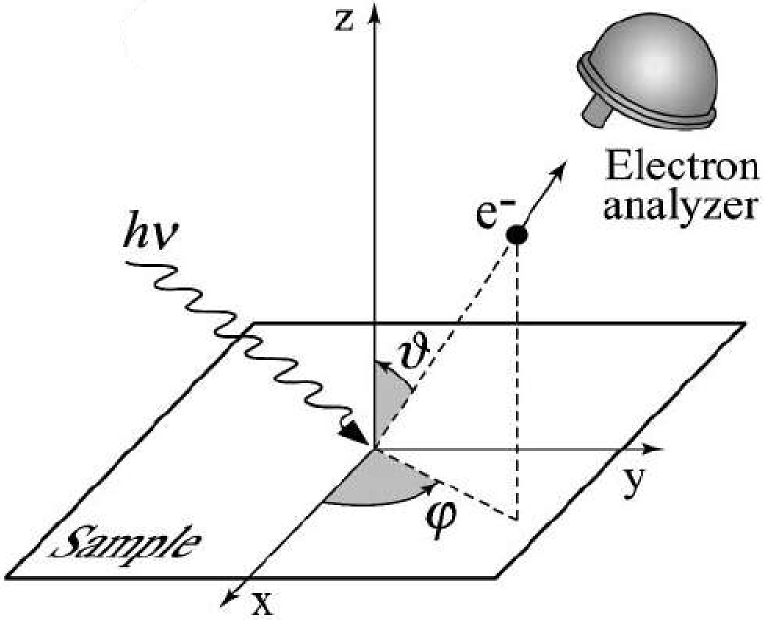
- Layered structure – non-negligible interface effect
- Short coherence length -- difficult to make a junction
- Anisotropy – requires momentum resolution
- No generally accepted mechanism for the superconductivity

Angle-resolved photoemission

The angle-resolved photoemission can directly map out the quasi-particle dispersion of a two-dimensional system.



Distortion induced by coupling with bosons



$$E_{kin} = h\nu - \phi - |E_B|,$$

$$\mathbf{p}_{\|} = \hbar \mathbf{k}_{\|} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$

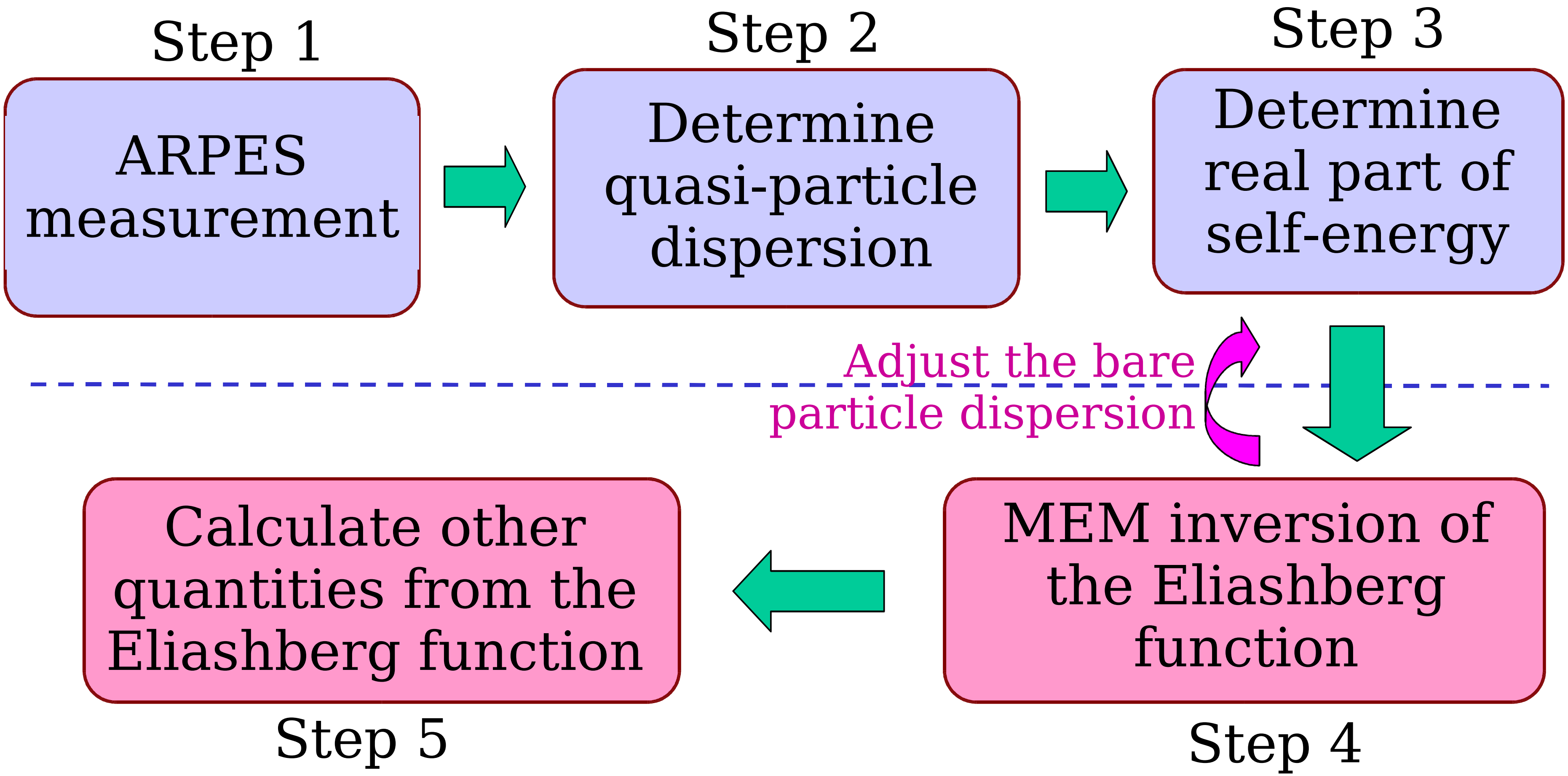
Damascelli *et al.*, RMP **75**, 473 (2003)

The detailed structure of the distortion should reveal more in-depth information – Eliashberg function!

Benefits

- Non-destructive technique – sample is probed as is
- Momentum resolution – anisotropy could be directly probed
- Wide applicability – samples are not required to be superconducting; it doesn't rely on a specific mechanism of the superconductivity...

