



Electronic Structure of High Temperature Superconductors Revealed by VUV Laser ARPES

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Dedicated to 70th Birthday of Prof. Zhaobin SU and Prof. Lu YU

Outline

- (1). Development of VUV Laser Based ARPES;**
- (2). Electronic Structure of High-Tc Superconductors:**
 - a. Extraction of Bosonic Spectral Function;**
 - b. Identification of a new form of electron coupling;**
- (3). Summary.**

Colleagues and Collaborators

ARPES System Development:

[Chuangtian Chen](#), Yong Zhu, Guochun Zhang, Xiaoyang Wang
Technical Institute of Physics and Chemistry, CAS, China

[Zuyan Xu](#), Guiling Wang, Hongbo Zhang, Yong Zhou, IOP, CAS, China

[Z. Hussain](#), John Pepper, Wanli Yang and others, ALS, Berkeley National Lab

[Z.-X. Shen](#), Donghui Lu, Nik Ingle and others, Stanford University

ARPES Samples:

Genda GU, Brookhaven National Lab

T. Sasagawa, Tokyo Institute of Technology

F. Zhou, Z.-X. Zhao, IOP, China

ARPES Theory:

Junren Shi, Institute of Physics, CAS, China

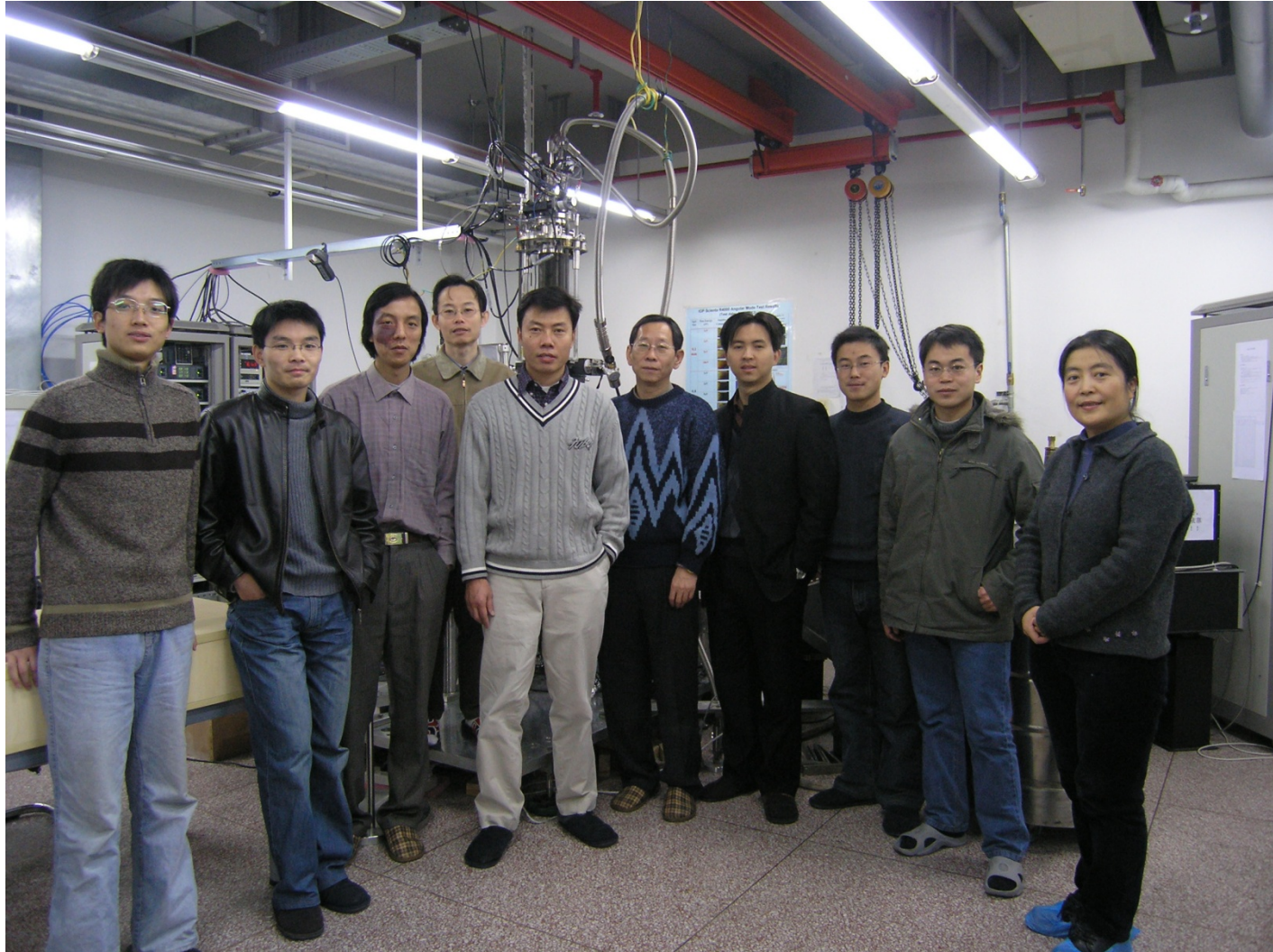
Colleagues and Collaborators: ARPES Group

Staff

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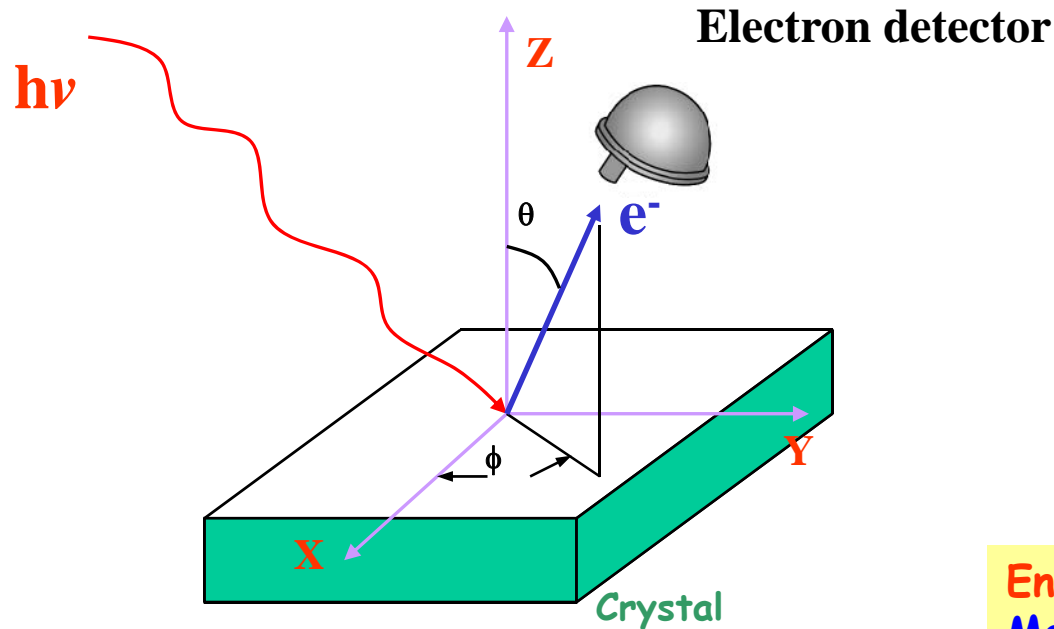
Jianqiao Meng
Lin Zhao
Haiyun Liu
Wentao Zhang
Xiaowen Jia
Daixiang Mu
Chanyu Liu



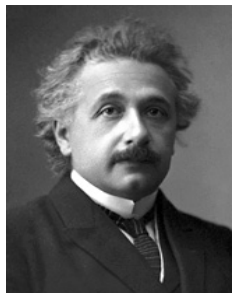
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Angle-Resolved Photoemission Spectroscopy (*ARPES*)



The Nobel Prize in Physics 1921



“For his services to Theoretical Physics, and especially for his discovery of the law of The Photoelectric Effect”

Photoemitted electrons in real space

$E_{\text{kin}}, K_{\parallel}$



Energy Conservation: $E_B = h\nu - E_{\text{kin}} - \Phi$

Momentum Conservation: $K_{\parallel} = k_{\parallel} + G_{\parallel}$

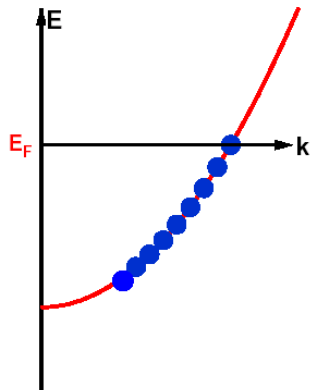


Electronic state in solid:

$\Psi(E_B, k_{\parallel})$

Power of ARPES:

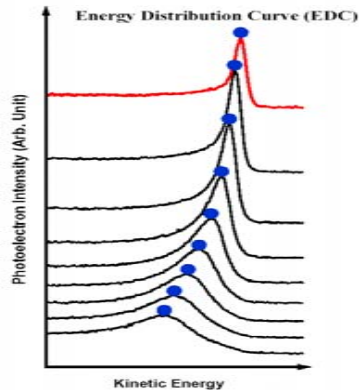
Direct Measurement of Fundamental Parameters



E-k relation

Velocity: $v = dE/dk$

Effective mass: $1/m^* \sim d^2E/dk^2$

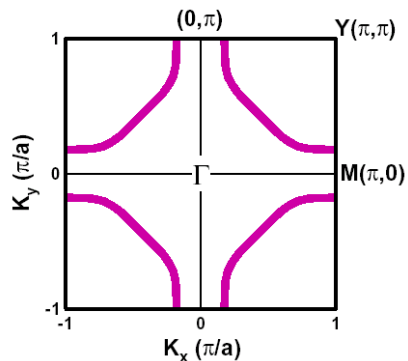


EDC lineshape

Scattering rate (τ): EDC Linewidth

Superconducting gap: EDC position

Pseudogap: EDC position



Fermi surface

Carrier density: Fermi surface volume

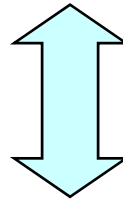
Nesting vector: Fermi Surface topology

Power of ARPES – A Probe for Many-Body Effects

Under the sudden approximation, photoemission measures
single-particle spectral function

