Why we need to model APRES
&
Why we need a modular approach

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Need: only modeling will bring us further

- ARPES is result of many coupled aspects

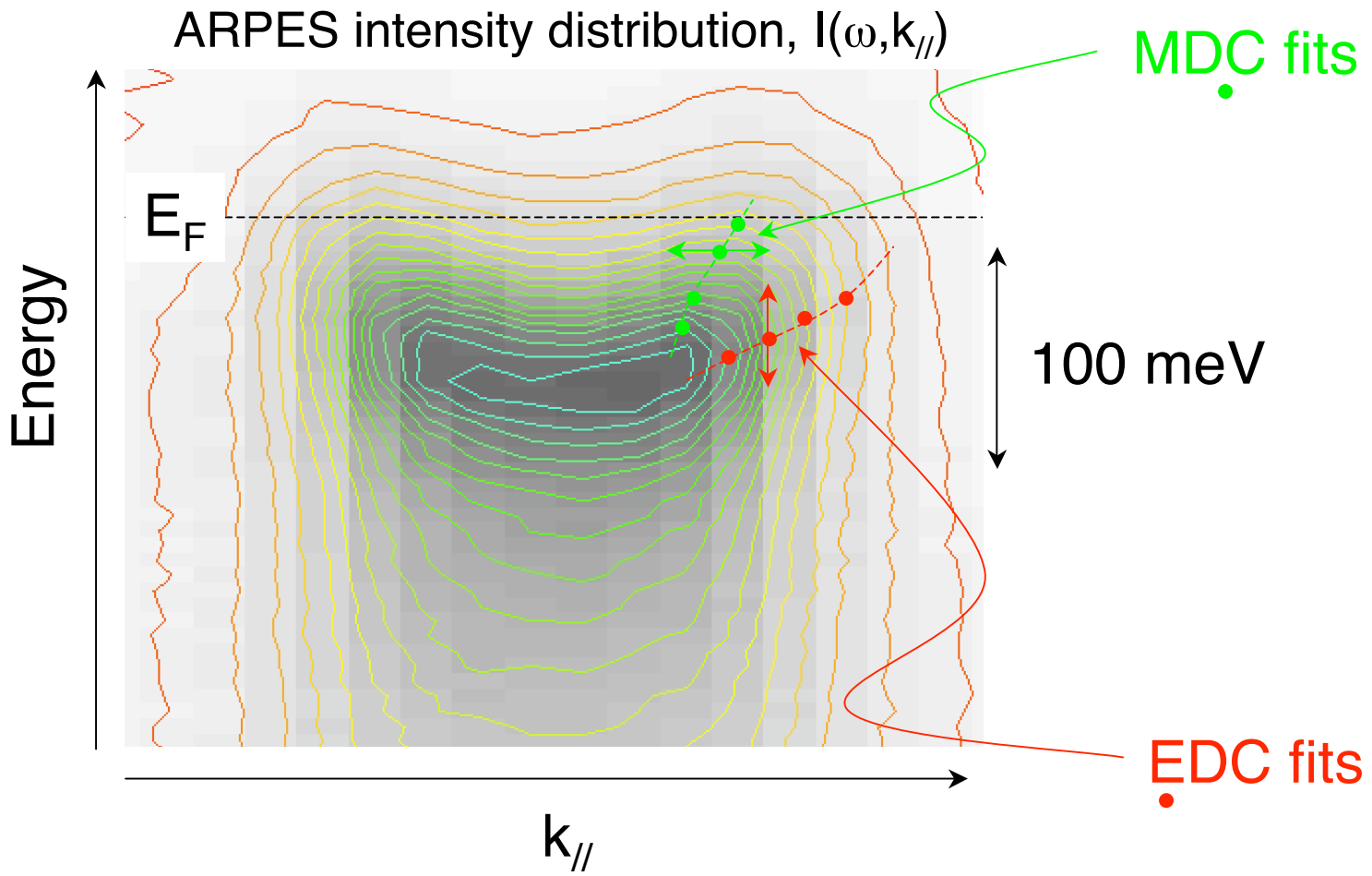
Modular approach: separately understand

- physics of initial state
- physics of final state
- physics of coupling (matrix elements)

C. Monney, H. Cercellier, C. Battaglia, L. Despont, M.G. Garnier

What is the quasi particle dispersion? (todays analysis!)
What are the Fermi vectors?

… only modeling will bring us further…



What is the truth? … k_F?