Our Procedure: Outline



Step 1

ARPES measurement

Step 2

Determine quasi-particle dispersion

Step 3

Determine real part of self-energy

Adjust the bare particle dispersion

MEM inversion of the Eliashberg function

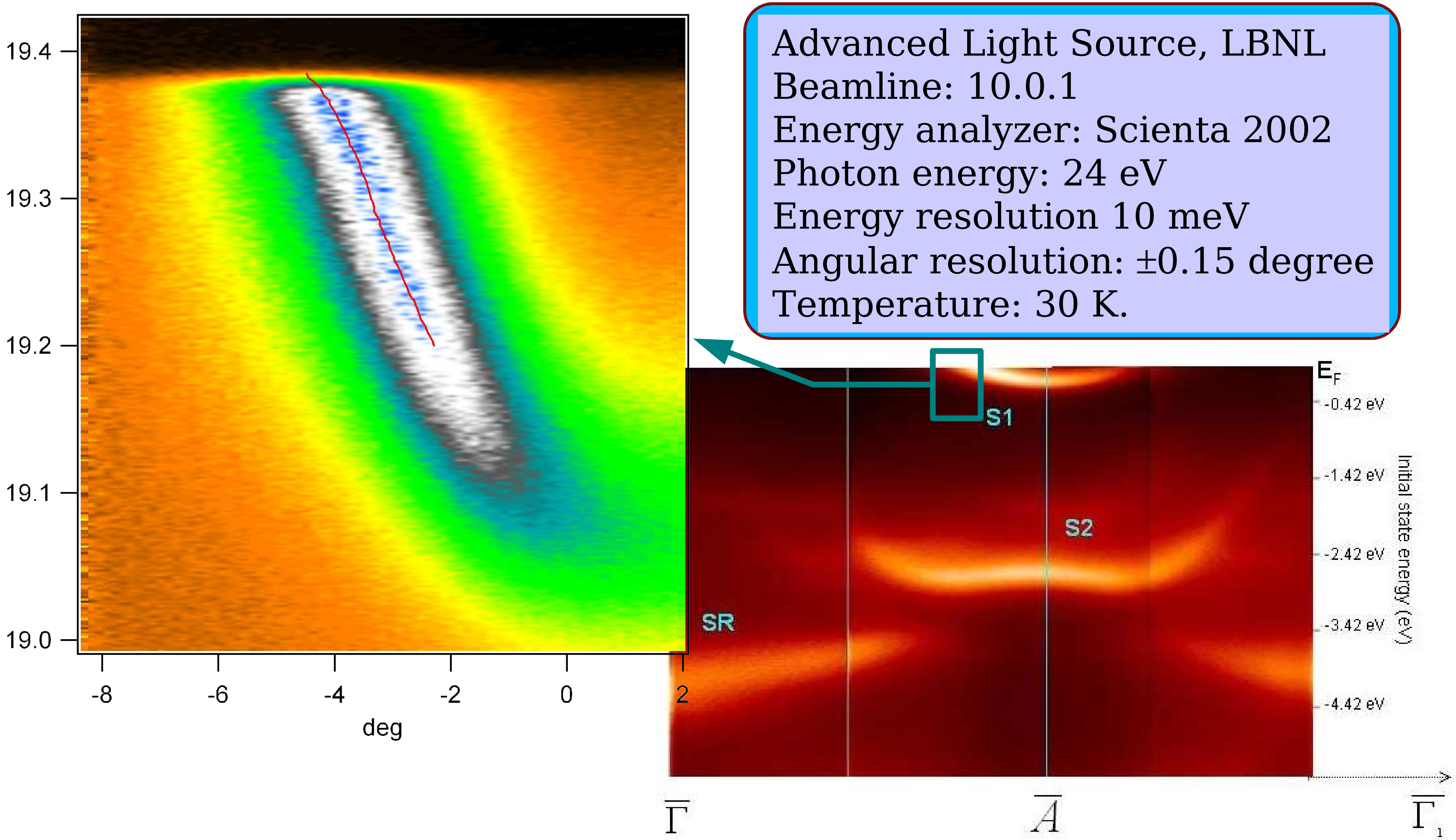
Step 4

Calculate other quantities from the Eliashberg function

Step 5

Test Case: Be(1010)

Step 1: ARPES measurement

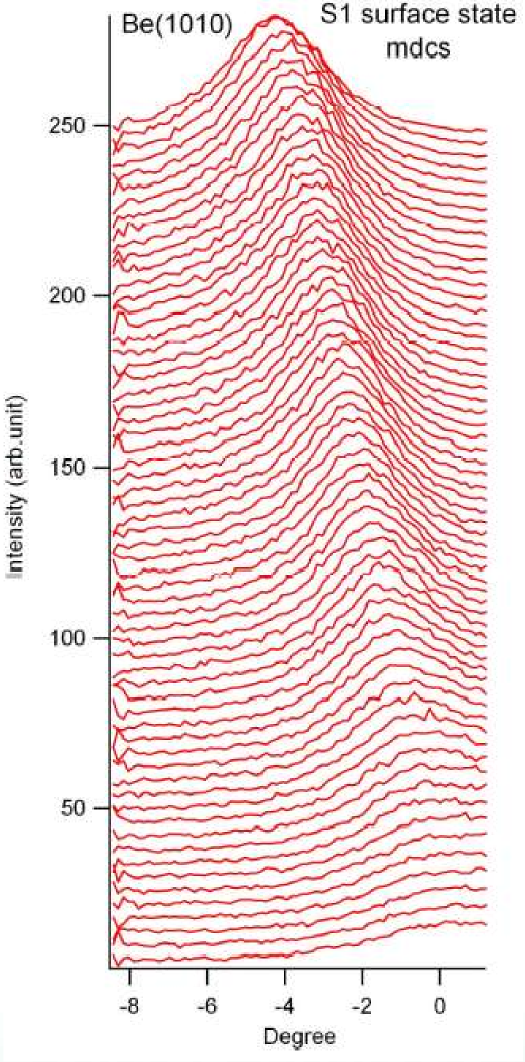


Advanced Light Source, LBNL
Beamline: 10.0.1
Energy analyzer: Scienta 2002
Photon energy: 24 eV
Energy resolution 10 meV
Angular resolution: ±0.15 degree
Temperature: 30 K.

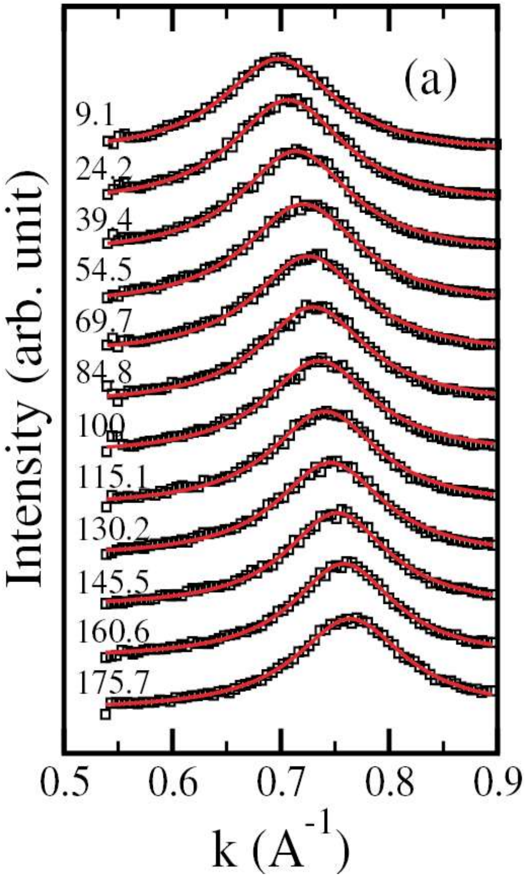
Photoemission image for Be(1010)