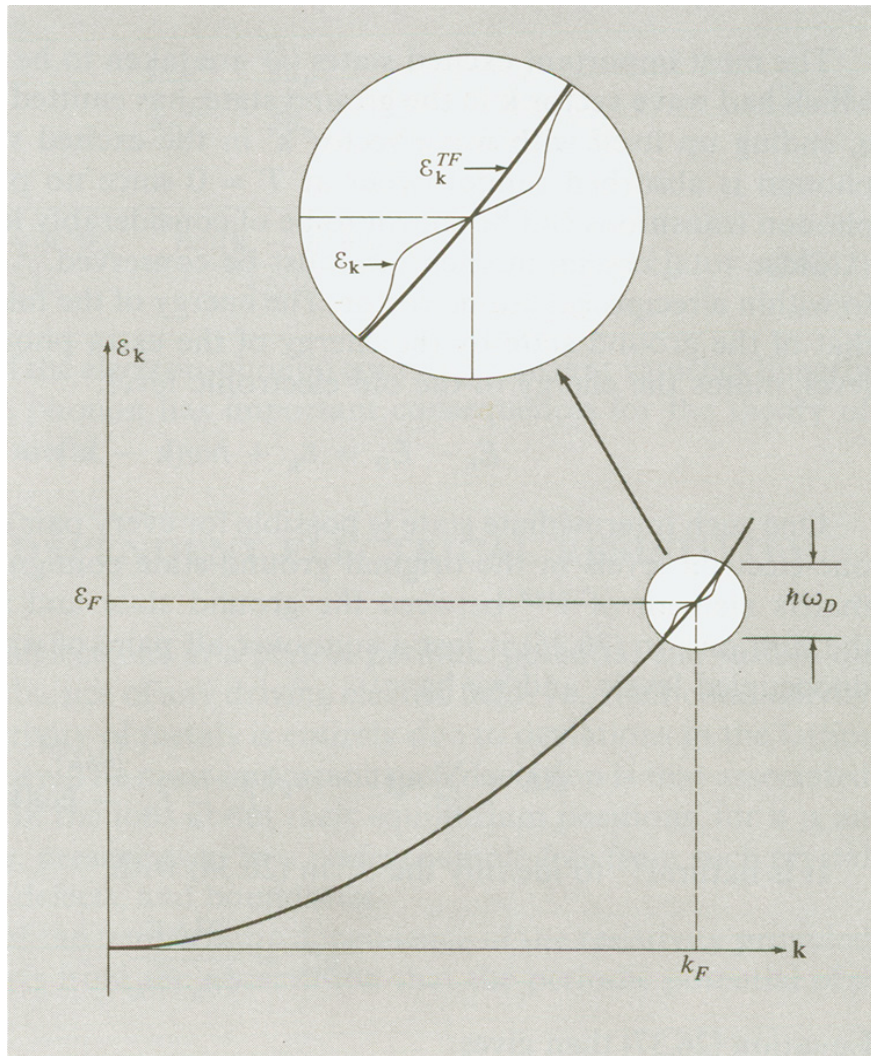
$$A(k, \omega) = \frac{1}{\pi} \frac{\text{Im} \Sigma}{[\hbar \omega - E_k^0 - \text{Re} \Sigma]^2 + [\text{Im} \Sigma]^2}$$

Electron self-energy: $\Sigma = \text{Re} \Sigma + i \text{Im} \Sigma$



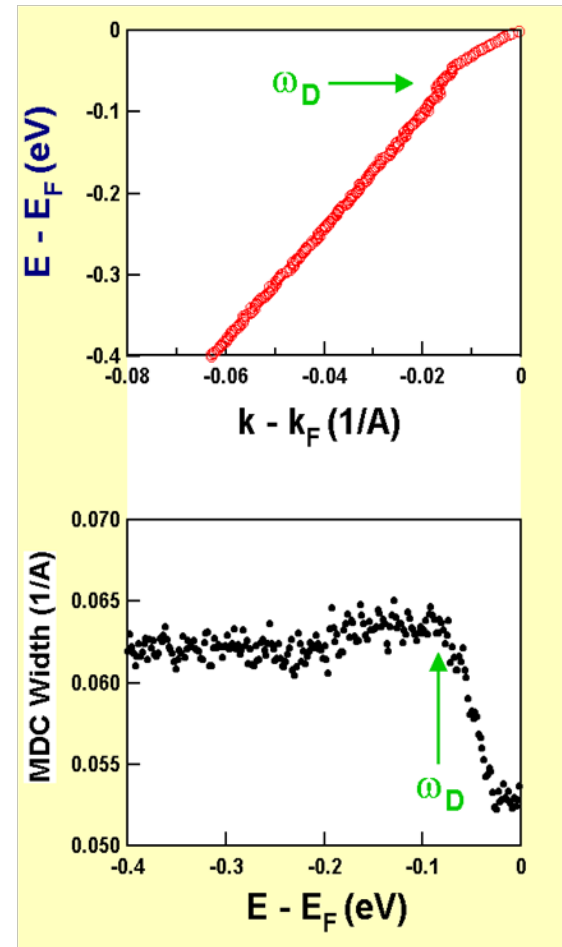
Many-Body Effects: Interaction of electrons with other entities
such as other electrons, phonons, magnons and etc.

Manifestation of Many-Body Effects: Band Renormalization



Ashcroft-Mermin, Solid State Physics

Be(0001) Surface State



Hengsberger et al., PRL 83(1999)592.

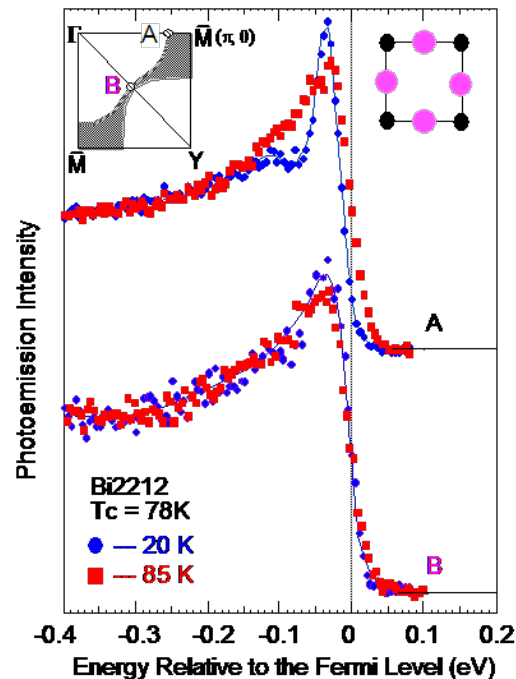
S. Lashell et al., PRB 61(2000)2371.

S. J. Tang et al., Phys. Stat. Solidi. 241(2004)2345.

ARPES on High Temperature Superconductors

d-wave S. C. gap

ARPES on Superconducting gap

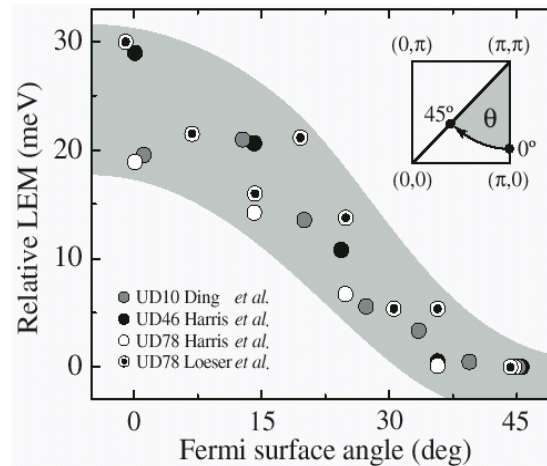


Z.-X. Shen *et al.*, *Phys. Rev.Lett.* **70**(1993)1553.

Pseudogap

ARPES on Pseudogap

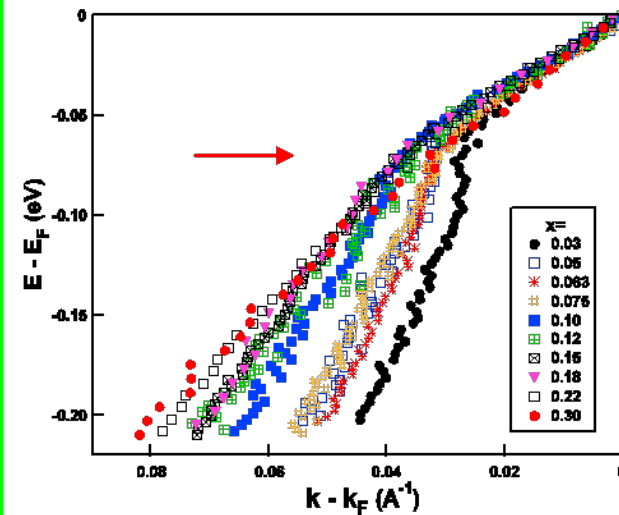
d-wave-like symmetry



Loeser *et al.*, *Science* **273**(1996)325.
Ding *et al.*, *Nature* **382**(1996) 51.

Electron-phonon coupling

ARPES on Kink



A. Lanzara *et al.*, *Nature* **412**(2001)510.
X. J. Zhou *et al.*, *Nature* **423**(2003)398.

ARPES—Prime Choice in Studying High-Tc Superconductors

2006 DOE Report

Emerging Experimental Techniques and Opportunities

- Angle-Resolved Photoemission Spectroscopy (ARPES). Wavelike quantum states of the electrons are defined in momentum space (k -space). ARPES allows direct determination of the complete momentum-space electronic structure, $A(k, E)$, with remarkable energy and momentum resolution.
- *Spectroscopic Imaging-Scanning Tunneling Microscopy (SI-STM)*. This is the complementary technique to ARPES that allows mapping of the energy-resolved quantum states in real space (r -space) with atomic resolution and yet over large sample areas.
- *Microwave/terahertz/infrared/optical spectroscopies*. These probe the electronic excitations and charge dynamics in both the frequency and time domains. This information is the key to understanding the dynamical interactions of the electrons.
- *Resonant elastic and inelastic x-ray spectroscopy*. Resonant elastic and inelastic x-ray scattering can now reveal spin and charge density waves and superlattices with tiny modulation amplitudes. This information is critically important for understanding spatially periodic electronic states of matter.
- *Neutron Scattering (NS)*. High-intensity NS — for example, from the Spallation Neutron Source — will allow precision measurements of both magnetic ground states and the complete spectrum of magnetic excitations in high-temperature and exotic superconductors.
- *NMR/NQR/ μ SR*. NMR measures spin dynamics, NQR measures the charge heterogeneity and dynamics, and μ SR measures nanoscale variation in local magnetic field strength. These are essentially local spin/charge probes, but without imaging capabilities.