Interpret line shape as

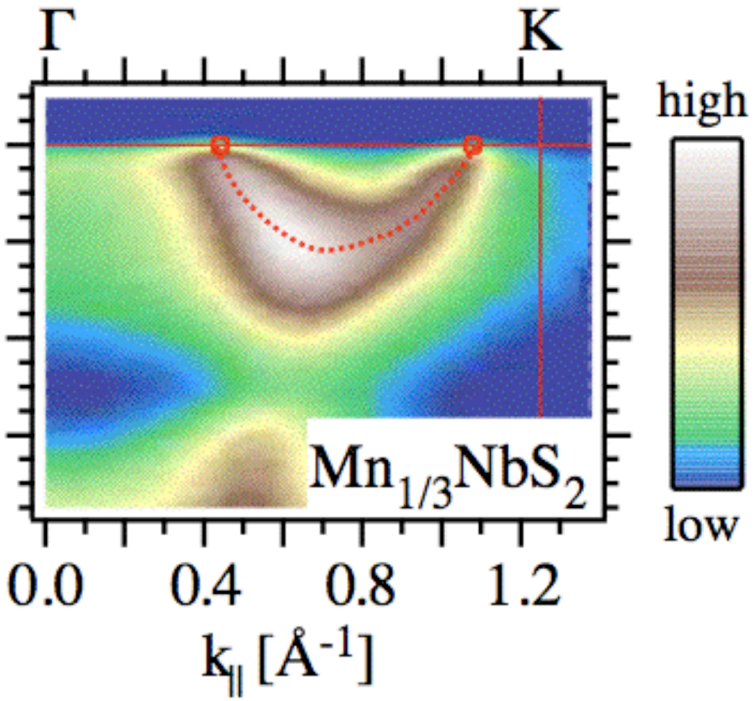
$$A(\vec{k},\omega) = \frac{1}{\pi} \frac{\Im m\Sigma(\vec{k},\omega)}{|\omega - \epsilon_{\vec{k}} - \Re e\Sigma(\vec{k},\omega)|^2 + |\Im m\Sigma(\vec{k},\omega)|^2}$$

Peak width: inverse life time

Band dispersion

Self Energy

$$\Sigma(\vec{k},\omega)$$



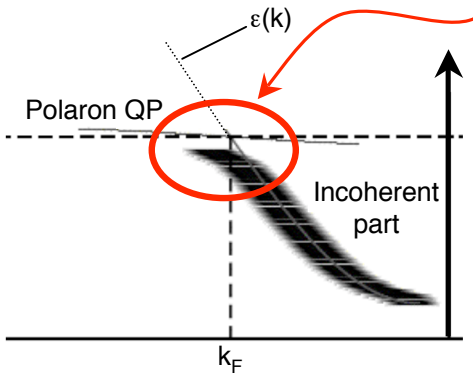
… only modeling will bring us further…

C. Battaglia et al.

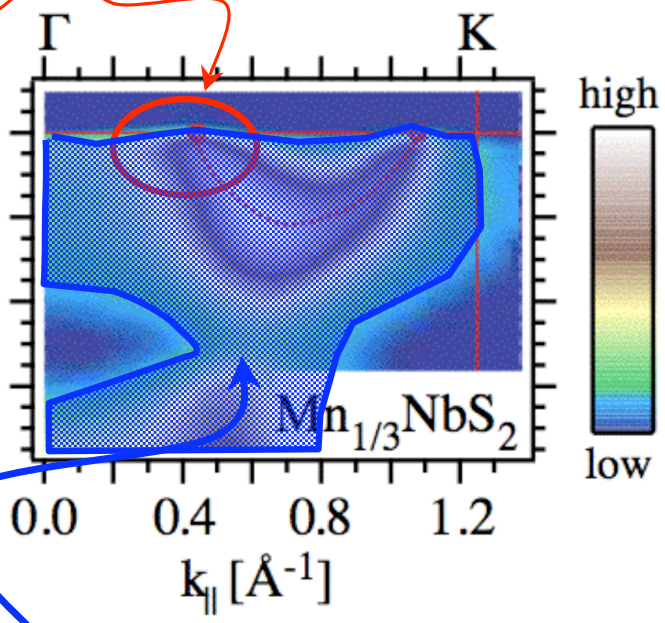
arXiv:cond-mat/0611215 v2 10 Nov 2006

… only modeling will bring us further…

A(k,ω) may be sufficient for local (in ω and $k_{//}$) analysis



Sketch of A(k,ω) derived from numerical solution of Holstein problem: Hohenadler PRB 71 '05



Intensity distribution over large areas
Needs inclusion of matrix elements

AND: k_{perp} integration needs to be considered including Matrix elements
for the residual 3D character of quasi-2D materials

Influence of the Third Dimension of Quasi-Two-Dimensional Cuprate Superconductors on Angle-Resolved Photoemission Spectra

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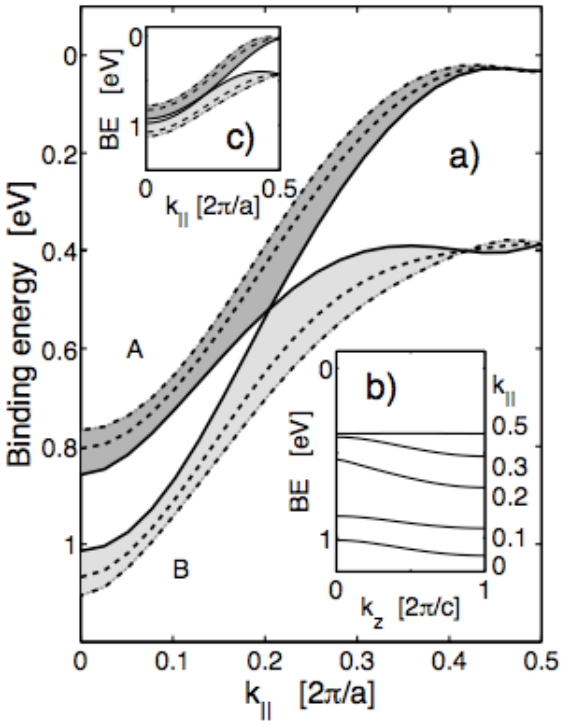
… only modeling will bring us further…



