Introduction to Angle-Resolved Photoelectron Spectroscopy

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Group: Electronic Structure of Solids

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Previous Collaborators

- **ARPES at Stanford:**

  K.M. Shen, D.H. Lu, D.L. Feng, N.P. Armitage, F. Ronning, C. Kim, **Z.-X. Shen**

- **Band Structure Calculations (NRL, Washington):**

  I.I. Mazin, D.J. Singh

- **Samples:**
  - **Sr_2RuO_4**

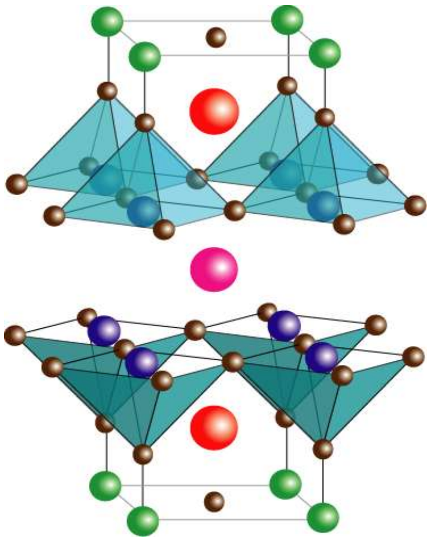
    S. Nakatsuji, T. Kimura, Y. Tokura, Z.Q. Mao, Y. Maeno
  - **$Bi_2Sr_2CaCu_2O_{8+\delta}$**

    H. Eisaki, R. Yoshizaki, J.-i. Shimoyama, K. Kishio, G.D. Gu, S. Oh, A. Andrus, J. O'Donnell, J.N. Eckstein
  - $YBa_2Cu_3O_{7-\delta}$

    D.A. Bonn, R. Liang, W.N. Hardy, A.I. Rykov, S. Tajima
  - $Nd_{2-x}Ce_xCuO_4$

    Y. Onose, Y. Taguchi, Y. Tokura; P.K. Mang, N. Kaneko, M. Greven
  - $Ca_{2-x}Na_xCu_2O_2Cl_2$

    L.L. Miller, T. Sasagawa, Y. Kohsaka, H. Takagi



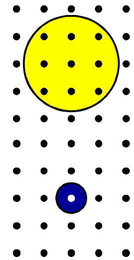
Outline

- Electronic structure of **complex systems**
- State-of-the-Art **ARPES**: the essentials
- **Sr_2RuO_4**
  - **Introduction**
    Interesting properties and open issues
  - **Experimental results**
    Bulk & surface electronic structure
- ARPES on **$Bi_2Sr_2CaCu_2O_{8+\delta}$**
- Conclusions and discussion

Strongly Correlated Electron Systems

d - f

open shells materials



U<<W
Charge fluctuations

U>>W
Spin fluctuations

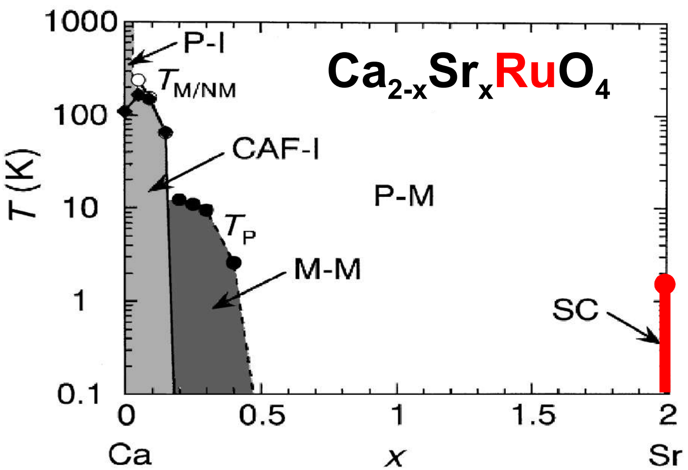
Control parameters

Bandwidth (U/W)
Band filling
Dimensionality

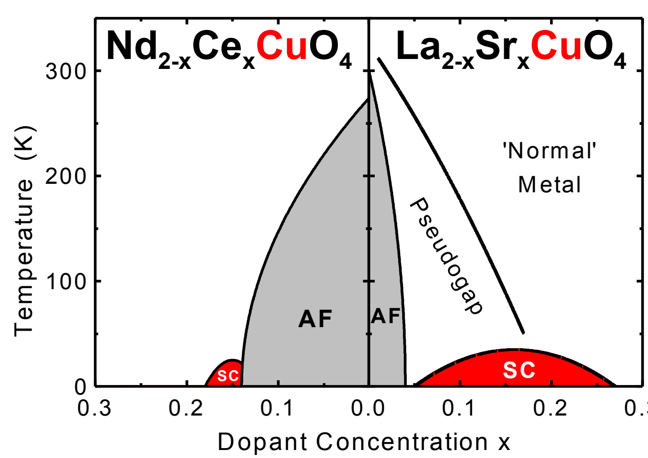
I	II	IIIb	IVb	Vb	VIb	VIIb	VIIIb			Ib	IIb	III	IV	V	VI	VII	0
H																	He
Li	Be											B	C	N	**O**	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	**Ti**	**V**	**Cr**	**Mn**	**Fe**	**Co**	**Ni**	**Cu**	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	**Ru**	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt									
Lanthanides*			**Ce**	**Pr**	**Nd**	**Pm**	**Sm**	**Eu**	**Gd**	**Tb**	**Dy**	**Ho**	**Er**	**Tm**	**Yb**	Lu	
Actinides**			Th	Pa	**U**	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

Degrees of freedom

Charge / Spin
Orbital
Lattice



- **Kondo**
- **Mott-Hubbard**
- **Heavy Fermions**
- **Unconventional SC**
- **Spin-charge order**
- **Colossal MR**