BASIC RESEARCH NEEDS FOR SUPERCONDUCTIVITY

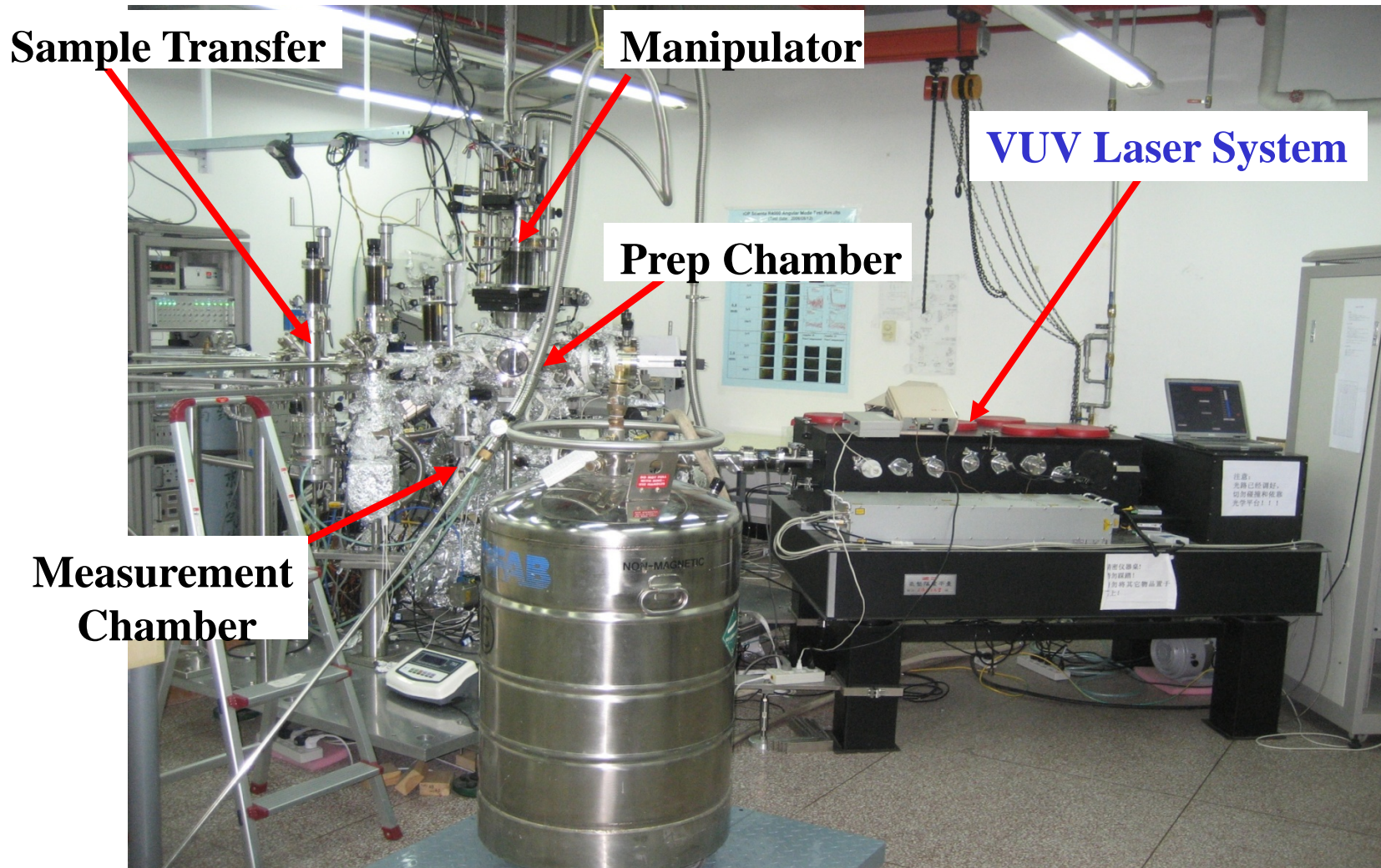
Report of the Basic Energy Sciences
Workshop on Superconductivity,
May 8-11, 2006



