united nations educational, scientific and cultural organization

international atomic energy agency

the
abdus salam
international centre for theoretical physics

SMR/1270-33

SCHOOL ON SYNCHROTRON RADIATION

6 November - 8 December 2000

Miramare - Trieste, Italy

Supported in part by the Italian Ministry of Foreign Affairs in connection with the SESEME project

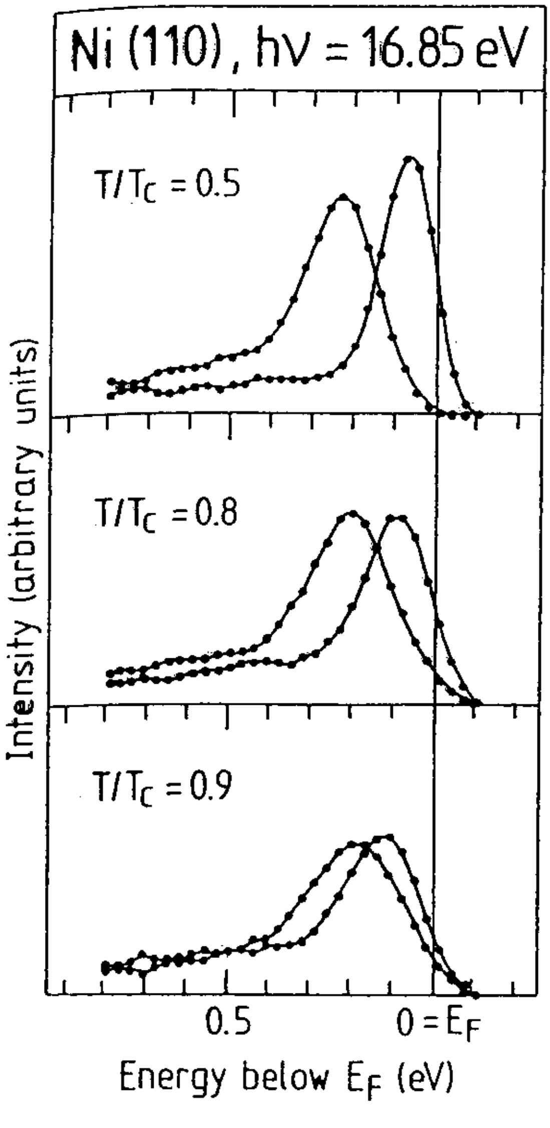
Co-sponsors: Sincrotrone Trieste, Società Italiana di Luce di Sincrotrone (SILS) and the Arab Fund for Economic and Social Development

Spin- and Angle-Resolved Photoemission / Manybody Effects

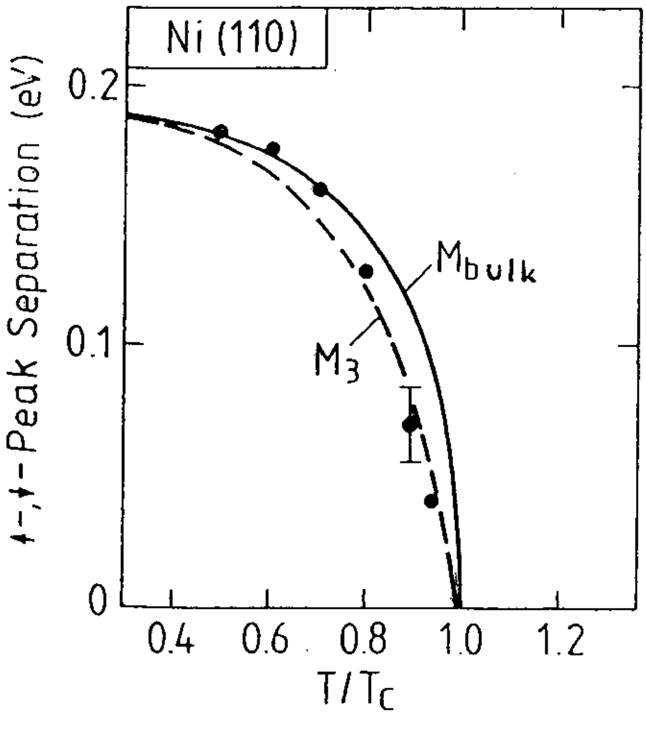
Juerg Osterwalder
Universitaet Zuerich-Irchel
Zurich, Switzerland