Step 2: Determine Quasi-Particle Dispersion

Momentum dist. curves

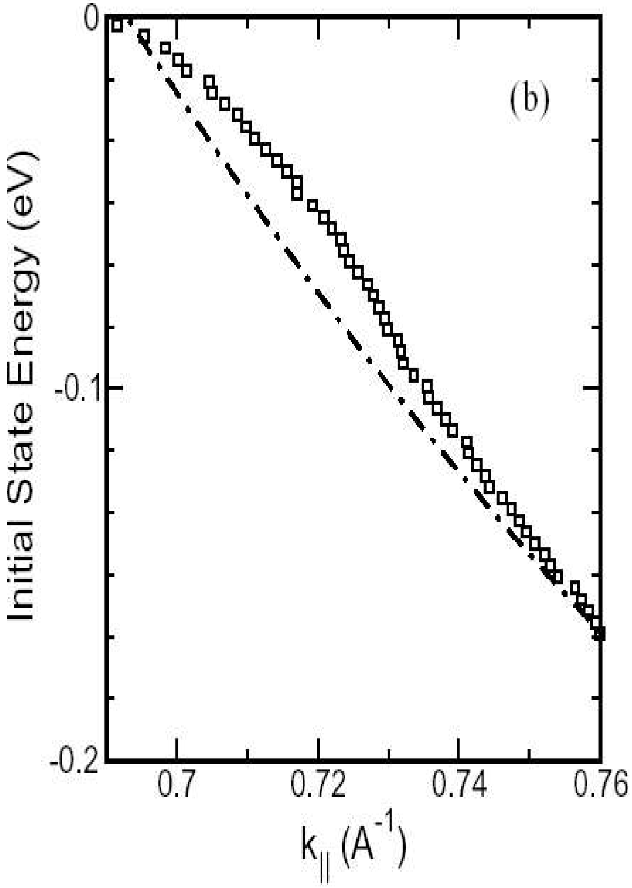


Lorentzian fitting

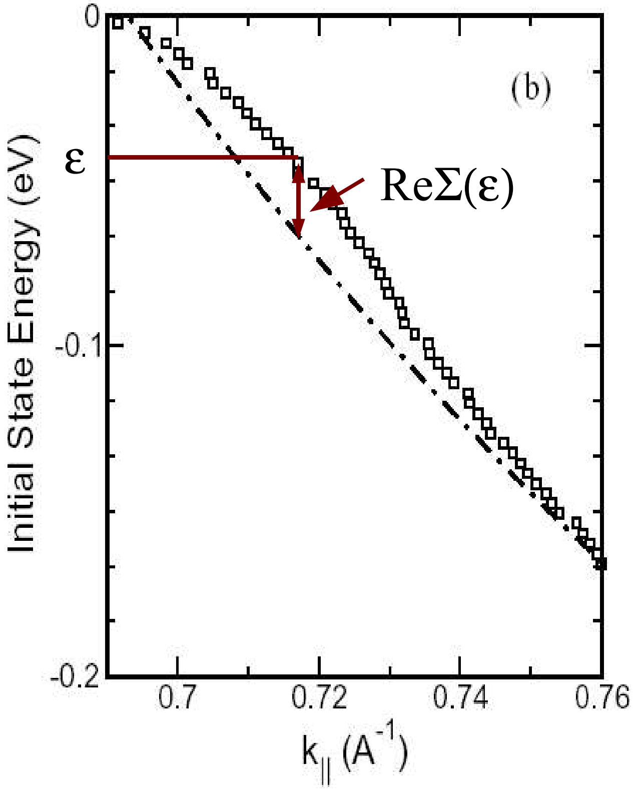


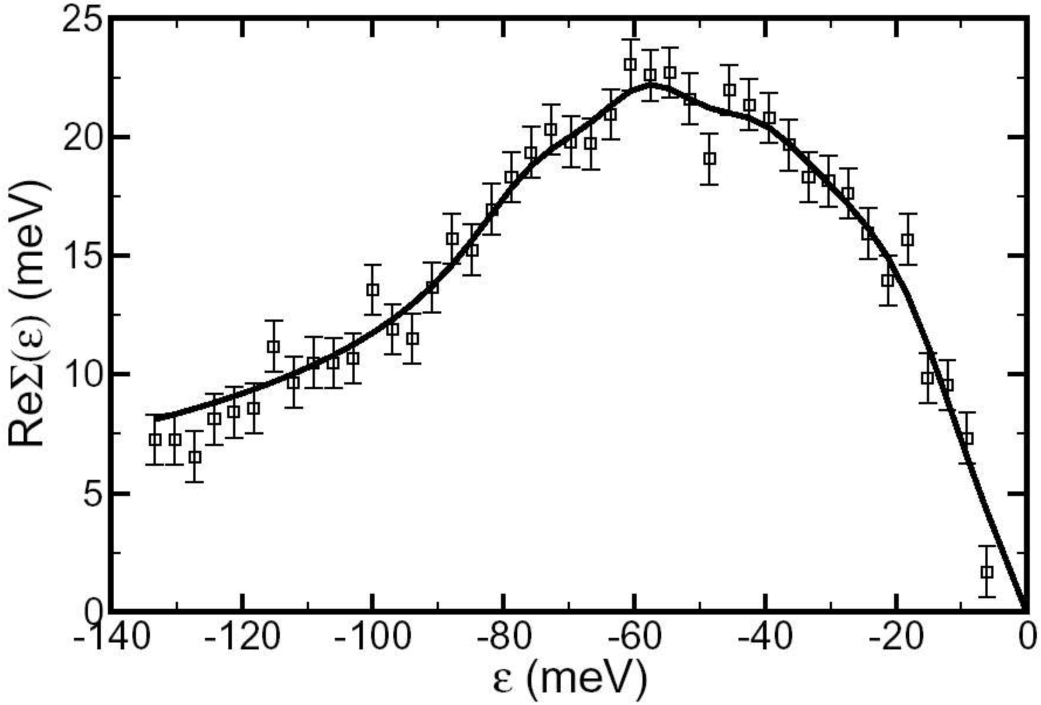
$$I \propto \frac{\Gamma}{[k - k(\epsilon)]^2 + \Gamma^2}$$

Dispersion



Step 3: Determine real part of self-energy





$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k}) + \mathrm{Re}\,\Sigma(\epsilon, \mathbf{k})$$

$$\epsilon_0(\mathbf{k}) = -\upsilon_F^0 (k - k_F) + \beta (k - k_F)^2$$

Unfold the Eliashberg function: Theory

$$\mathrm{Re}\,\Sigma(\epsilon,\hat{\mathbf{k}};T)=\int_0^\infty d\omega\,\alpha^2F(\omega;\epsilon_F,\hat{\mathbf{k}})\,K\left(\frac{\epsilon}{kT},\frac{\omega}{kT}\right)$$