Office of
Science
U.S. DEPARTMENT OF ENERGY

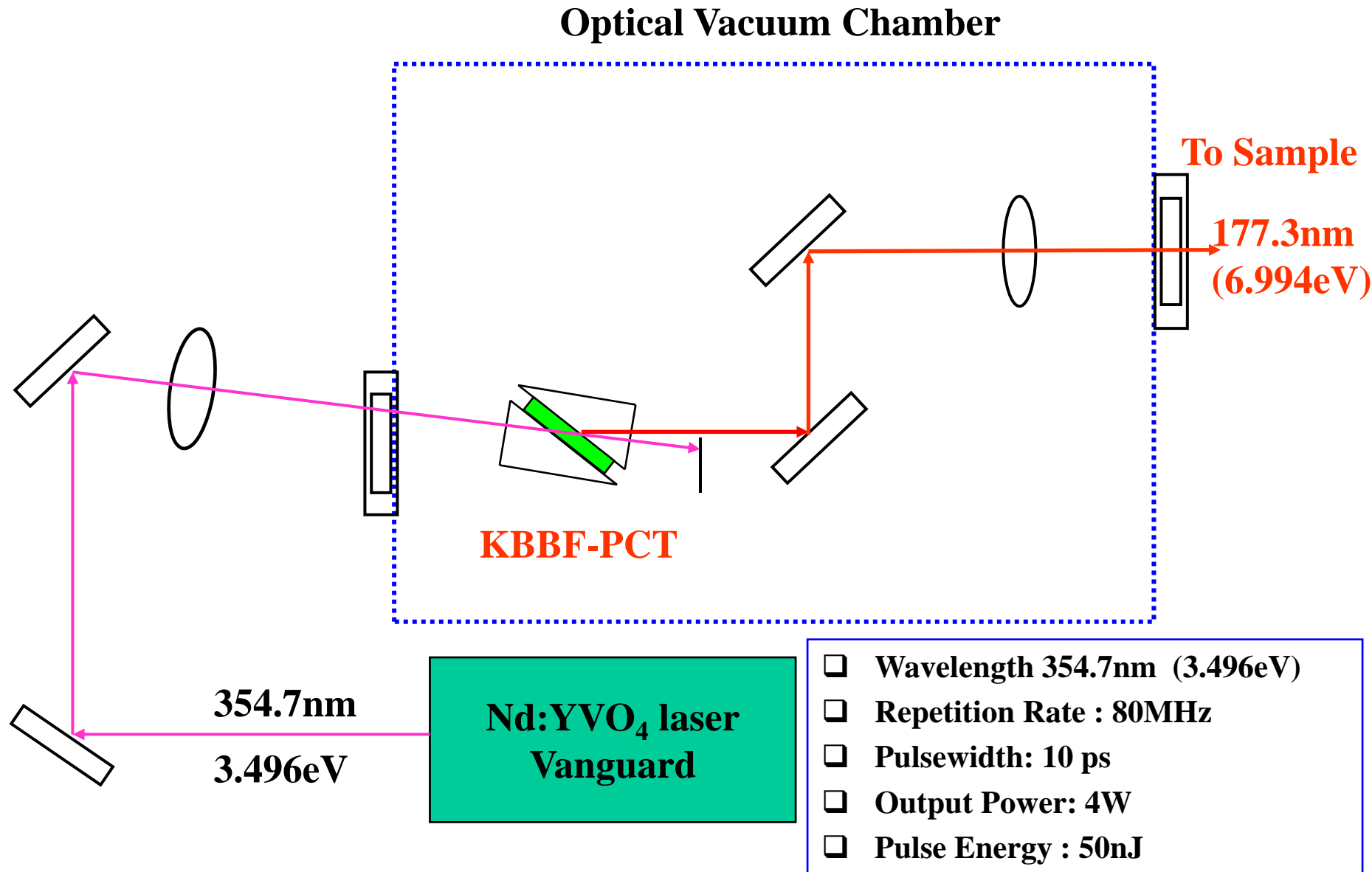


VUV Laser Angle-Resolved Photoemission System

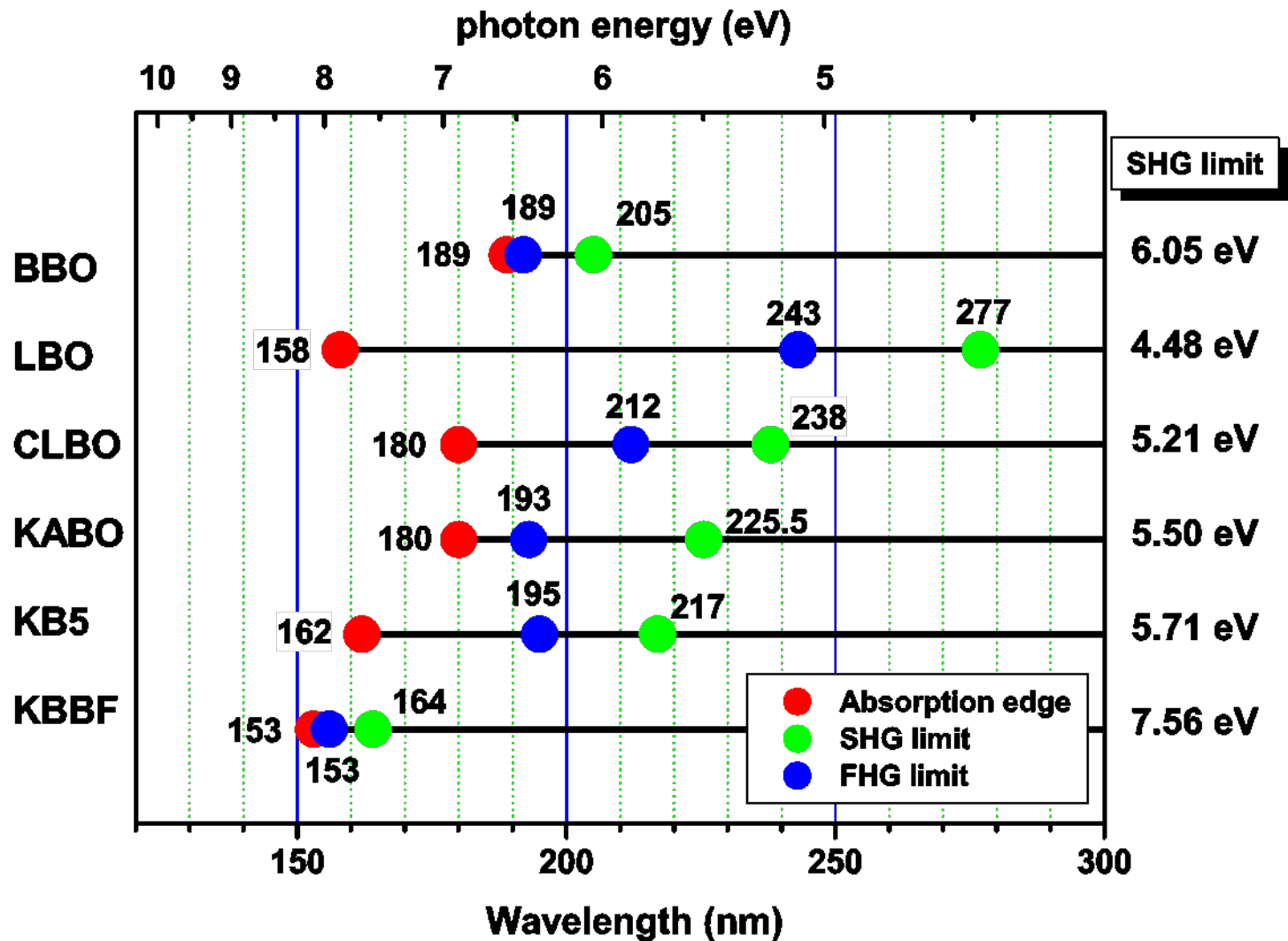


Institute of Physics, Chinese Academy of sciences

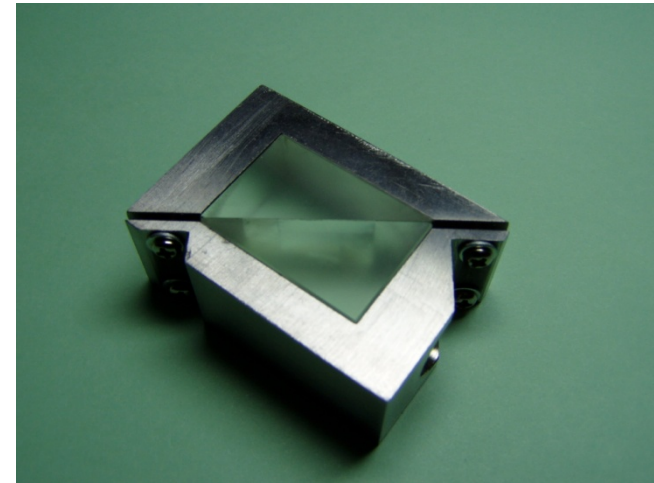
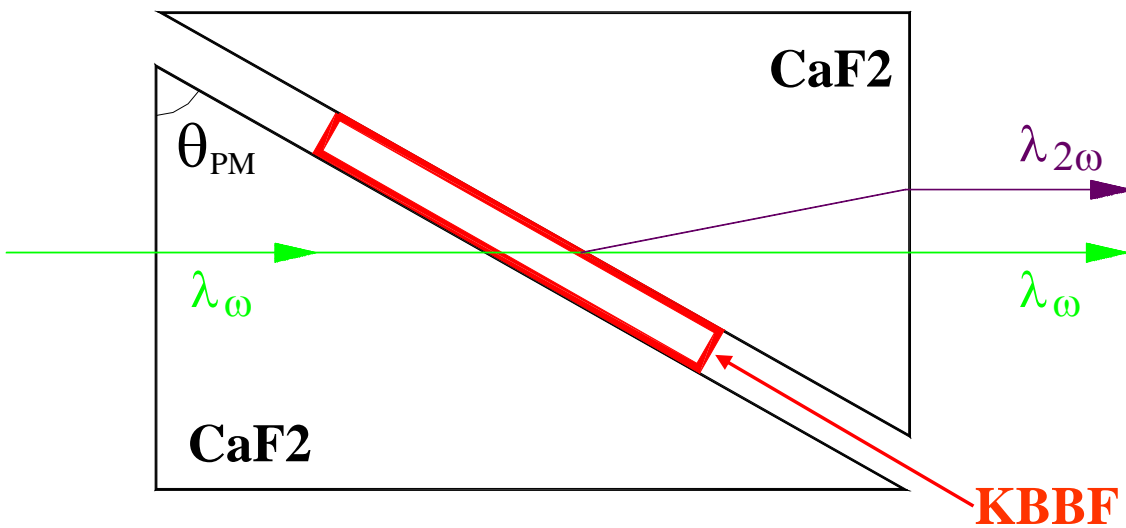
Generation of VUV Laser ($h\nu=6.994$ eV)



$\text{KBe}_2\text{BO}_3\text{F}_2$ (KBBF): New Non-Linear Optical Crystal



Laser Frequency Doubling Device—Prism Coupling



C. T. Chen, Z. Y. Xu et al., Chin. Phys. Lett. 18(8), 1081 (2001).

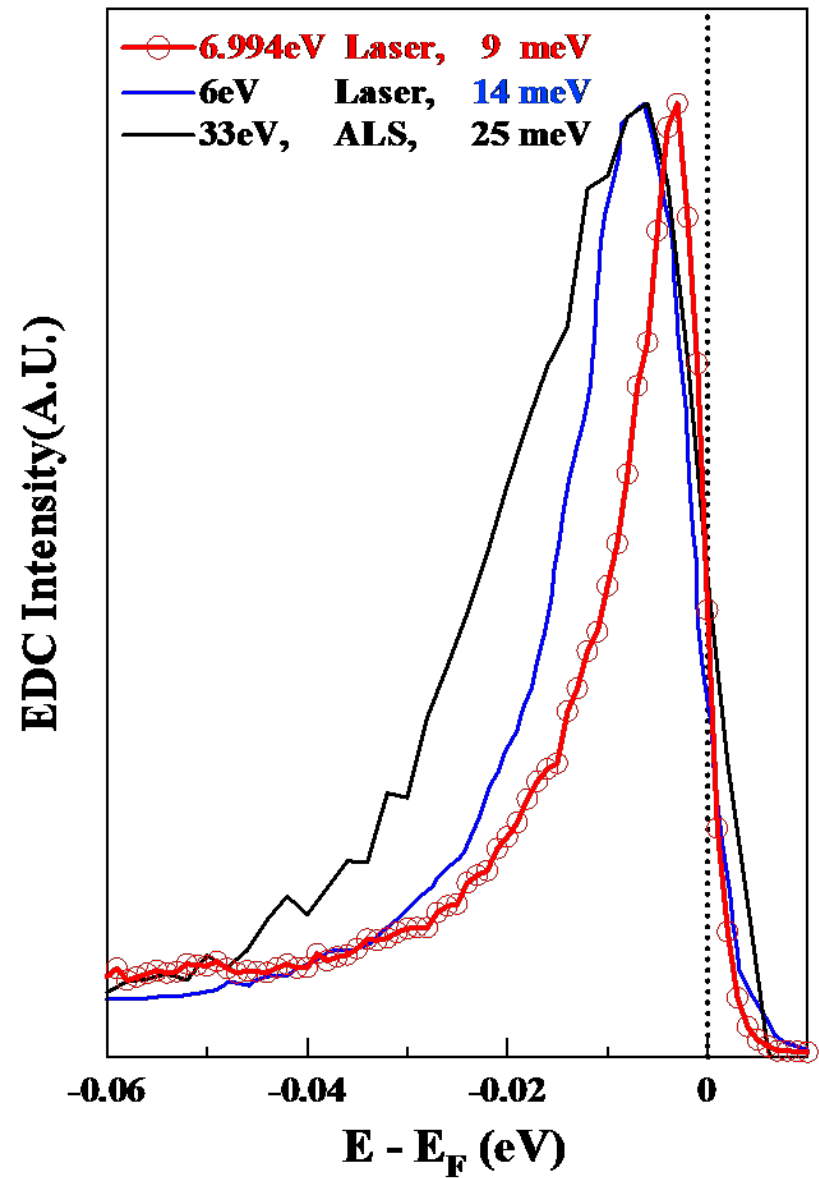
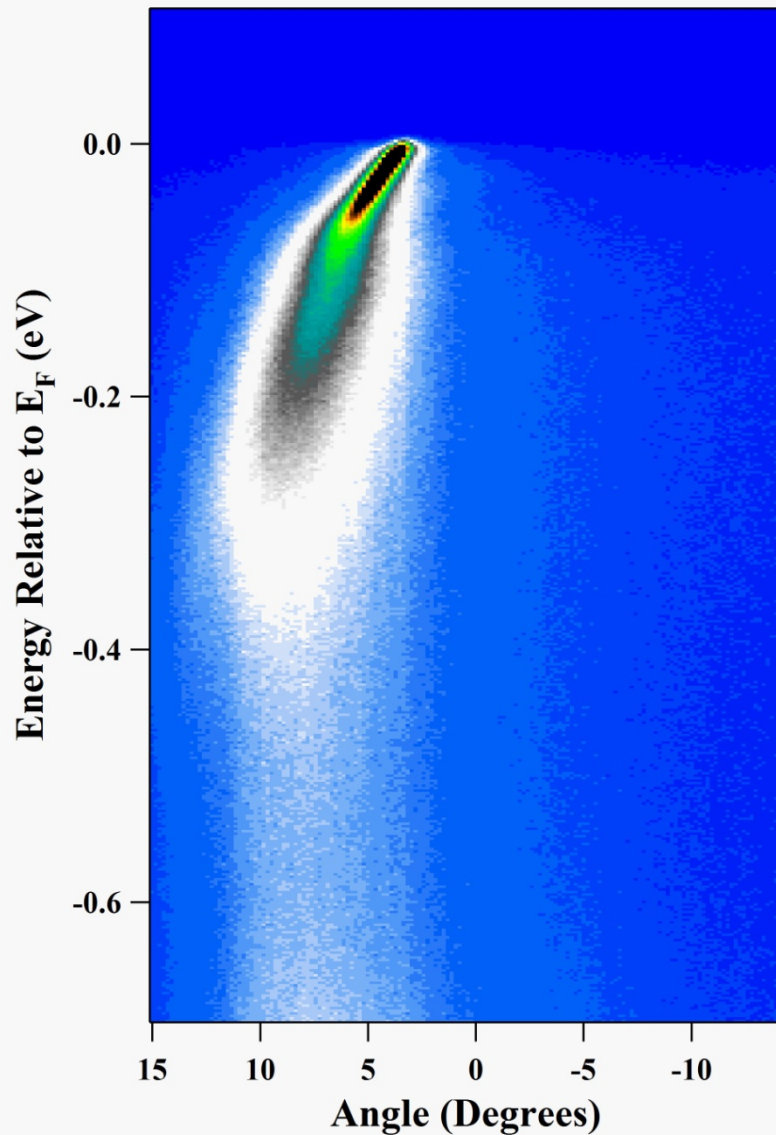
Advantages of VUV Laser ARPES

Light Source	VUV Laser	Synchrotron
Energy Resolution (meV)	0.26	~10
Momentum Resolution (\AA^{-1})	0.0036 (6.994eV)	0.0091 (21.2eV)
Photon Flux(Photons/s)	$10^{14}\sim 10^{15}$	$10^{12}\text{-}10^{13}$
Electron Escape Depth (\AA)	30~100	5~10

Elevated ARPES Technique to a New Level

Sharp Photoemission Spectrum

Bi2212, OP90K



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Prominent Issue: Mechanism of High-Tc Superconductivity

■ BCS theory for conventional superconductivity (1957)

- Tc has a limit ($< 40\text{K}$);
- Isotropic s-wave superconducting gap.

Electron pairing through phonon exchange

■ High-Tc superconductors:

- Tc is high (Tc max=135K for Hg1223
Tc max=160K under pressure);
- Anisotropic d-wave Superconducting gap.