Strongly Correlated Electron Systems

Understand the

macroscopic electronic properties

and the role of

competing degrees of freedom

↓

Study the low-energy electronic excitations

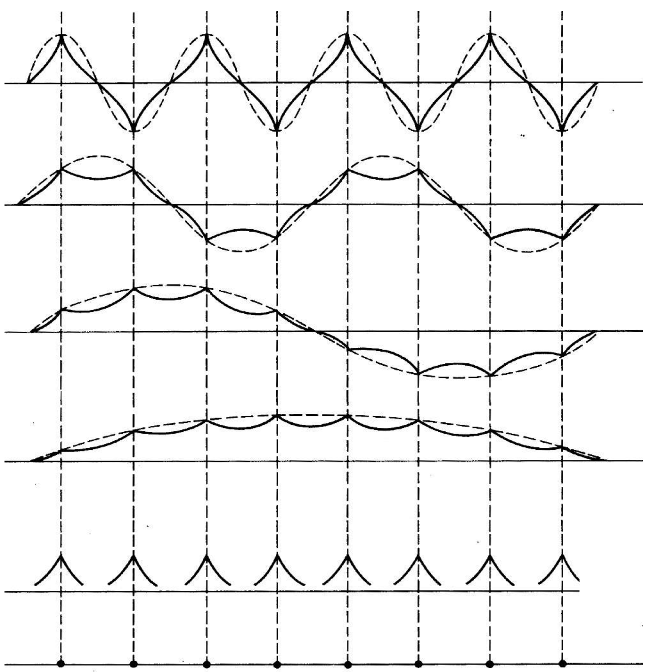
↓

ARPES

Velocity and direction of the electrons in the solid

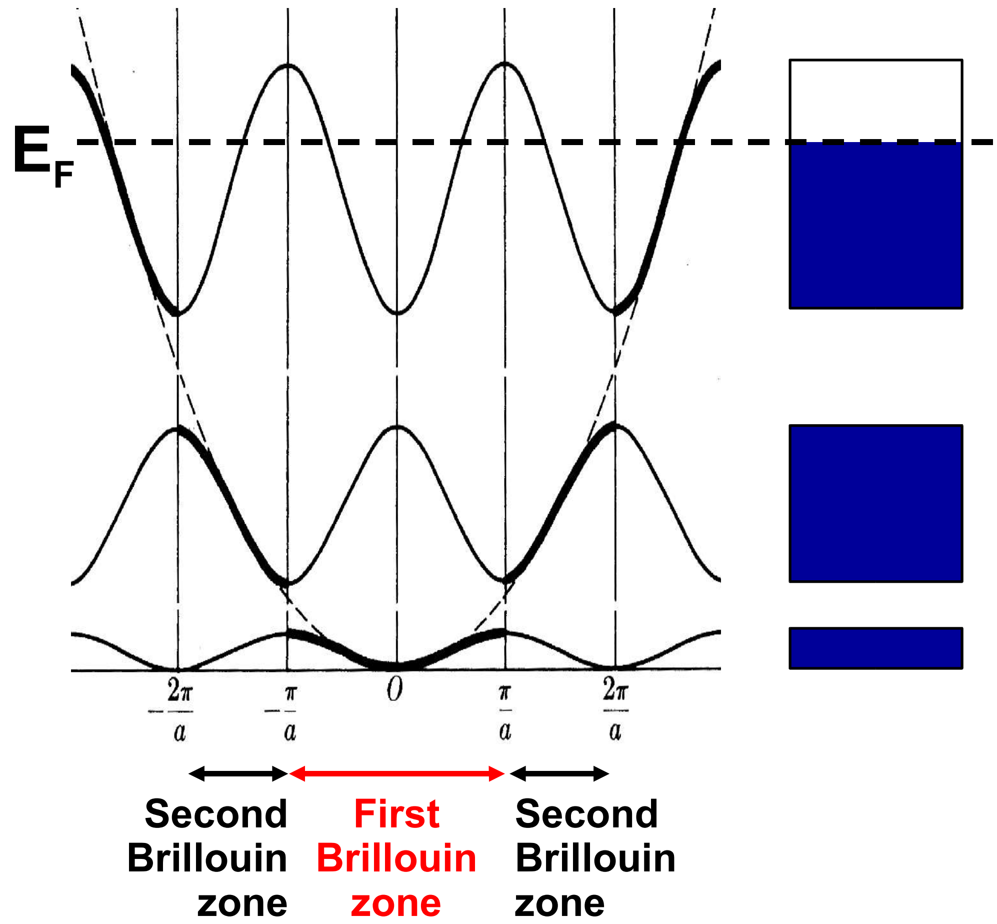
Electrons in a 1D periodic potential

Wave functions
in a 1D lattice



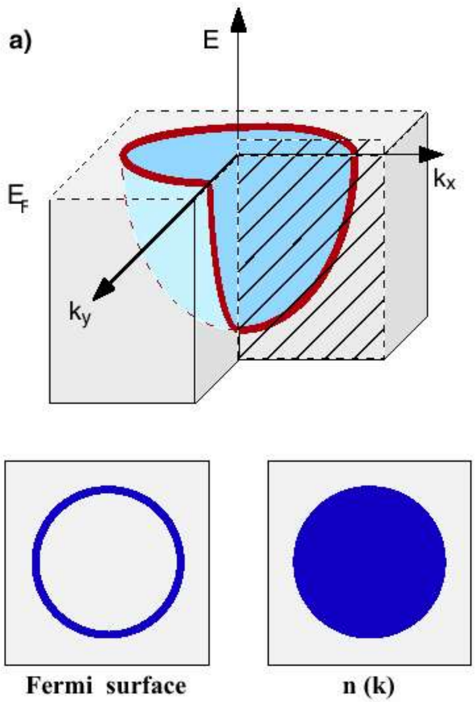
1D chain of atoms

Allowed electronic states
Repeated-zone scheme



Electrons in a 1D periodic potential

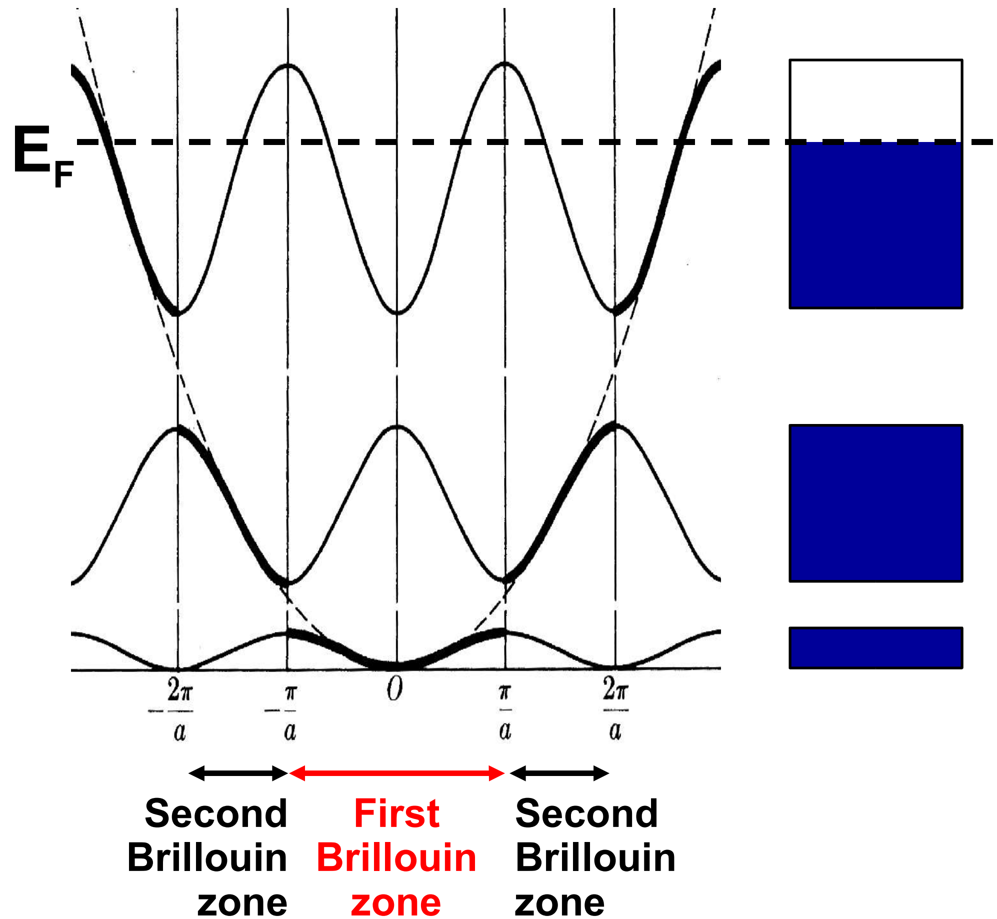
Many **properties** of a solids are determined by **electrons near E_F** (conductivity, magnetoresistance, superconductivity, magnetism)



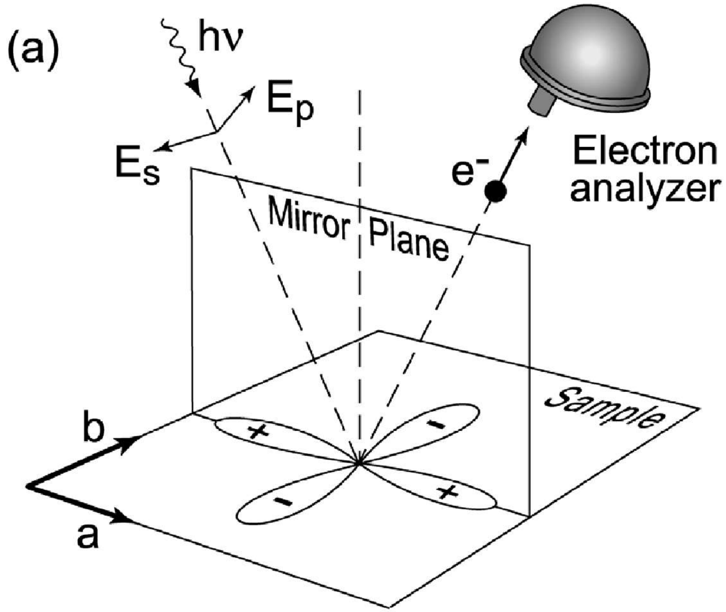
Only a **narrow energy slice** around E_F is relevant for these properties (**~kT=25 meV** at room temperature).

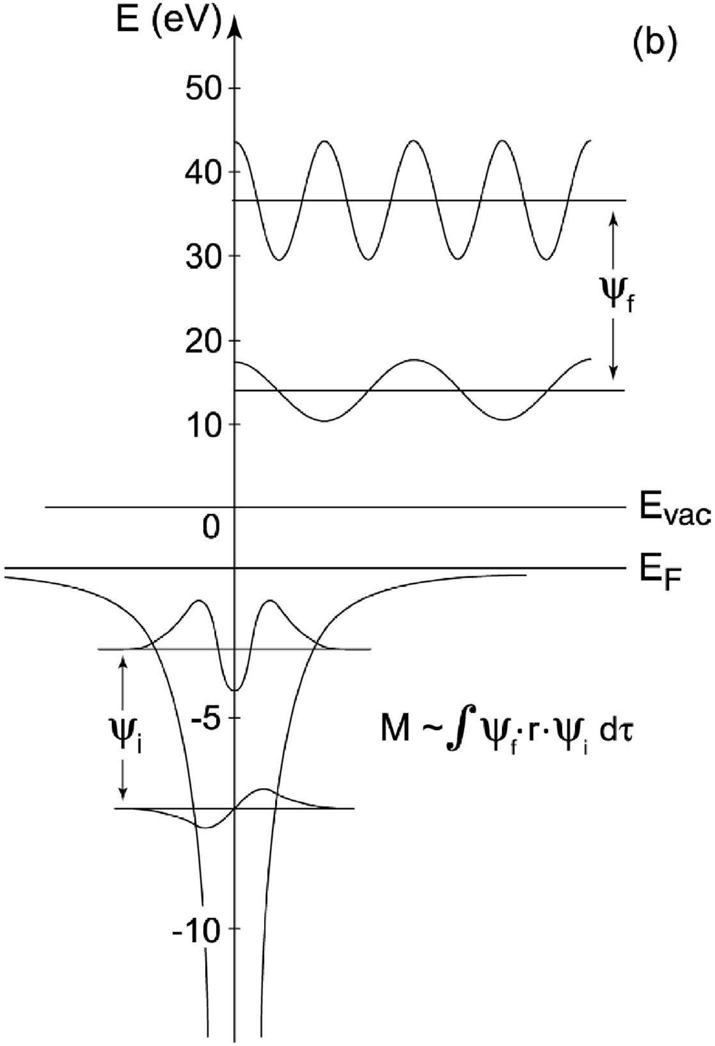
Allowed electronic states

Repeated-zone scheme



Angle-Resolved Photoemission Spectroscopy

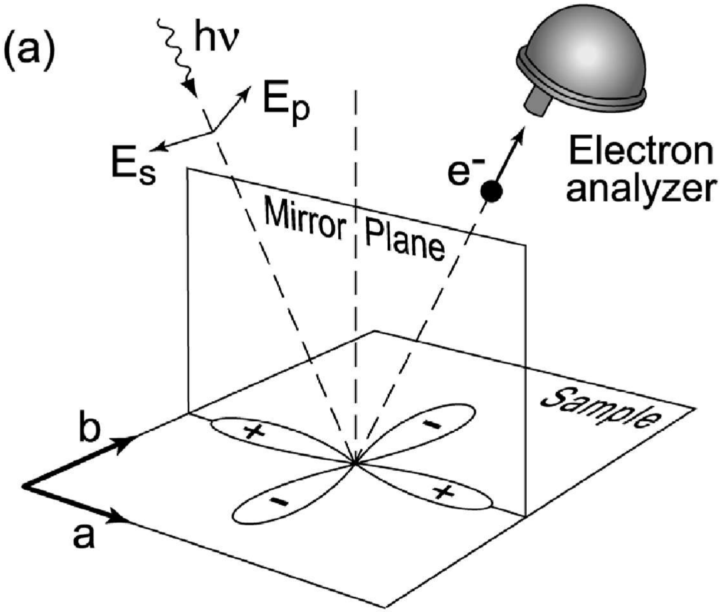


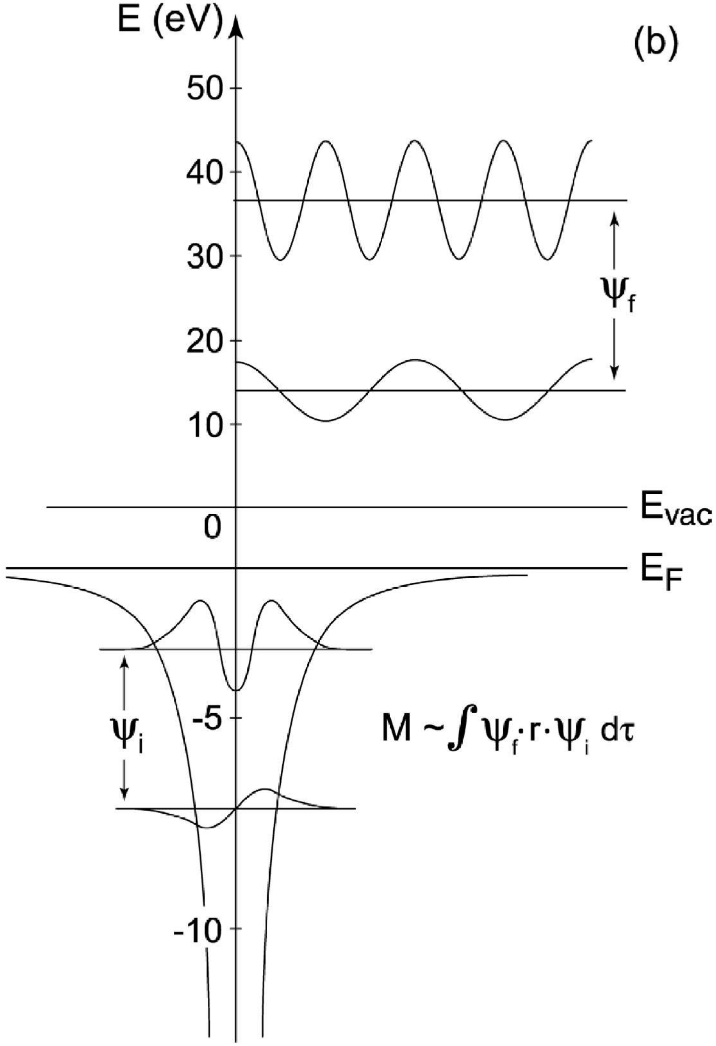


$$w_{fi} = \frac{2\pi}{\hbar} \left| \langle \Psi_f^N | H_{int} | \Psi_i^N \rangle \right|^2 \delta(E_f^N - E_i^N - h\nu)$$

$$H_{int} = -\frac{e}{2mc}(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}) = -\frac{e}{mc}\mathbf{A}\cdot\mathbf{p}$$