$$K(y,y')=\int_{-\infty}^{\infty}\frac{2y'}{x^2-y'^2}f(x+y)$$

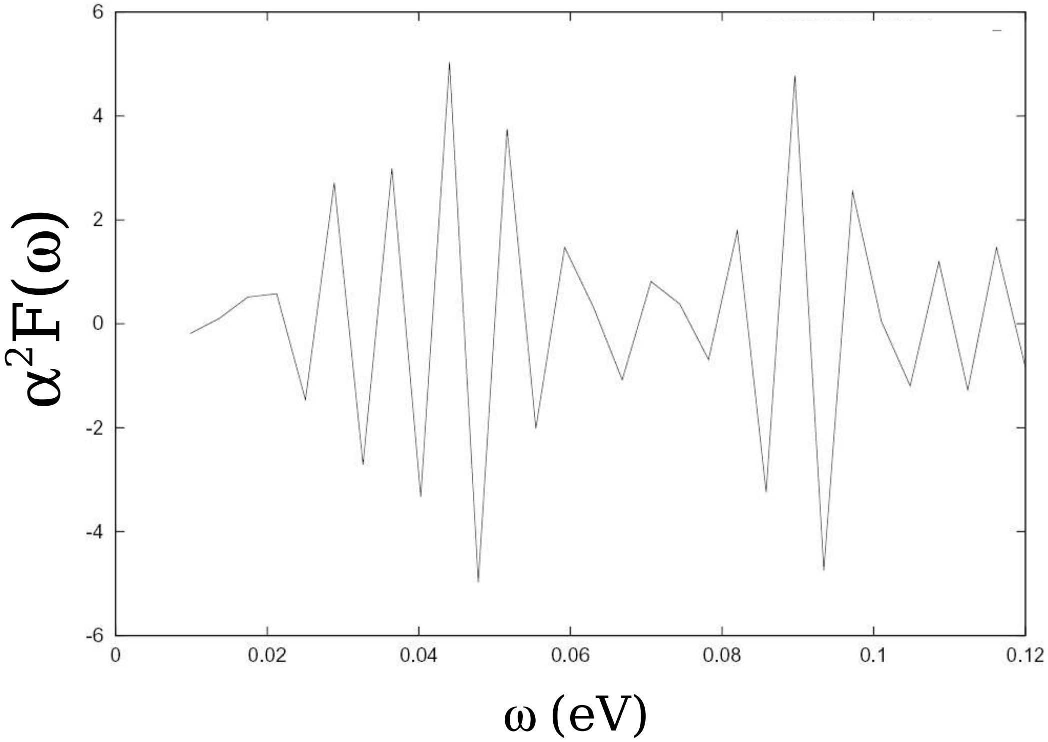
Fermi function

- The relation is valid for systems with quasi-electrons coupling with bosons (phonon) – <u>the details of electron structure are irrelvant</u>.
- Electron structure should not have abrupt change near the fermi surface within the energy scale of the phonon bandwidth.
- It is an integral inversion problem to unfold the Eliashberg function from the data of the real part of self energy:

$$\mathrm{Re}\,\hat{\Sigma}=\hat{K}[\alpha^2F] \Rightarrow [\alpha^2F]=\hat{K}^{-1}\mathrm{Re}\,\hat{\Sigma}$$

the least square approach, minimizes $\chi^2=\sum_i\frac{\left|\mathrm{Re}\,\hat{\Sigma}-\hat{K}[\alpha^2F]\right|_i^2}{\sigma_i^2}$

Difficulty of the direct inversion



Reasons:

- The inversion problem is mathematically unstable
- We do not incorporate the necessary constraint into the inversion – the Eliashberg function must be positive!

Maximum Entropy Method

$$\chi^2 \Rightarrow L = \frac{\chi^2}{2} - a\,S$$

Entropy: $$S = \int_0^\infty d\omega \left[\alpha^2 F(\omega) - m(\omega) - \alpha^2 F(\omega) \ln \frac{\alpha^2 F(\omega)}{m(\omega)} \right]$$

- constraints are imposed by the entropy term
- specific constraints are encoded in the default model: $m(\omega)$ – the entropy term is maximized when $\alpha^2 F(\omega) = m(\omega)$
- a balances between the data and the constraints – the optimal value of a can be determined by using the “classic method”

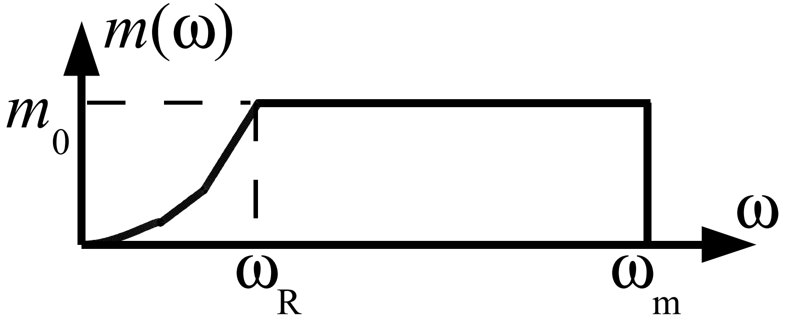
Reference: M. Jarrell *et al.*, Phys. Rep. **269**, 133 (1996)

Default model

Choosing a default model:

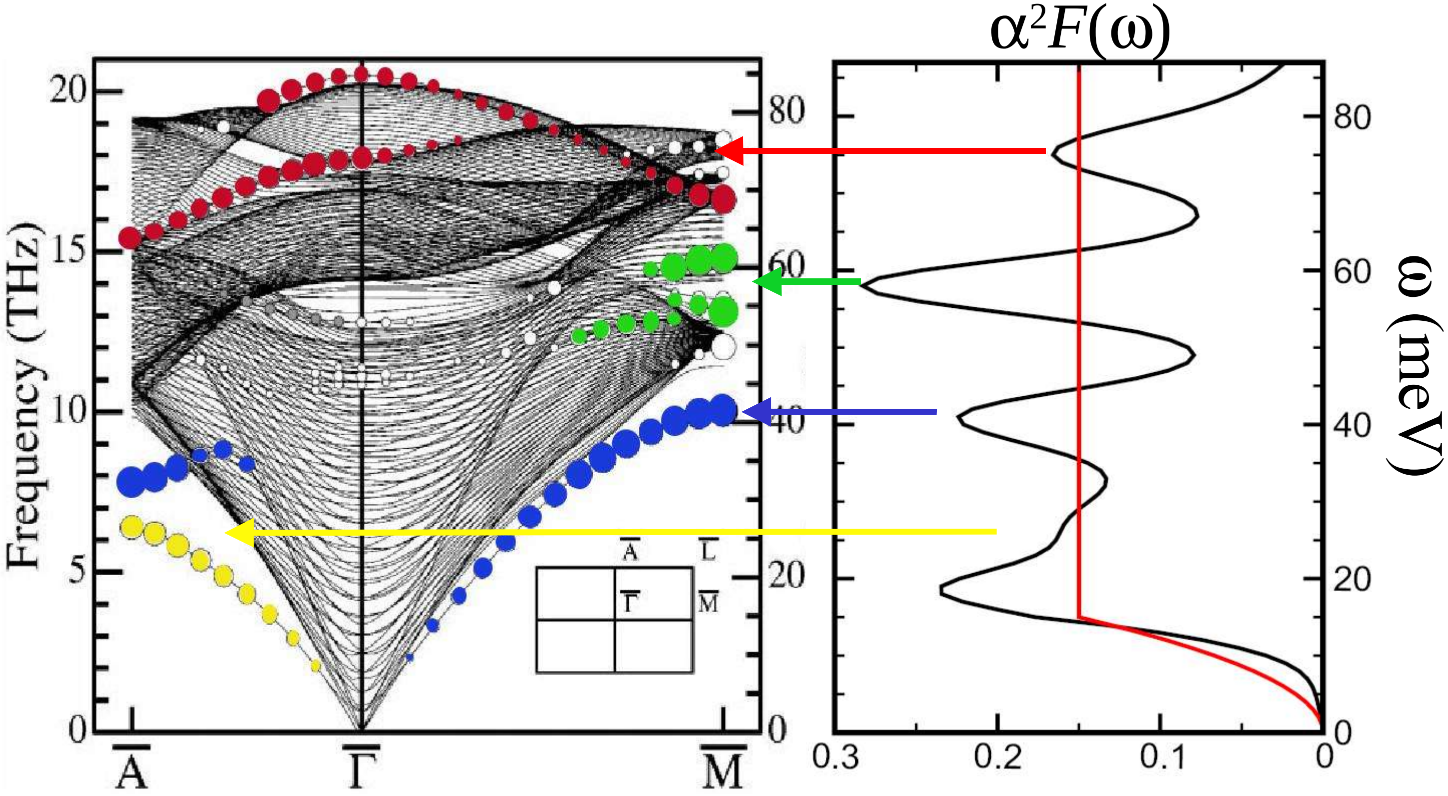
- Include known knowledge as much as possible
- If nothing is known, just use a constant to keep the fitting unbiased

$$m(\omega) = \begin{cases} m_0 \, (\omega/\omega_R)^2 \, , & \omega \leq \omega_R \\ m_0 \, , & \omega_R < \omega \leq \omega_m \\ 0 \, , & \omega > \omega_m \end{cases}$$



