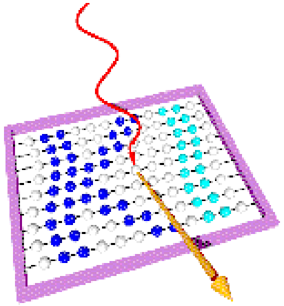
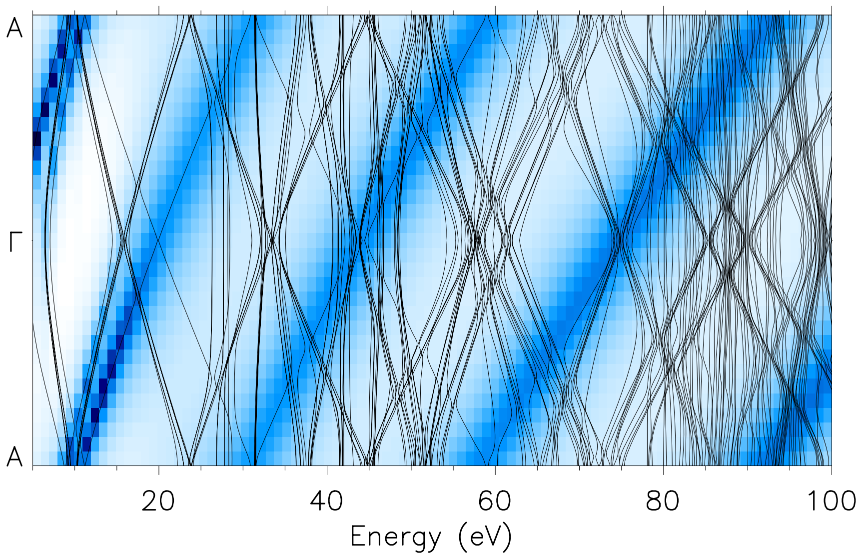


# ARPES (and FEL)

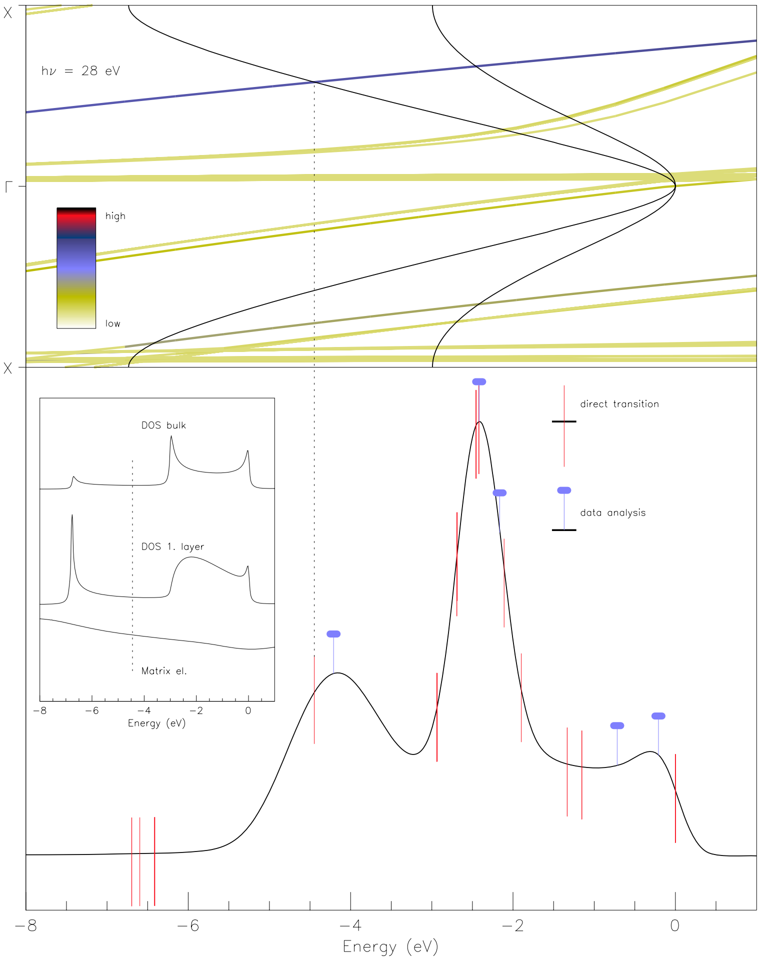
W. Schattke, Theoret. Physik und Astrophysik, Universität Kiel

CORPES05, Dresden, 18.04.05




band structure, final and intermediate states, spectra ?

# Compare: energy-momentum conservation (top)
# with
# electron distribution curve (bottom)




“Solid-State Photoemission and Related Methods” ed. by WS, VanHove, WILEY-VCH (2003)
Progr. Surf. Sci. 54, 211 (1997), WS

# Some examples of ARPES

- i) GaAs(110), ($TiSe_2$)

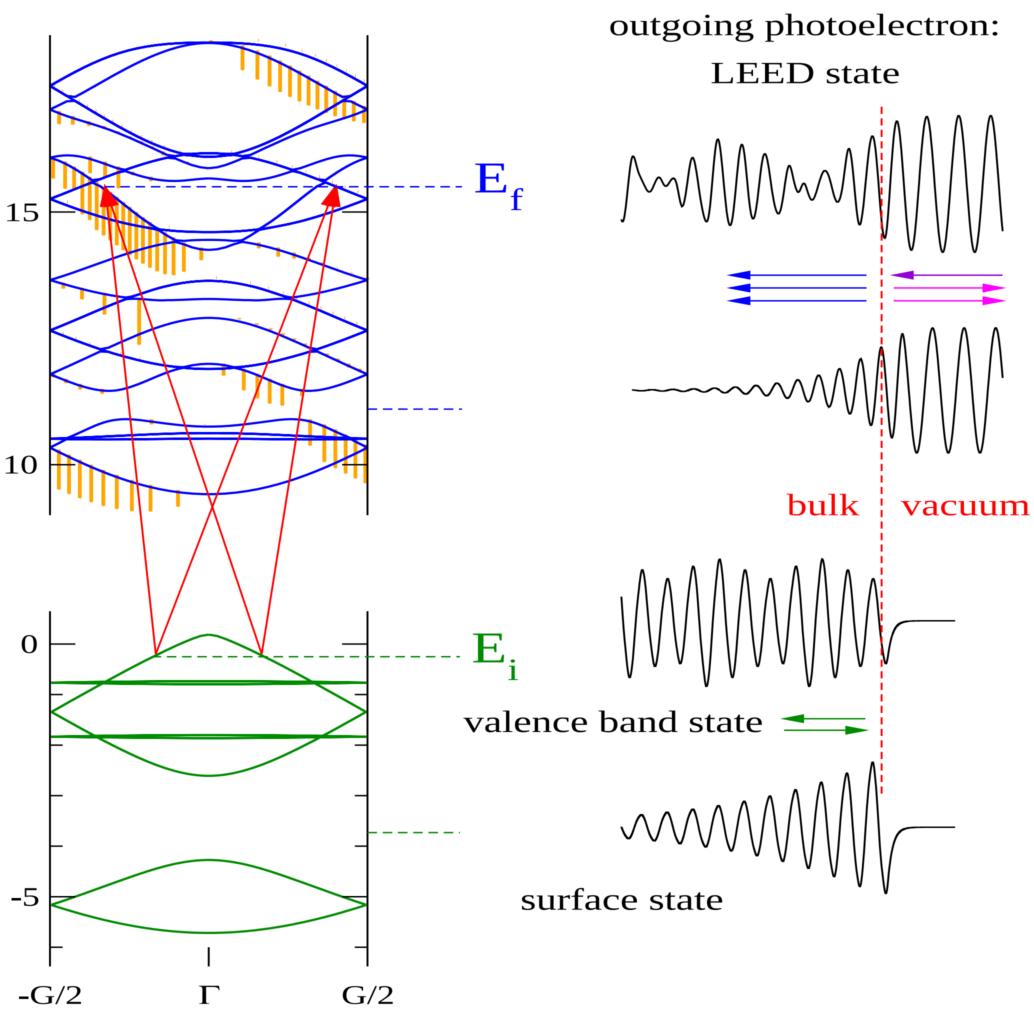
  angular distributions
- ii) S/GaAs (001) – (2x6)

  spectral series
- iii) Cu (111), Al(100)