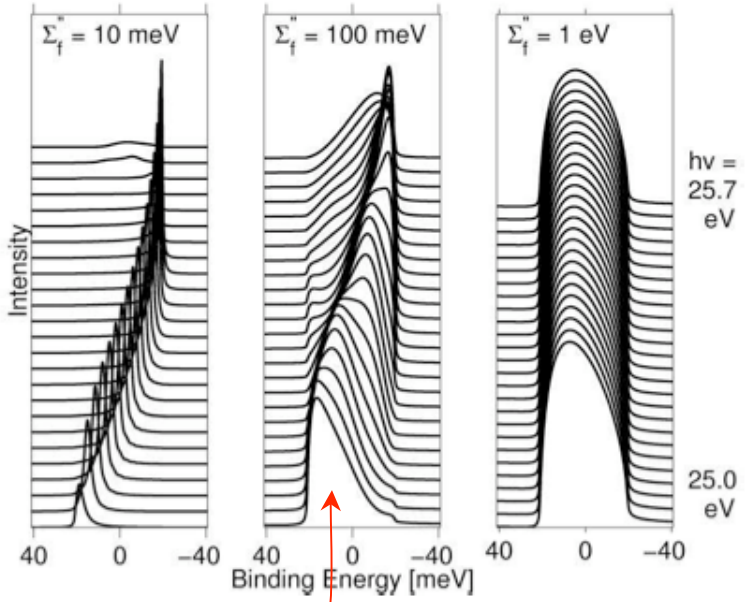


FIG. 2: Simulated ARPES lineshapes (EDCs) in Bi2212 for a series of photon energies ($h\nu = 25 - 25.7$ eV) at a *fixed* $k_{\|} = (0.34, 0.09)2\pi/a$-point using three different values of the final state broadening given by the indicated imaginary parts of the self-energy, Σ_f''. In order to highlight the influence of k_z-dispersion, the initial state broadening is chosen to be very small, $\Sigma_i'' = 0.2$ meV.[17]

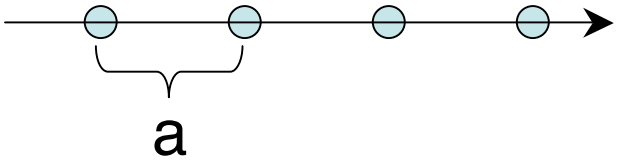
Line shape?