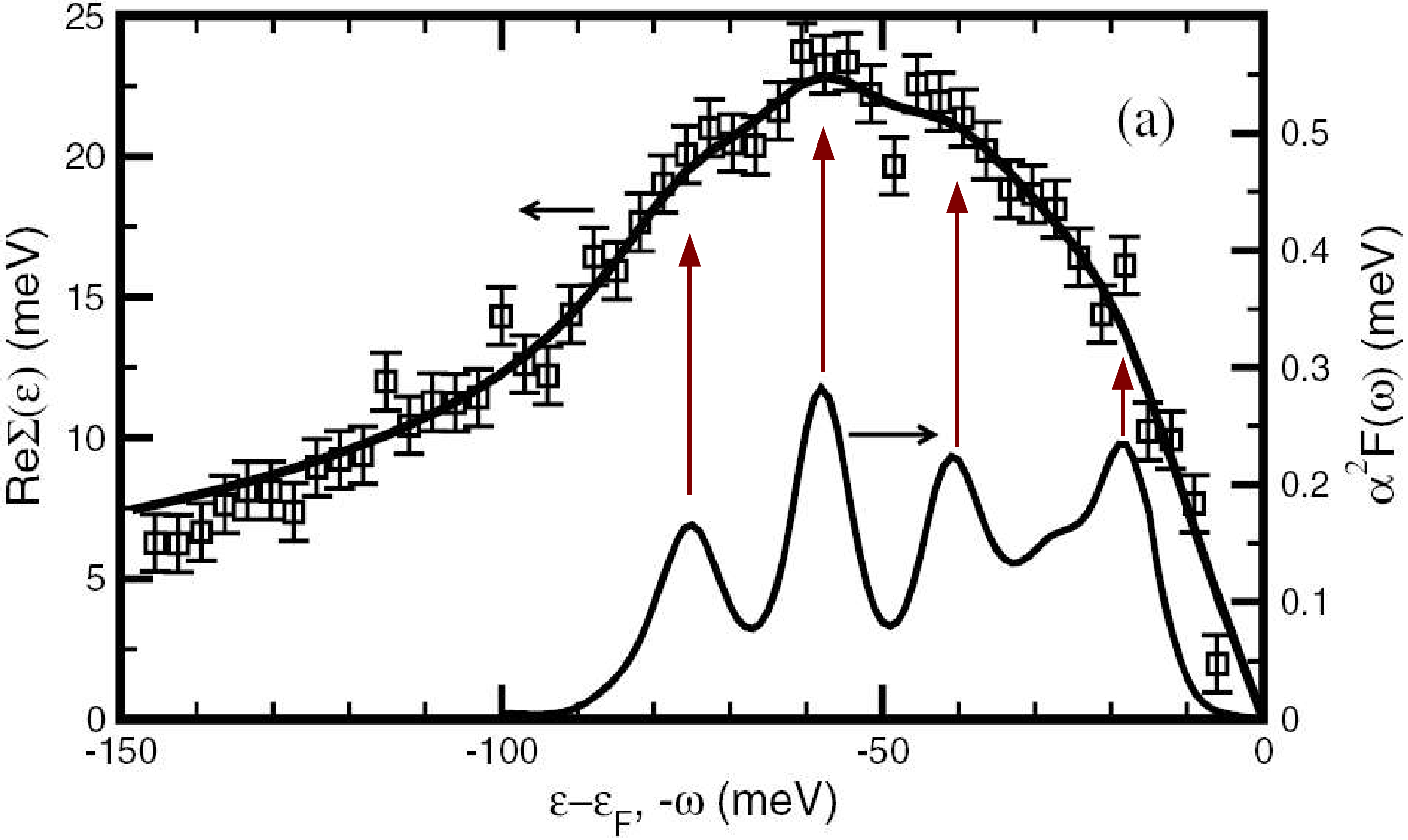
- The Eliashberg function is positive;
- The Eliashberg function vanishes at the limit $\omega \rightarrow 0$;
- The Eliashberg function vanishes above the maximal phonon frequency.

Step 4: Eliashberg function of Be(1010)



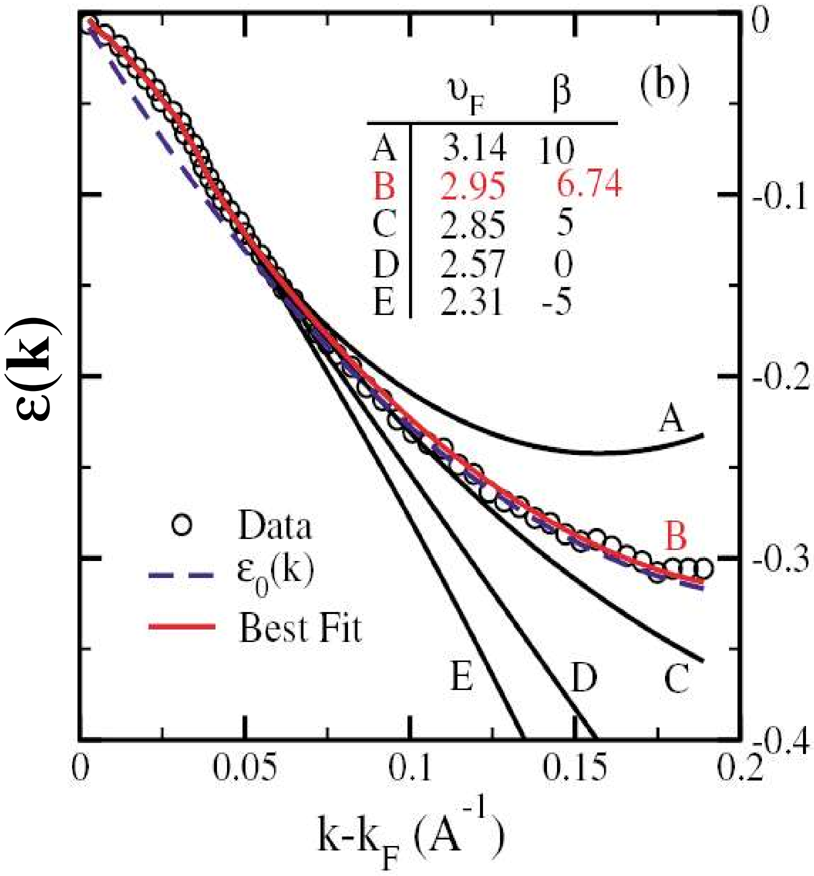
First principles calculation: M. Lazzeri and S. de Gironcoli, Surf. Sci. **454 - 456**, 442 (2000)