Angle-Resolved Photoemission Spectroscopy



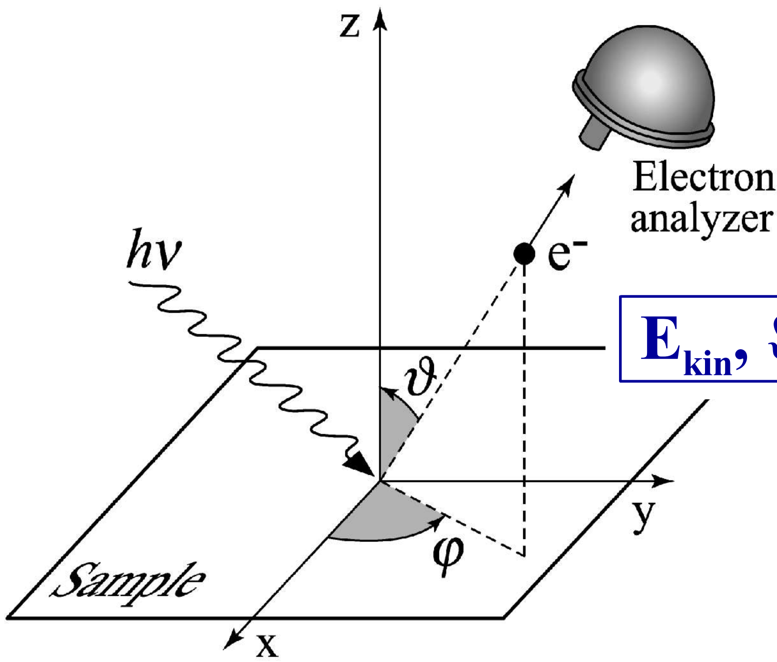


$$w_{fi} = \frac{2\pi}{\hbar} |\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle|^2 \delta(E_f^N - E_i^N - h\nu)$$

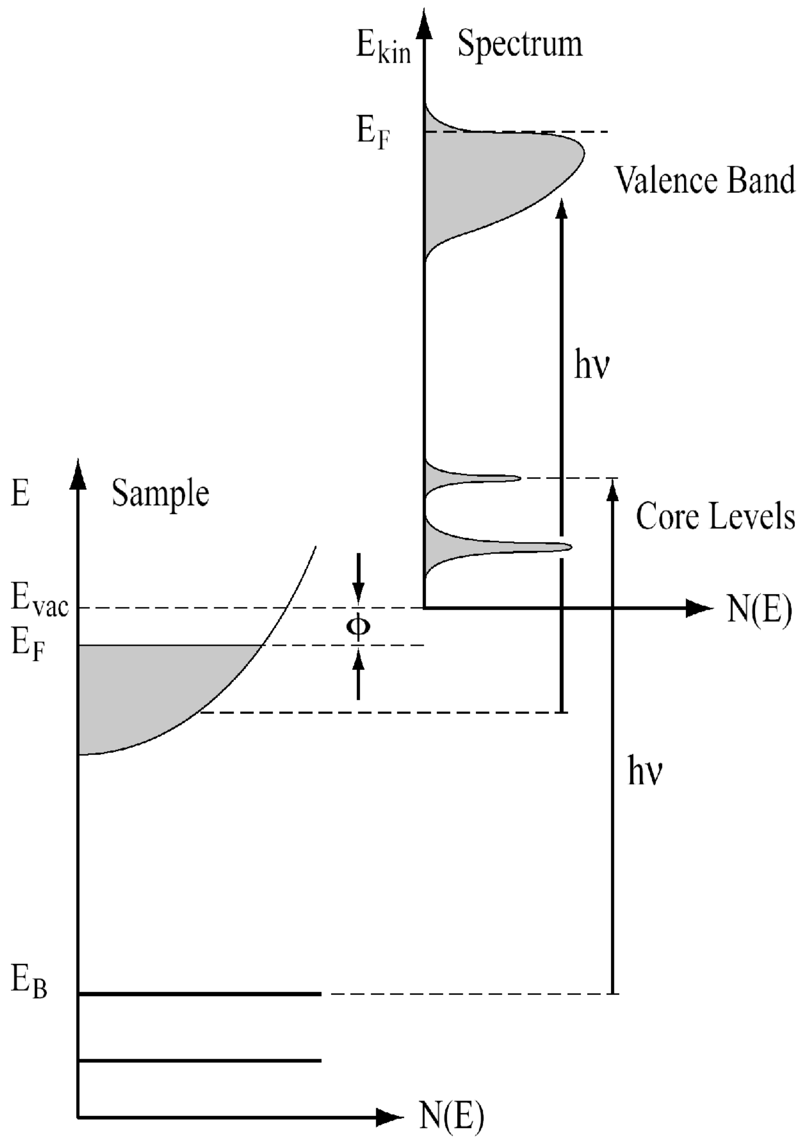
$$\Psi_i^N = \mathcal{A}\, \phi_i^{\mathbf{k}} \Psi_i^{N-1} \qquad \Psi_f^N = \mathcal{A}\, \phi_f^{\mathbf{k}} \Psi_f^{N-1}$$

$$\langle \Psi_f^N | H_{int} | \Psi_i^N \rangle = \langle \phi_f^{\mathbf{k}} | H_{int} | \phi_i^{\mathbf{k}} \rangle \langle \Psi_m^{N-1} | \Psi_i^{N-1} \rangle$$

Angle-Resolved Photoemission Spectroscopy



E_{kin}, ϑ, φ



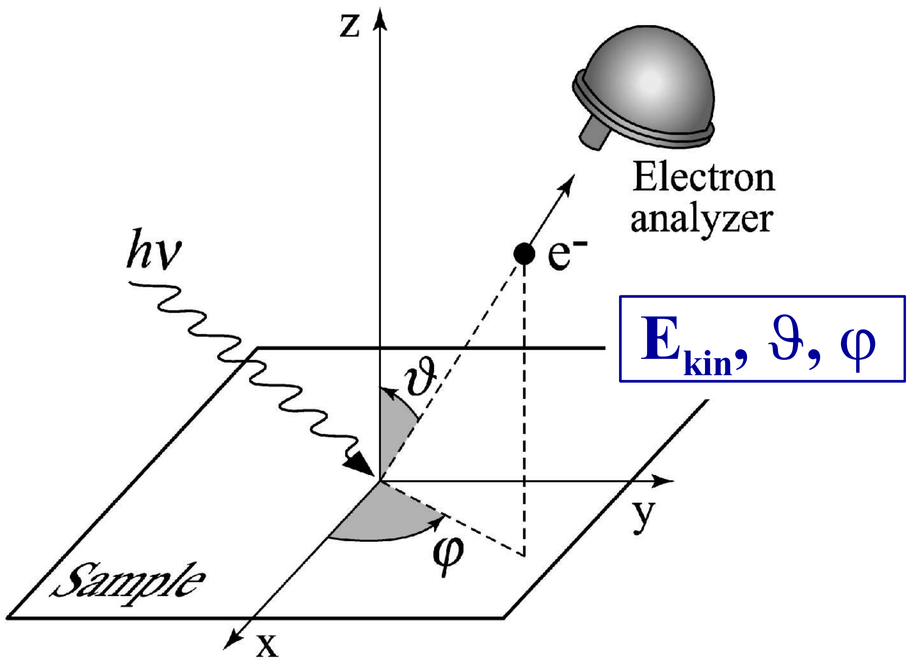
Energy Conservation

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

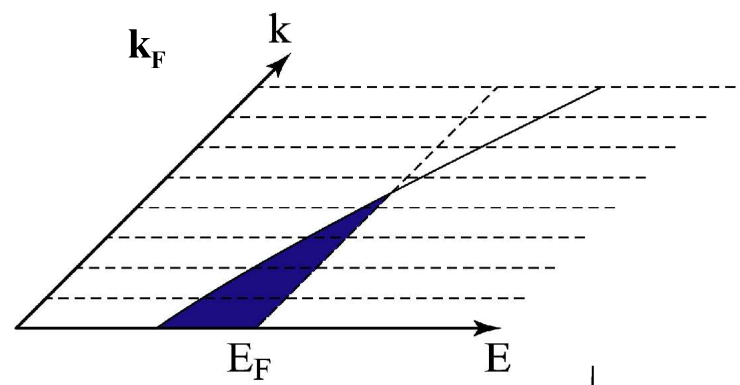
Momentum Conservation

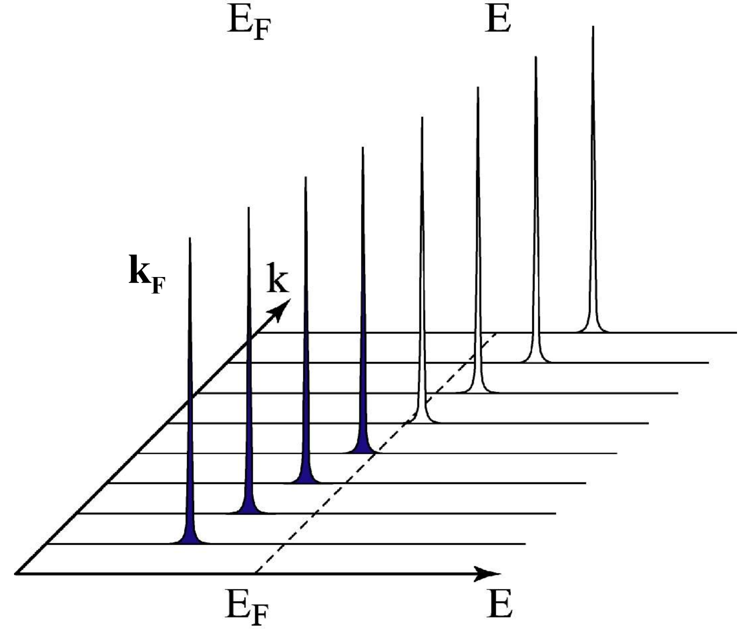
$$p_{\parallel} = \hbar k_{\parallel} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$