How to know what is A(k,ω) & what is from different k_{perp}

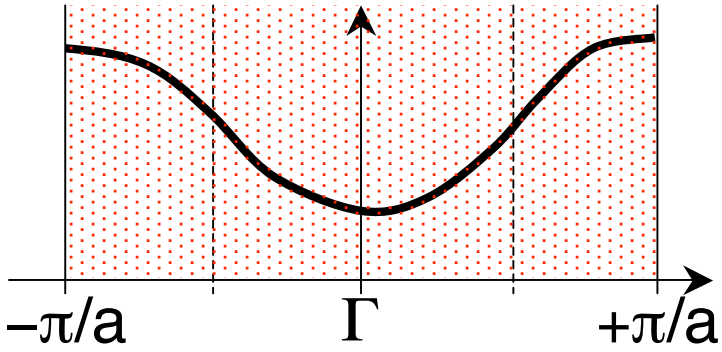
Modulation of the crystal potential

… only modeling will bring us further…

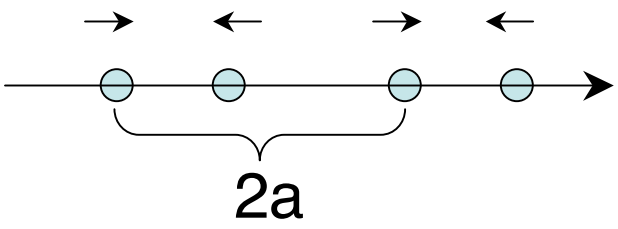
Real space



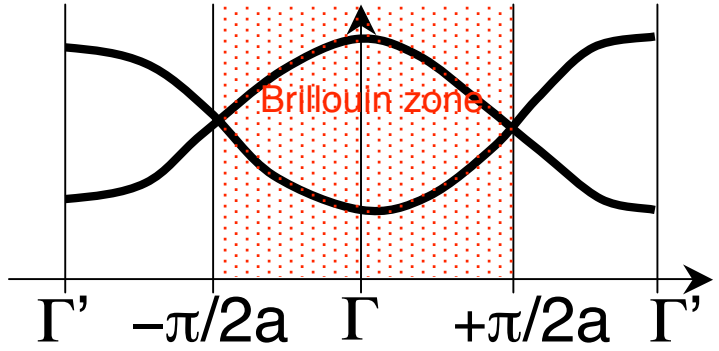
Reciprocal space



Real space



Reciprocal space

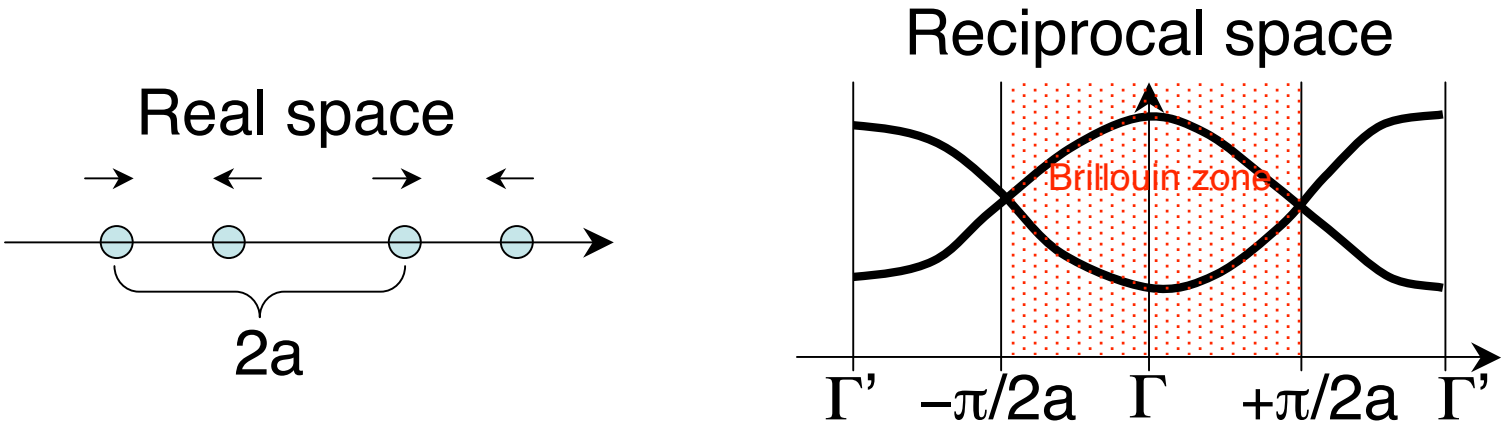


Even for an infinitesimal lattice modulation

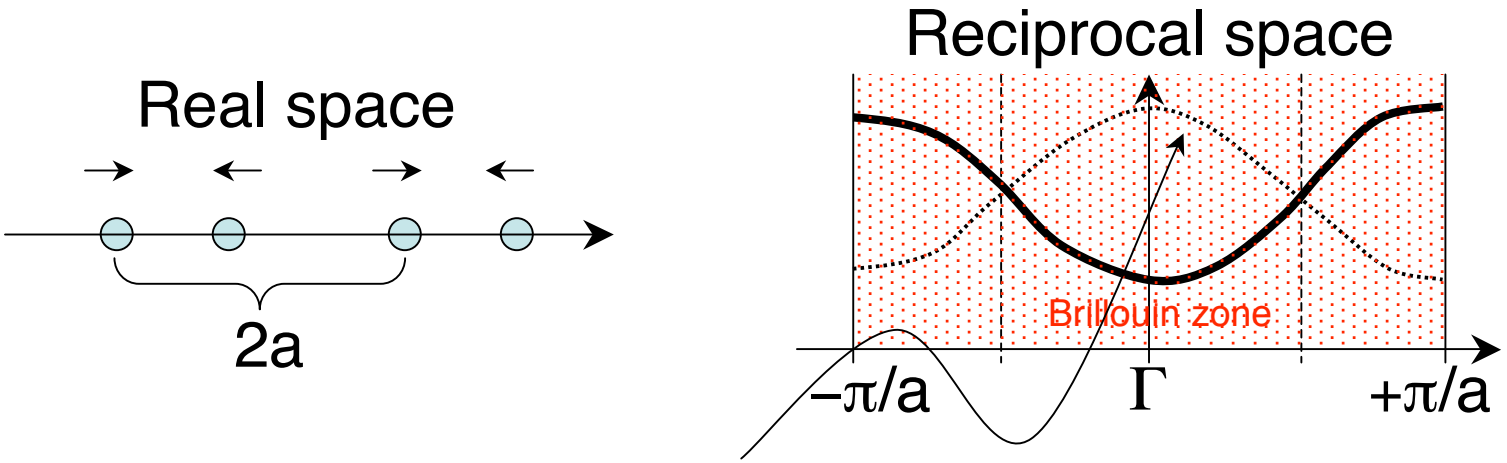
Band structure is immediately reconstructed