  accuracy
- iv)$TiSe_2$, $NbSe_2$

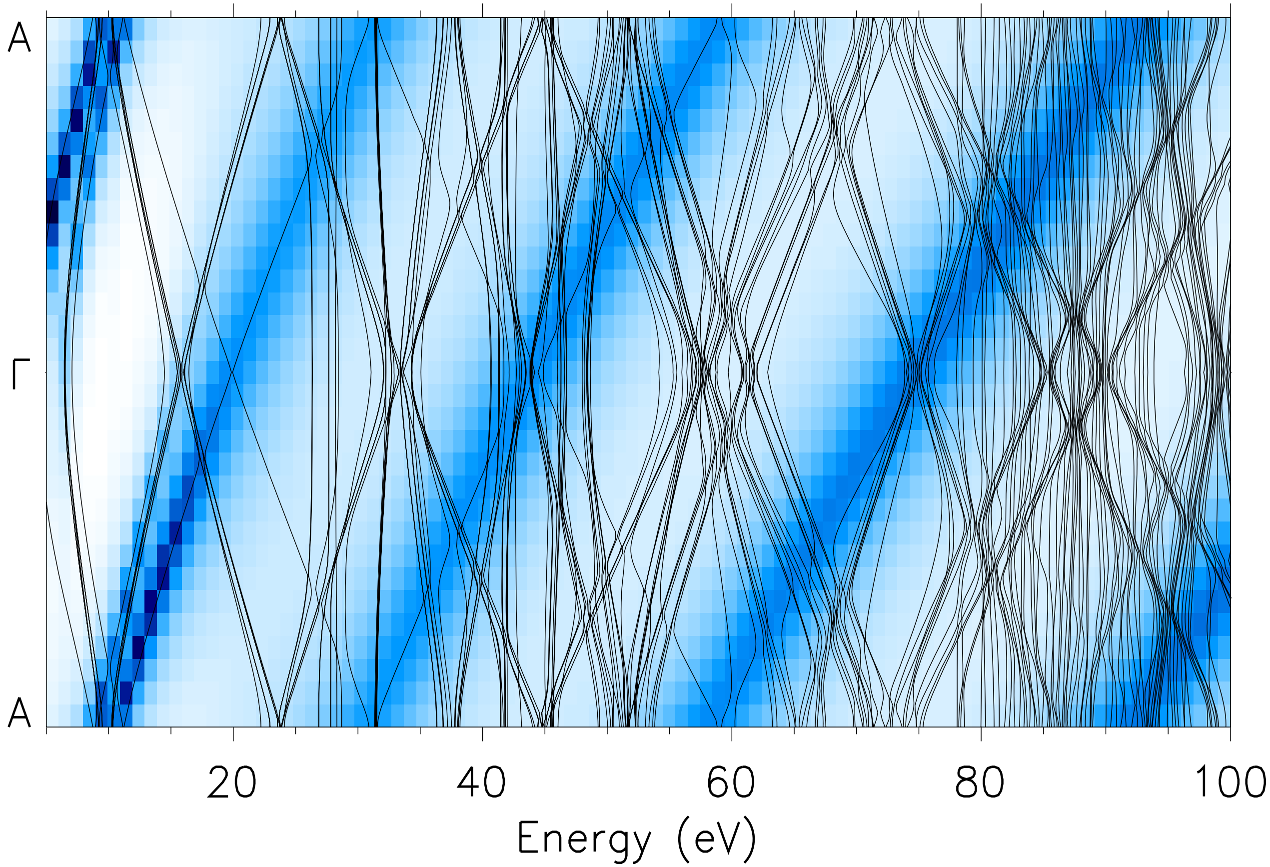
  inelastic effects

# One-Step Theory of Photoemission



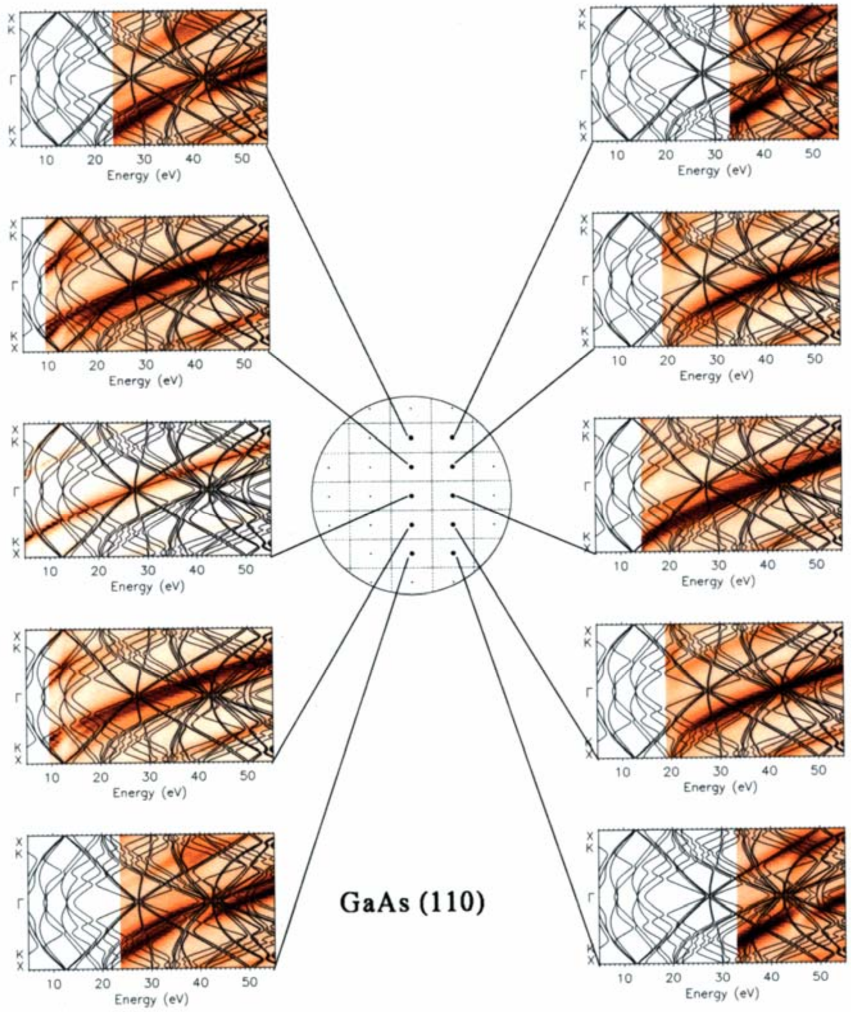
# True final states Fourier decomposed (blue)

$TiSe_2$ bandstructure (black) in surface perpendicular direction




close to parabolic band, backfolded by $2\pi/c$ *n

# Side bands for higher Γ points



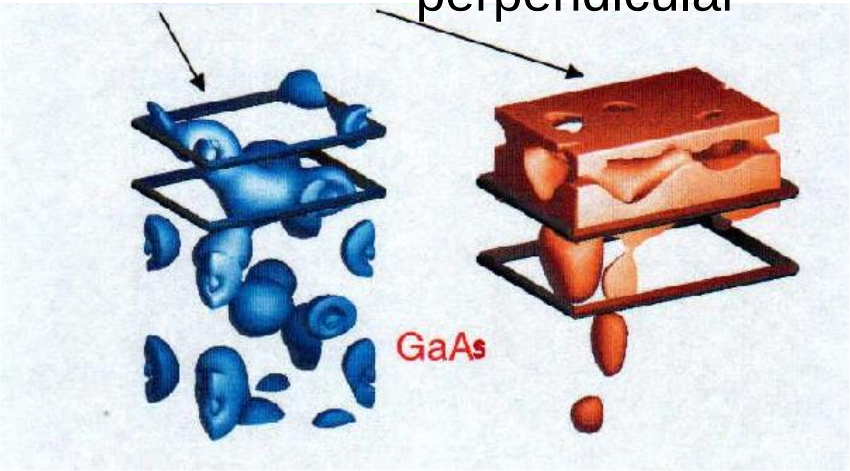
# Photocurrent reflects integrated product of initial with final state