SPIN-RESOLVED ARUPS DATA FROM Ni(110)*

Energy Distribution Curves

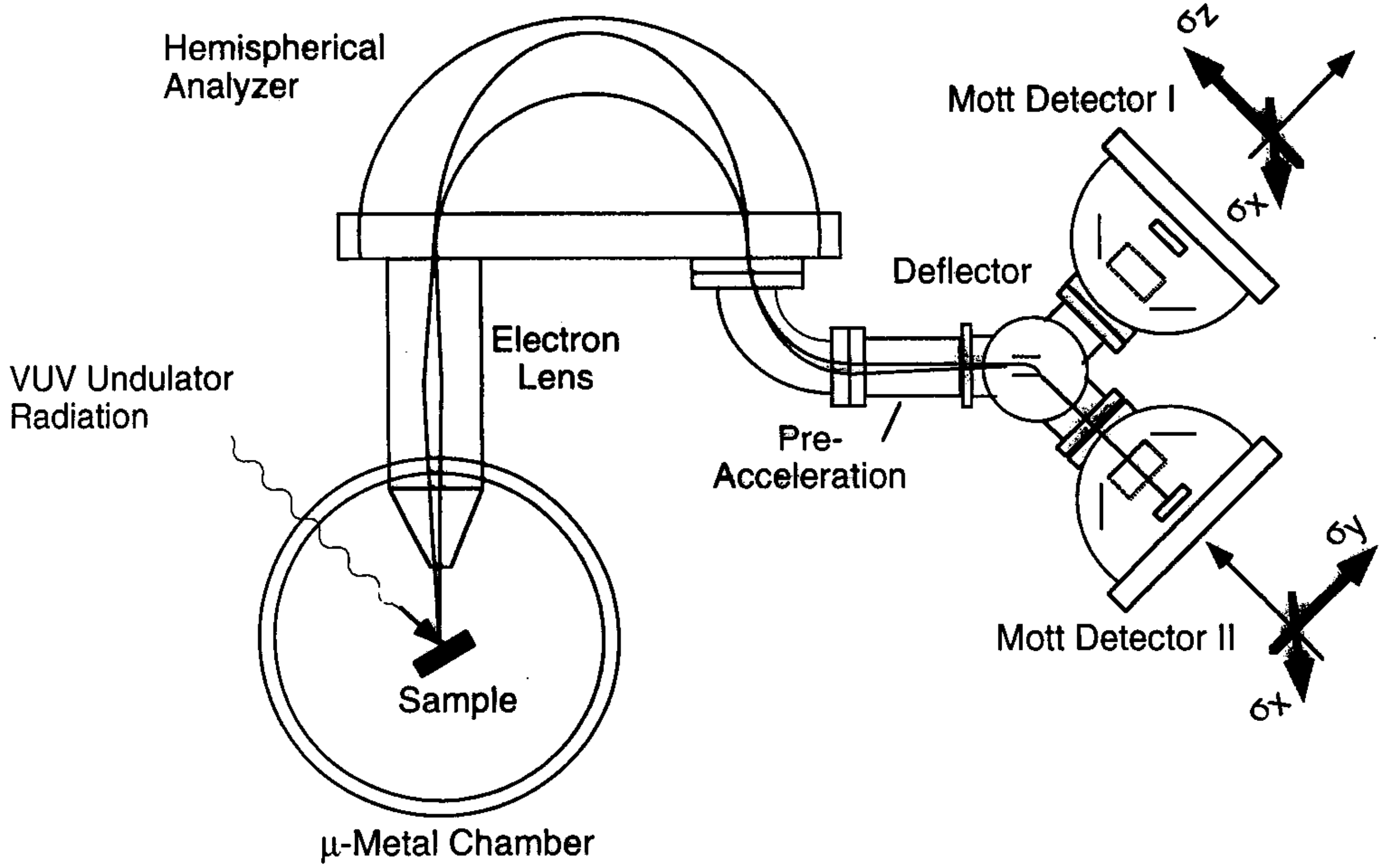


Temperature-Dependent Exchange-Splitting

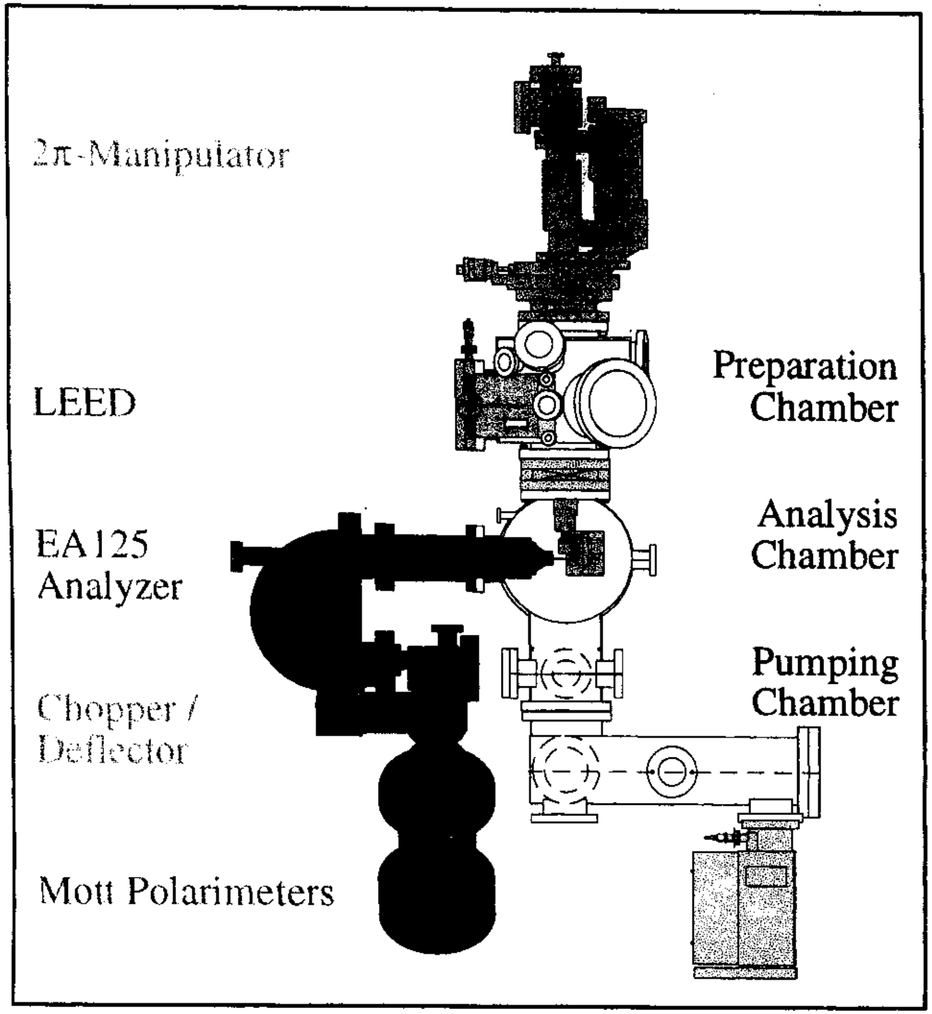


* **From: R. Raue, H. Hopster, R. Clauberg, Z. Phys. B 54, 121, (1984)**

SPIN-RESOLVED FERMI SURFACE MAPPING



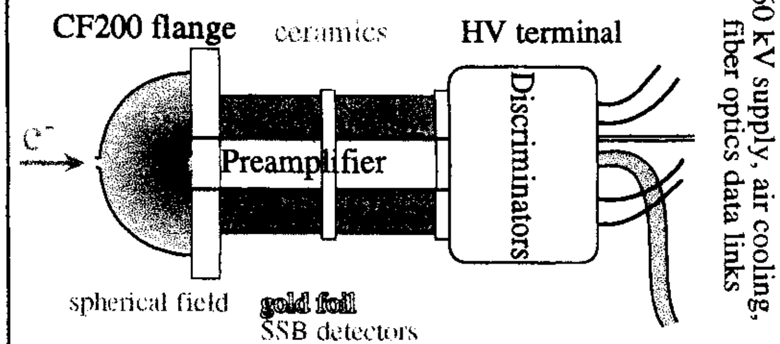
Set-up of COPHEE



1. Set-up at University Zürich-Irchel
2. Installation at APE beamline of Elettra
3. Use at second port of SIS-beamline at SLS

Mott-Polarimeters

- Mott scattering at 60 keV
- 800 Å gold foil
- energy resolved detection by four silicon surface barrier detectors

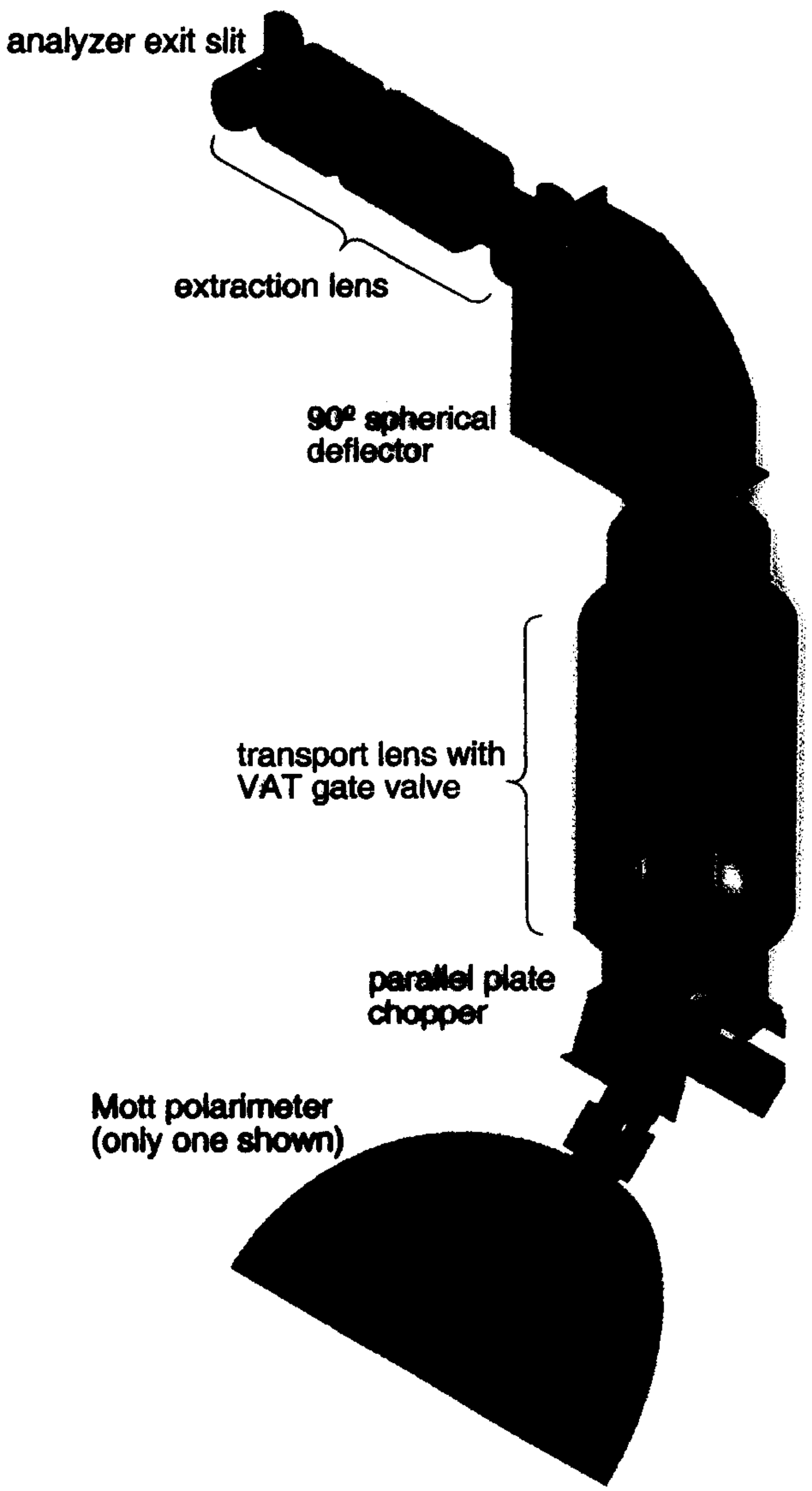


Ref: V.N.Petrov, M.S.Galaktionov *et al.* Techn. Phys. **43** (1998) 125

Status of COPHEE

March 2000

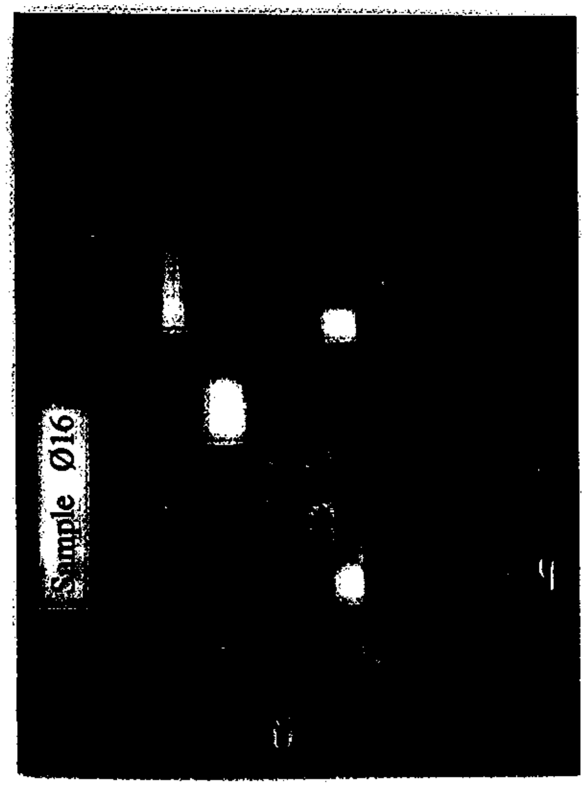
Electrostatic Lens Scheme for COPHEE



Calculation made by SIMION 3D Vers. 6.0 by D. Dahl

Manipulator

- 2π rotation
- liquid He cooling (40K)
- heating contacts (900K)
- switchable sample magetization



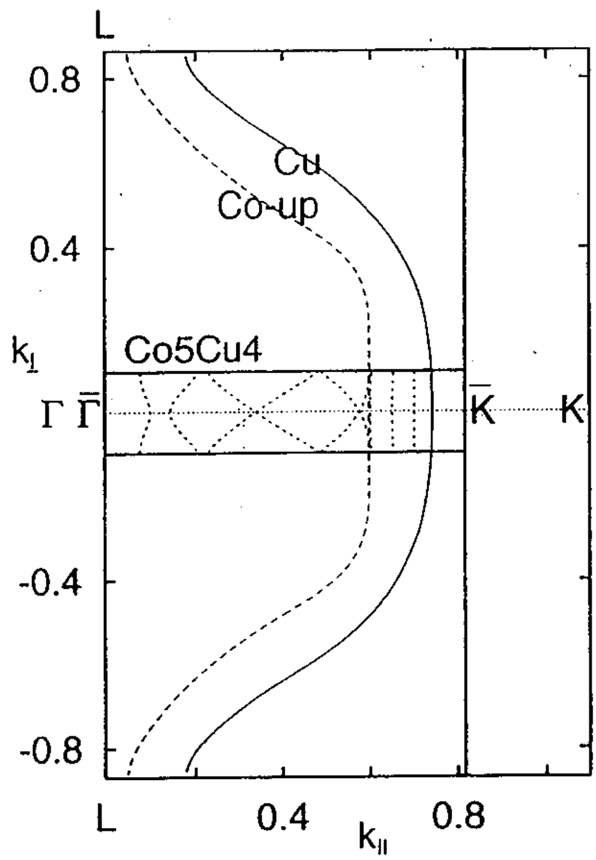
Swiss Stub sample holder

Giant Magnetoresistance from an Electron Waveguide Effect in Cobalt-Copper Multilayers