Modulation of the crystal potential

… only modeling will bring us further…



In practice… the experiment may show …



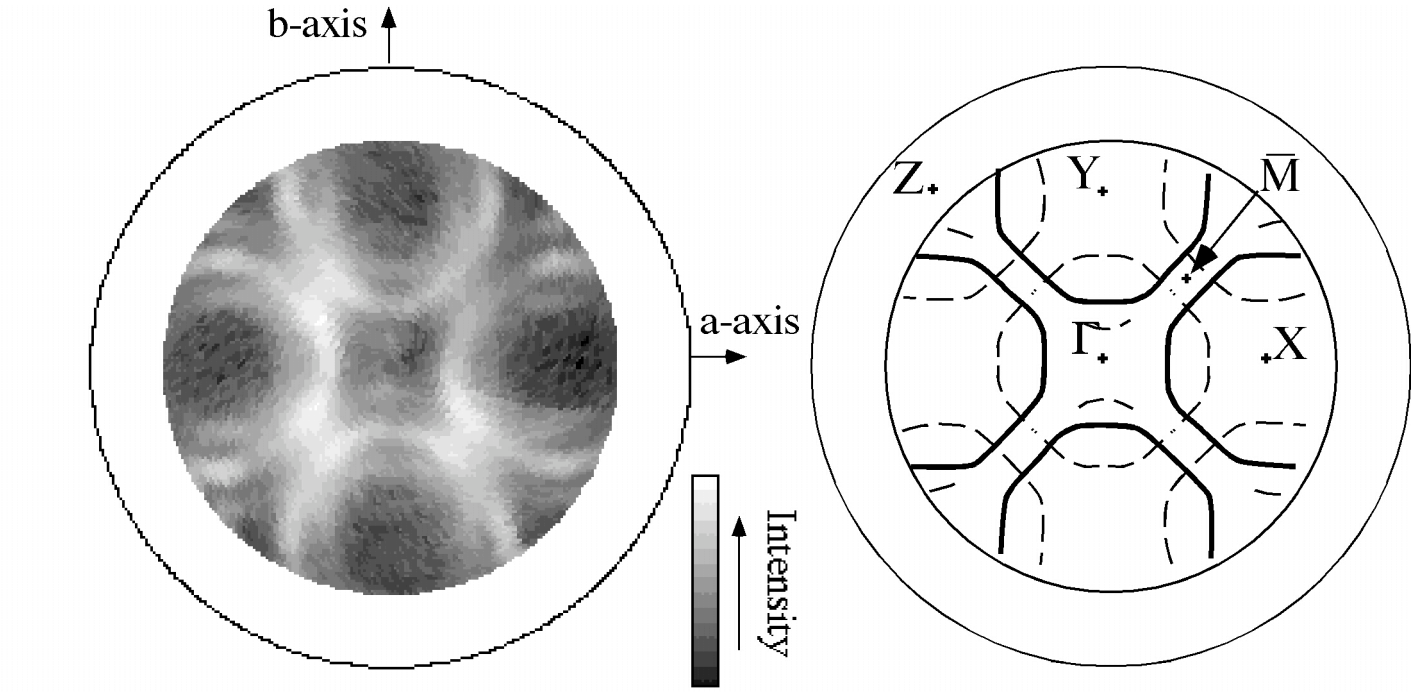
…**negligible** spectral weight on Umklapp bands

… unless there is strong electronic coupling with the new wave vector (see H. Cercellier)

Quasi 2D system, a well-known example …

… only modeling will bring us further…

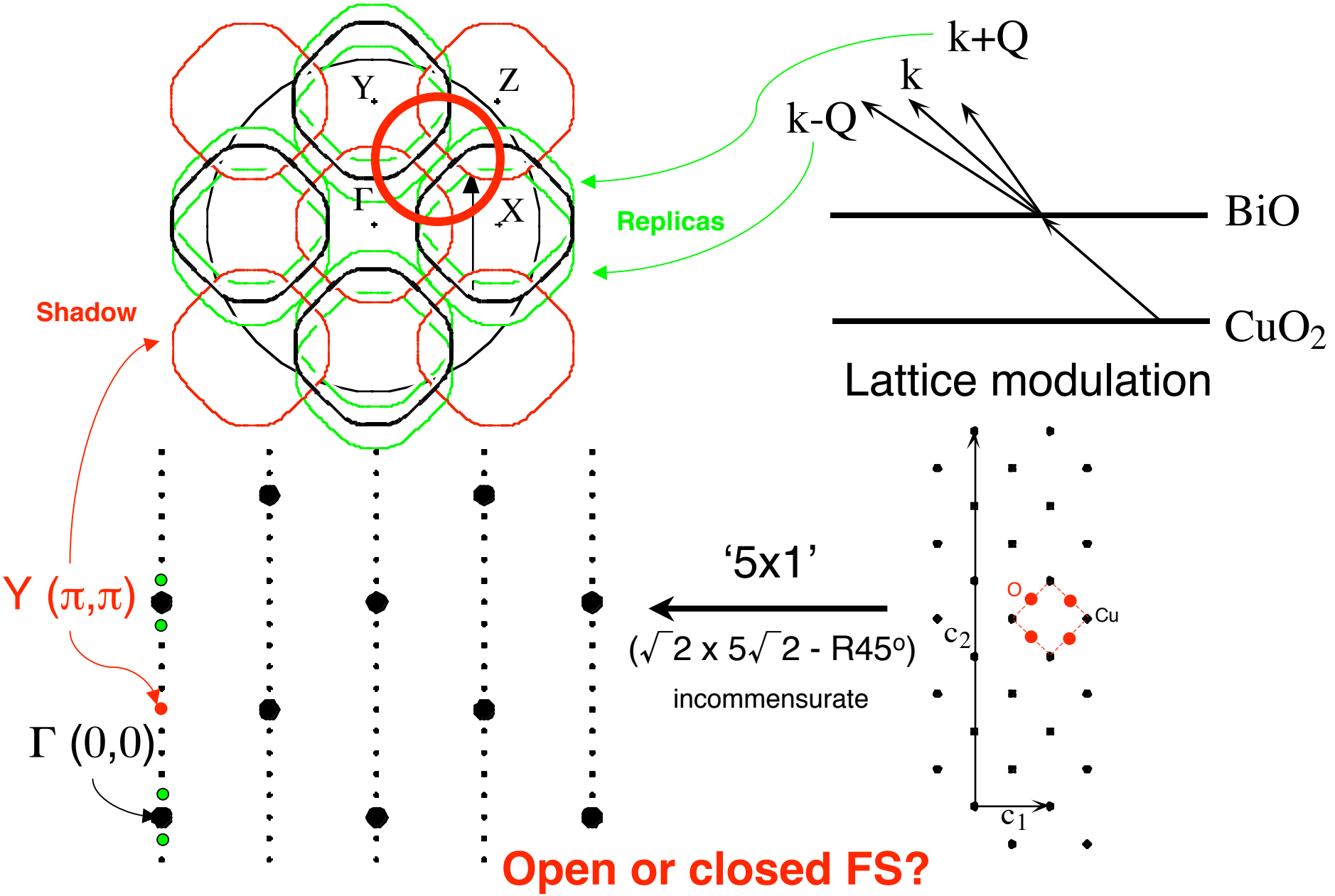
Bi2212: The joys of Fermi surface mapping …