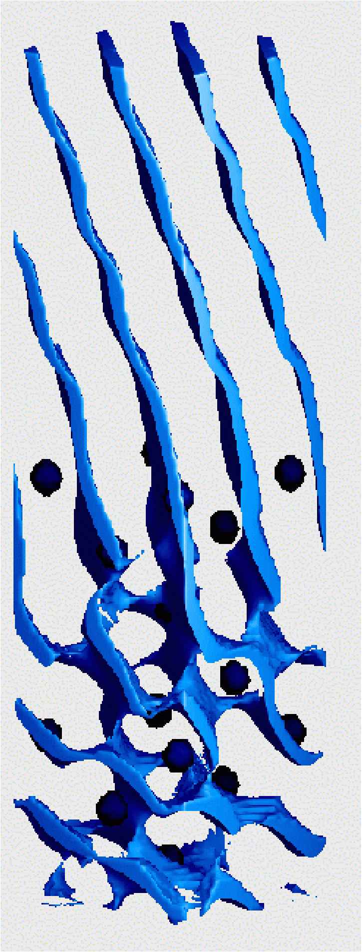
final states

inclined

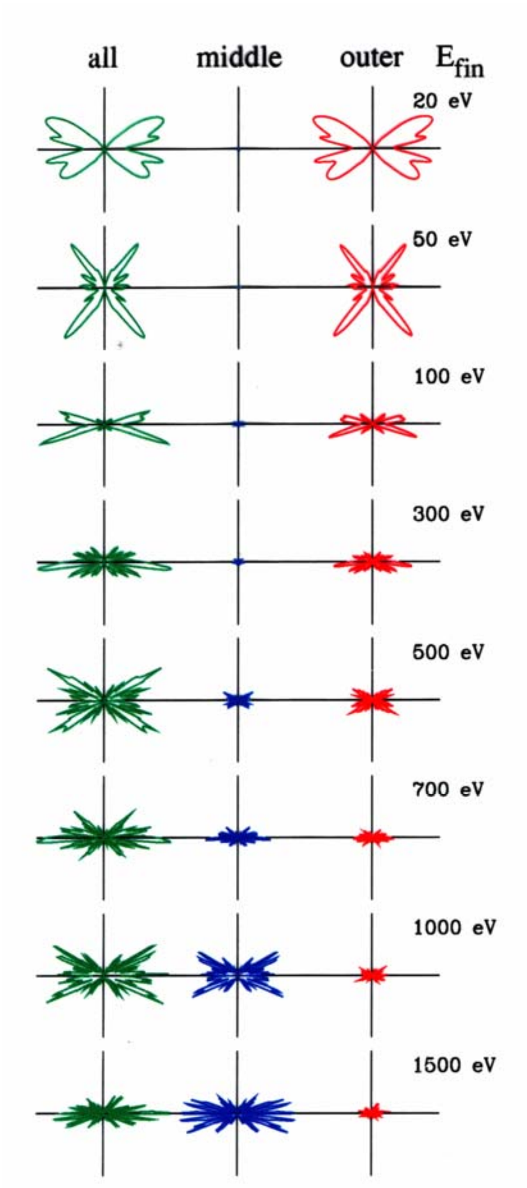
initial state

perpendicular



# Sensitivity of photocurrent on emitting region



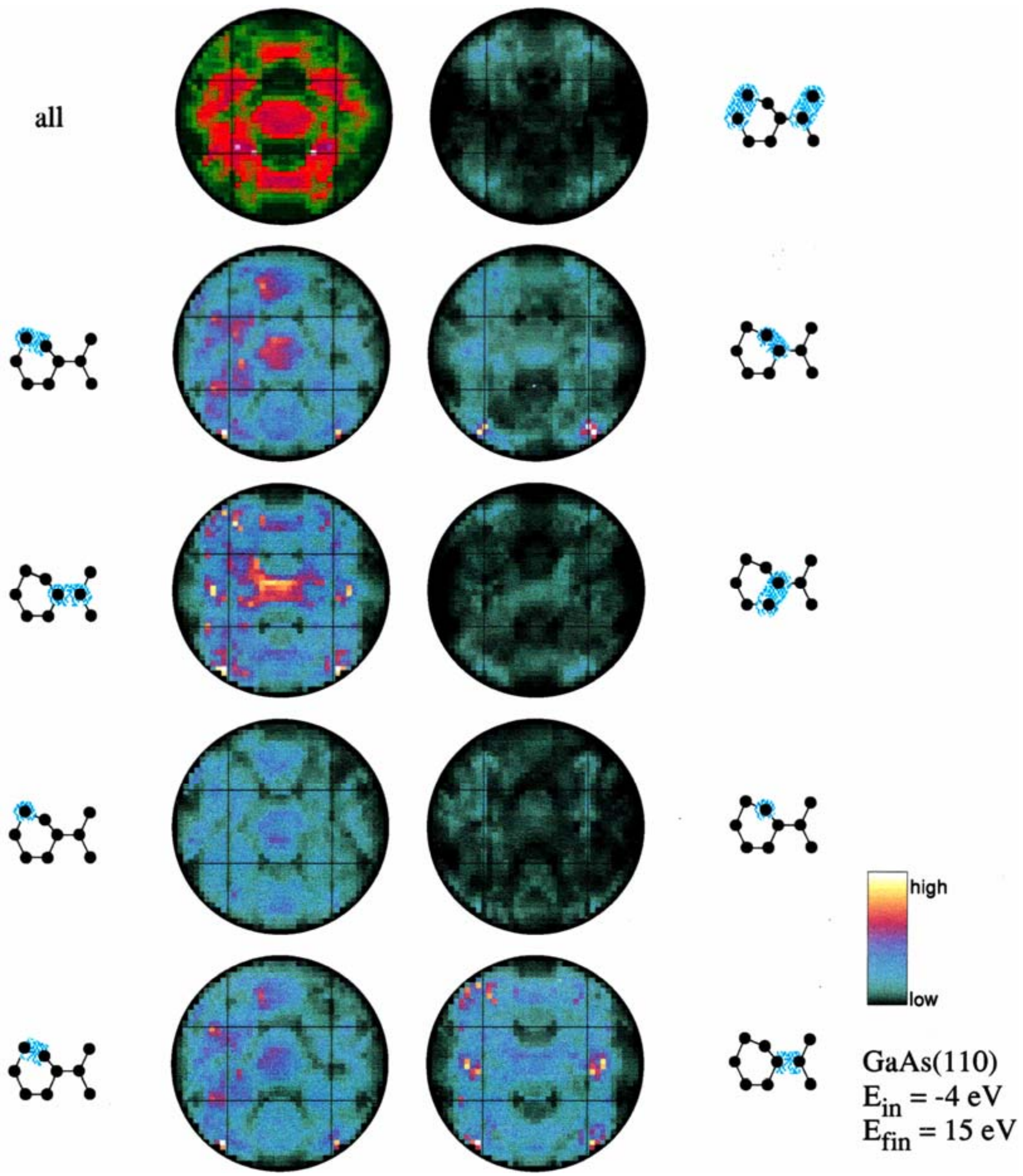

middle and outer region separated by a sphere of 0.3 A radius from nucleus

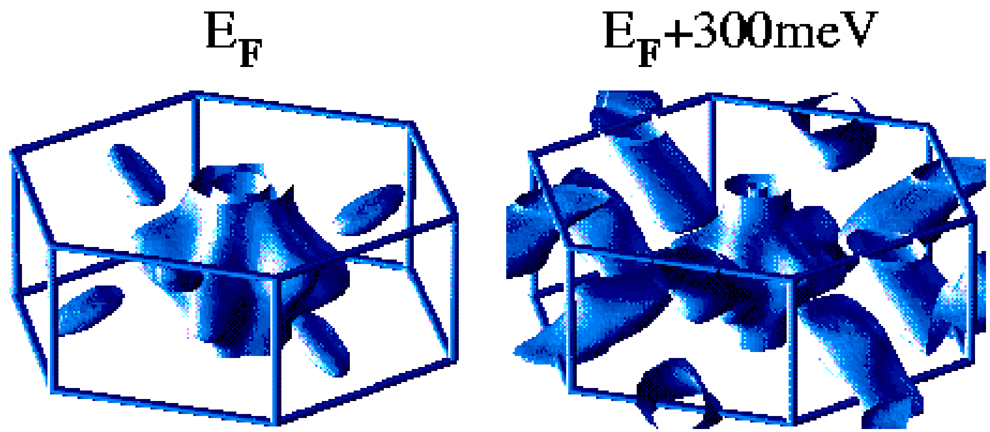
detects:

interstitial at low photon energy

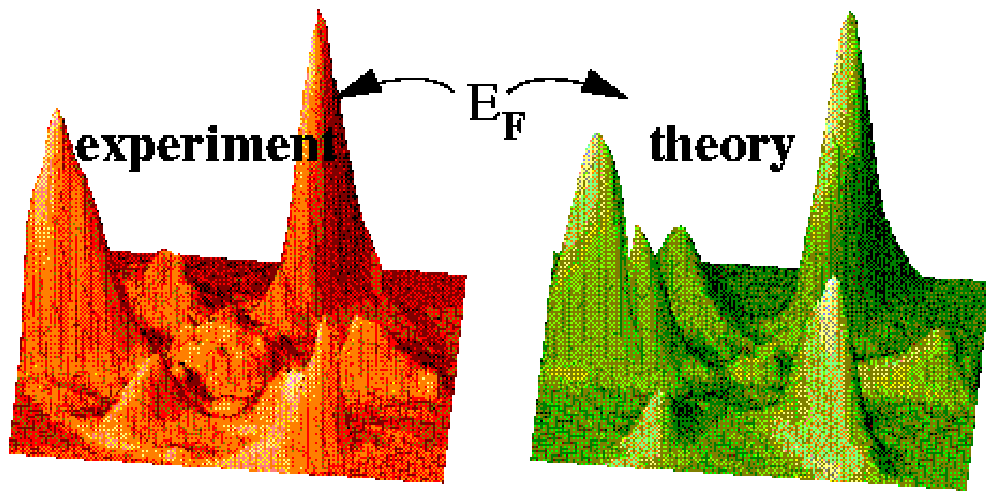
core region at high energy

# Associate emitting region



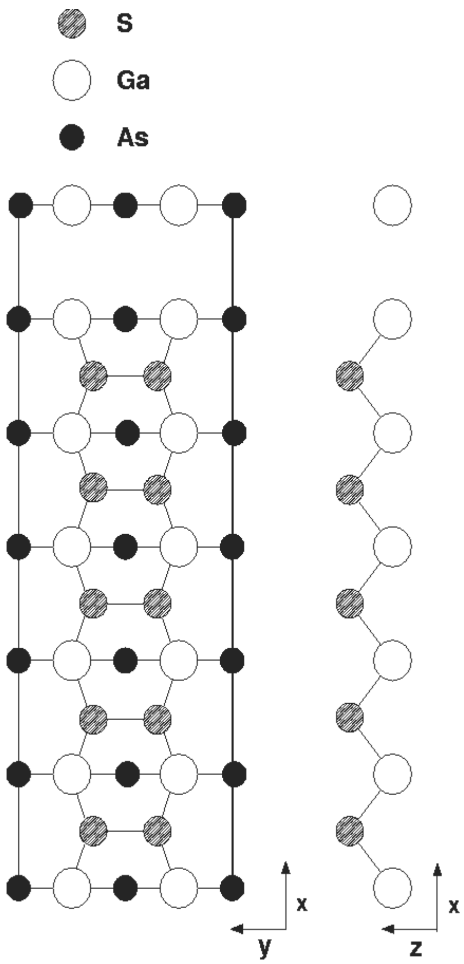


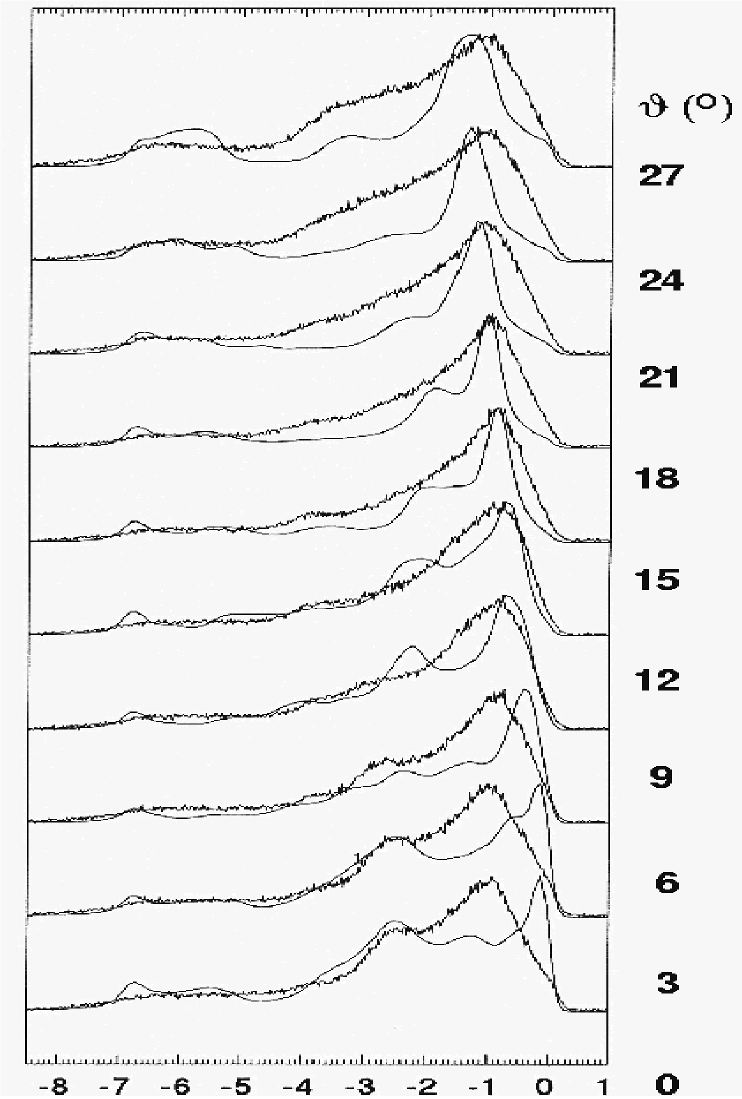

**energy surfaces**



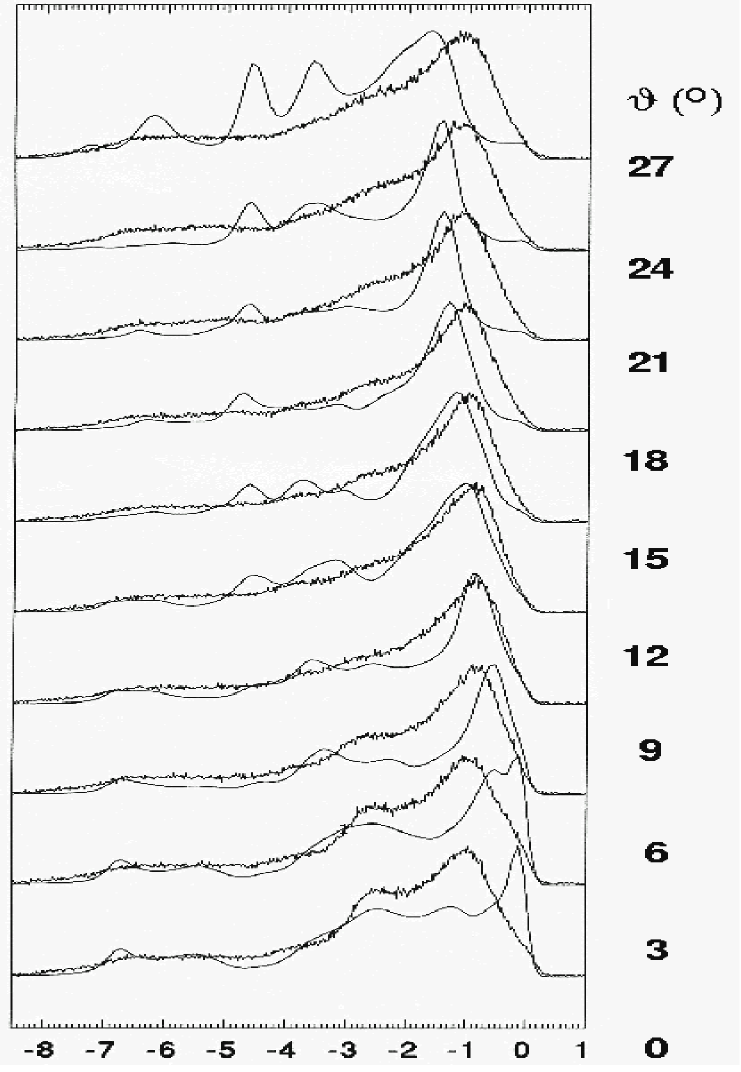

**photocurrent**

# ARPES from S/GaAs(001)-2x6

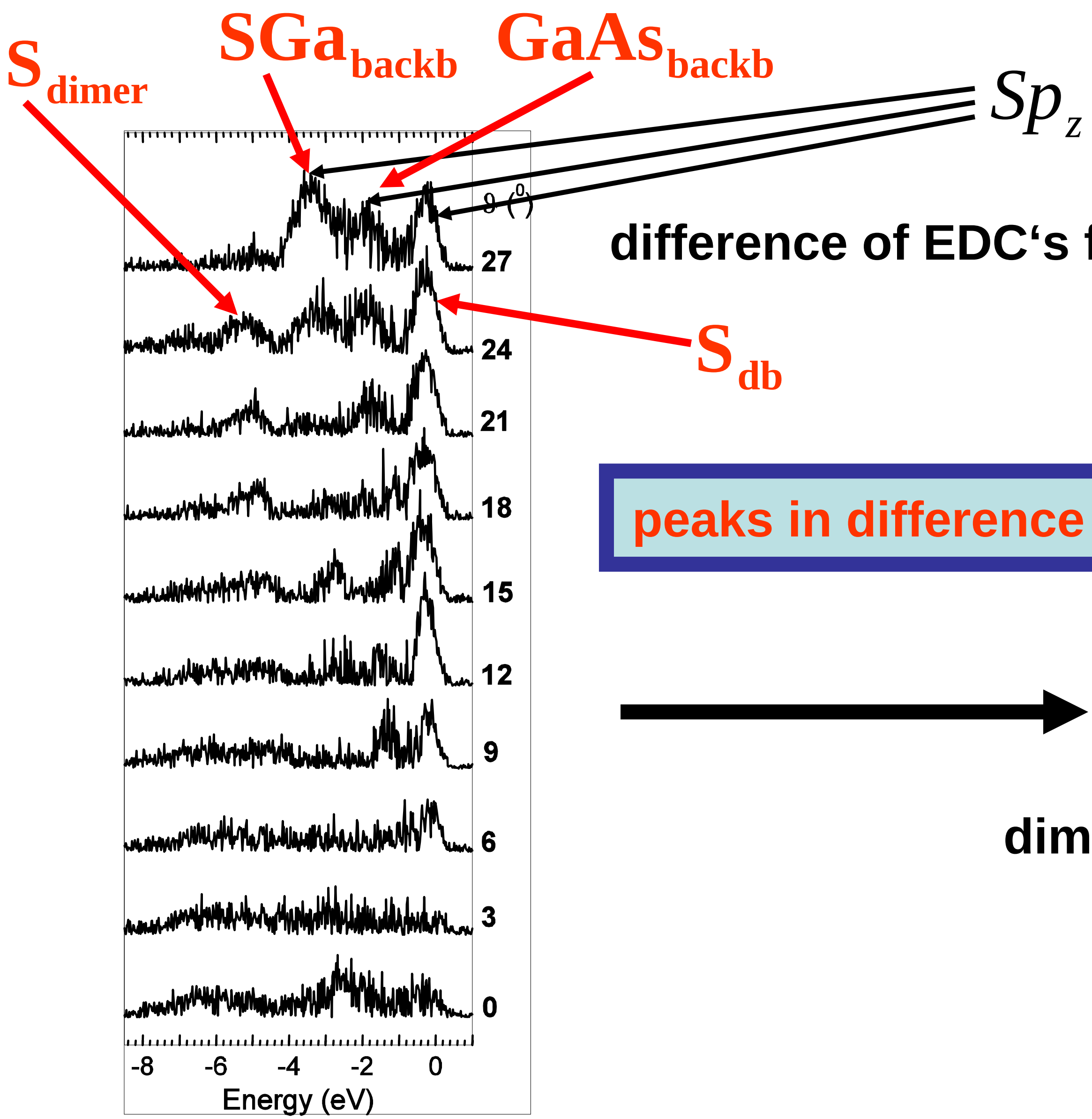