W. H. Butler, X.-G. Zhang, and D. M. C. Nicholson
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114

T. C. Schulthess
Lawrence Livermore National Laboratory, Livermore, California 94551

J. M. MacLaren
Department of Physics, Tulane University, New Orleans, Louisiana 70118
(Received 24 October 1995)



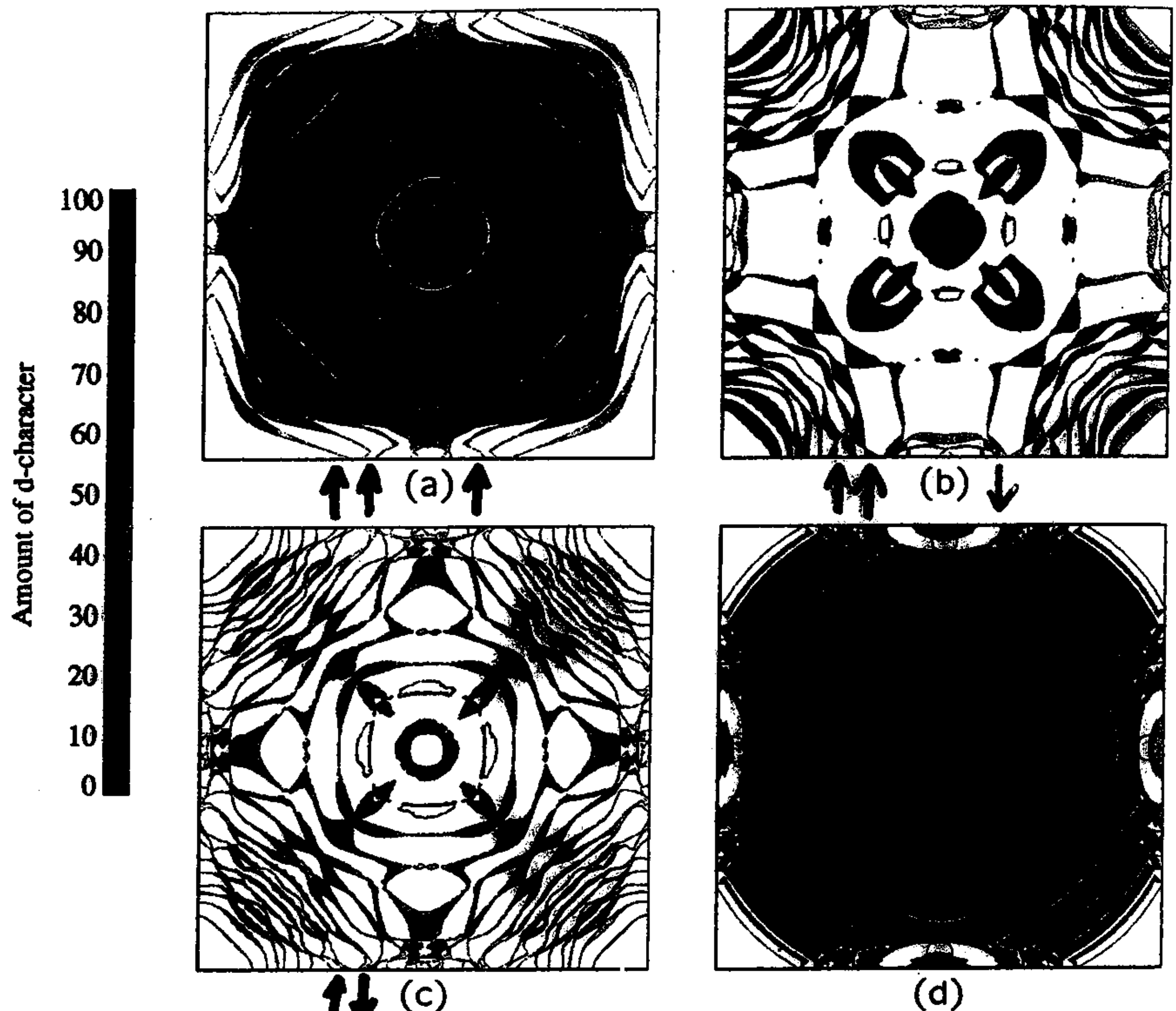
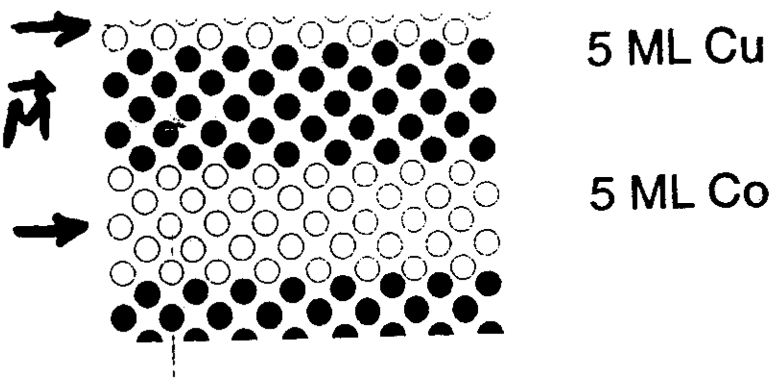


FIG. 1. Projections inside the first Brillouin zone of different Fermi surfaces for a (100) oriented Co_5/Cu_5 multilayer on a plane parallel to the interfaces. The amount of *d* character is given by the color code on the left-hand side of the figure. The Γ point is at the center of each panel. (a) Majority spin and (b) minority spin in the parallel configuration. (c) Either spin in the antiparallel configuration, (d) minority spin in the parallel configuration where the *sp-d* hybridization is omitted. The quantum well *d* states are just visible as thin blue lines.

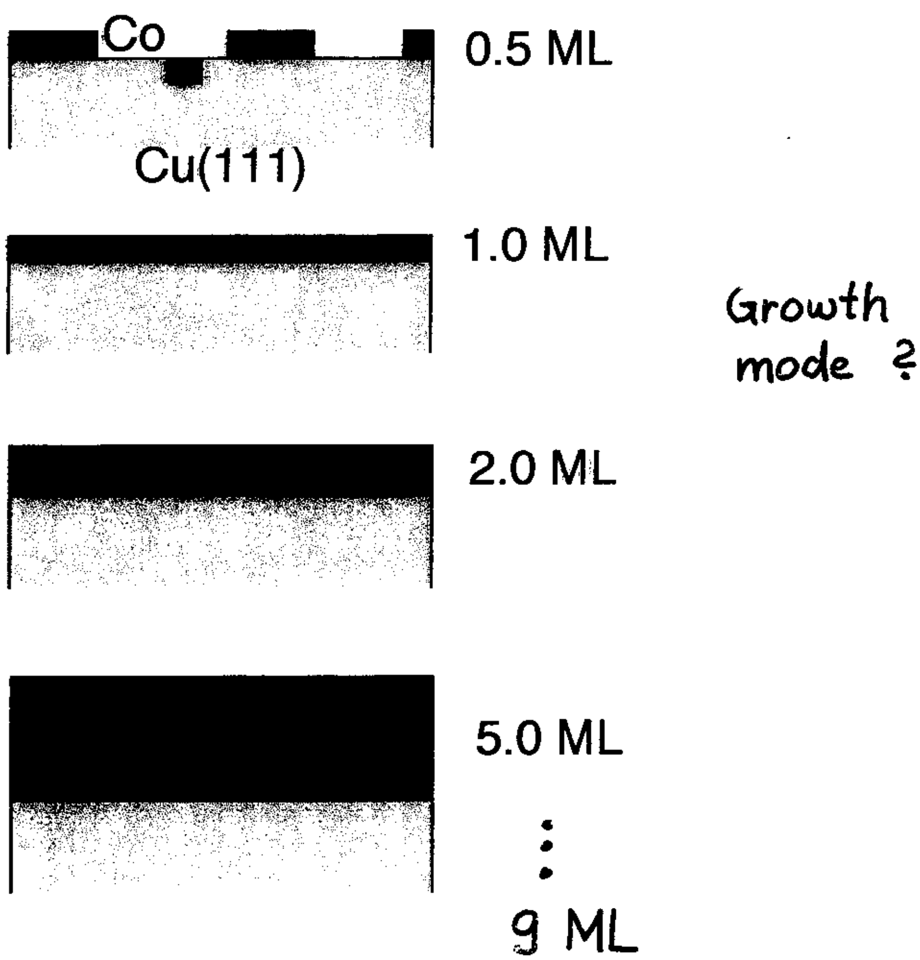


K. M. Schep, P. J. Kelly, G. E. W. Bauer, PRL 74, 586 (1995)

Co / Cu(111)

- The layer-by-layer evolution of a magnetic Fermi surface on a non-magnetic substrate.
- The room-temperature Fermi surface of hcp-Cobalt:

  How many layers does it take to converge?