The Nobel Prize in Physics 1972

"for their jointly developed theory of superconductivity, usually called the BCS-theory"



John
Bardeen



Leon
Neil
Cooper



John
Robert
Schrieffer

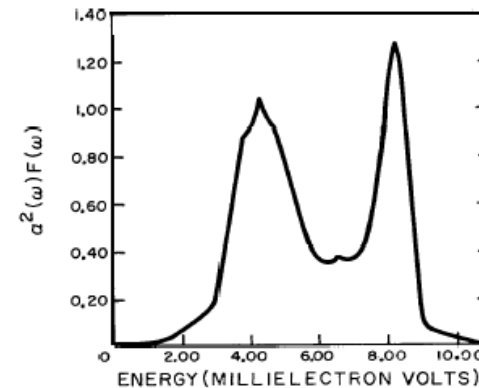
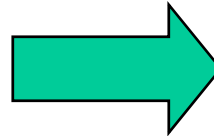
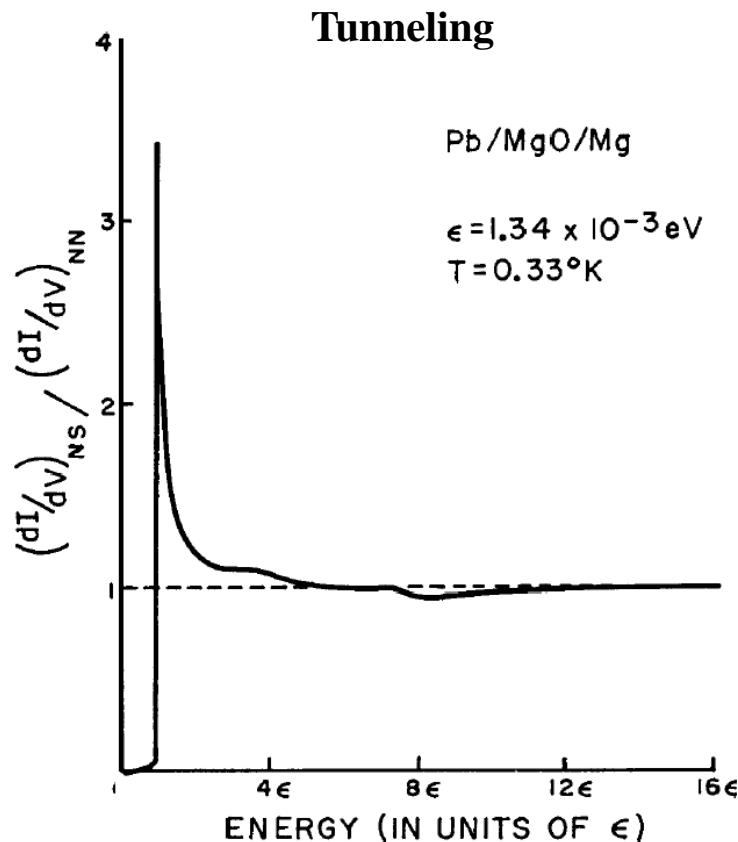


Who is next?

High-Tc superconductivity still involves Cooper pairs
What is the GLUE for the pairing?

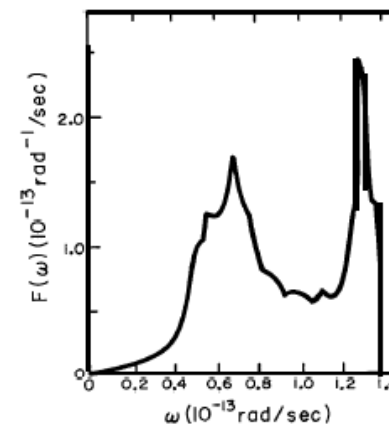
Experimental “Smoking Gun” in Unveiling Mechanism of Conventional Superconductivity

Extraction of Bosonic Spectral Function



$\alpha^2 F(\omega)$

Comparison of $\alpha^2 F(\omega)$ and $F(\omega)$ for Pb (after McMillan and Rowell)

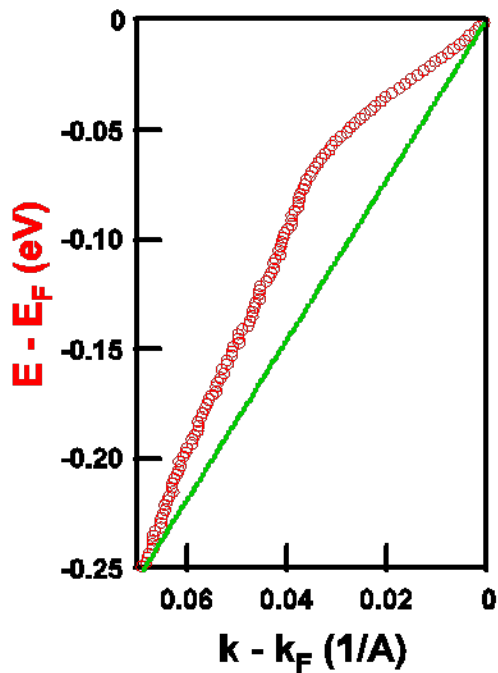


$F(\omega)$

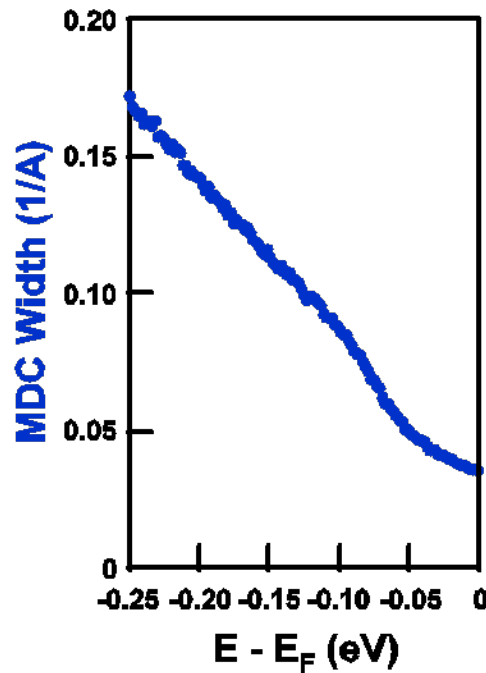
Bardeen, Nobel Lecture, 1972.

ARPES Directly Measures Electron Self-Energy Σ

Dispersion from
MDC position $k_0(E)$



MDC Width
 $\Gamma(E)$



$$\begin{aligned} \text{Re } \Sigma &= E - k_0 v_0 \\ \text{Im } \Sigma &= (\Gamma / 2) * v_0 \end{aligned}$$

Extraction of Bosonic Spectral Function from ARPES

In metals, the real part of self-energy is related to the bosonic spectral function b

$$\text{Re } \Sigma(k, \varepsilon, T) = \int_0^{\infty} d\omega \alpha^2 F(\omega; \varepsilon, k) K\left(\frac{\varepsilon}{kT}, \frac{\omega}{kT}\right)$$

where

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

with $f(x)$ being the Fermi-Dirac distribution Function

The direction inversion is mathematically unstable because of data noise.

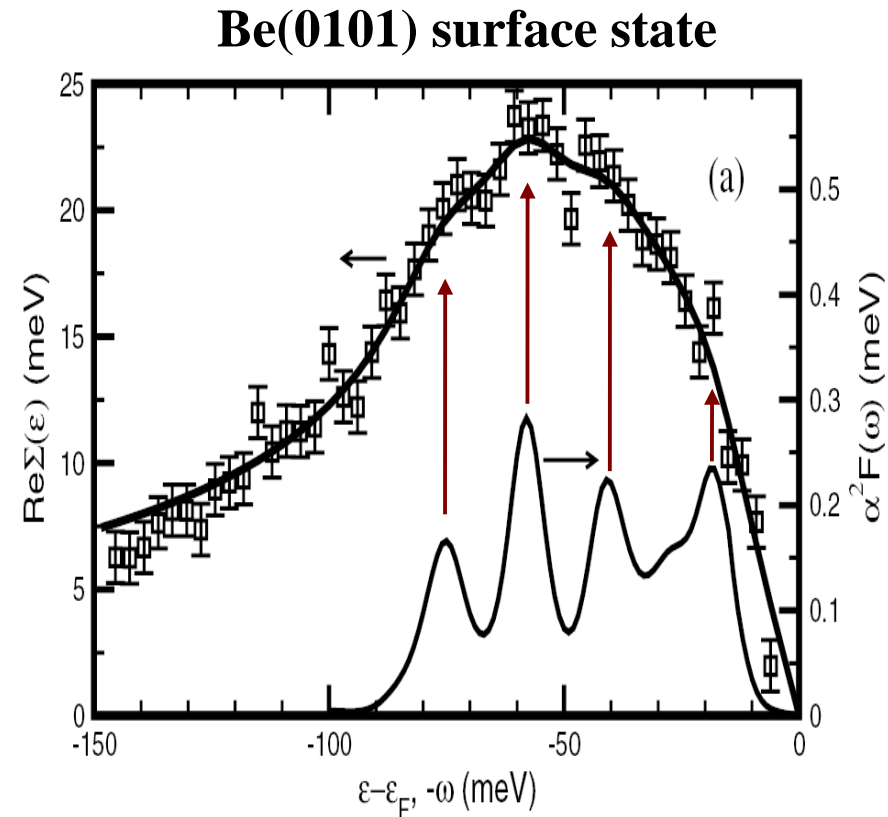
Theoretical Progress: Maximum Entropy Method (MEM)

Advantages of MEM over Least Square:

(1). Statistical method;

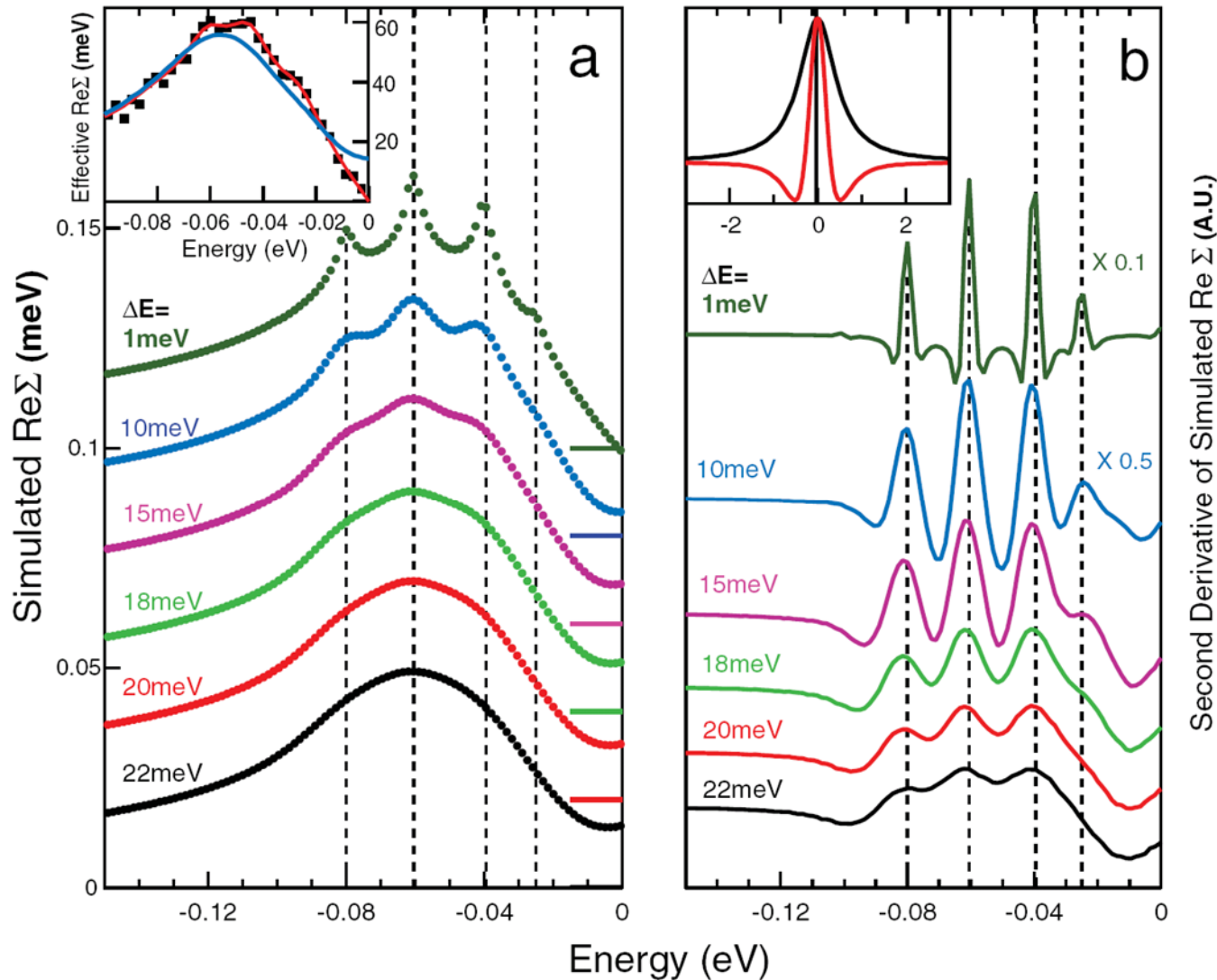
(2). It can incorporate *a priori* knowledge

- ☐ $\alpha^2 F(\omega)$ is positive;
- ☐ It vanishes as $\omega \rightarrow 0$;
- ☐ It vanishes above a maximum energy.