# ARPES from S/GaAs(001)-2x6



# ARPES from S/GaAs(001)-2x6



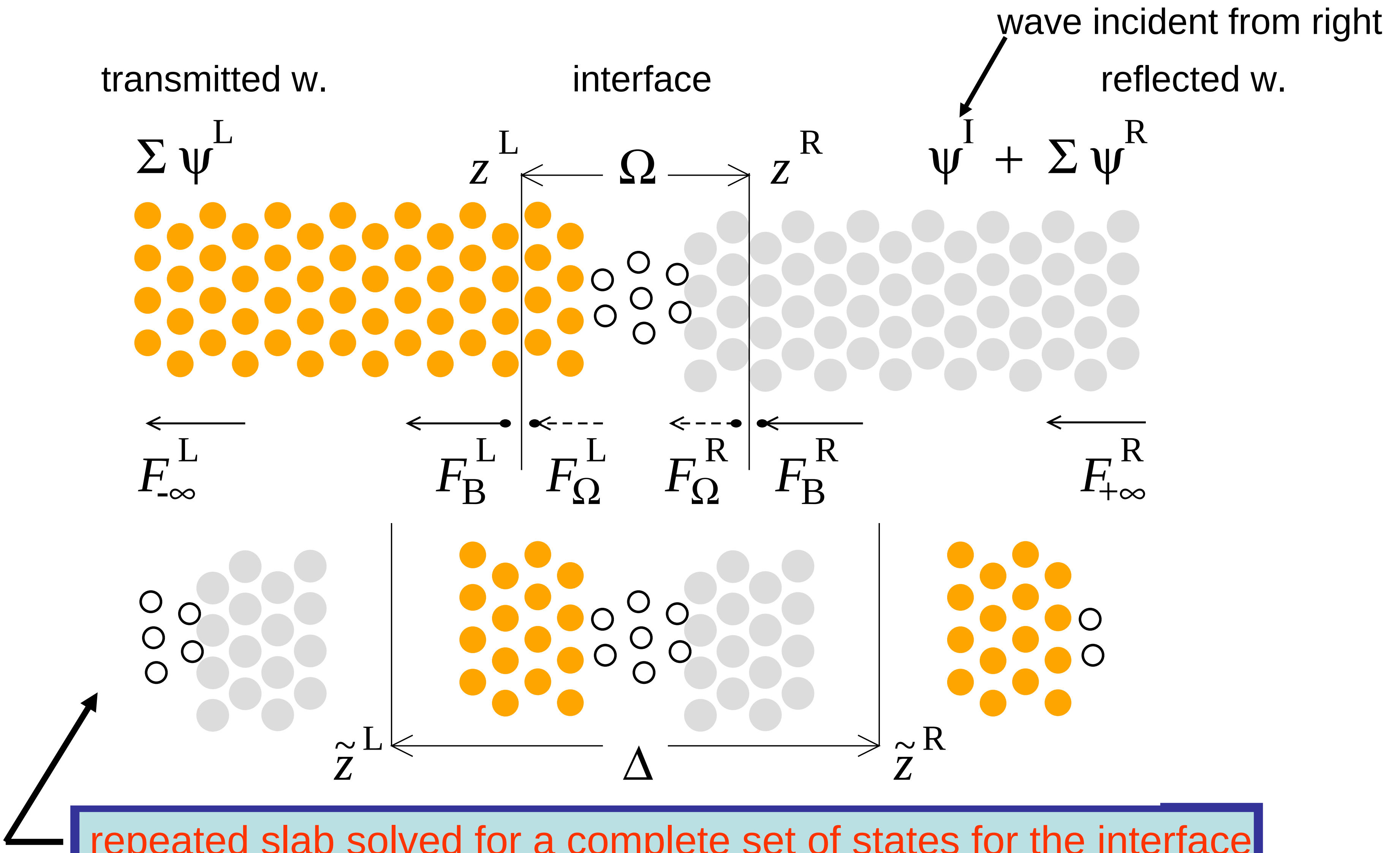

**difference of EDC's for 0 and 90 azimuth**

**peaks in difference due to anisotropy**

→ **S px,py orbitals**

**dimer bond, dangling bond**

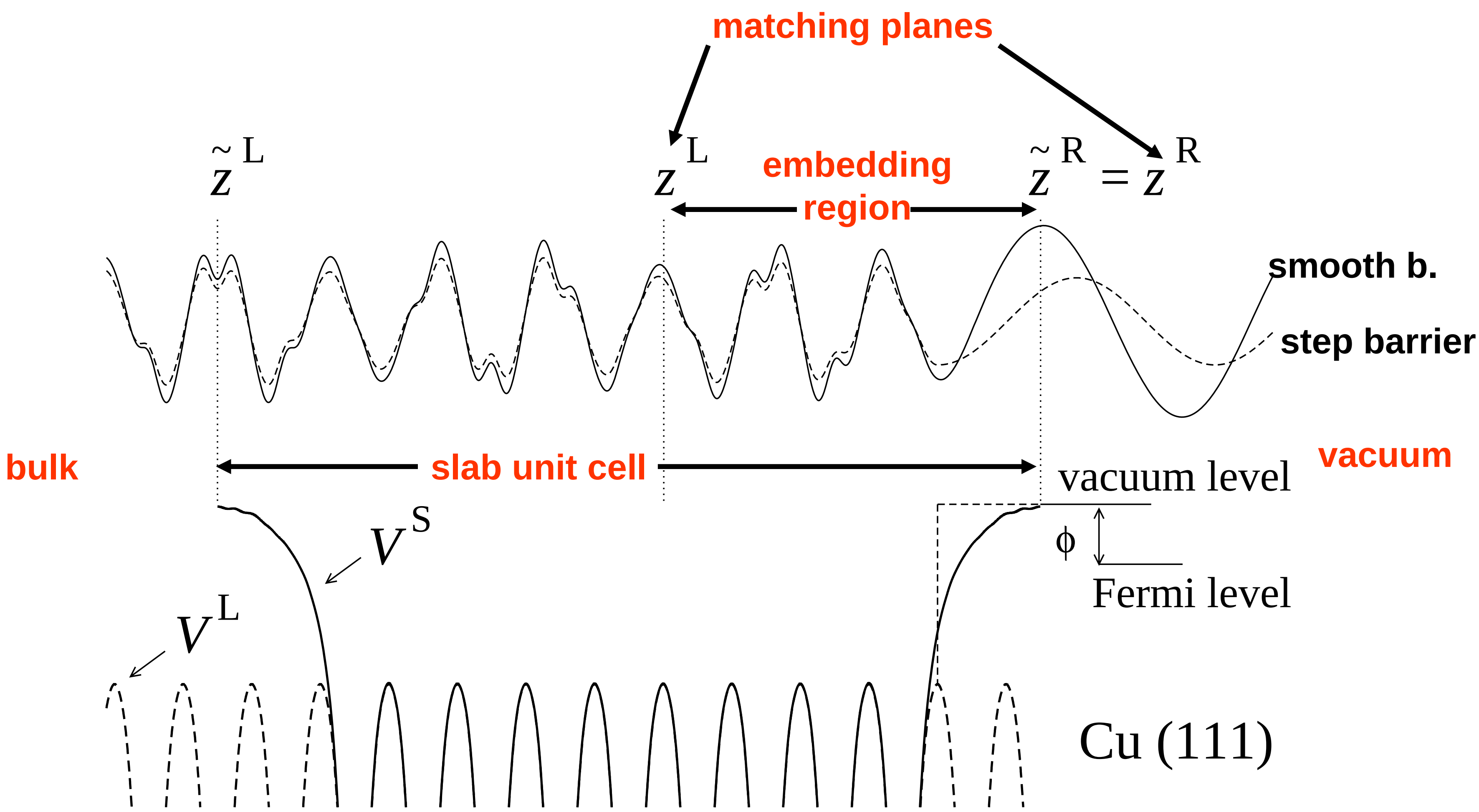
# One-step photocurrent by APW: LEED




repeated slab solved for a complete set of states for the interface