Angle-Resolved Photoemission Spectroscopy



Electrons in Reciprocal Space





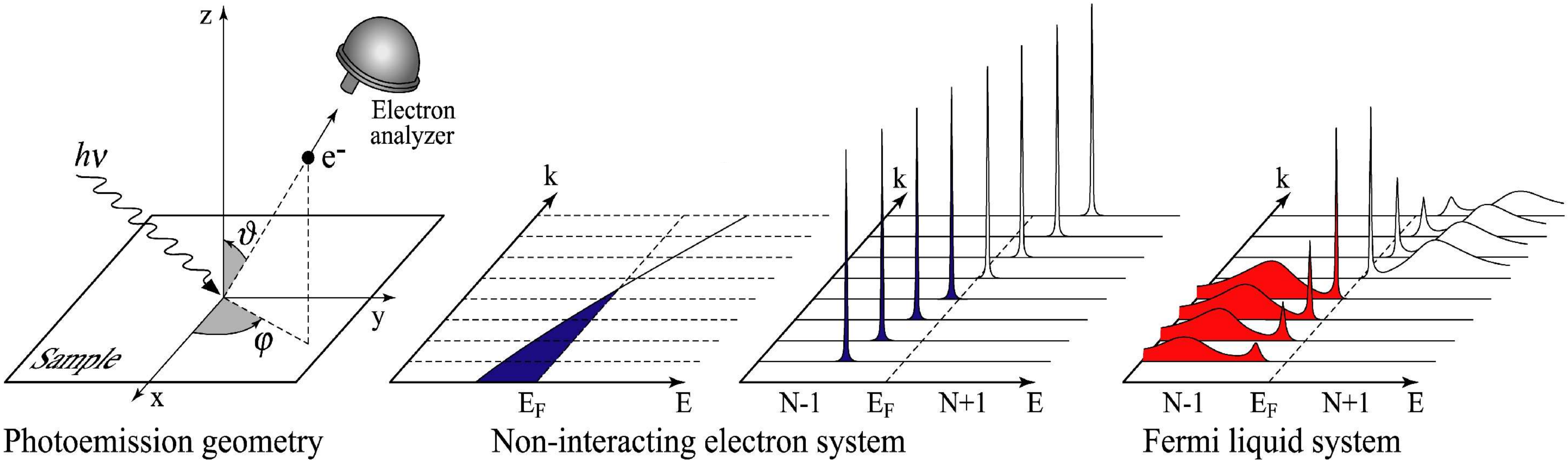
Energy Conservation

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

Momentum Conservation

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

Angle-Resolved Photoemission Spectroscopy



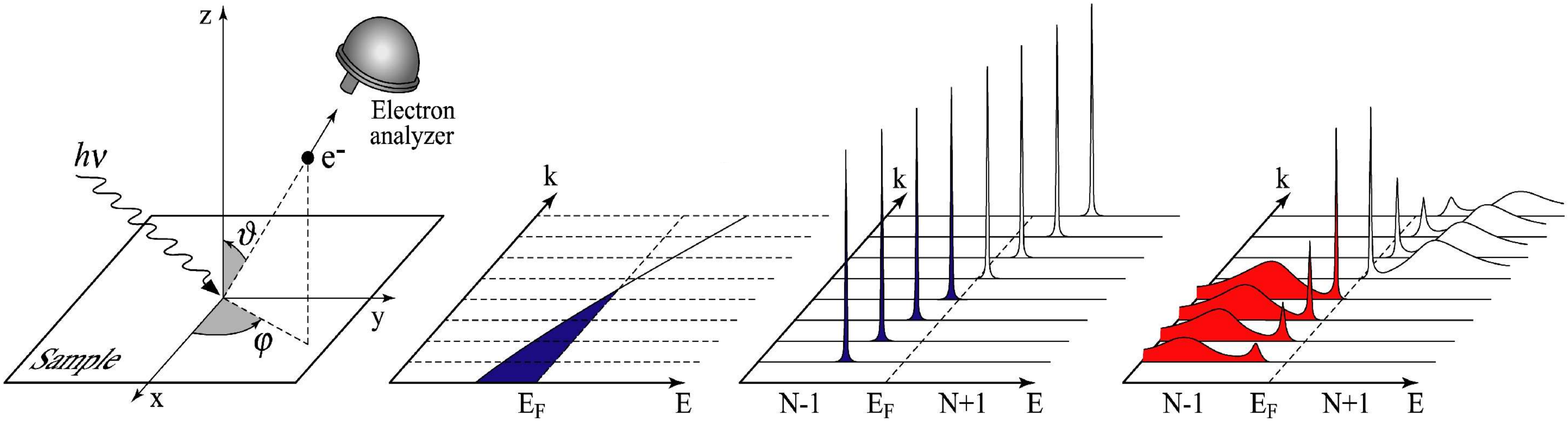
Photoemission intensity: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\,A(k,\omega)$

Single-particle spectral function

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

$\Sigma(k,\omega)$: the "self-energy" - captures the effects of interactions

Angle-Resolved Photoemission Spectroscopy



Photoemission geometry

Non-interacting electron system

Fermi liquid system

Photoemission intensity: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\,A(k,\omega)$

Non-interacting

$$A(\mathbf{k},\omega)=\delta(\omega-\epsilon_k)$$

No Renormalization

Infinite lifetime

Fermi Liquid

$$A(\mathbf{k},\omega)=Z_{\mathbf{k}}\frac{\Gamma_{\mathbf{k}}/\pi}{(\omega-\varepsilon_{\mathbf{k}})^2+\Gamma_{\mathbf{k}}^2}+A_{inc}$$

$$m^*>m \qquad |\varepsilon_{\mathbf{k}}|<|\epsilon_{\mathbf{k}}|$$

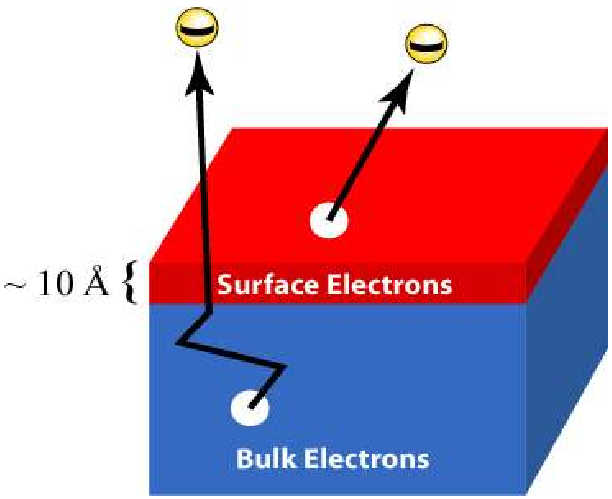
$$\tau_{\mathbf{k}}=1/\Gamma_{\mathbf{k}}$$

ARPES: advantages and limitations

Advantages

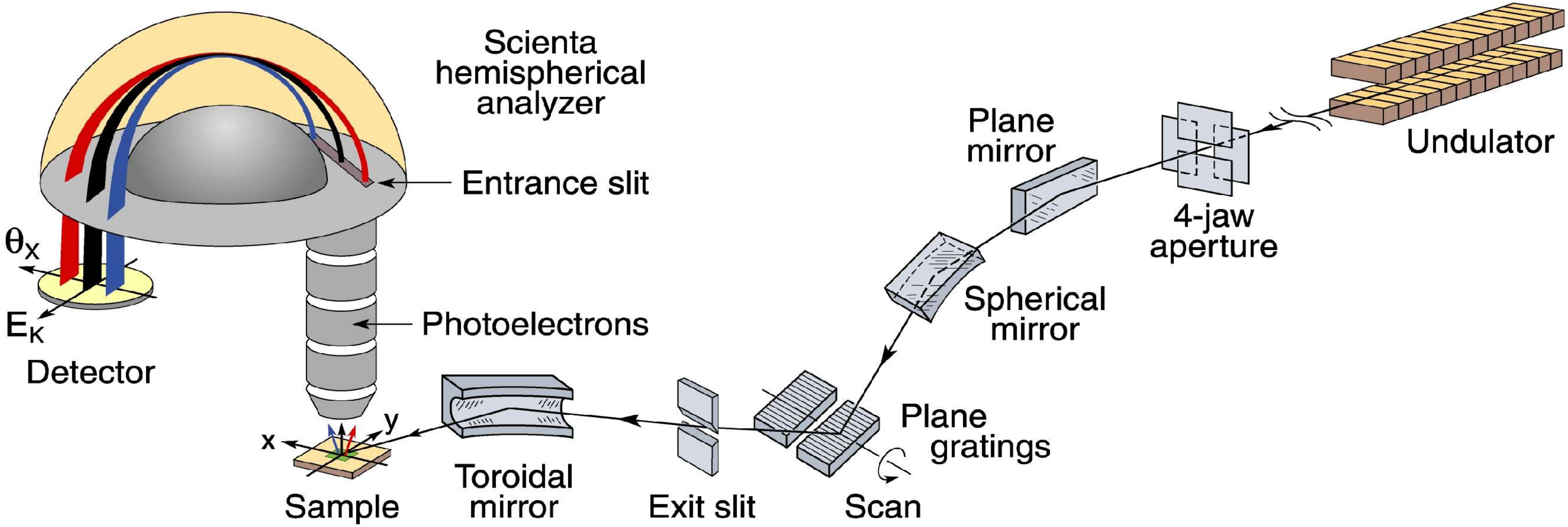
- **Direct information about electronic states!**
- Straightforward comparison with theory - little or no modelling.
- High-resolution information about **BOTH energy** and **momentum**
- **Surface-sensitive probe**
- Sensitive to “many-body” effects
- Can be applied to small samples (100 μm x 100 μm x 10 nm)

Limitations



- **Not bulk sensitive**
- Requires clean, atomically flat surfaces in **ultra-high vacuum**
- Cannot be studied as a function of pressure or magnetic field

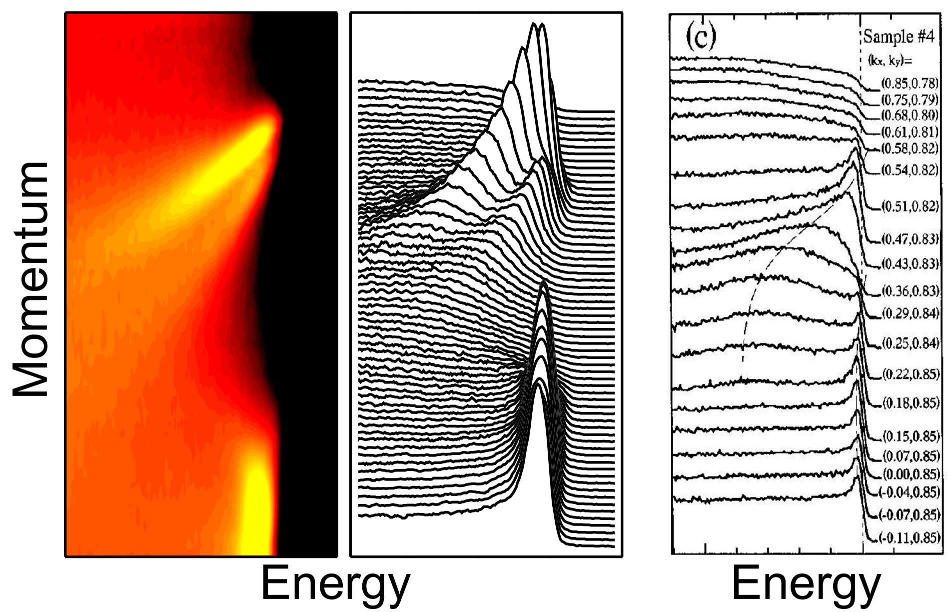
Angle-Resolved Photoemission Spectroscopy



Parallel multi-angle recording

- Improved **energy resolution**
- Improved **momentum resolution**
- Improved **data-acquisition efficiency**

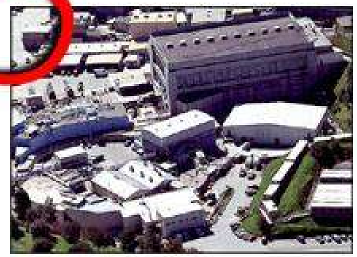
	ΔE *(meV)*	$\Delta\theta$
past	*20-40*	*2°*
now	*2-10*	*0.2°*