Data fitting

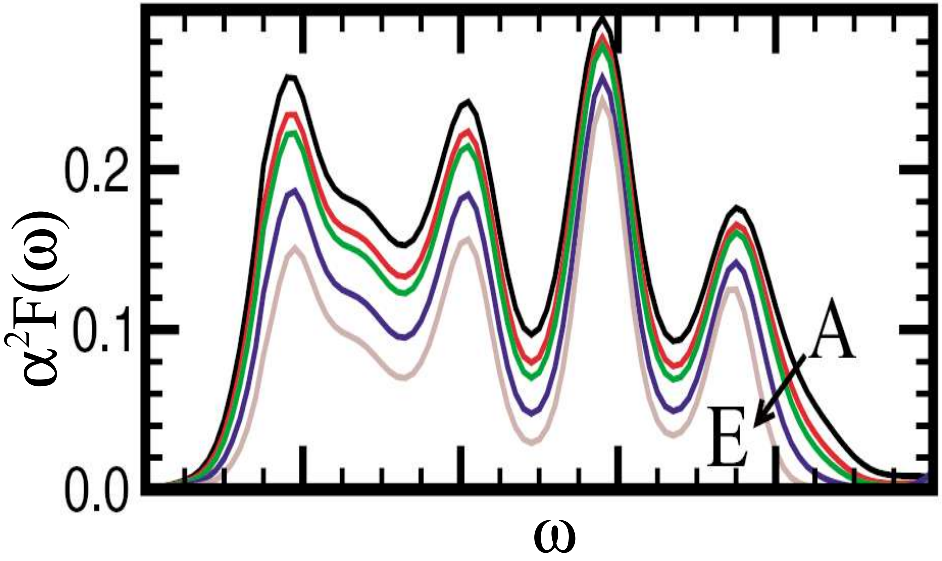


Determine the bare particle dispersion

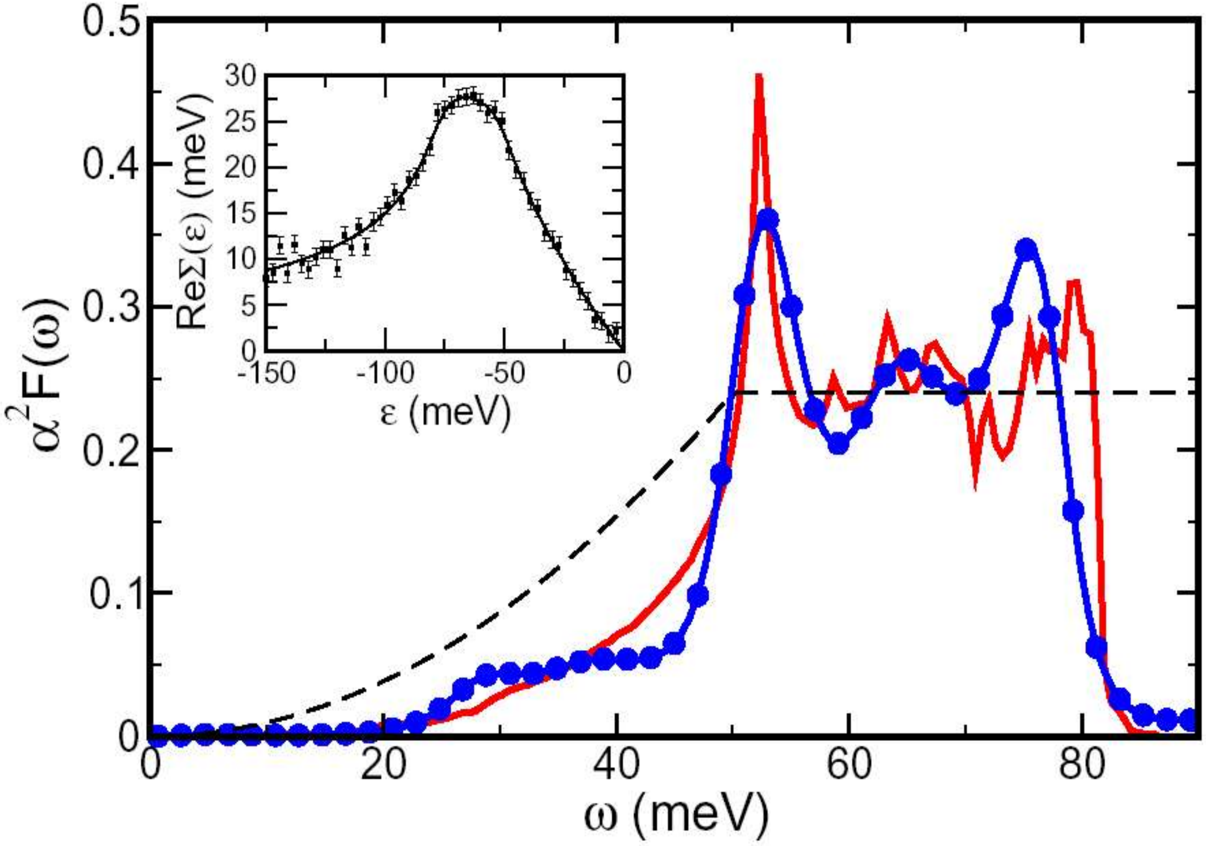
$$\epsilon_0(\mathbf{k}) = -\upsilon_F^0(k-k_F)+\beta(k-k_F)^2$$