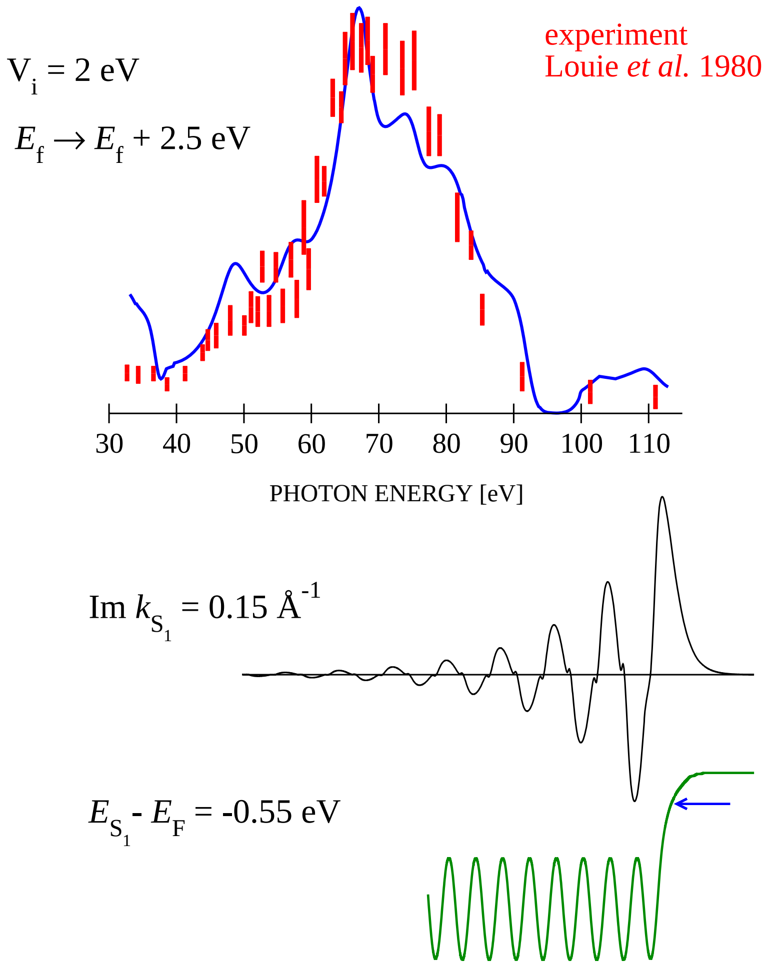
Phys. Rev. B **70**, 245322 (2004), Krasovskii

# Potential and wavefunction for surface system

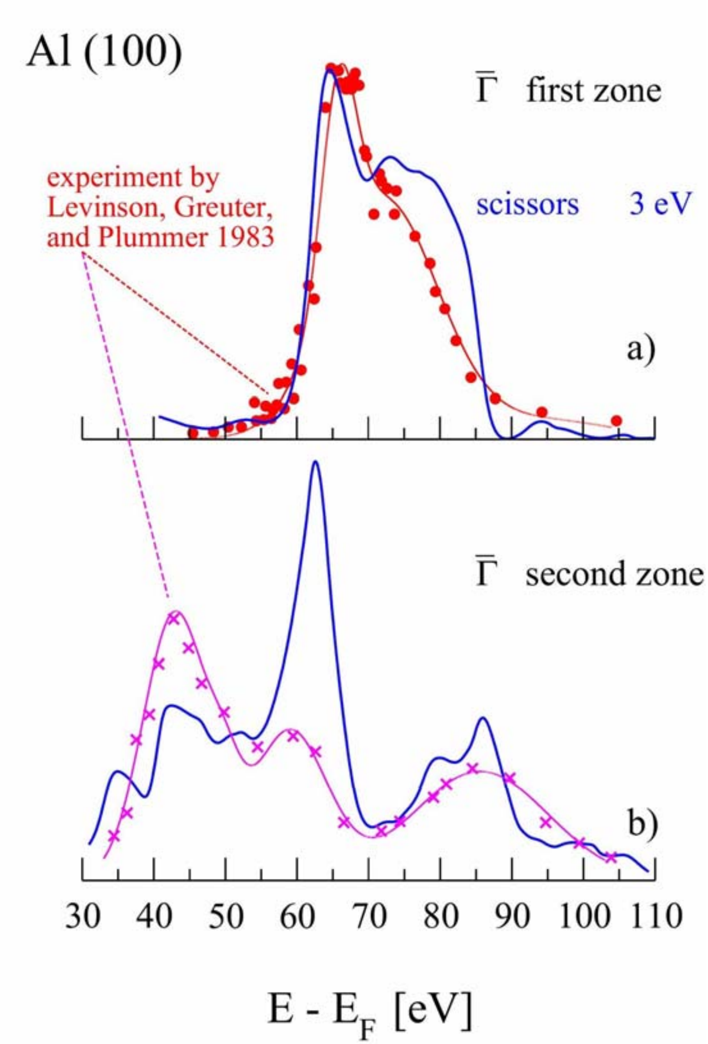


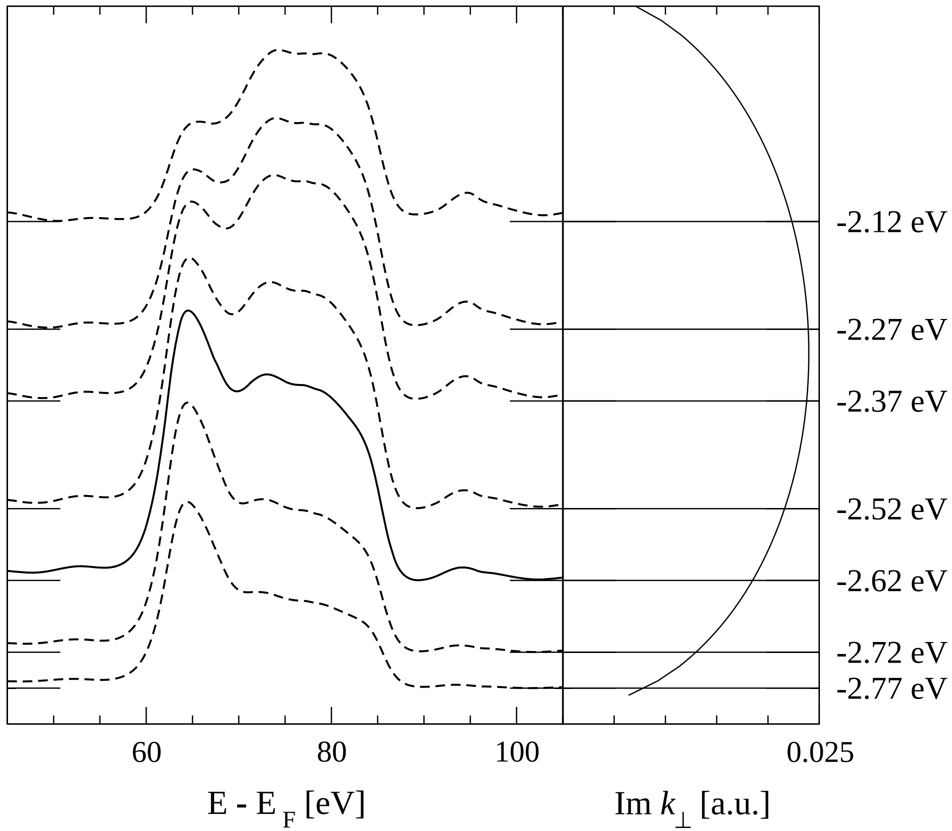

Phys. Rev. B **70**, 245322 (2004), Krasovskii

Photoemission from the surface state $S_1$ on Cu (111)