SSRL Beamline 5-4 : NIM / Scienta System

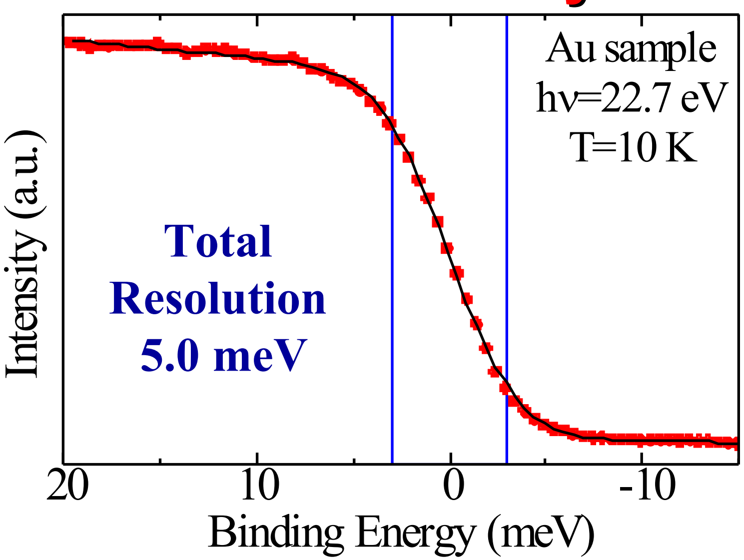
STANFORD SYNCHROTRON RADIATION LABORATORY

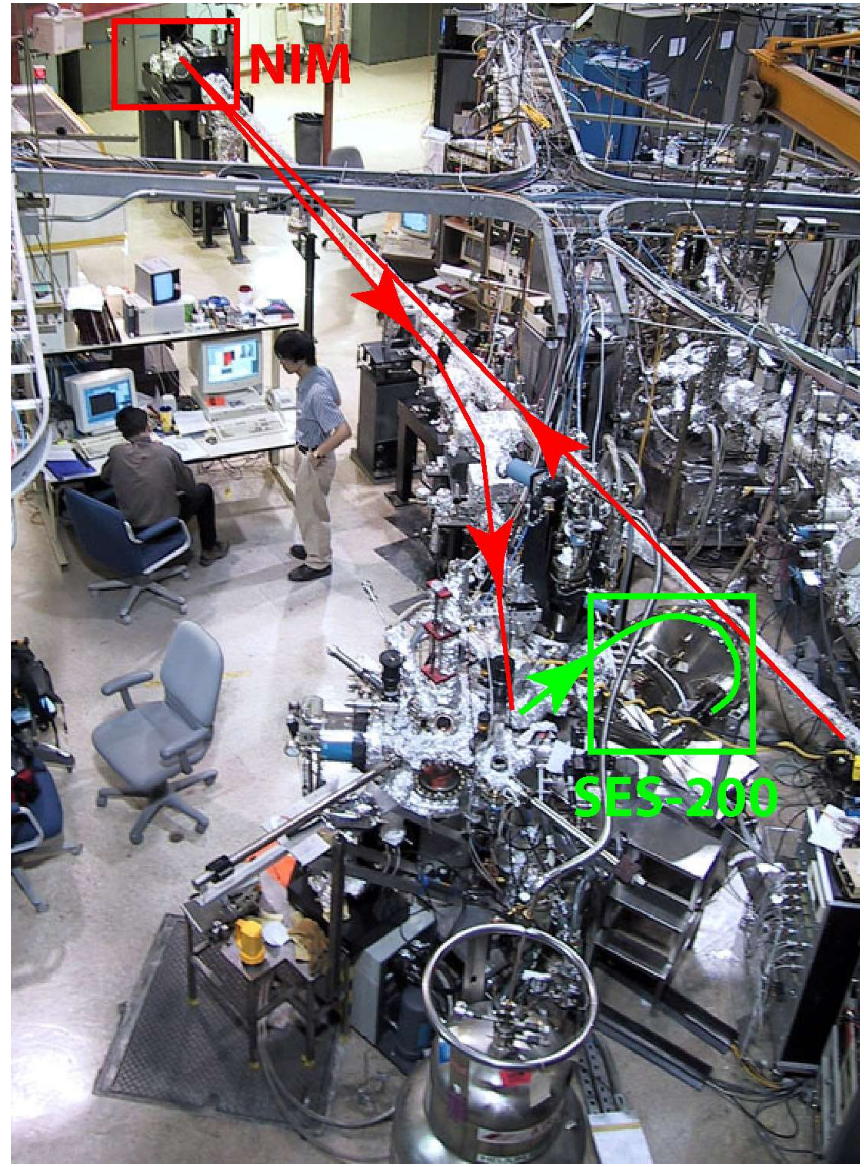
SSRL



ΔE (meV)	Δθ
2-10	*0.2°*

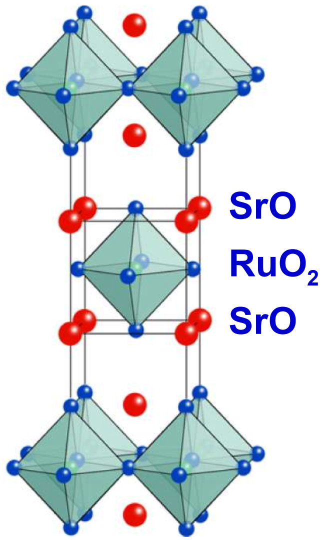
NIM/SCIENTA System





Sr_2RuO_4: basic properties

2D perovskite

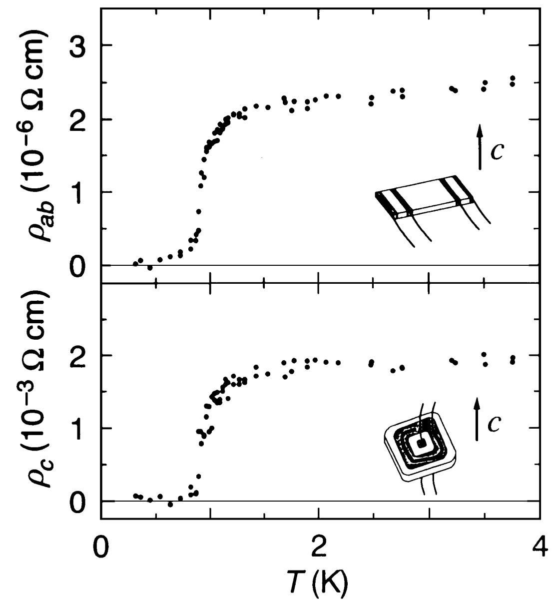


Unconventional superconductivity

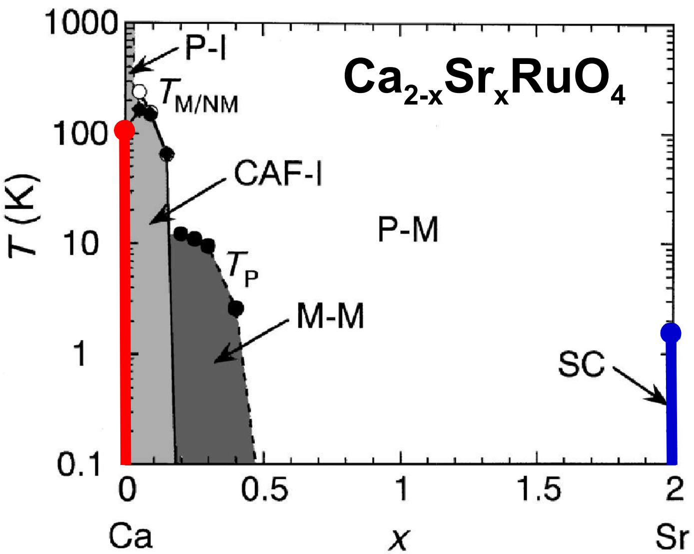
- Pairing mechanism ?
- Order parameter ?
- FM-AF fluctuations ?

Rice & Sigrist, JPCM **7**, L643 (1995)

Maeno *et al*., Nature **372**, 532 (1994)



Nakatsuji & Maeno, PRL **84**, 2666 (2000)



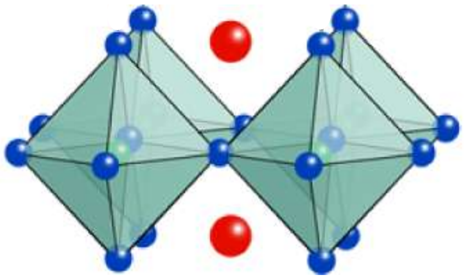
Lattice-magnetism interplay
Orbital degrees of freedom

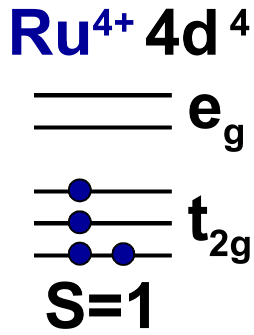
Sr_2RuO_4 : 2D **Fermi Liquid** (ρ_c/ρ_{ab}=850)

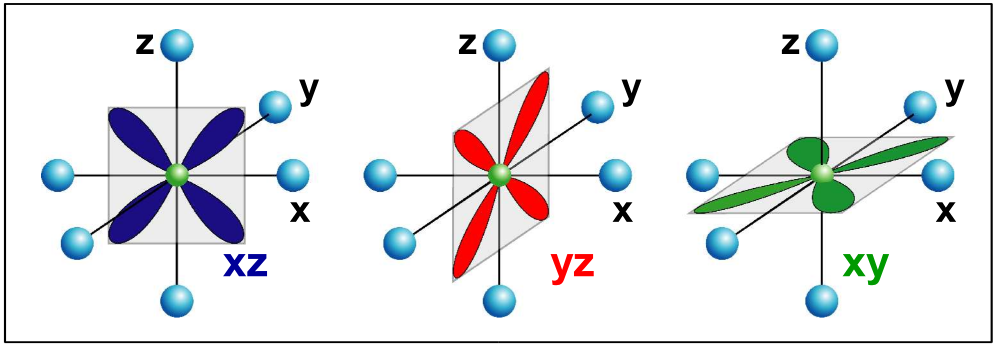
Ca_2RuO_4 : insulating **Anti-FerroMagnet**