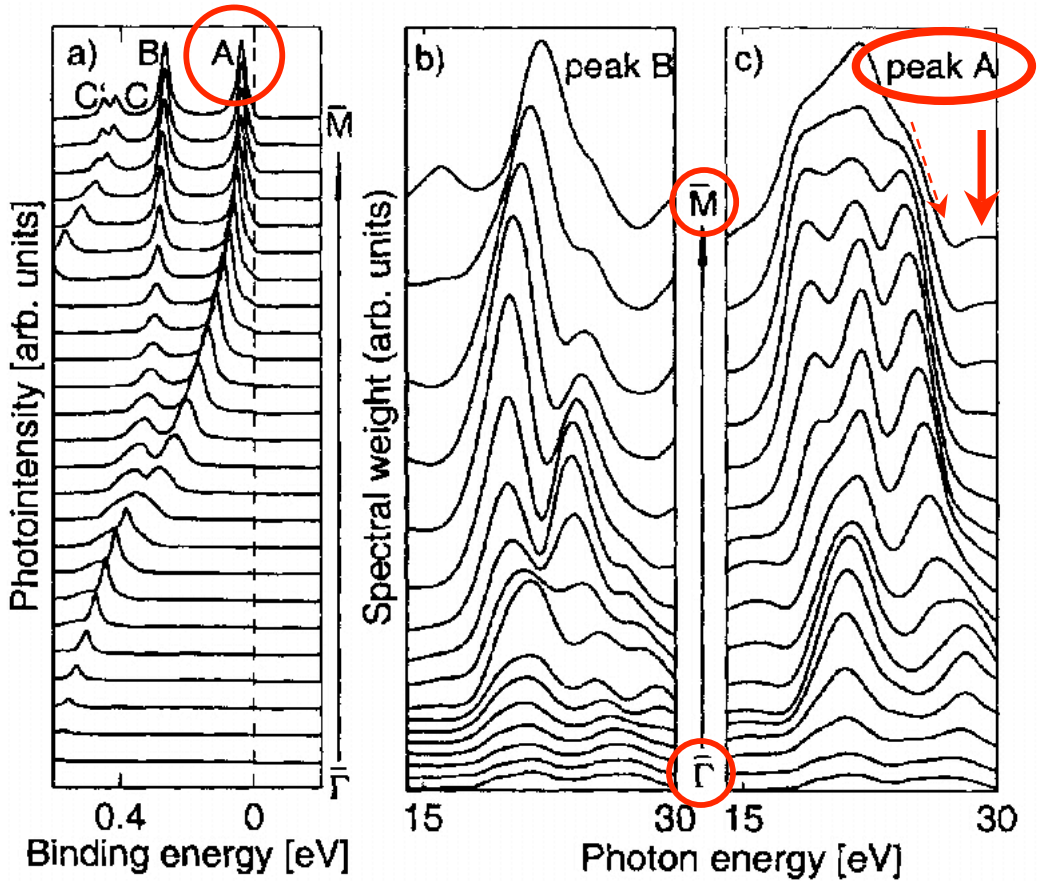


… may turn into pitfalls ….