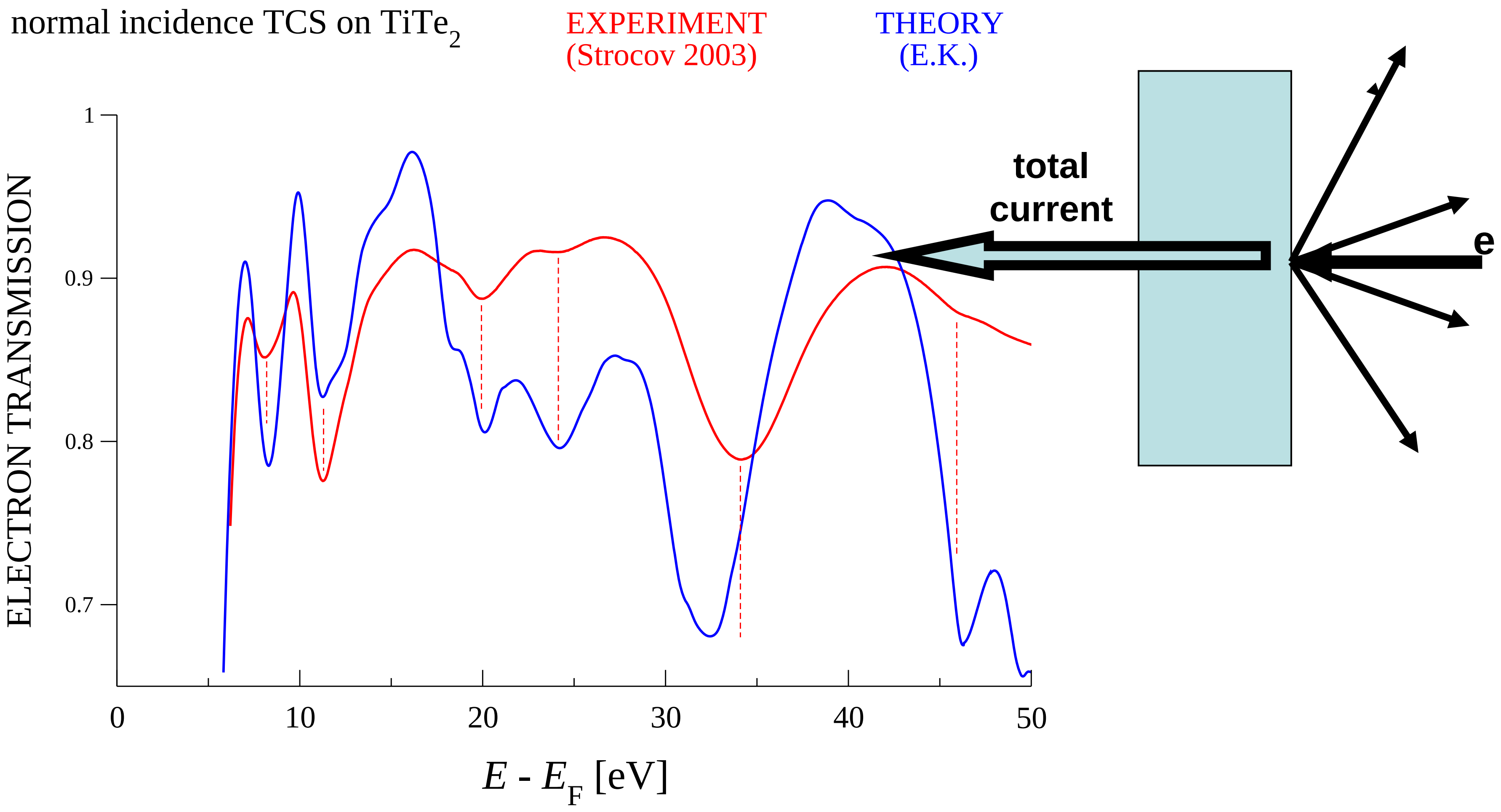
# Energy Accuracy of ARPES



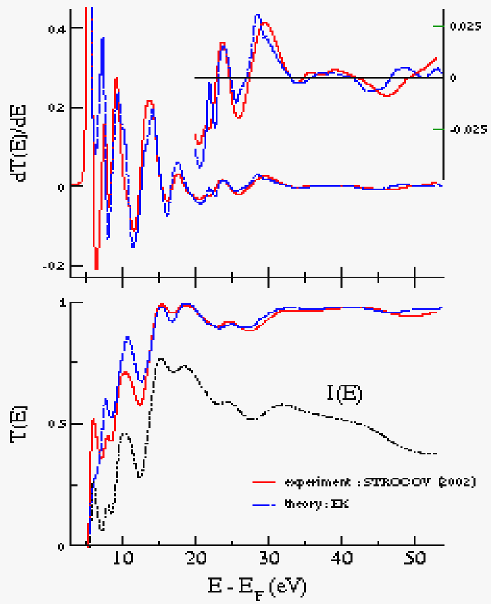

Phys. Rev. Lett. **93**, 027601 (2004), Krasovski,WS

# Total current spectroscopy

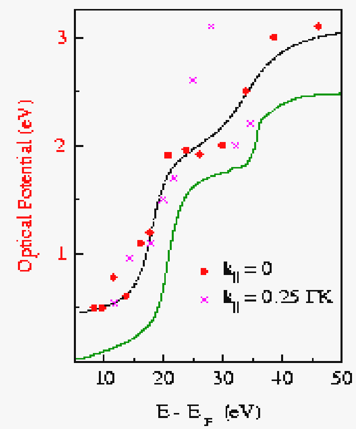


# Inelastic Effects in Target Current Spectroscopy of $NbSe_2$

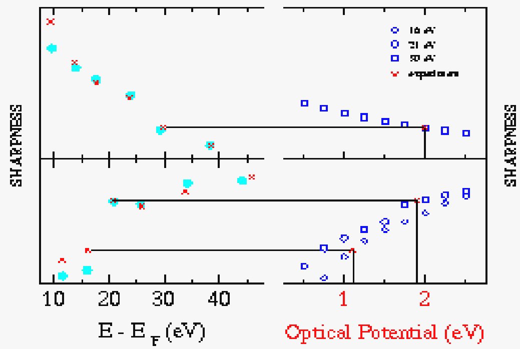
## Normal Incidence Spectrum



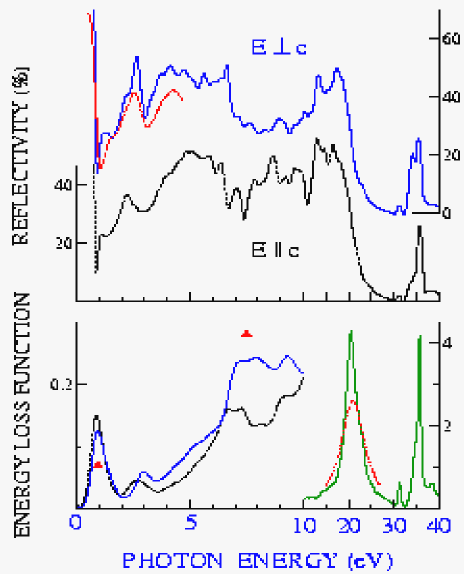

## $V_i(E)$ compared to $\int_0^E \mathrm{Im}[-1/\epsilon(\omega)]\, d\omega$




## Determining the optical potential from the sharpness of $dT/dE$ spectral structures.




## Optical Properties of $NbSe_2$




Phys. Rev. B **66**, 235403 (2002), Krasovskii et al

# FEL photoemission

- free electron laser (VUV-FEL, at DESY Hamburg) ➔

  source of high photon intensity

  → higher order terms of electromagnetic field, golden rule to be extended

  lateral focus

  → lateral spatial inhomogeneities, keeps with traditional golden rule

# FEL photoemission

**source of high photon intensity:**

**A large** → quantum kinetics a la Kadanoff-Baym (M. Bonitz)
→ time dependent DFT (E. Pehlke)
→ higher order perturbation in $H_1(t)$ (WS)