$SrRuO_3$: metallic **FerroMagnet**

Low-Energy Electronic structure of Sr_2RuO_4

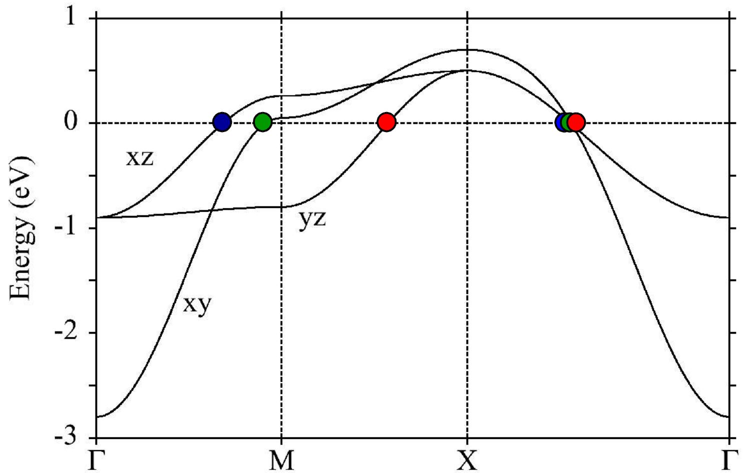




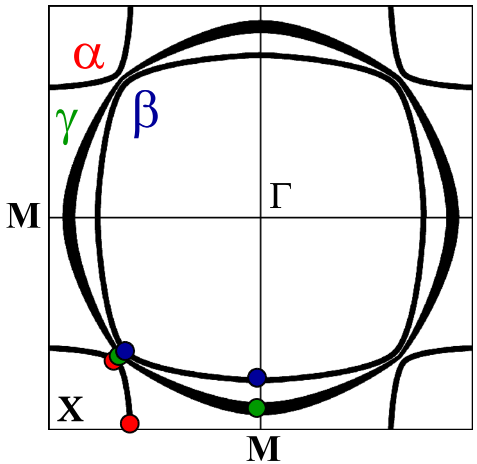


▶ Band structure calculation: **3** $\mathbf{t_{2g}}$ bands crossing $\mathbf{E_F}$

➡ 3 sheets of FS { α (hole-like)
β and γ (electron-like)



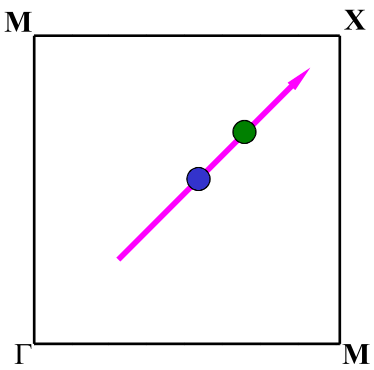
A. Liebsch *et al*, PRL **84**, 1591 (2000)

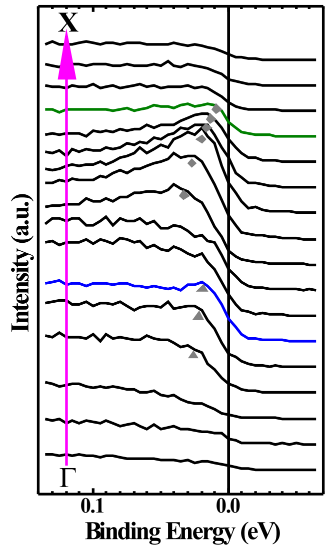


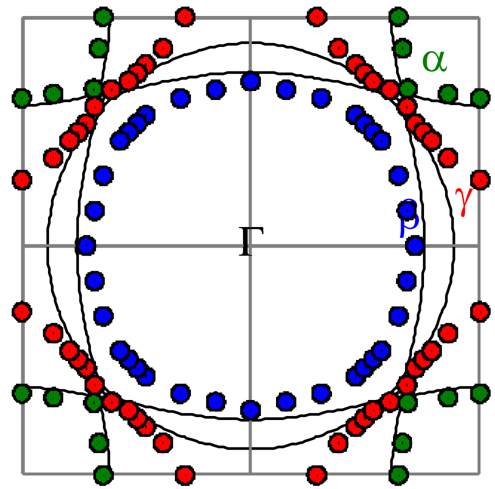
I.I. Mazin *et al*, PRL **79**, 733 (1997)

Fermi Surface Topology of Sr_2RuO_4

ARPES : circa 1996

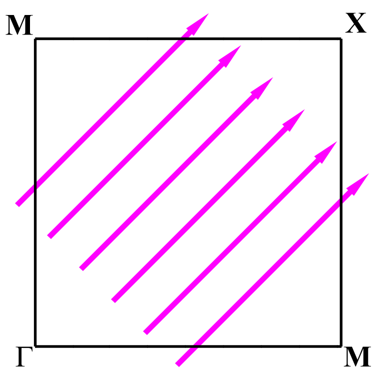


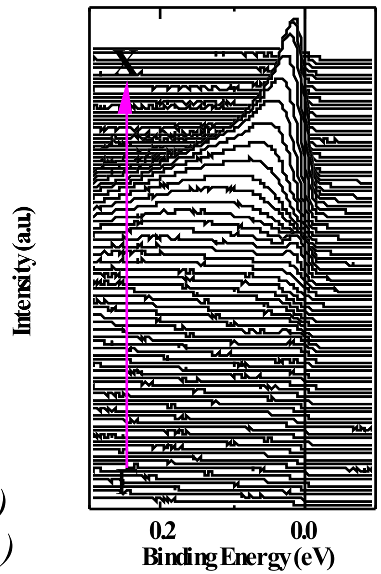


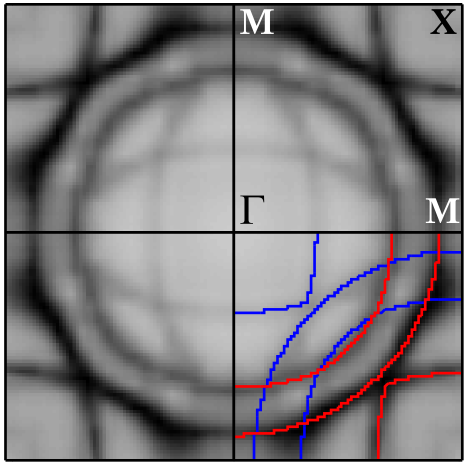


*D.J. Singh, PRB **52**, 1358 (1995)*

ARPES : present day

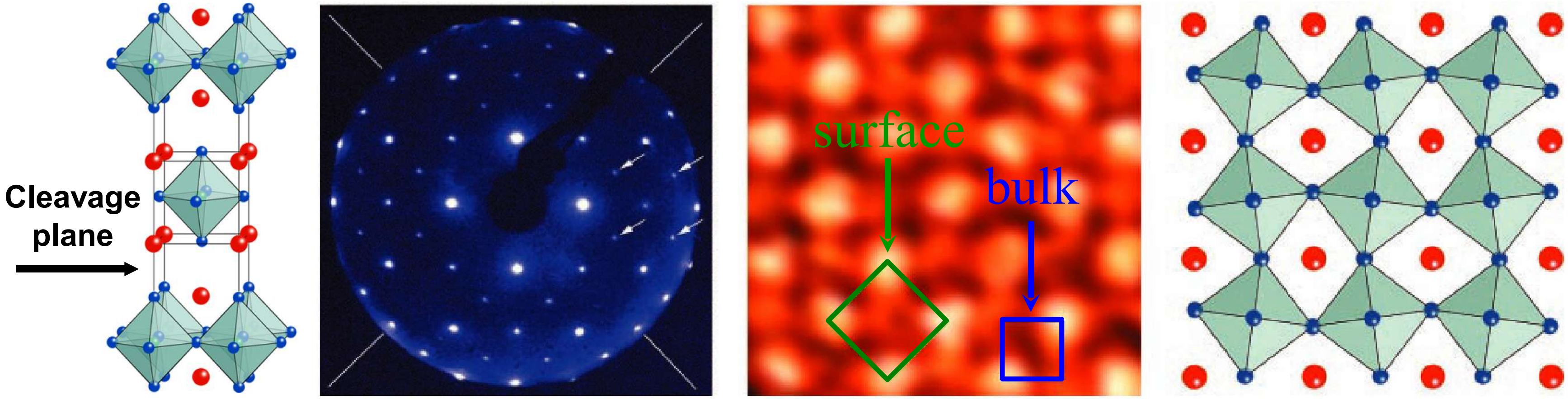






*A. Damascelli et al., PRL **85**, 5194 (2000)*
*K.M. Shen et al., PRB **64**, 180502R (2001)*

Surface reconstruction of cleaved Sr_2RuO_4

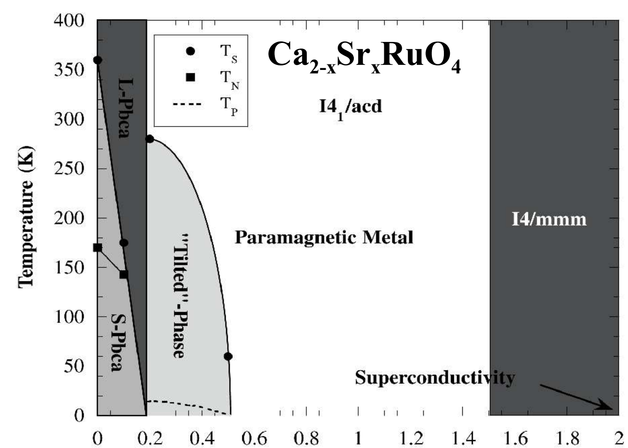


R. Matzdorf *et al.*, Science **289**, 746 (2000)

Rotation of the RuO_6 octahedra around the c axis

Soft phonon branch

Structural instability of $Ca_{2-x}Sr_xRuO_4$



O. Friedt *et al.*, PRB **63**, 174432 (2001)

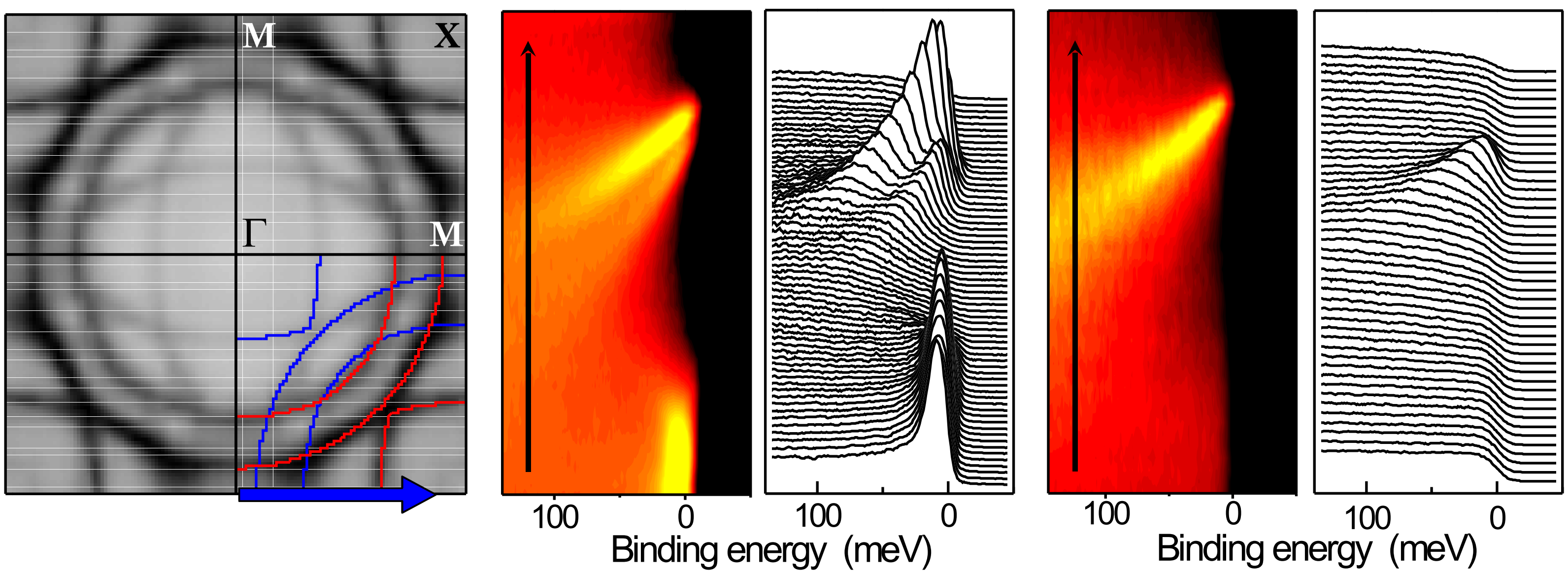
Surface electronic structure of Sr_2RuO_4