Preparation by in-situ vapour deposition

Characterized by XPS, XPD

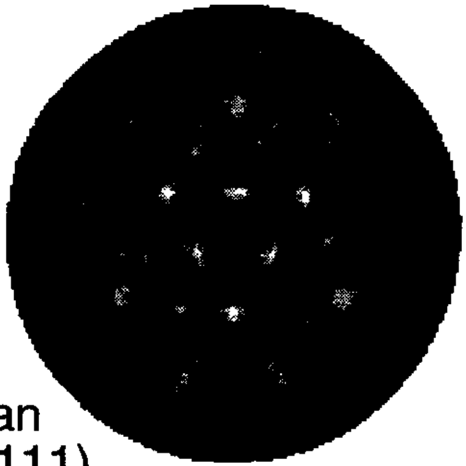
Co / Cu(111)

Growth
Morphology
(STM)

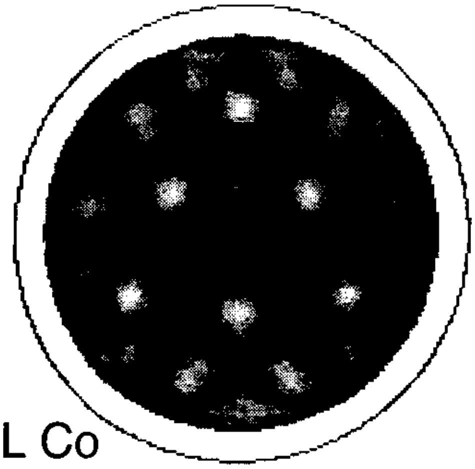
~ 0.05 ML

~ 1 ML

~ 4 ML



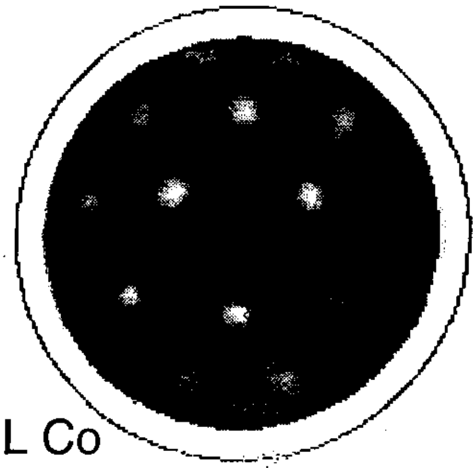
Clean
Cu(111)
Cu 2p (808 eV)



0.8 ML Co

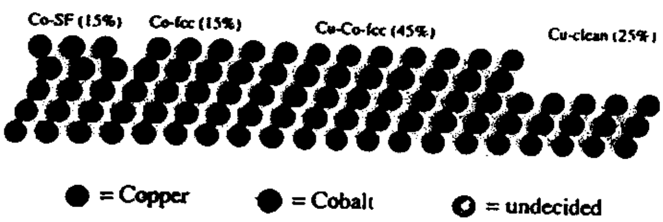
Co / Cu(111)

Photoelectron Diffraction
Co 2p (963 eV)

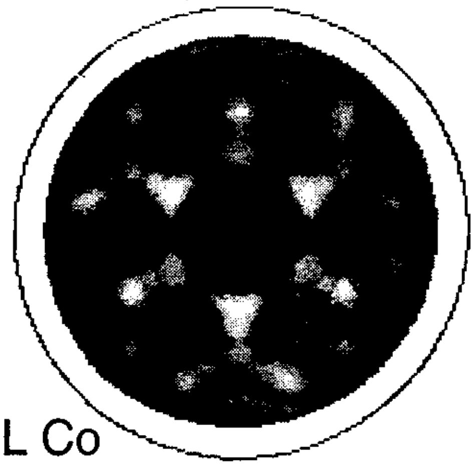


1.8 ML Co

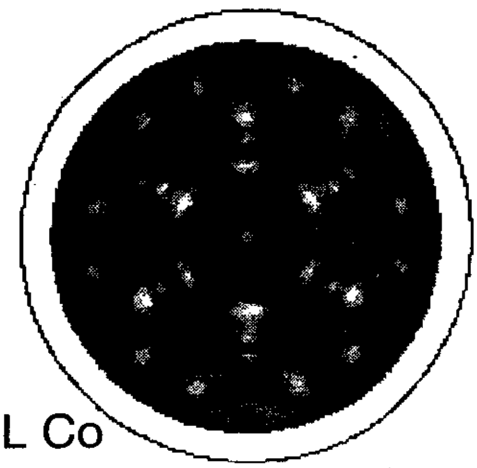
(a)



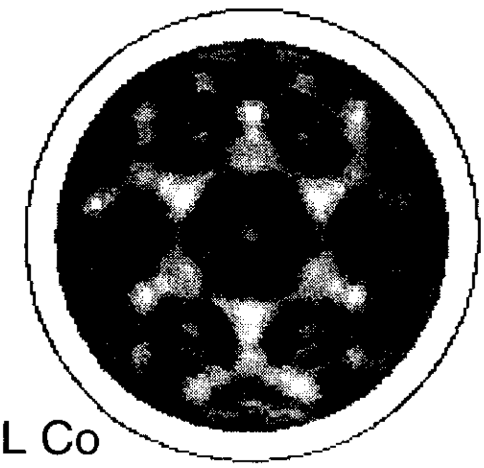
Ch. Rath et al.
PRB 55, 10791 (1997).



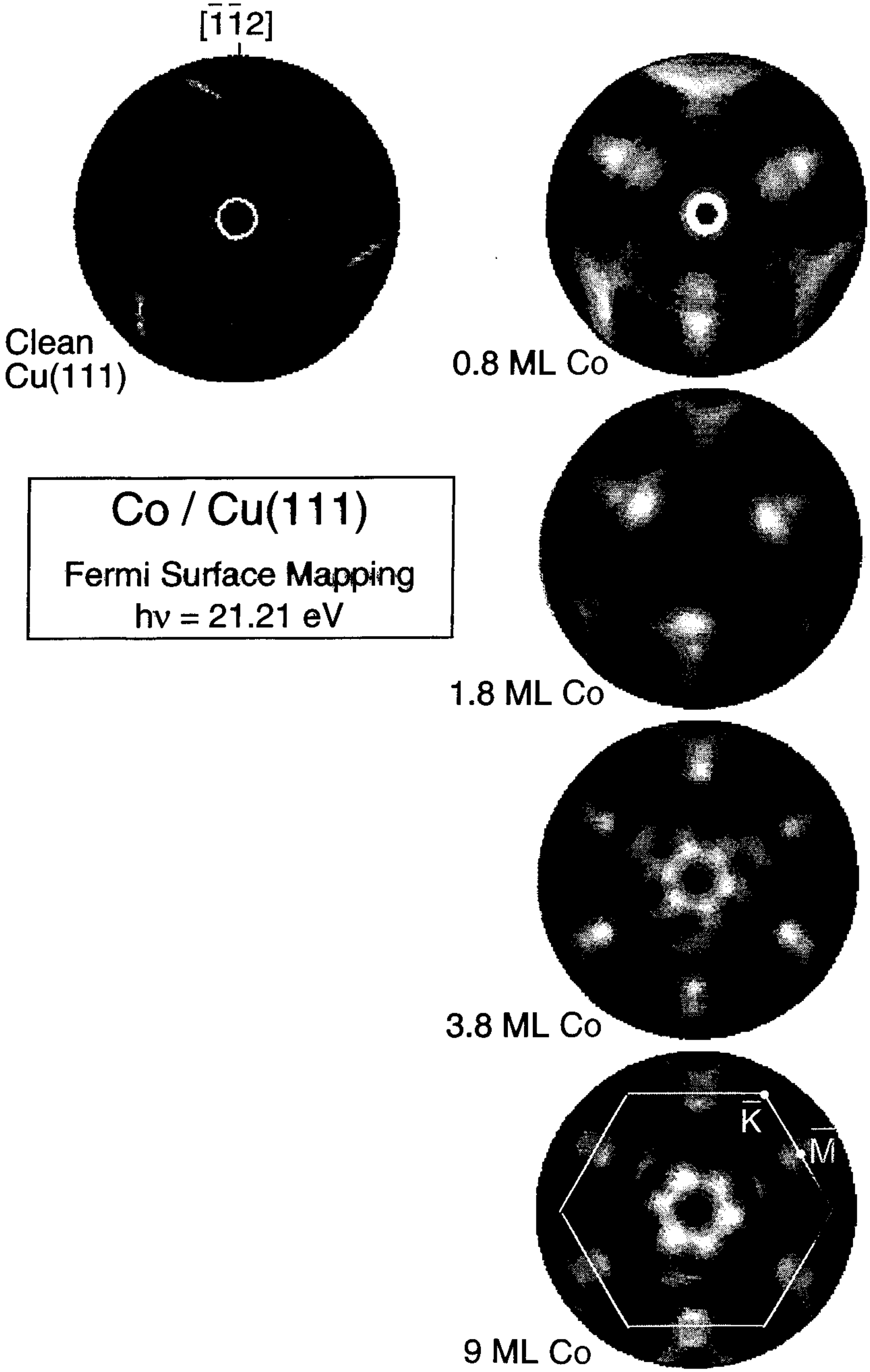
3.8 ML Co



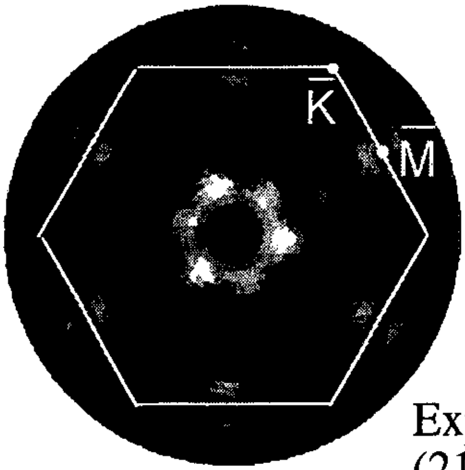
28 ML Co



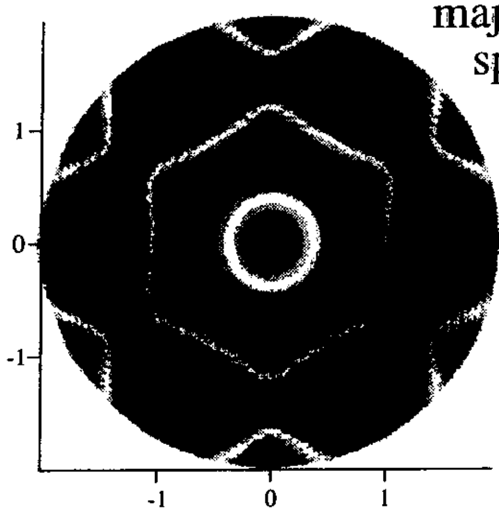
9 ML Co

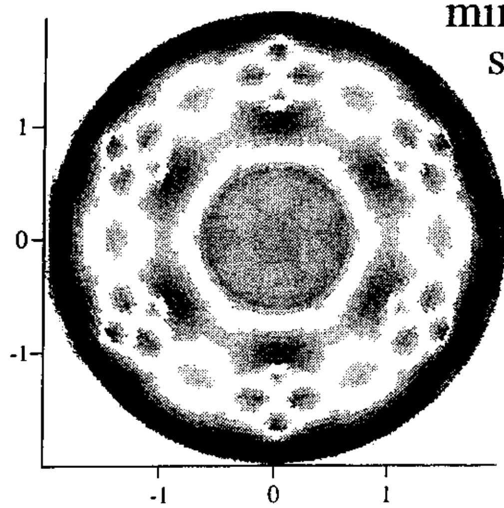

[$\bar{1}\bar{1}$2]
Clean
Cu(111)
0.8 ML Co
Co / Cu(111)
Fermi Surface Mapping
hν = 21.21 eV
1.8 ML Co
3.8 ML Co
$\bar{K}$
$\bar{M}$
9 ML Co