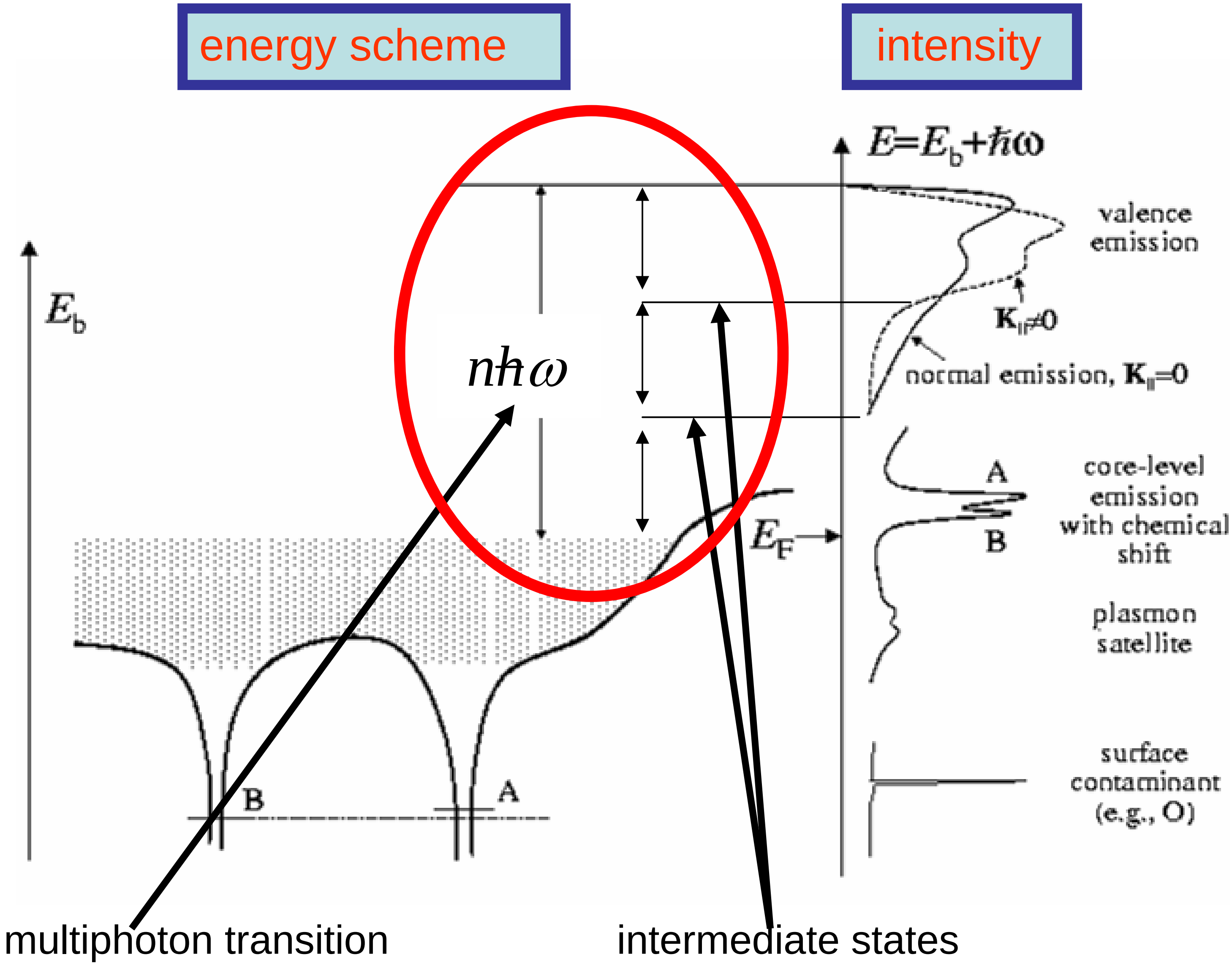
$$\varphi(t) = \varphi(0) - \tfrac{i}{h}\int_0^t dt' V(t')\varphi(t')$$

$$V(t) = \exp(\tfrac{i}{h} H_0 t) H_1(t) \exp(-\tfrac{i}{h} H_0 t),$$

$$H_1(t) = -\frac{e}{2m}(\mathbf{pA} + \mathbf{Ap}) + \frac{e^2}{2m}\mathbf{A}^2$$

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{E}\sin(\mathbf{qr} - \omega t) / \omega$$

# photoemission in higher order



## FEL photoemission

# ´´golden rule´´ with next order perturbation:

**photocurrent** *in dipole approximation (● large)*

$$j \approx \frac{\pi}{4\hbar}\sum_i \left| < \varphi_f \,|\, \mathbf{A_0}\cdot\mathbf{p} \,|\, \varphi_i > \right|^2 \delta(E_f - E_i - \hbar\omega) +$$

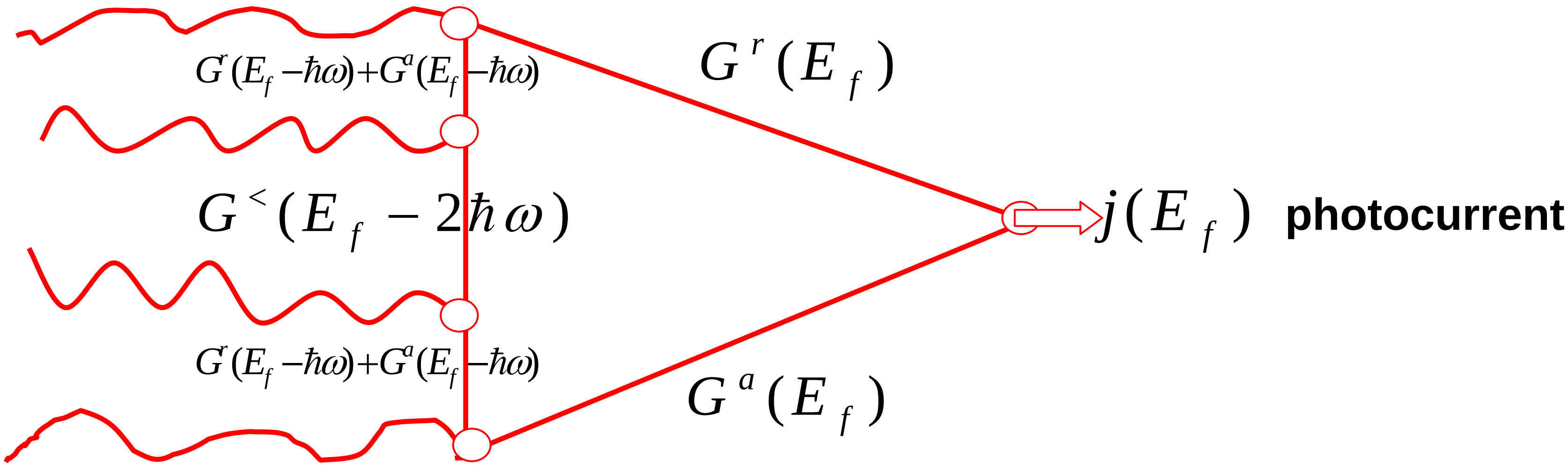
$$+\frac{\pi}{16\hbar}\sum_i \left| \sum_n P\left(\frac{<\varphi_f|\mathbf{A_0}\cdot\mathbf{p}|n><n|\mathbf{A_0}\cdot\mathbf{p}|\varphi_i>}{E_f - E_n - \hbar\omega}\right) \right|^2 \delta(E_f - E_i - 2\hbar\omega)$$

*P(…),* principal part |n>, intermediate states

$$j = j_{gr}(E_f, \hbar\omega) + j_{ngr}(E_f, \hbar\omega)$$

# FEL photoemission

## vertex graph




**furthermore**

extrinsic effects: renormalize outgoing LEED state by $\mathbf{A_0p}$

$\longrightarrow$ $G^r(E_f), G^a(E_f), \varphi_f$ and similarly $G^<(E_f-2\hbar\omega), G^{r/a}(E_f\pm\hbar\omega)$

*via time independent perturbation or scattering theory*

# FEL photoemission

beyond 2(3…)-photon transitions:

What is the initial state, $\varphi_i$ ? → time dependent DFT calculations: following electrons from ground state to the excited plasma and to photoemission (E. Pehlke)

How does the excited many-body system evolve?

→ quantum kinetic equations under excitation by electromagnetic radiation (M. Bonitz)