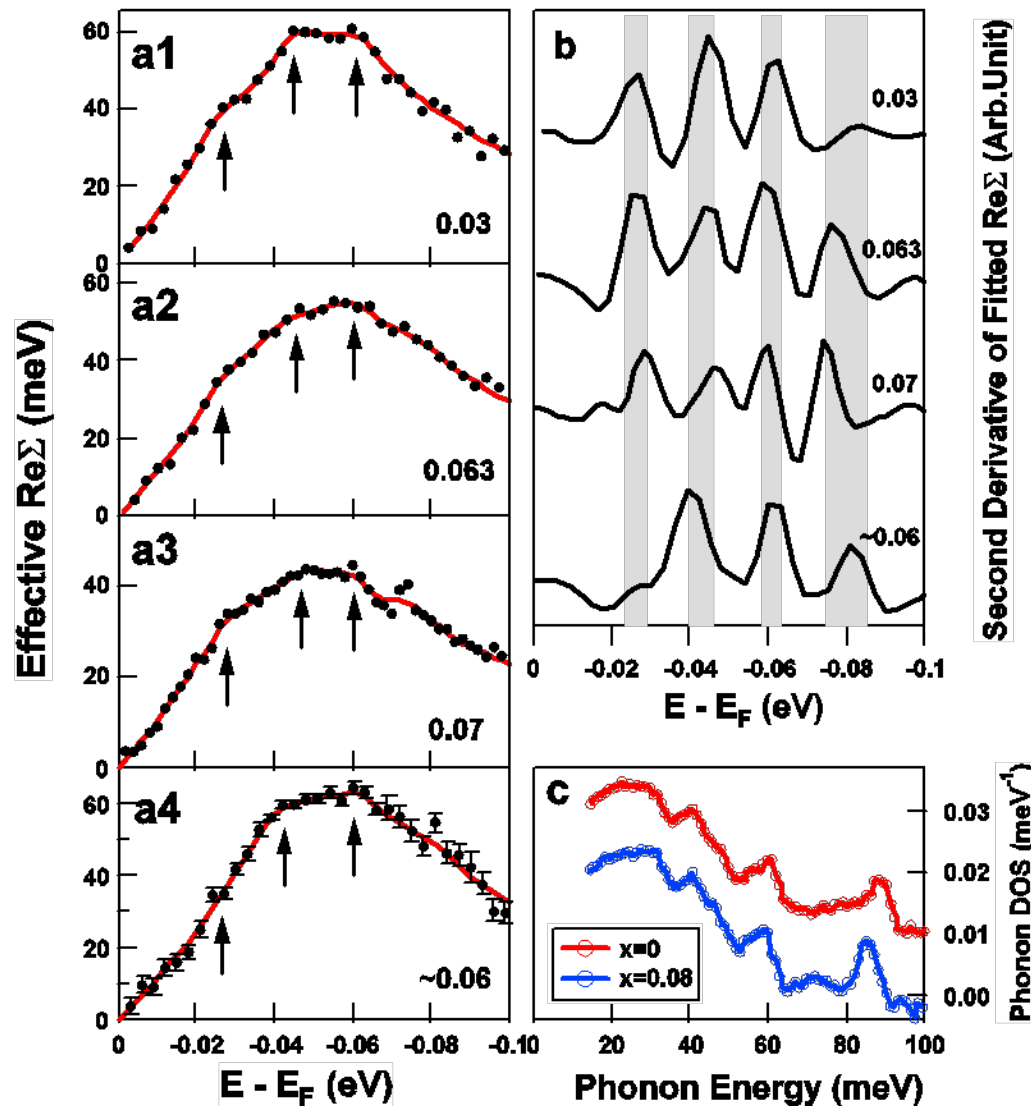
J. R. Shi et al., Phys. Rev. Lett. 92, 186401 (2004).

Experimental Requirement: High Energy Resolution



X. J. Zhou et al., Phys. Rev. Lett. 96(2006)119702.

First Trial of Fine Structure Extraction in High-Tc Cuprates



$(\text{La}_{2-x}\text{Sr}_x)\text{CuO}_4$

Synchrotron ARPES:
Advanced Light Source

- (1). Further evidence for electron-phonon coupling;
- (2). Multiple phonon modes;

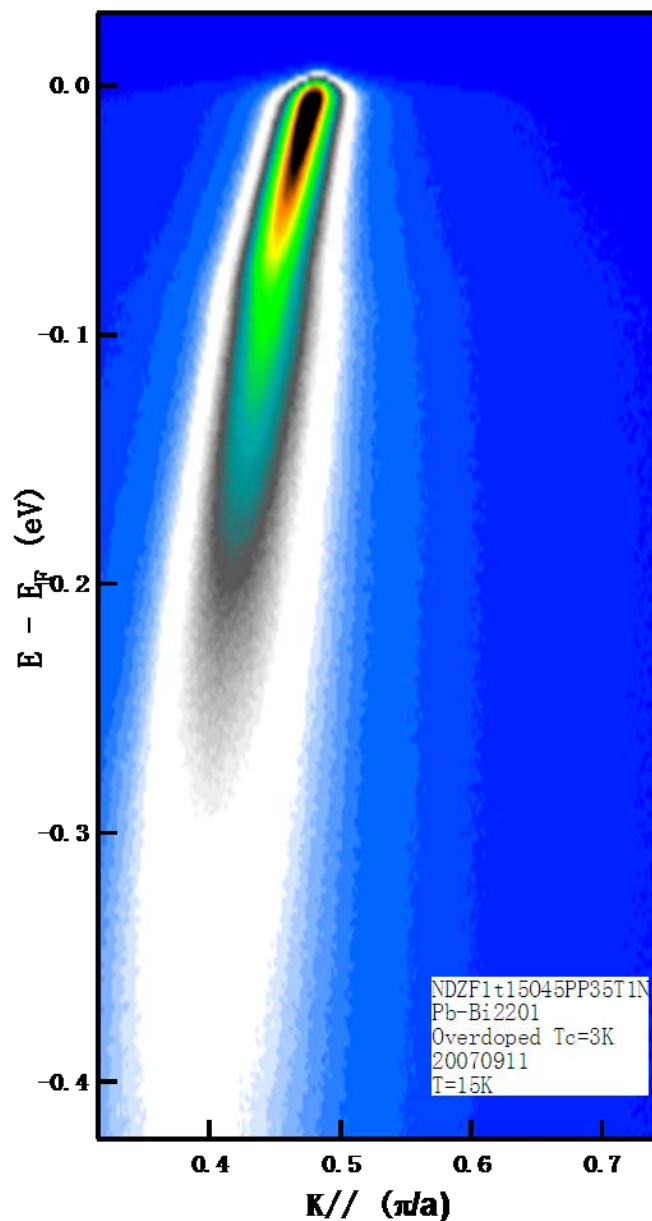
Experimental Challenges: Searching for Finer Structure in Fine Structure

Essentials for identifying Fine Structure

- (1). High resolutions;
- (2). High data statistics (High signal).

	Synchrotron	VUV Laser
Photon Energy	55 eV	6.994 eV
<u>Beamline resolution:</u>	<u>12~15 meV</u>	<u>0.26 meV</u>
<u>Photon flux (photons/second) :</u>	<u>$\sim 3 \times 10^{13}$</u>	<u>$\sim 10^{14-15}$</u>
Analyzer energy resolution:	10 meV	0.5 meV
Momentum resolution (1/A):	0.014	0.0036
Collection time	~ 1 hour	~ 0.5 hr