Fermi surface of 9 ML Co / Cu(111)

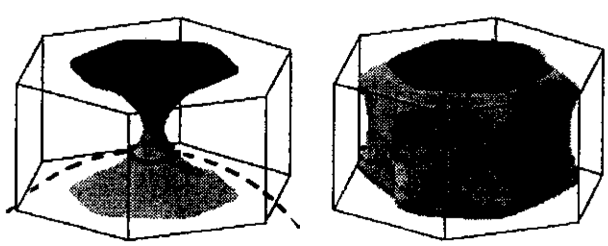


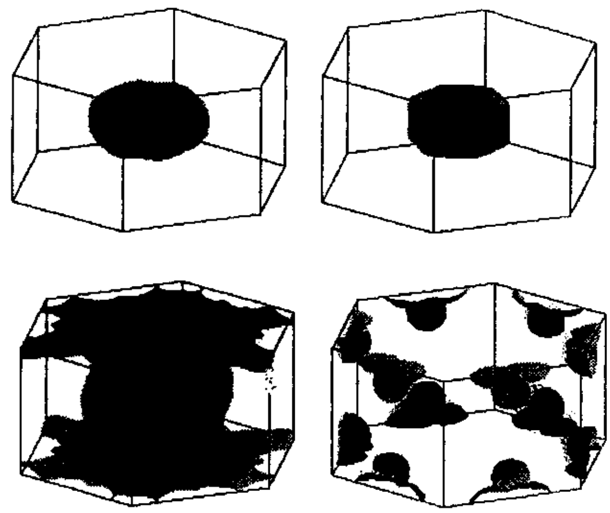
Experiment
(21.2 eV)





FLAWP (by P. Aebi)





Fermi surface figures from
http://physik.phy.tu-dresden.de/~fermisur/

Manybody Effects in Photoemission

So far: one-electron picture (Fermi gas !)

But: electrons interact with electrons
with phonons
with ...

Two types of phenomena:

- e^-- interaction in the initial state

  -> hot topic in solid state physics
  (strongly correlated materials,
  Fermi liquids -> non-Fermi liquids)

- e^-- interaction during the photoemission process

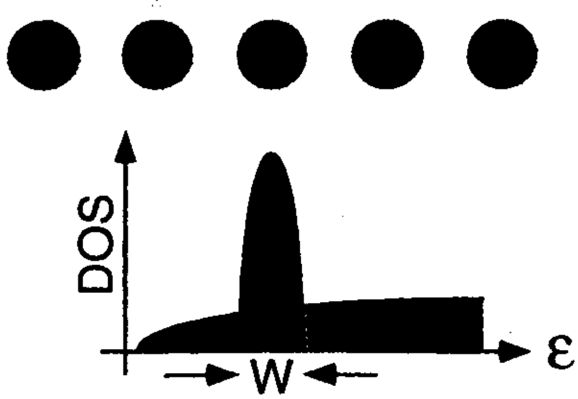
  -> satellites, line shapes, line positions

  important for interpretation of spectra !

Two extreme types of states

$R \approx d$: large overlap (s,p)
large dispersion $\varepsilon(k)$
nearly free electrons

=> one-electron picture !



$R \ll d$: little overlap (d,f)
little dispersion
tight binding

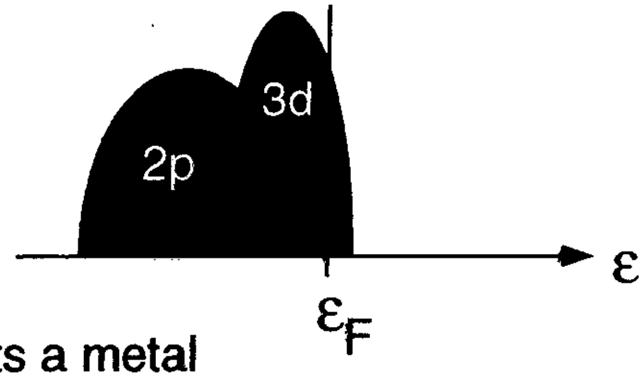
=> correlation effects !

NiO: an Example for a Strongly Correlated System

NiO

$3d^8$ $2p^6$

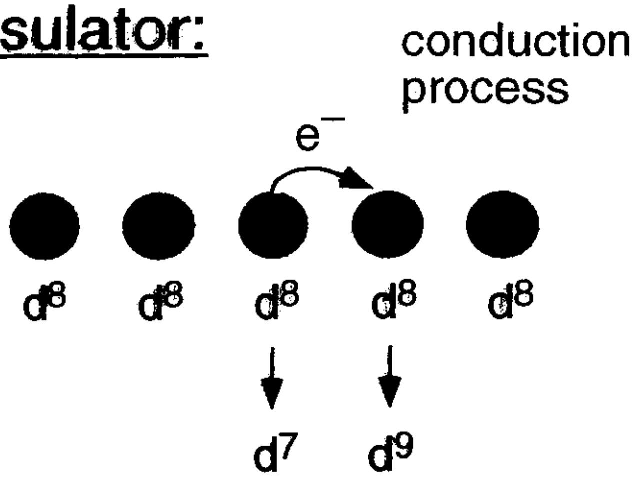
band theory:



=> predicts a metal

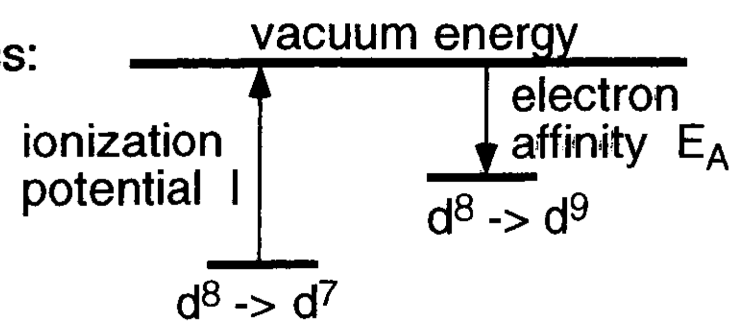
But: experiment shows insulating gap (4 eV) !

Mott Insulator:



"reaction": $2\,d^8 \dashrightarrow d^7 + d^9 - U$

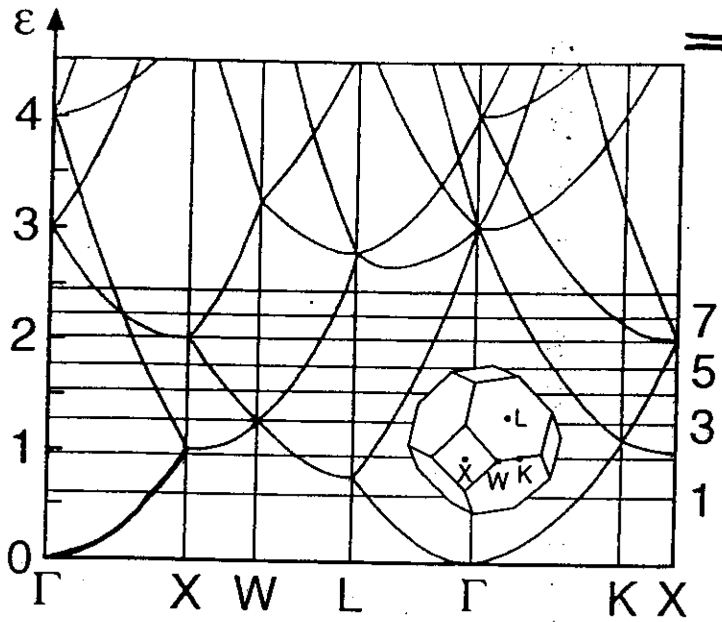
energetics:



$U = I - E_A$

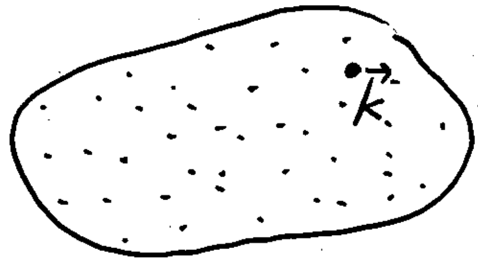
free ions : U = 18 eV
solid state : reduced (O charge transfer)

Theoretical Concepts



Theory:
⇒ energy eigenvalues:

Koopman's Theorem:

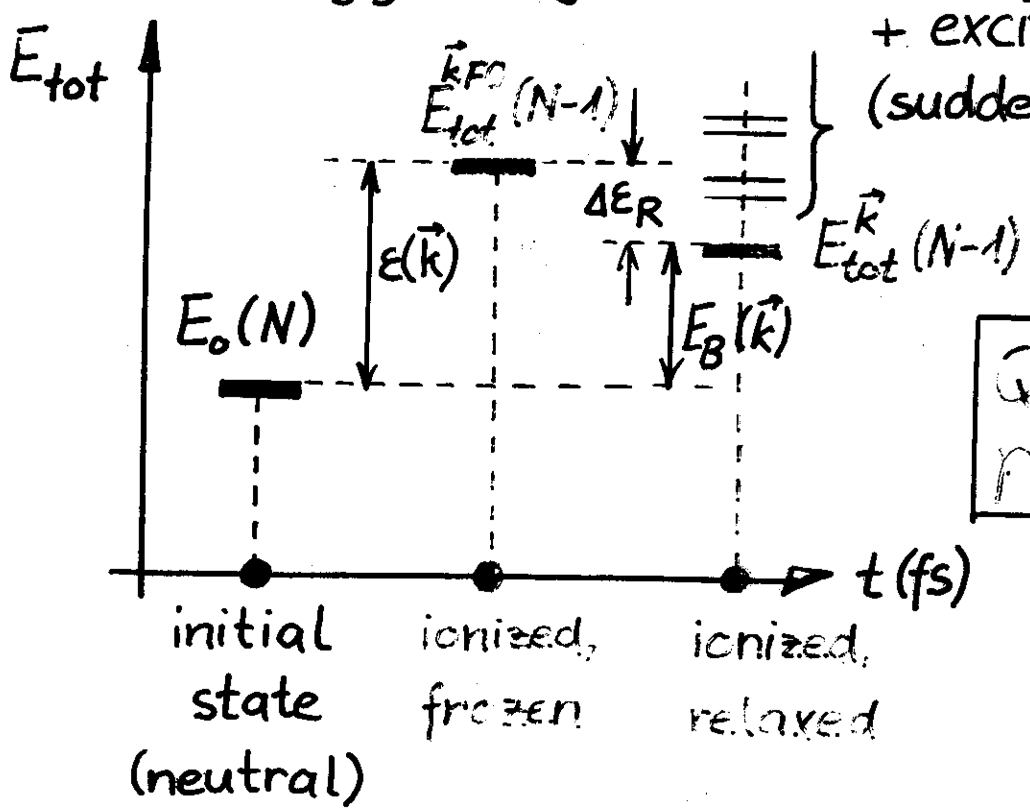


N electrons

$$\varepsilon(\vec{k}) = E_{tot}^{\vec{k},SCF}(N) - E_{tot}^{\vec{k},FO}(N-1) < 0$$

"frozen orbitals"

Total-Energy Diagram:



Quasi-particle $\vec{k}$

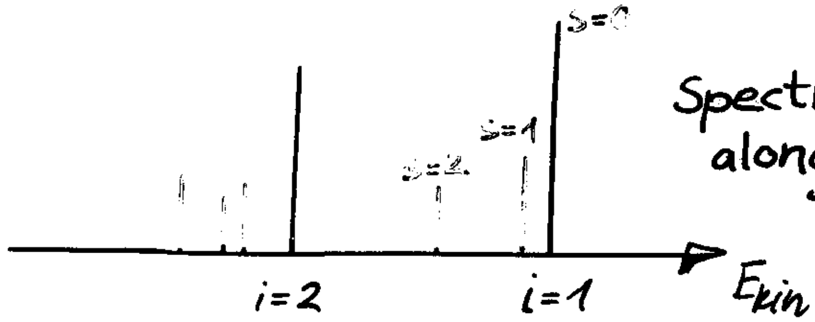
(core levels: adiabatic line)

The Photocurrent I

Atoms, Molecules:

$$I \sim \sum_{f,i,k} \left|\langle \phi_{f,E_{kin}} | \vec{r}_k \cdot \vec{\varepsilon} | \phi_{i,k}(\vec{r}_k) \rangle\right|^2 \sum_s |c_s^{i,k}|^2 \, \delta(E_{kin} + E_s(N-1) - E_0(N) - h\nu)$$

- f: various final states (angles, ...)
- i: various orbitals
- k: various atoms
- $\sum_s |c_s^{i,k}|^2$: excited final states "satellites"

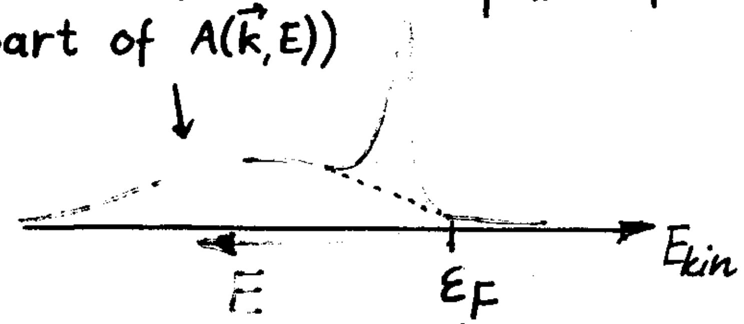


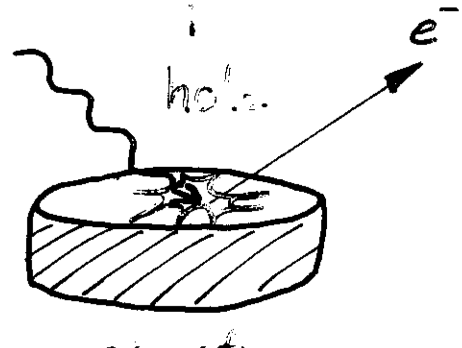
Spectrum along $(\theta, \phi) = f$

Solids:

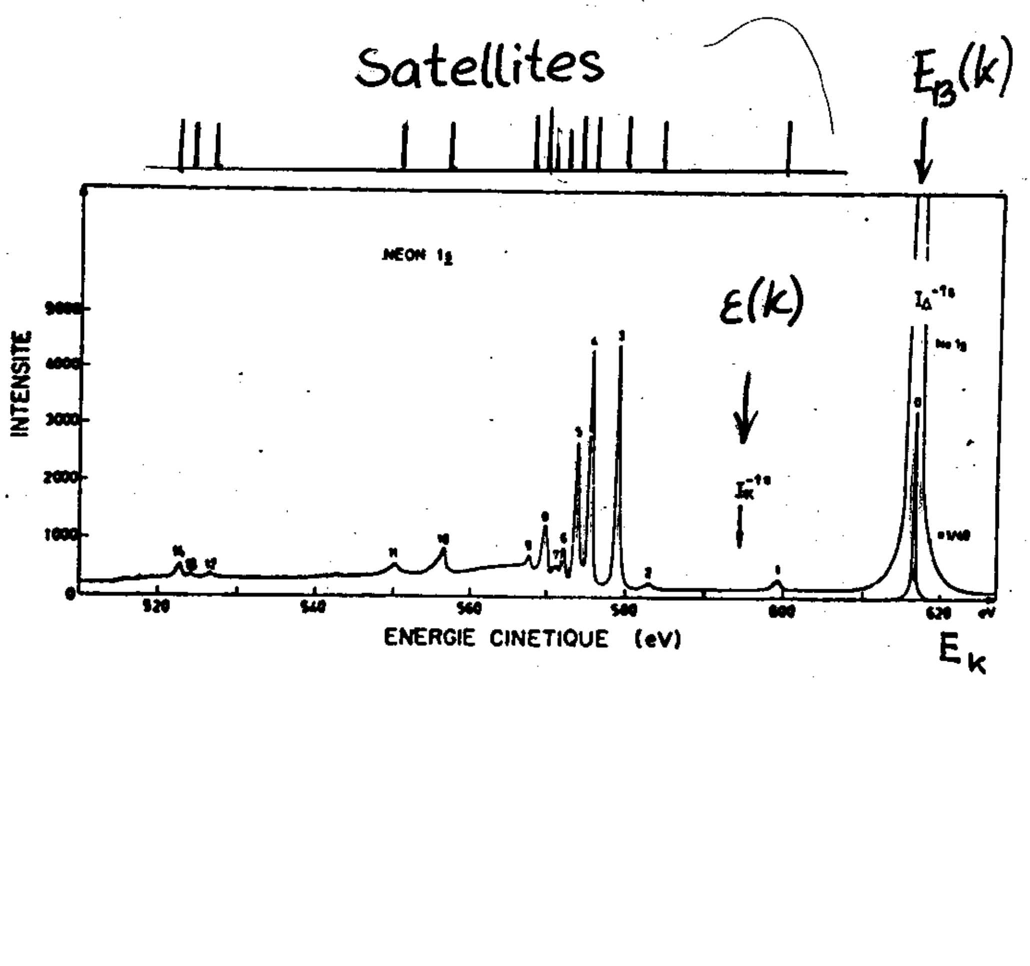
$$I \sim \sum_{f,i,\vec{k}} \left|\langle \phi_{f,E_{kin}} | \vec{r}_k \cdot \vec{\varepsilon} | \phi_{i,\vec{k}} \rangle\right|^2 A(\vec{k}, E)$$

"Spectral Function"





sea of excitations


Satellites
$E_B(k)$
NEON 1s
$\varepsilon(k)$
INTENSITE
ENERGIE CINETIQUE (eV)
E_k

Spectral Functions

... can be calculated by Greens Function Formalism:

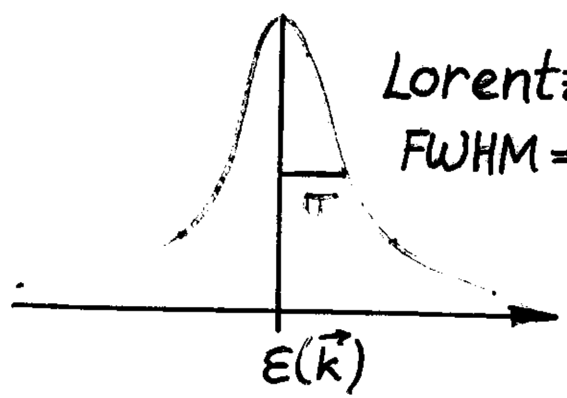
$$A(\vec{k},E) = \frac{1}{\pi}\,\mathrm{Im}\left\{G_+(\vec{k},E)\right\}$$

independent particles (no interactions):

$$G_+^0(\vec{k},E) = \frac{1}{E - \varepsilon(\vec{k}) - i\sigma}$$

$$\Downarrow$$

$$A(\vec{k},E) = \frac{1}{\pi}\,\frac{\sigma}{(E-\varepsilon(\vec{k}))^2 + \sigma^2}$$