Phys. Rev. Lett. 72, 2757-2760 (1994)

… complicated situation due to FS contour manifolds





Bansil, Lindroos, PRL 83 (1999) 5154

Matrix elements play a crucial role

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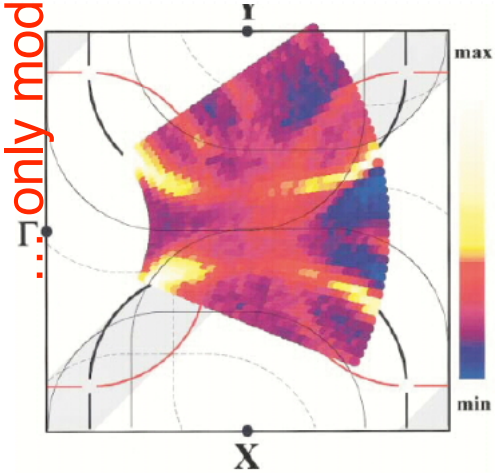
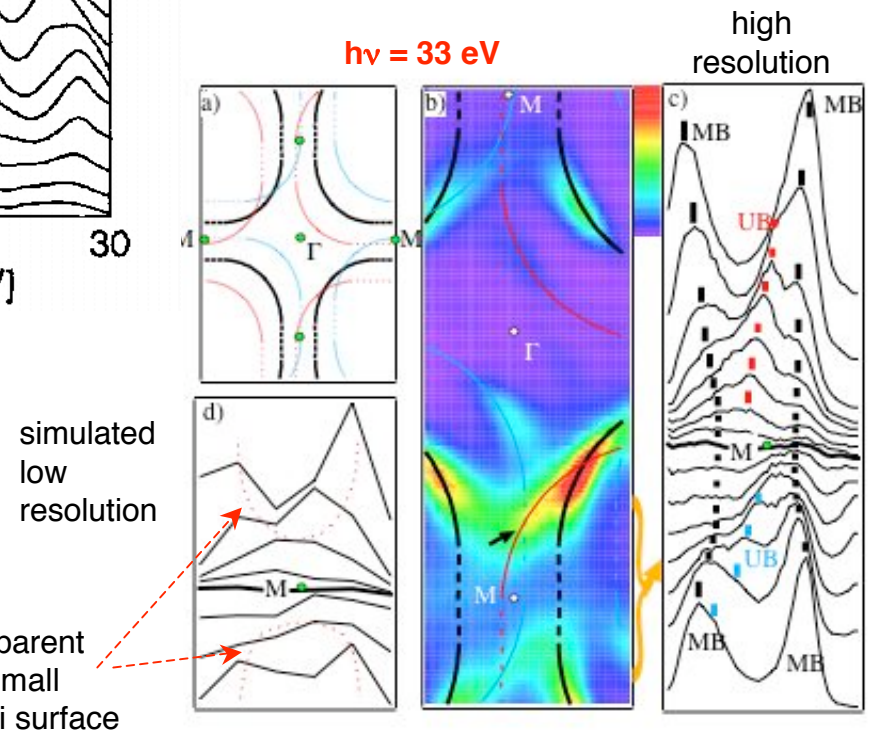


Borisenko et al., PRL 84 (2000) 4453

High resolution experiments



Fretwell et al., PRL 84 (2000) 4449

Bi2212: the situation is complicated despite its 2D character

… only modeling will bring us further…

?How to know?

-what is due to large unit cell (CDW) in initial state

-what is due to large unit cell (CDW) in final state

-whether low intensity is due to absence of QP or ME

-what is due to A(k,ω) / quasi particles

We need to consider

-final state scattering (‘5x1’)-reconstruction

-matrix elements (hν - dependence)

Matrix elements depend on k, ω, hν, polarization

It will be possible to explore influence of parameters:

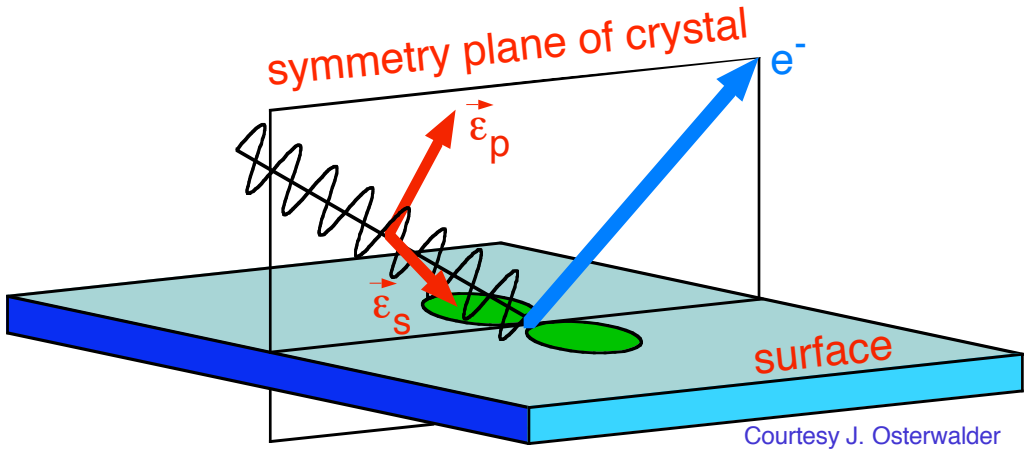
… only modeling will bring us further…

Choose parameters:

to have maximal sensitivity
for:
-certain Atomic elements,
-orbital symmetries,
-special effects of the μ-model

Intensities in Valence Photoemission - Symmetry Effects

... only modeling will bring us further...