Laser ARPES on Nodal Dispersion of Pb-Bi2201

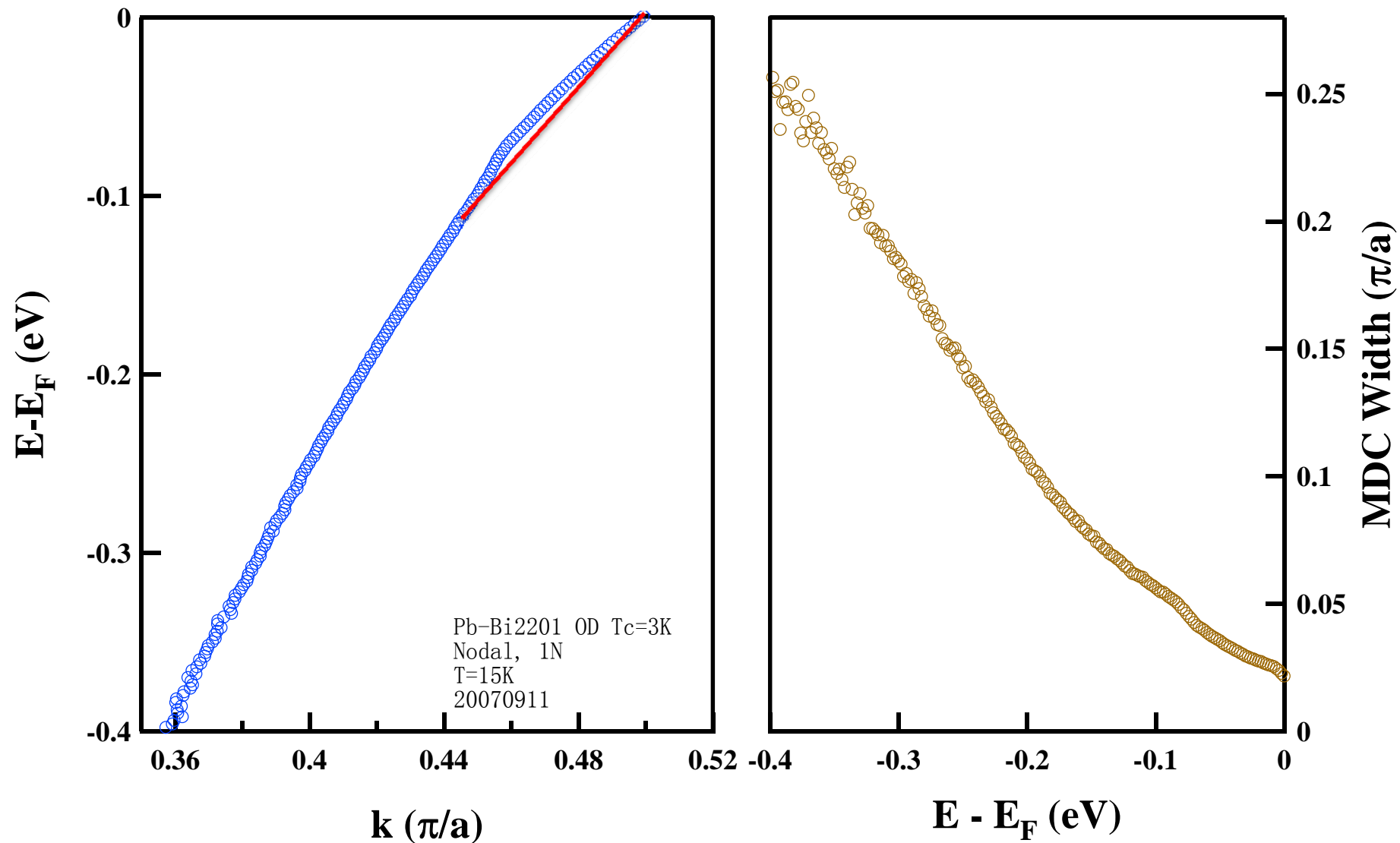


Overdoped, $T_c=3K$

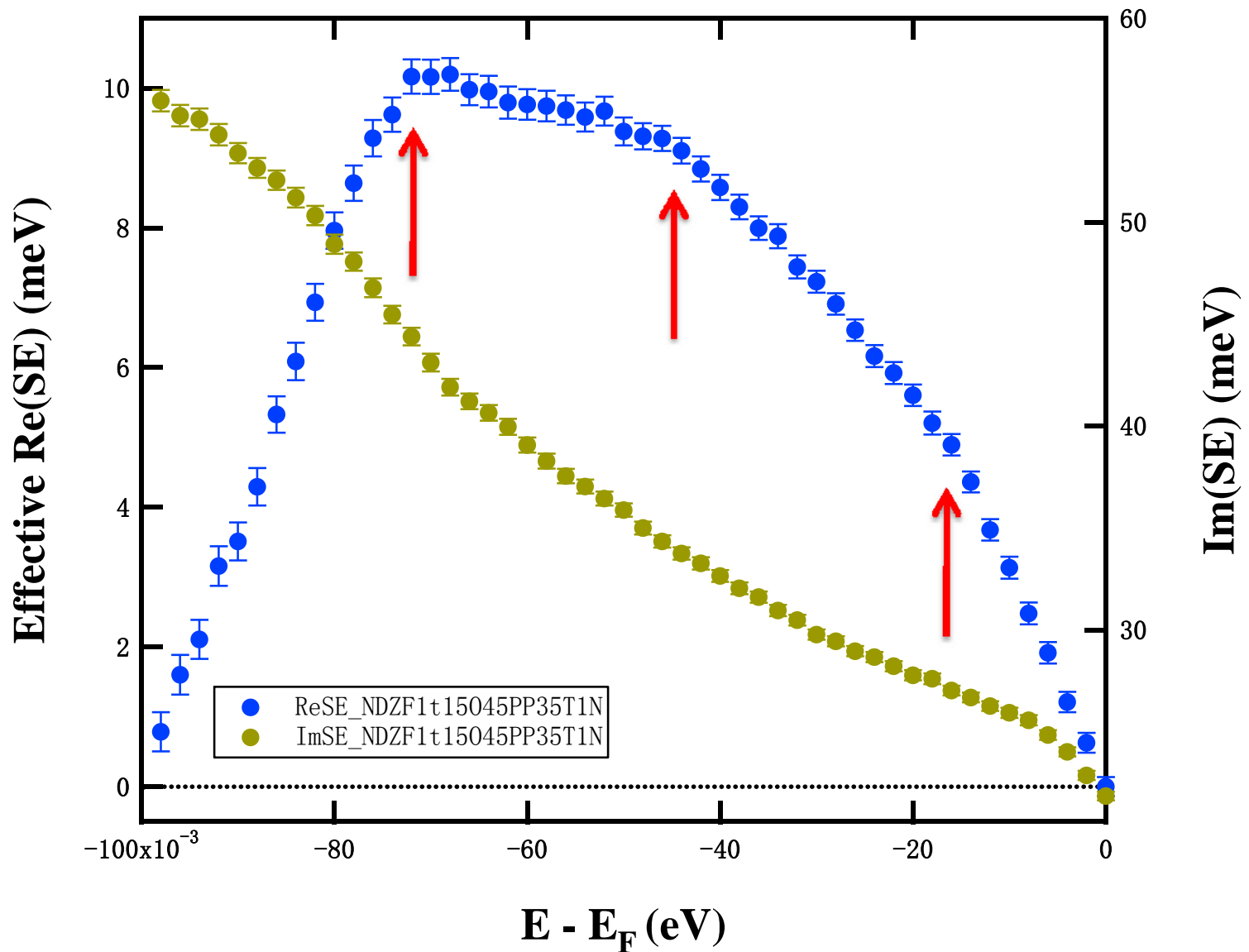
$T=15K$

Energy Resolution: 0.56meV

MDC Dispersion of Pb-Bi2201 (Overdoped, $T_c=3K$)



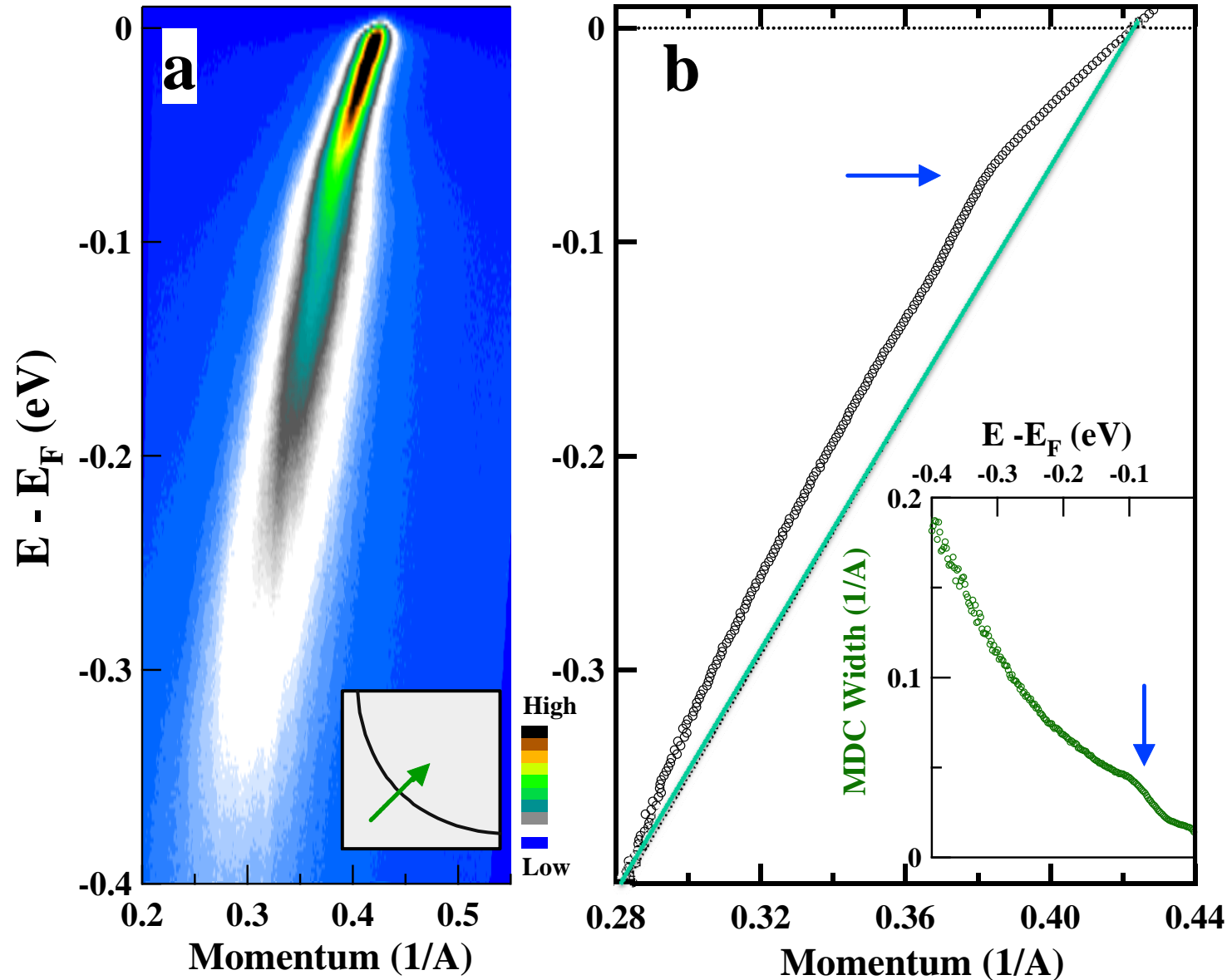
Fine Structure in Electron Self-Energy of Pb-Bi2201