On samples cleaved at **180 K** the **surface**-related features are **suppressed**

E_F mapping ±10 meV

Cold cleave T=10 K

Hot cleave T=180 K

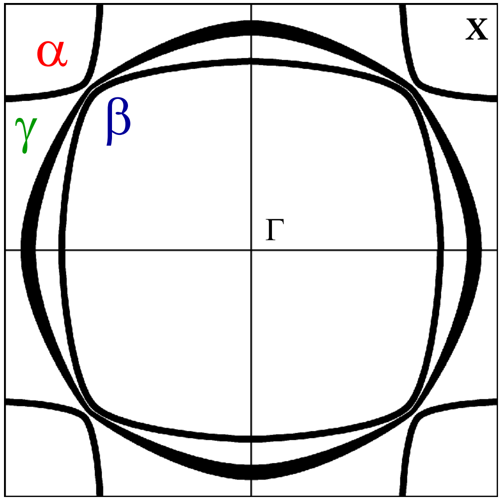


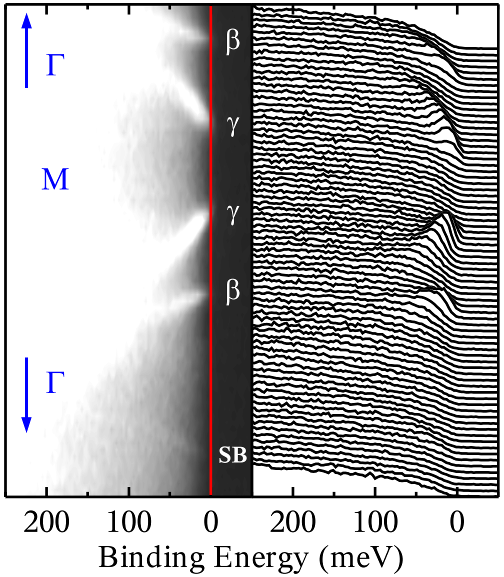
Bulk electronic structure of Sr_2RuO_4

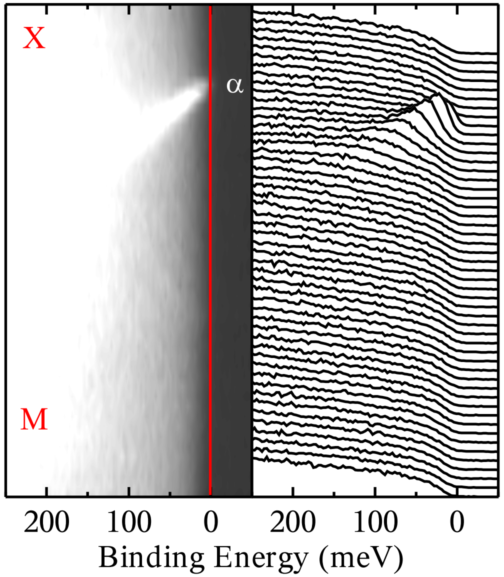
On samples cleaved at **180 K** the **surface**-related features are **suppressed**

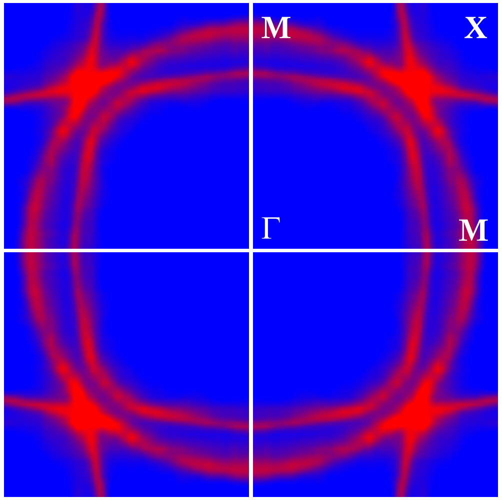
Thus, the **ARPES - FS** is consistent with **de Haas-van Alphen** and **LDA** results

I.I. Mazin *et al.*, PRL **79**, 733 (1997)





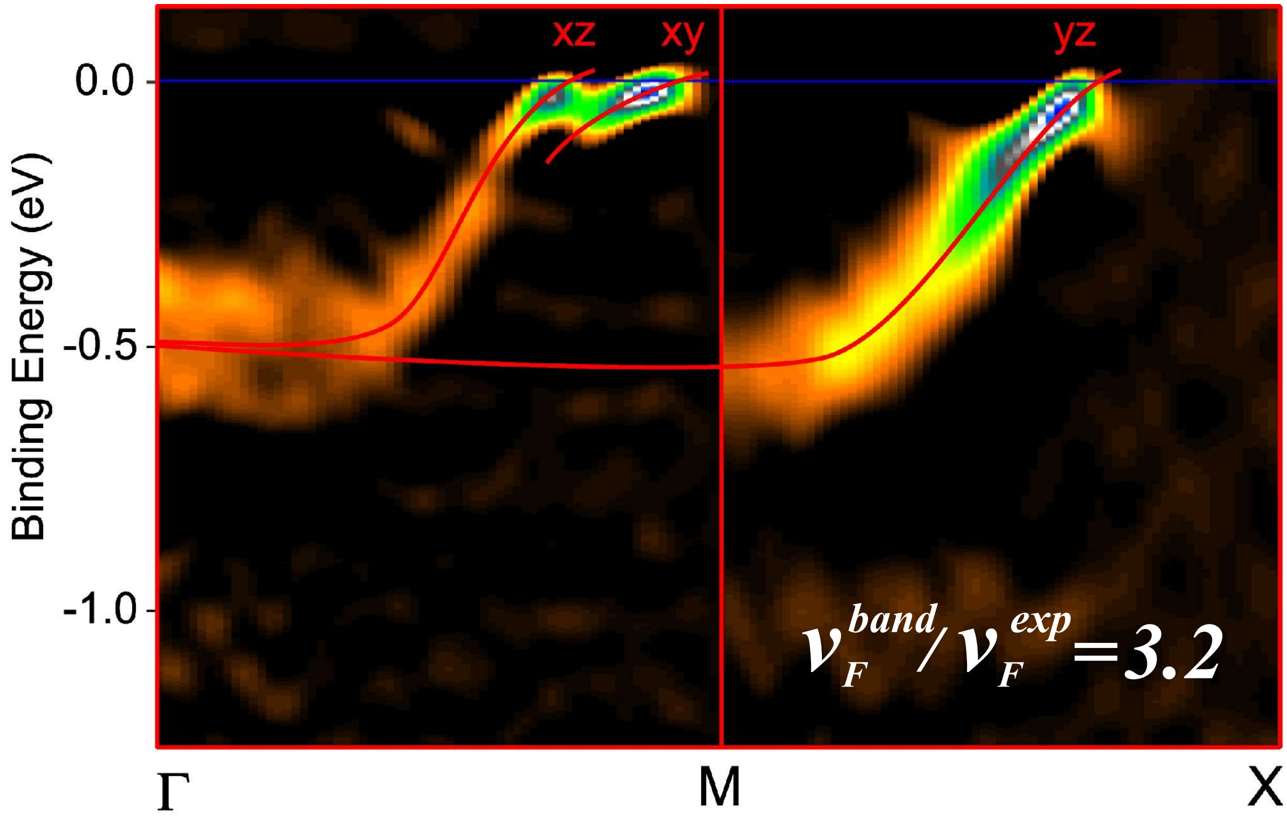




Sr_2RuO_4 cleaved at 180 K

T= 10 K hν=28 eV

Dispersion of the bulk electronic bands

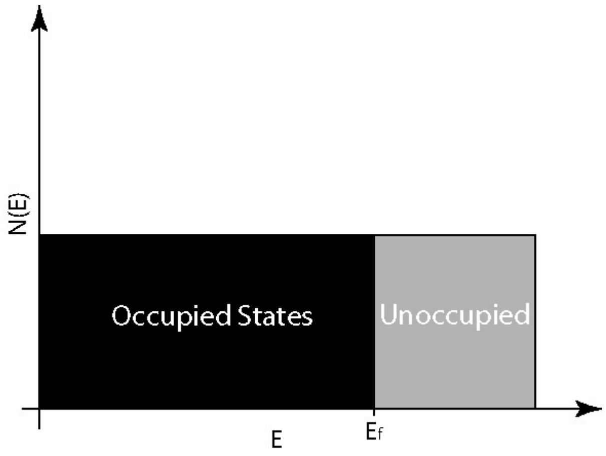


Experiment compares well with LDA+U calculations

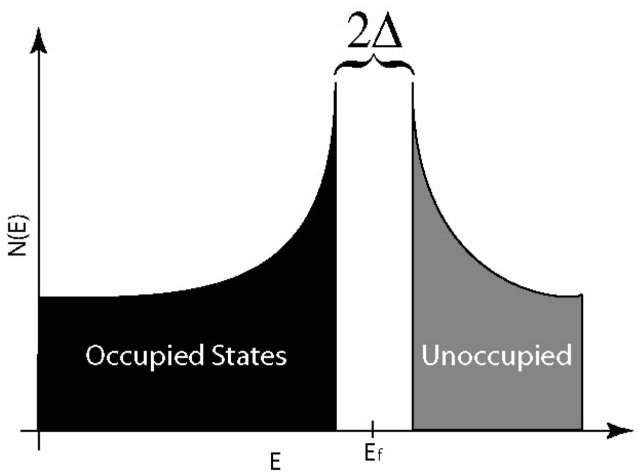
A. Liebsch & A. Lichtenstein, PRL **84**, 1591 (2000)

"Classic Low-temperature" Superconductors

Metallic Density of States

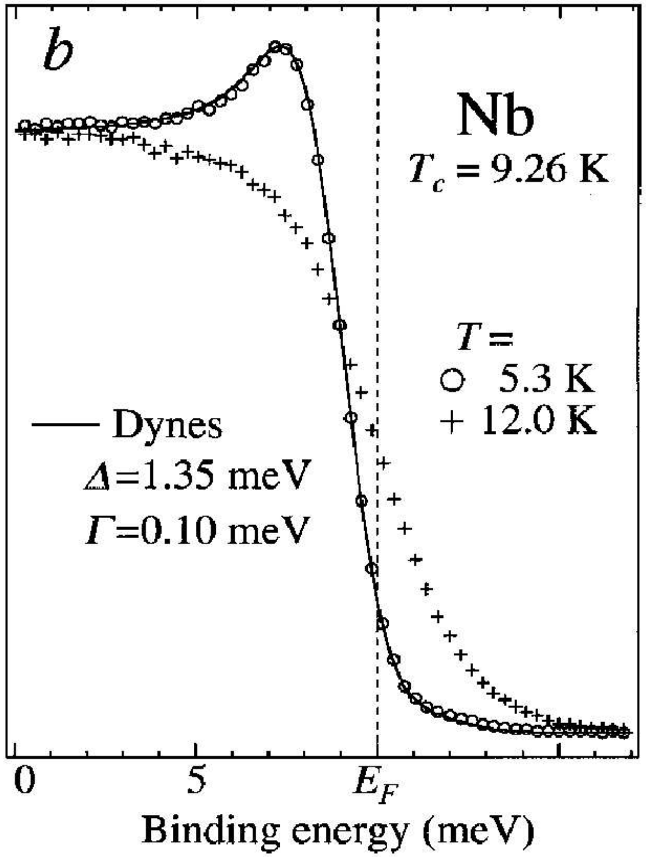


Superconducting Density of States



Superconductivity can only be seen on low energy scales and needs **high resolution**!