$\vec{\varepsilon}_p$ photon polarization in...

$\vec{\varepsilon}_s$ ...perpendicular ("senkrecht") to...scattering plane

photoemission matrix element: $\left| \langle \phi_{f,kin} | \vec{r}_k \cdot \vec{\varepsilon} | \phi_{i,k(\vec{r}_k)} \rangle \right|^2 \rightarrow$ Intensity

projection of r_k onto ε

Overlap integral depends on
final state E_{kin} ($h\nu$), polarization, experimental geometry
---> selective mapping of specific orbitals, states ...

... only modeling will bring us further...

The modeling has to be modular
between
initial and final state physics

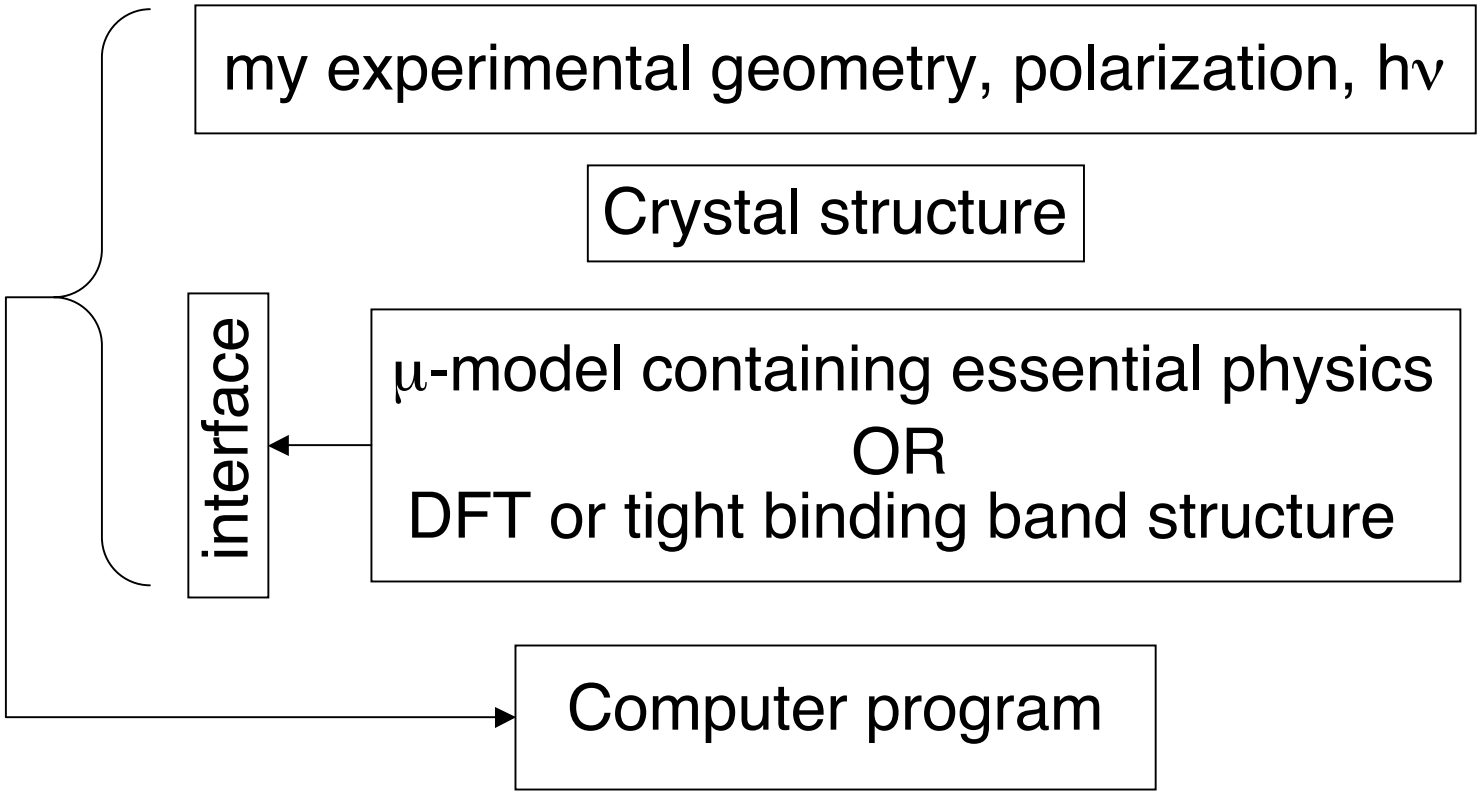
Open for
the most different models for initial state physics

Separate
matrix elements & final state scattering

Have to define the interfaces:
Hedin Lundquist formula?!

**It has to be used by the experimentalists,
each time giving credit
to the persons working on the project**

As an experimentalist, come with



… but also for a theoretician:
what experiment will be best for verifying my μ-model?