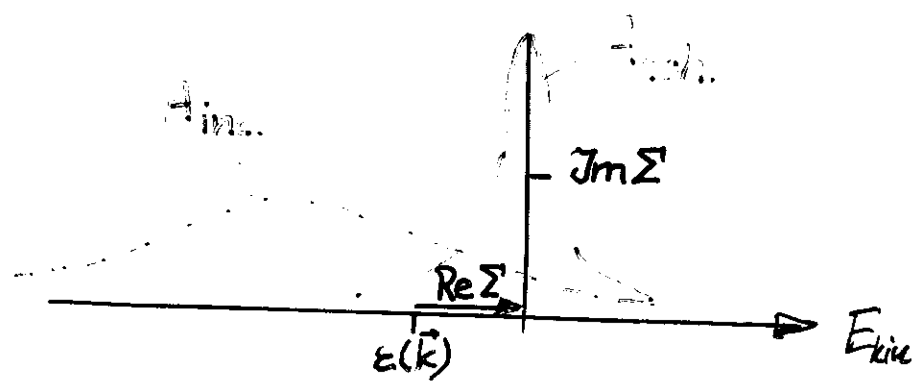
Lorentzian
FWHM = 2σ

with interactions:

$$G_+(\vec{k},E) = \frac{1}{E - \varepsilon(\vec{k}) - \Sigma(\vec{k},E)}$$

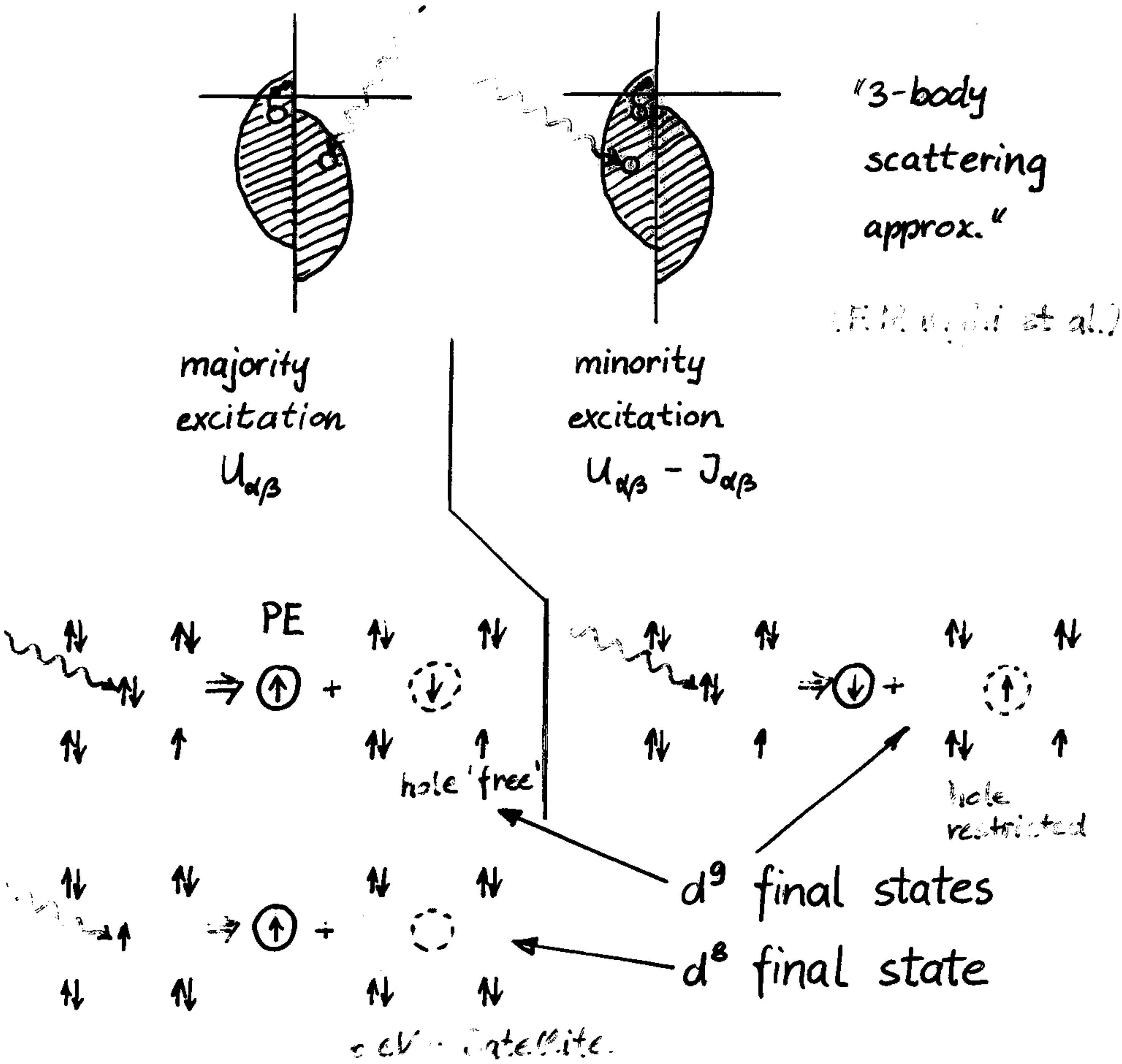
Self energy → need Hamiltonian of system!

$$A(\vec{k},E) \sim \frac{\mathrm{Im}\{\Sigma(\vec{k},E)\}}{[E - \varepsilon(\vec{k}) - \mathrm{Re}\,\Sigma]^2 + [\mathrm{Im}\,\Sigma]^2}$$