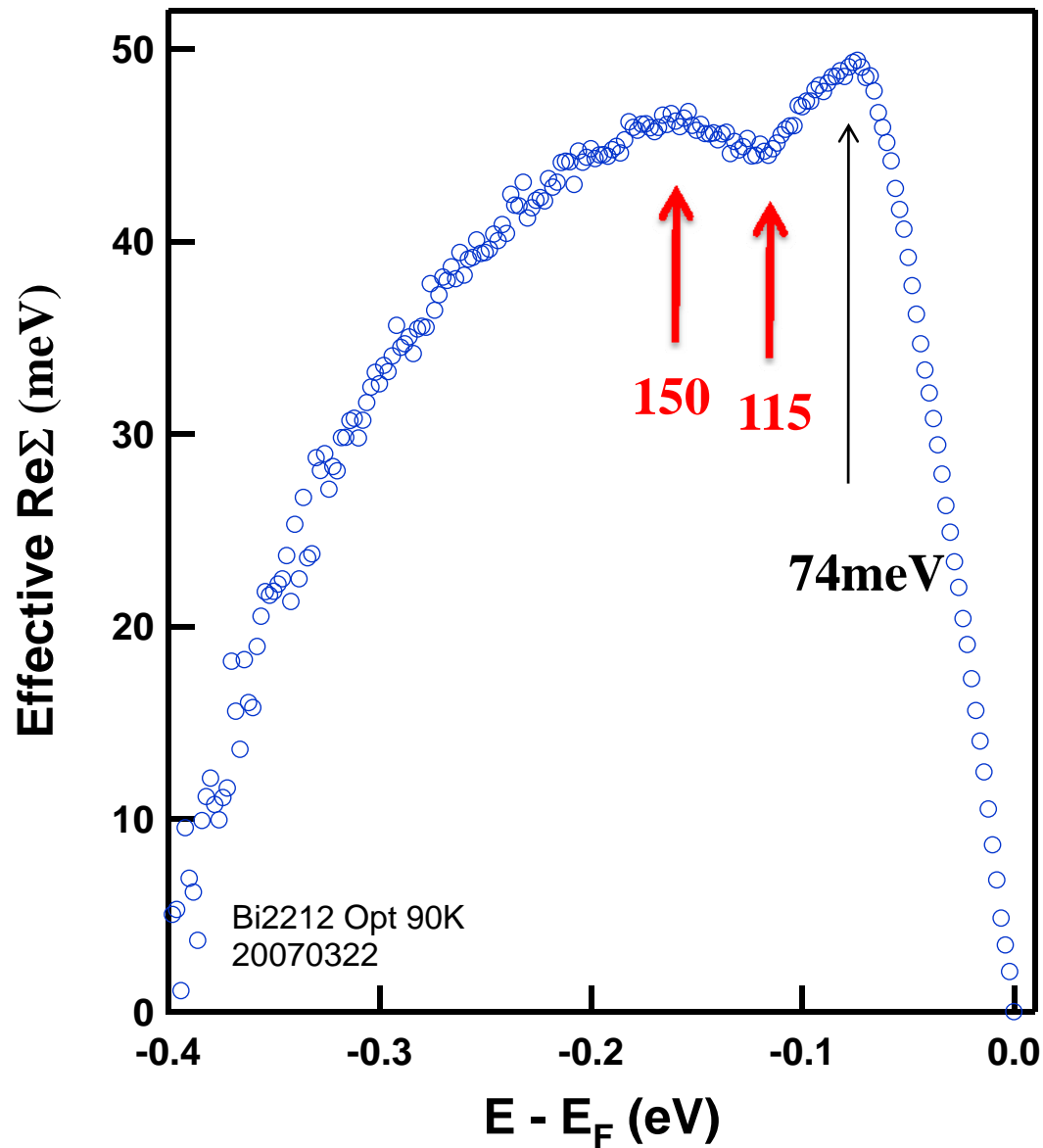
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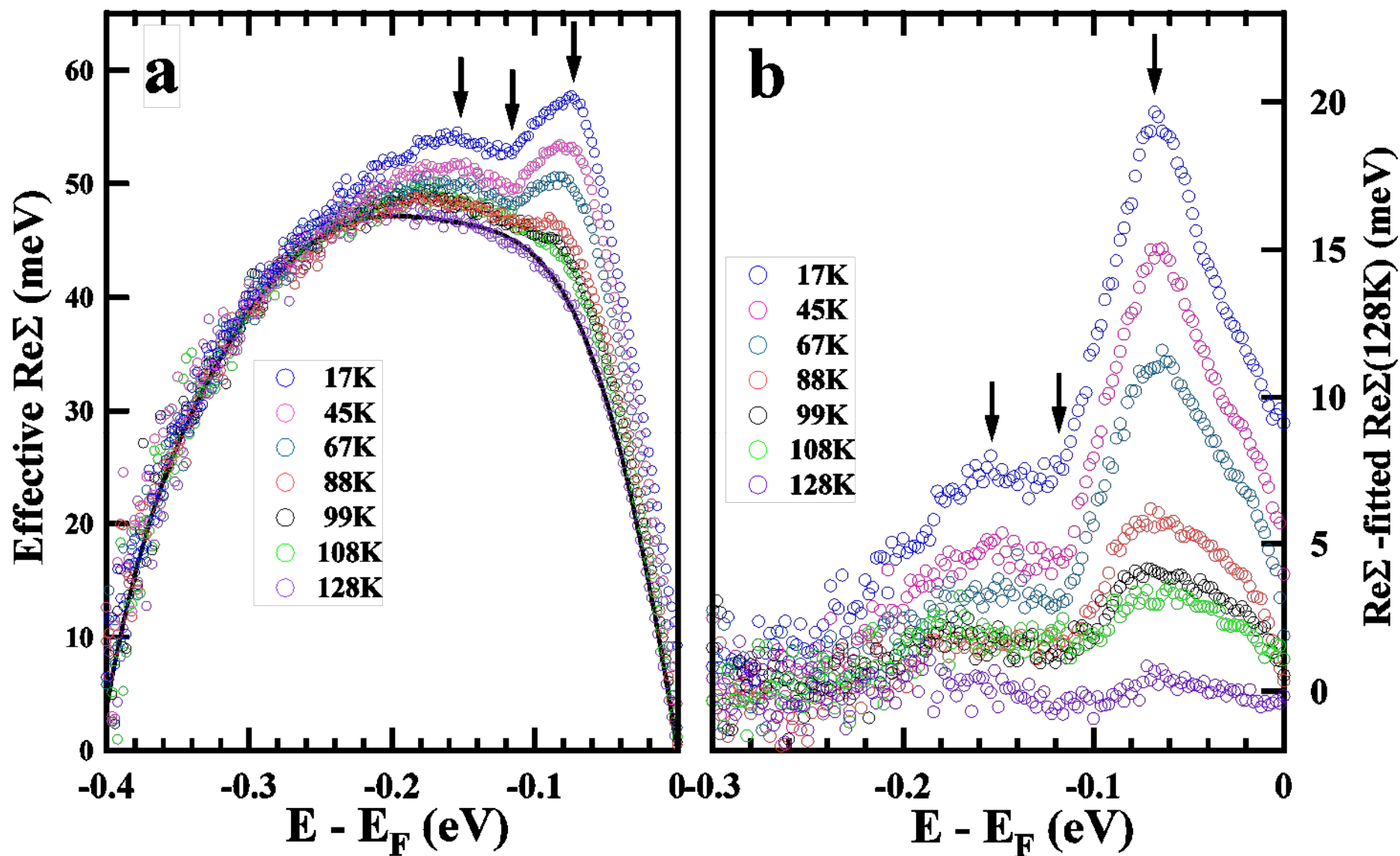
Nodal Dispersion in Bi2212 ($T_c=91\text{K}$, $T=17\text{K}$)



Identification of New High Energy Features in Self-Energy



Temperature Evolution of Nodal Electron Self-Energy in Bi2212



What is the origin

of

the new high energy features at 115 and 150 meV?

A New Form of Electron Coupling

~70 meV: Observed before

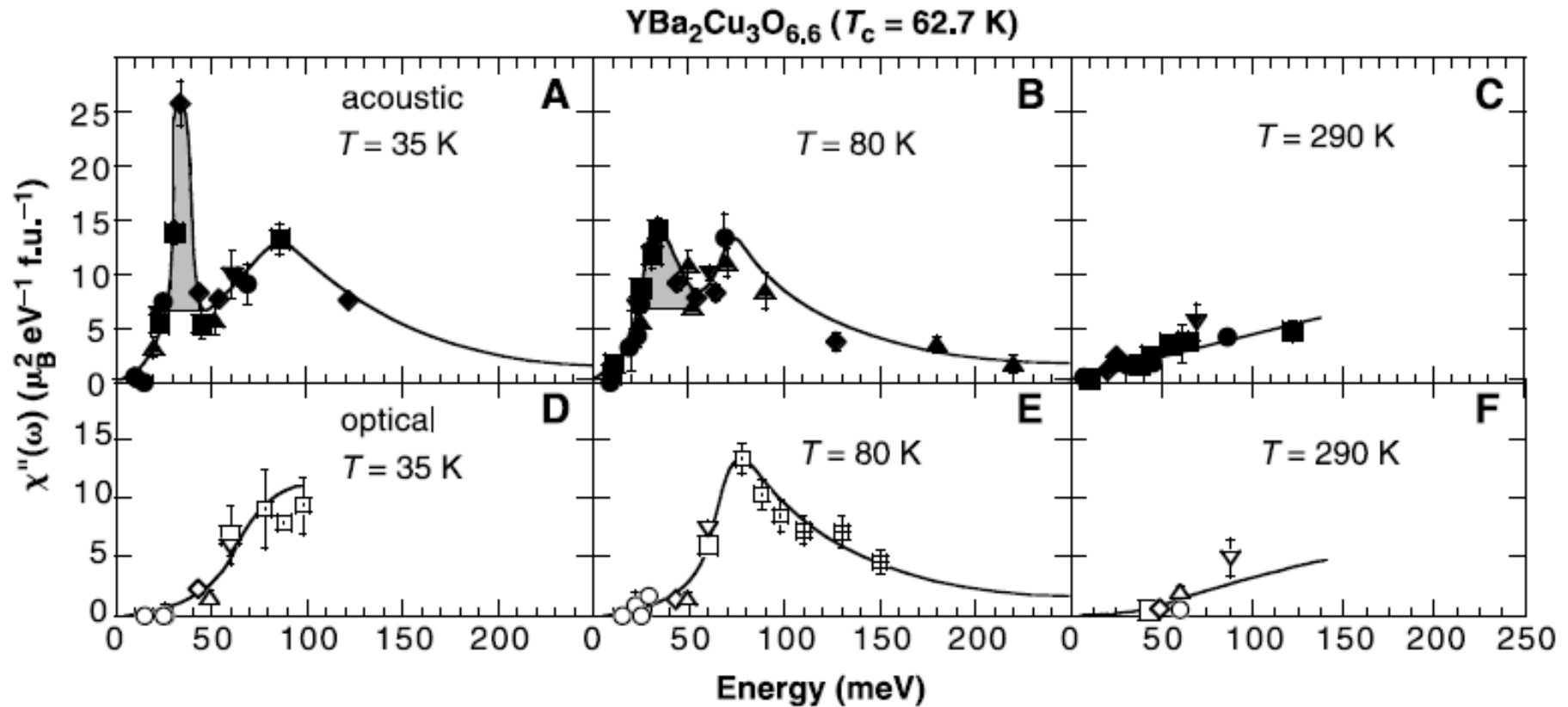
Electron coupling with Phonons or Magnetic resonance mode

~115meV and ~150meV: New form of electron coupling

Possibilities: Electron coupling with:

- | | |
|--|-----------------|
| 1). Single phonon; | Impossible |
| 2). Magnetic resonance mode; | Impossible |
| 3). Mode+Superconducting gap | Unlikely |
| 4). Multi-phonons; | Less likely |
| 5). Other high energy excitations, like spin fluctuations. | Possible |

Magnetic Excitation Spectra in $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$



P. C. Dai et al., Science 284 (1999) 1344.

Summary

- 1). Super-high resolution VUV laser-based ARPES system has been developed;**
- 2). It has revealed that:**
 - Electron coupling with multiple phonon modes;**
 - A new form of electron coupling**
It is probably a coupling with high energy excitations, related with spin fluctuation.



Thank you