	υ_F	β
A	3.14	10
B	2.95	6.74
C	2.85	5
D	2.57	0
E	2.31	-5

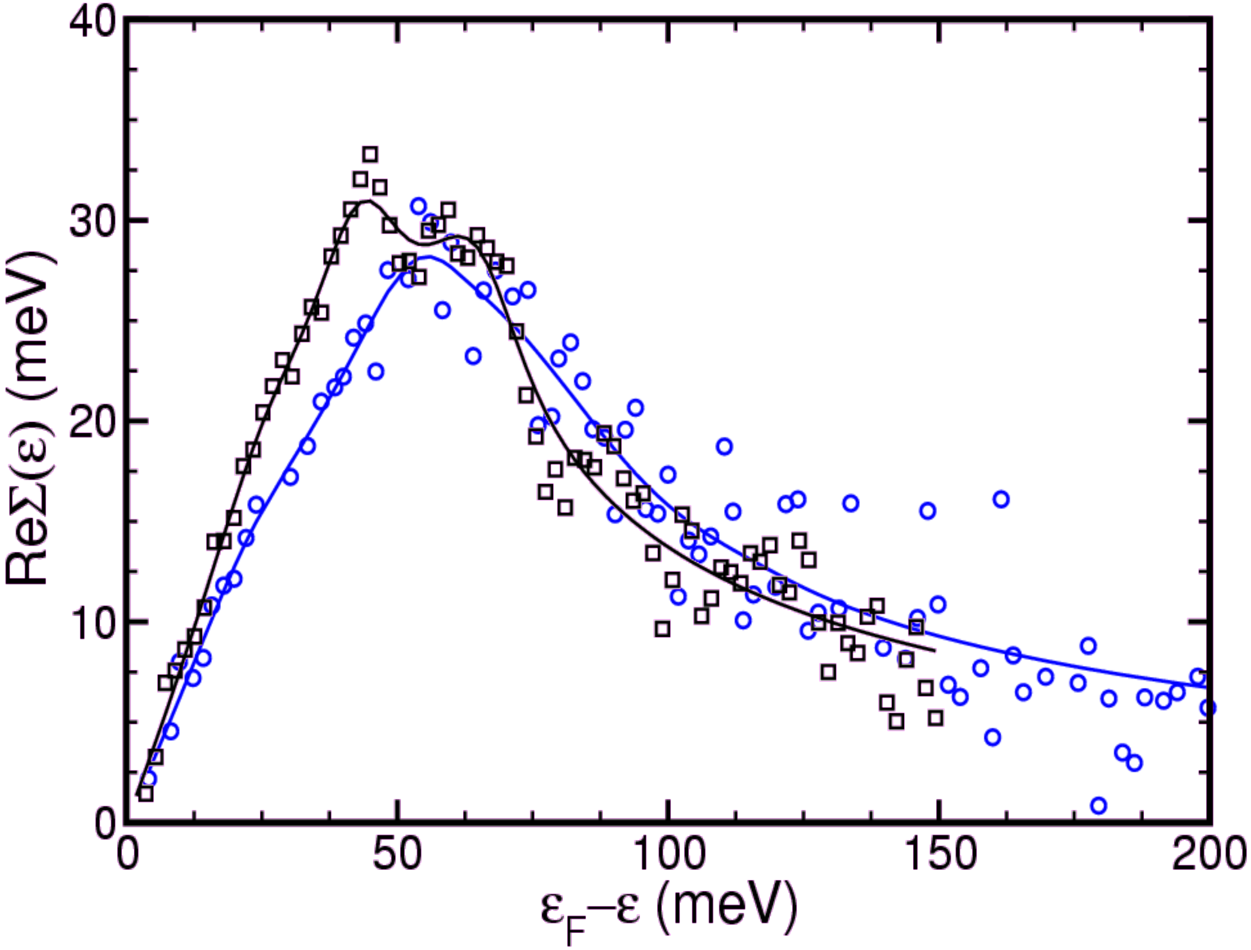


A test to the MEM



Predefined Eliashberg function ⇒ Real part of self energy ⇒ Add noise ⇒ MEM extraction

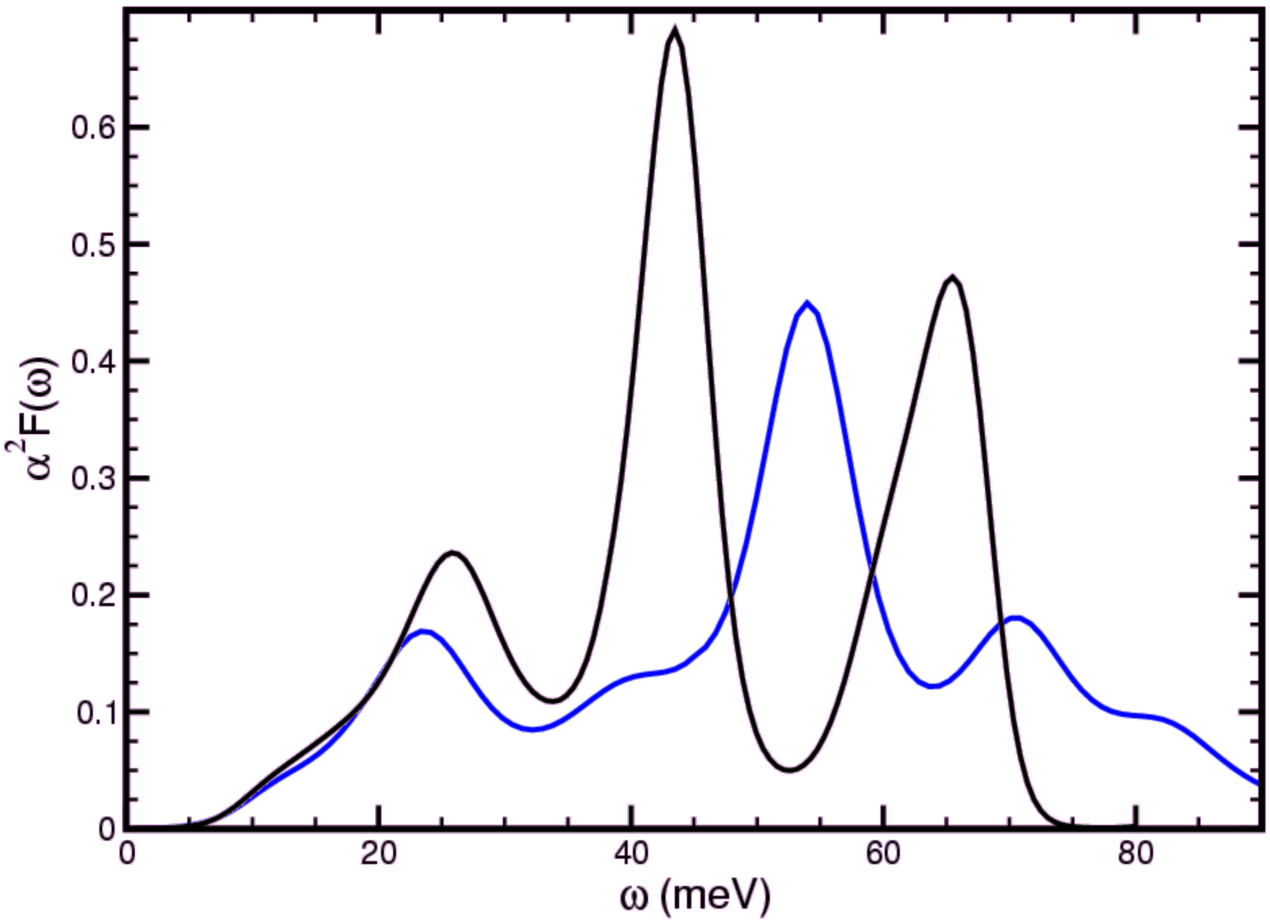
Application I: Be(0001)



LaShell *et al.* Phys. Rev. B **61**, 2371 (2000)