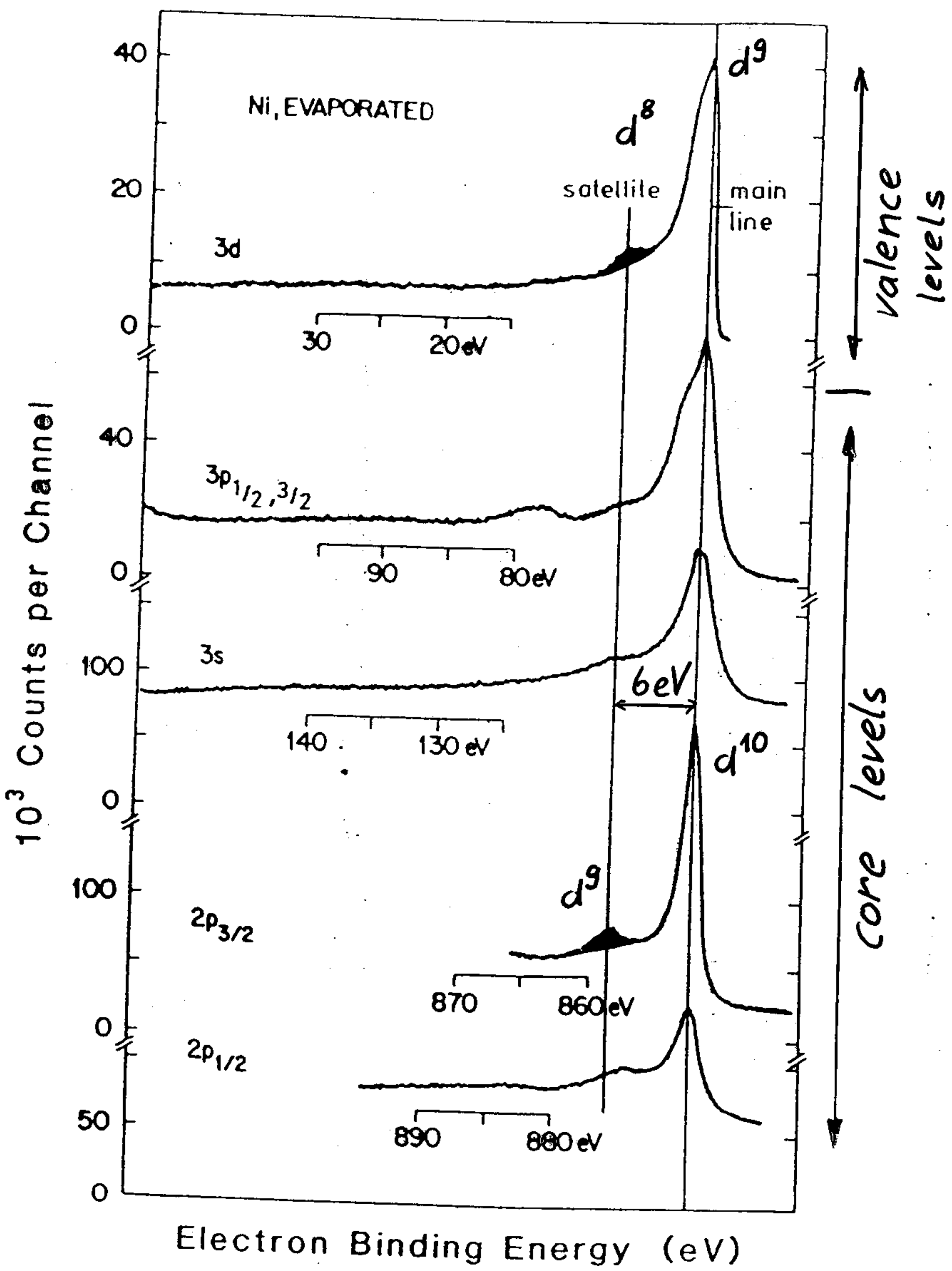


Valence Photoemission in Ni

$3d^{9.4}$ → Correlation Effects in 3d-Channel



The 6eV - Satellite in Ni - Metal

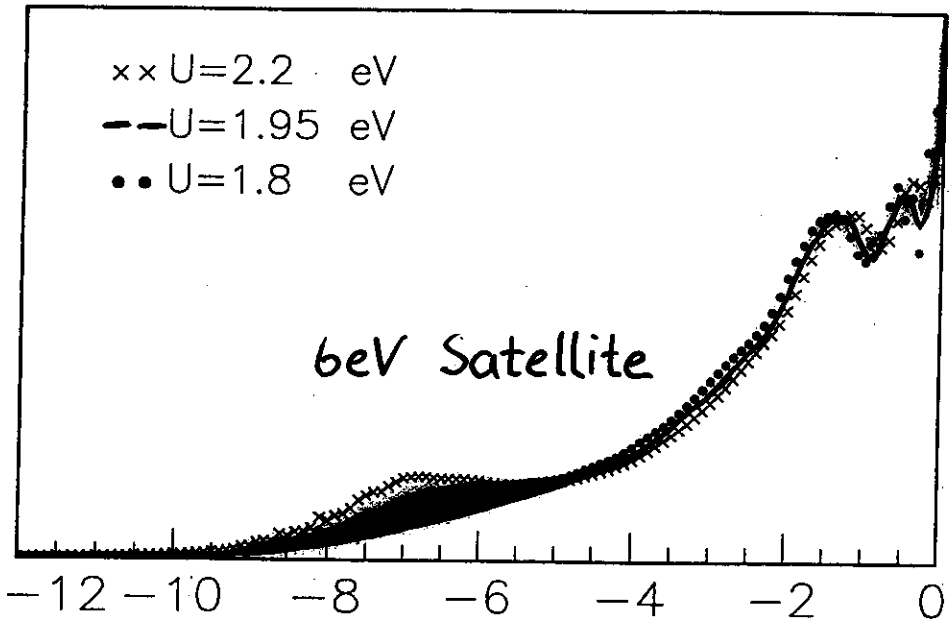


from Hüfner 1994

Quasiparticles DOS

$$n_{QP}(E) = \int_{BZ} A(\vec{k},E)\, d^3k$$

for Ni-metal:



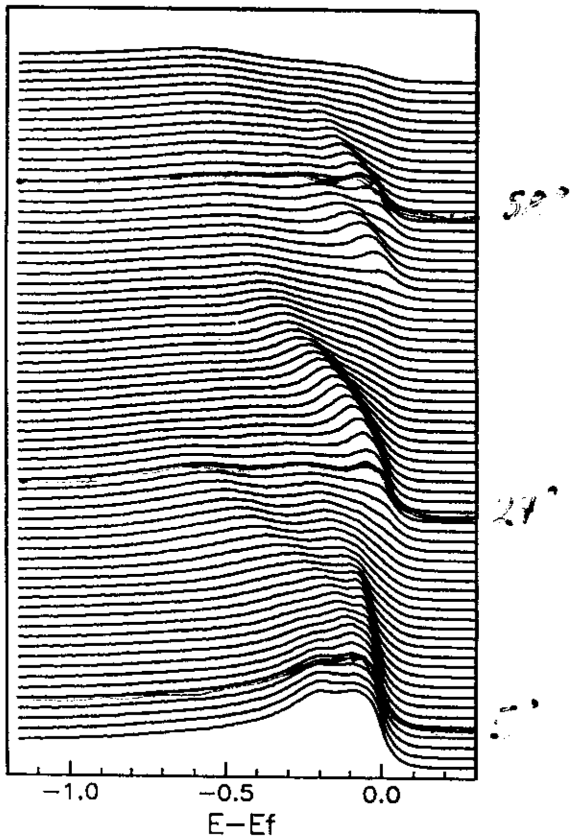
↑ no dispersion in $A(\vec{k},E)$
⇒ incoherent part

F. Manghi et al. Fig. 2
PRB 59 ('99) R10409

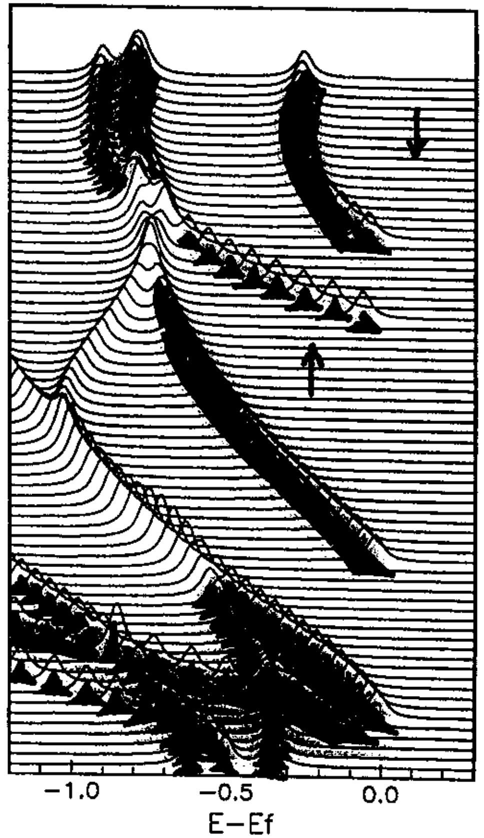
Low energy excitations - NICKEL

F. Manghi et al.
PRB 59 (1999)

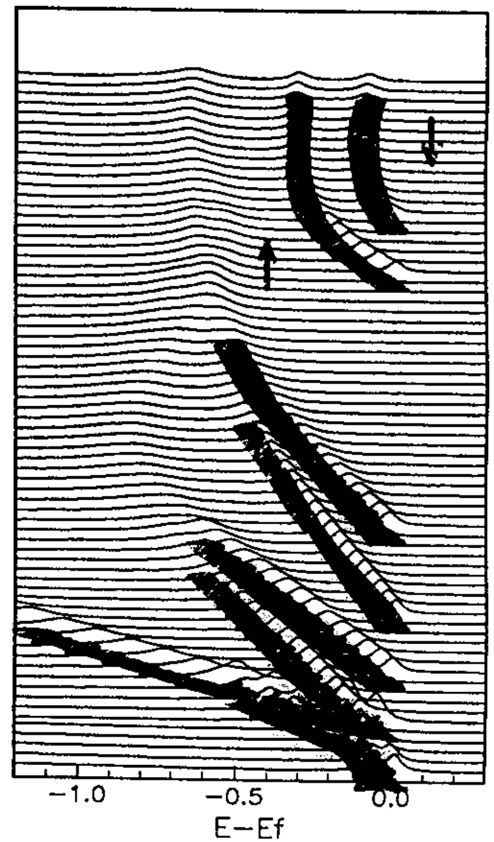
Experiments

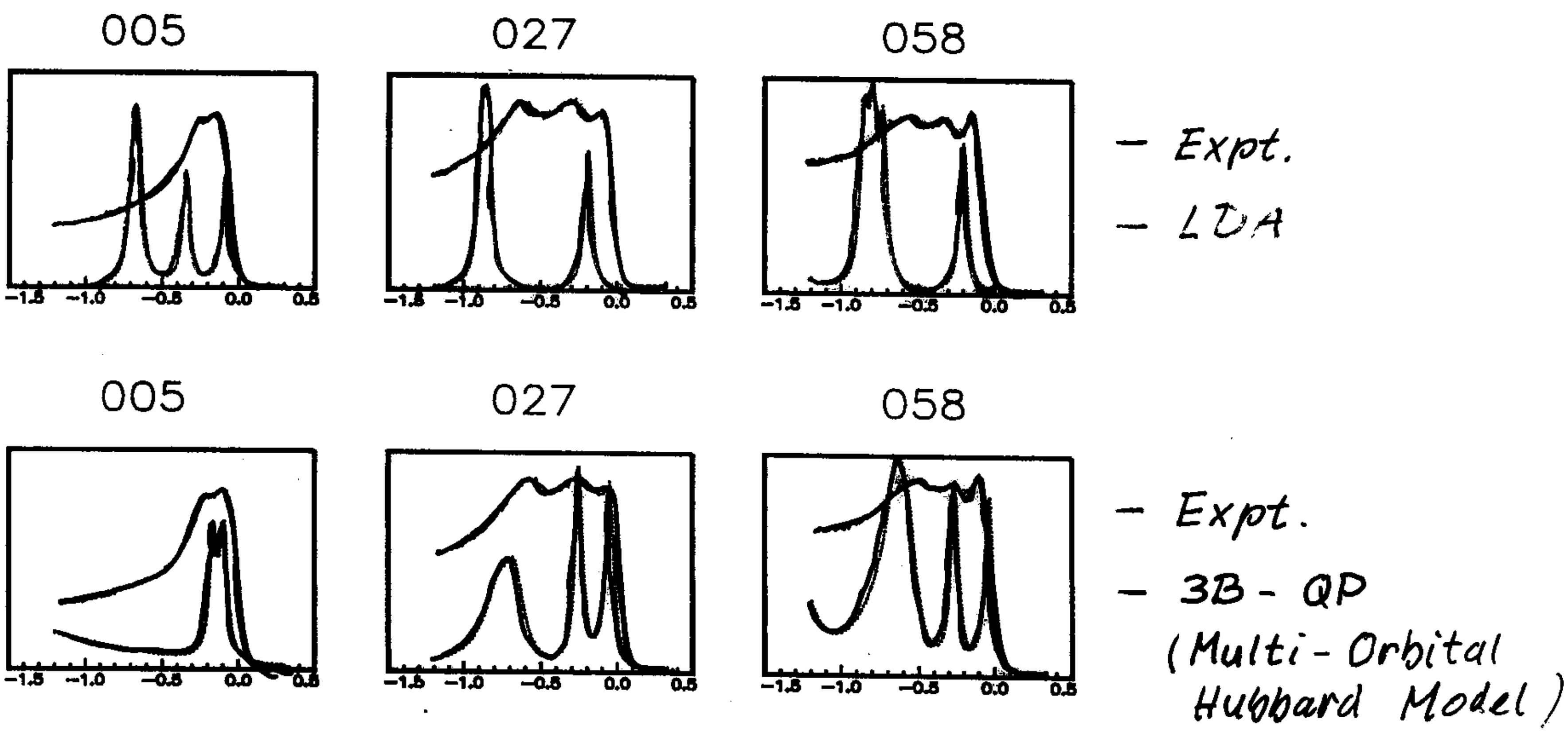


Theory (LDA)



Theory (Q.P.)




005
027
058
−1.5 −1.0 −0.5 0.0 0.5
– Expt.
– LDA
005
027
058
– Expt.
– 3B - QP
(Multi-Orbital
Hubbard Model)