A. Chainani et al., PRL 85 (2000)

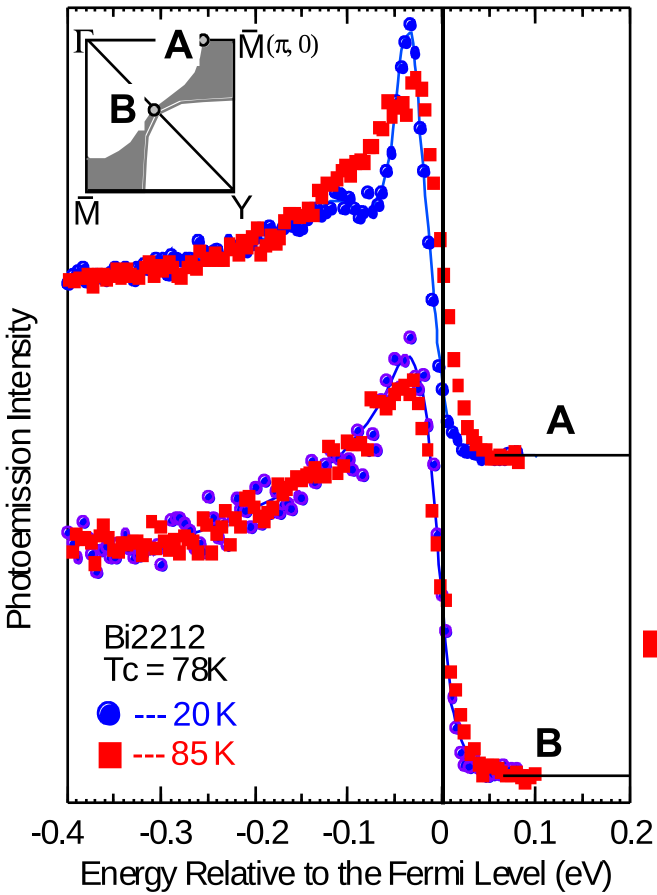


High-Temperature Superconductors

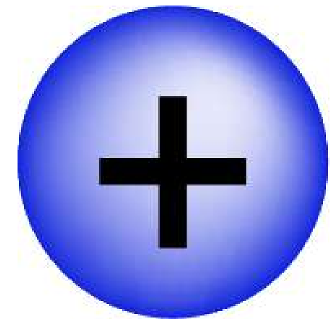
VOLUME 70, NUMBER 10 PHYSICAL REVIEW LETTERS 8 MARCH 1993

Anomalously Large Gap Anisotropy in the *a-b* Plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$

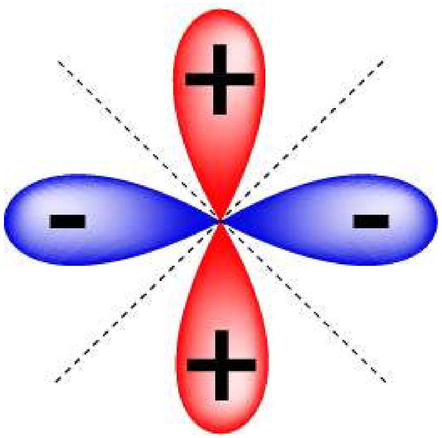
Z.-X. Shen,[1,2] D. S. Dessau,[1,2] B. O. Wells,[1,2,a] D. M. King,[2] W. E. Spicer,[2] A. J. Arko,[3] D. Marshall,[2] L. W. Lombardo,[1] A. Kapitulnik,[1] P. Dickinson,[1] S. Doniach,[1] J. DiCarlo,[1,2] A. G. Loeser,[1,2] and C. H. Park[1,2]



"*s*-wave"

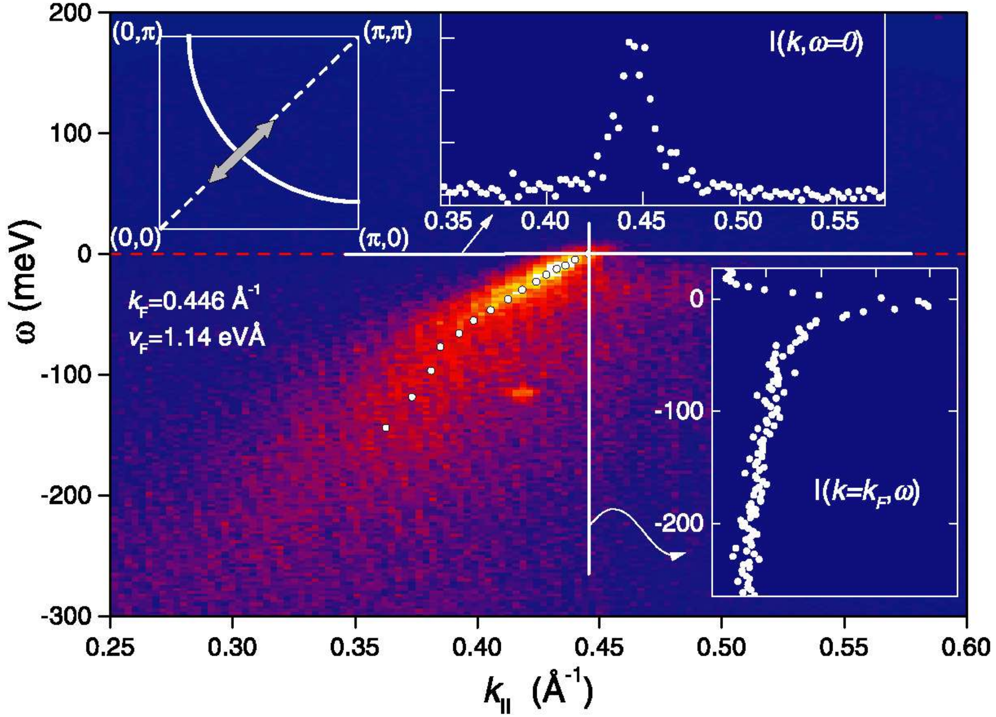


"*d*-wave"



Many Body effects in the Quasiparticle Dispersion

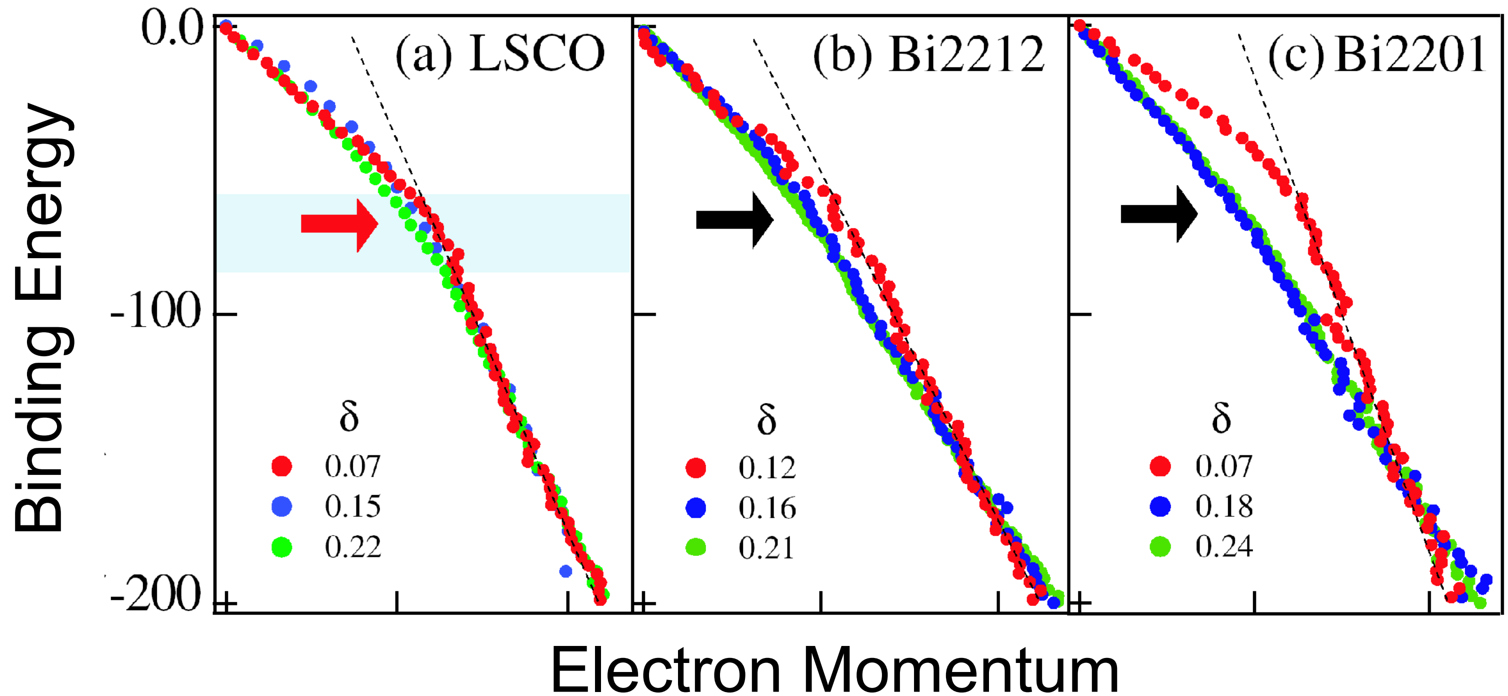
Valla *et al.*, Science **285**, 2110 (1999)



Mechanism for High-T_c { **Magnetic fluctuations ?**
Electron-phonon coupling ?

Many Body effects in the Quasiparticle Dispersion

Lanzara *et al.*, Nature **412**, 510



Mechanism for High-T_c { **Magnetic fluctuations ?** / **Electron-phonon coupling ?**

Conclusions

ARPES results from Sr_2RuO_4

- **FS in unprecedented detail**
- **Fermi velocity and effective mass**
- **Investigate the issue of surface FM**

- **Superconducting (d-wave) gap**
- **Many-body effects in the QP dispersion**

ARPES is a powerful tool for the study of the electronic structure of complex materials

A. Damascelli *et al.*, PRL **85**, 5194 (2000); PRL **87**, 239702 (2001)
K.M. Shen, A. Damascelli, *et al.*, PRB **64**, 180502(R) (2001)

For a review article see:

A. Damascelli, Z. Hussain, and Z.-X Shen, Rev. Mod. Phys. **75**, 473 (2003)