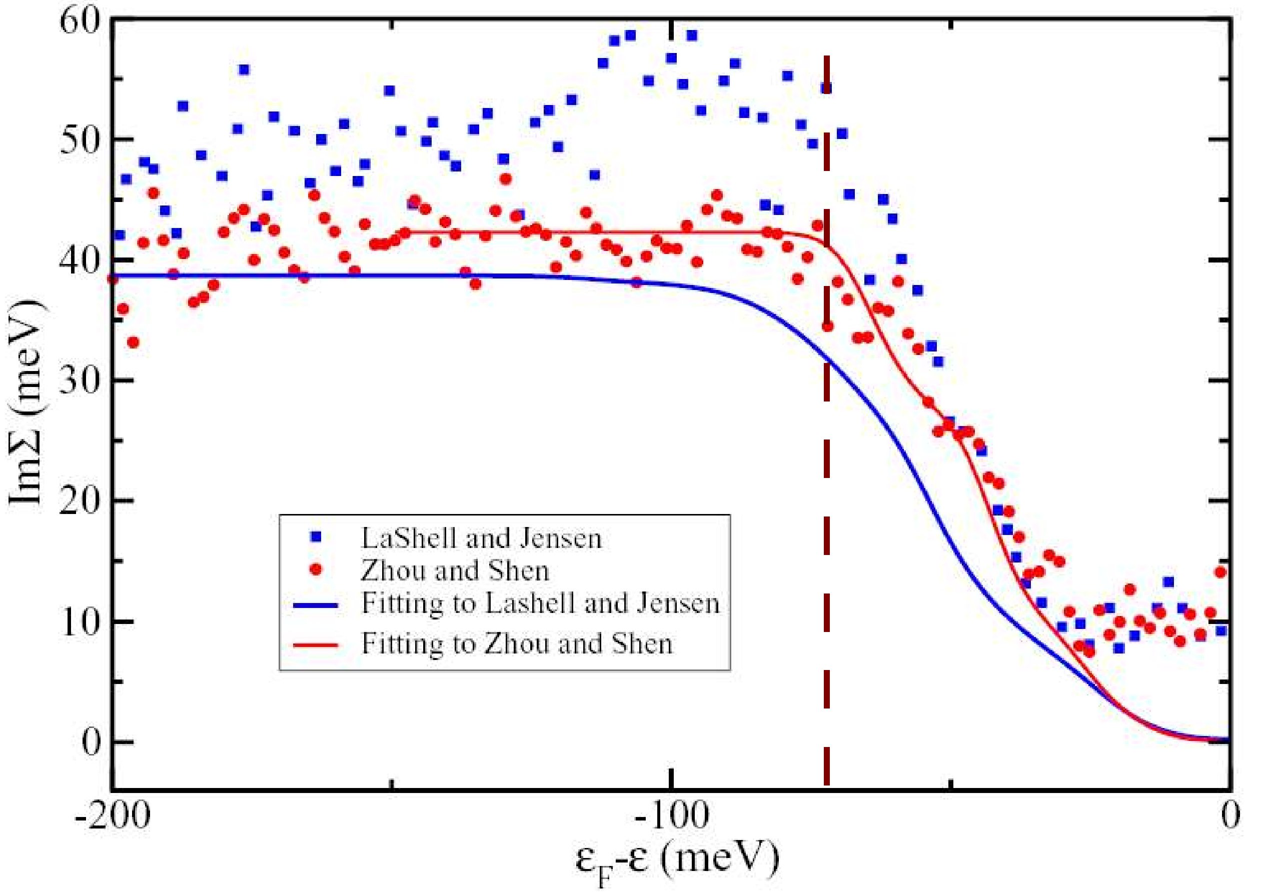
Z.X. Shen's group

Discrepancy



Reliable extraction of the Eliashberg function requires high data quality!

Imaginary part of self energy



Application II: High Tc cuprates

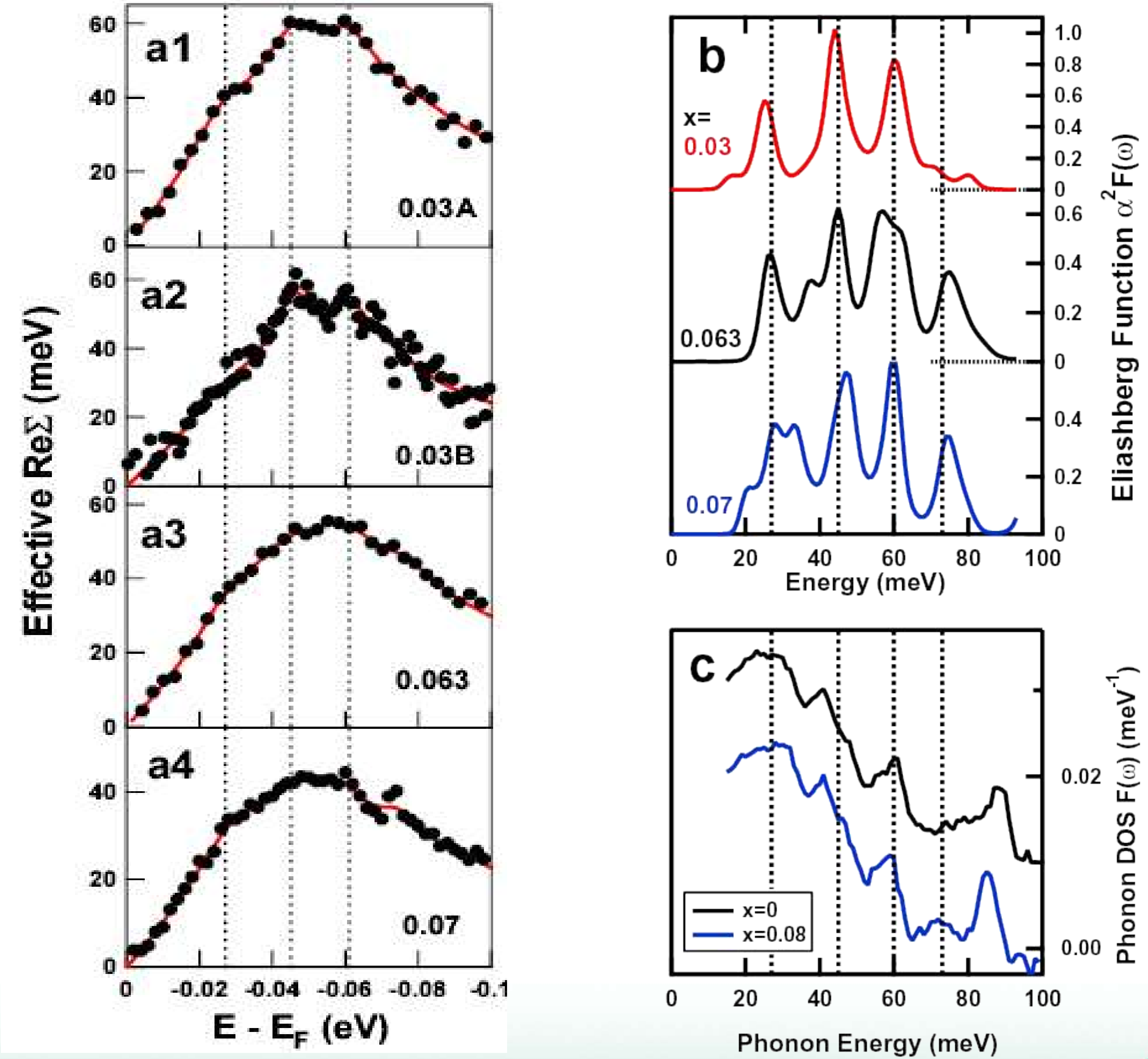
Difficulties:

- The applicability of the Fermi liquid theory is questionable in these strongly correlated systems
- Existence of the pseudo-gap complicates the matter

Our approach:

- An empirical approach: we just fit the data in the standard way and see what happens.
- Pay extreme attention to the data consistency.
- The resulting Eliashberg function may be renormalized in some ways that require further theoretical interpretation .

LSCO ($La_{2-x}Sr_xCuO_4$)



neutron data

Summary

- It is possible to extract the Eliashberg function from the photoemission data.
- Better data quality is highly desirable: better statistics, higher resolution (both energy and momentum), more rigorous data analysis procedures ...

References:

- Junren Shi, S.-J Tang, Biao Wu, P.T. Sprunger, W.L. Yang, V. Brouet, X.J. Zhou, Z. Hussain, Z.-X. Shen, Zhenyu Zhang, E.W. Plummer, Phys. Rev. Lett. **92**, 186401 (2004).
- X. J. Zhou, Junren Shi, T. Yoshida, T. Cuk, W.L. Yang, V. Brouet, J. Nakamura, N. Mannella, S. Komiya, Y. Ando, F. Zhou, W. X. Ti, J. W. Xiong, Z. X. Zhao, T. Sasagawa, T. Kakeshita, H. Eisaki, S. Uchida, A. Fujimori, Zhenyu Zhang, E. W. Plummer, R. B. Laughlin, Z. Hussain, and Z.-X. Shen, preprint, cond-mat/0405130.