Center for
Electronic Correlations and Magnetism
University of Augsburg

Theory of correlated fermionic condensed matter

1. Correlated electrons made simple

a. What are electronic correlations and where do they show up?

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 5, 2009

Dieter Vollhardt

Supported by Deutsche Forschungsgemeinschaft through SFB 484

Outline:

- "Correlations"
- Electronic correlations in the periodic table
- Fermi liquid theory
- Electronic correlations in solids: Examples
- How to detect electronic correlations:
  e.g., photoemission spectroscopy
- Model approaches to correlated electon systems:
  Hubbard model

"Correlations"

Correlation [lat.]: *con* + *relatio* *("with relation")*

Grammar: *either ... or*

Mathematics, natural sciences:

$$\boxed{\langle AB\rangle \neq \langle A\rangle\langle B\rangle}$$

e.g., densities:

$$\boxed{\langle \rho(\mathbf{r})\rho(\mathbf{r}')\rangle \neq \langle \rho(\mathbf{r})\rangle\langle \rho(\mathbf{r}')\rangle}$$

Beyond (standard) mean-field theory [Weiss/Hartree-Fock,...]

correlation $\neq$ causality

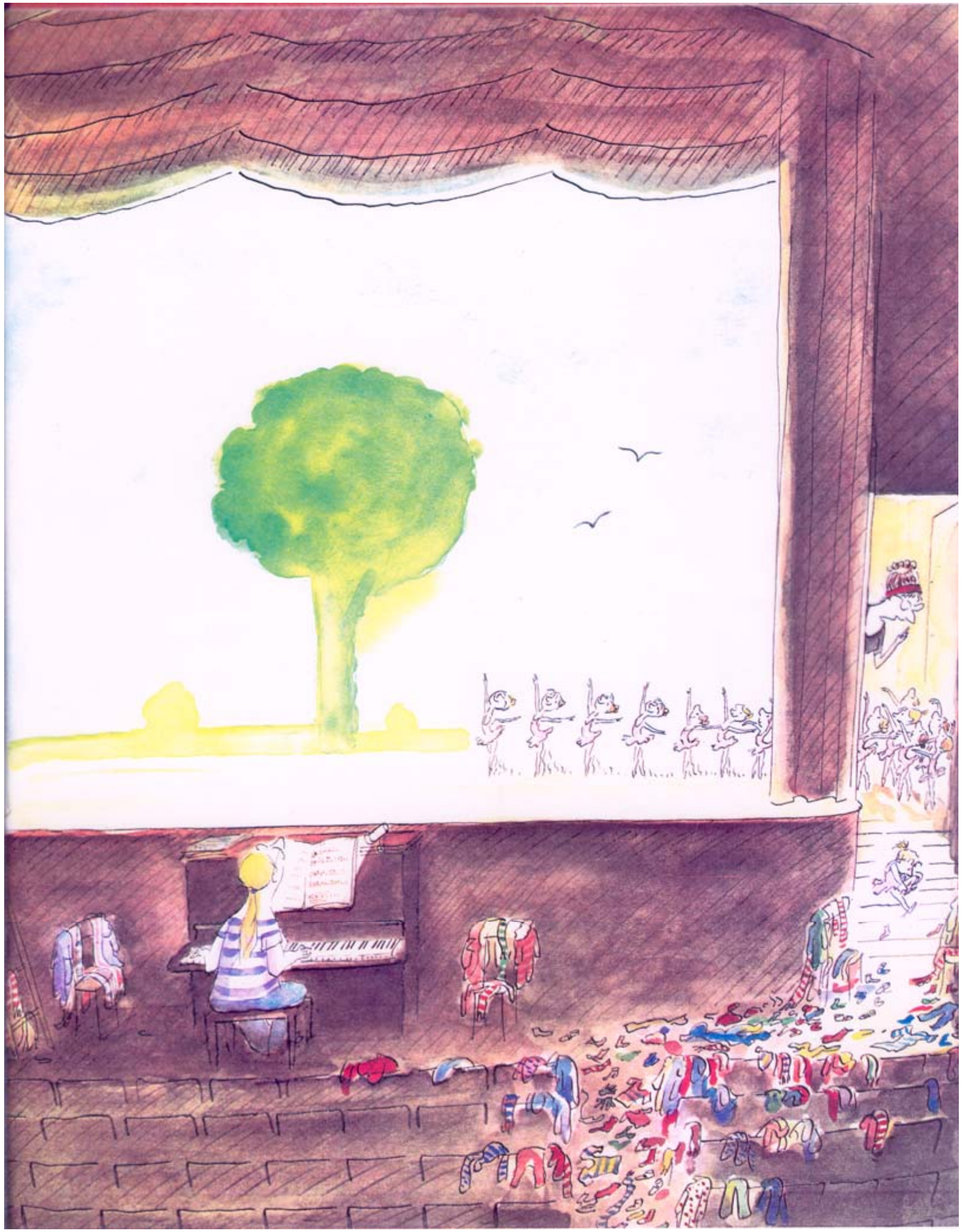
Short-range spatial correlations in everyday life

Time average insufficient

Correlations

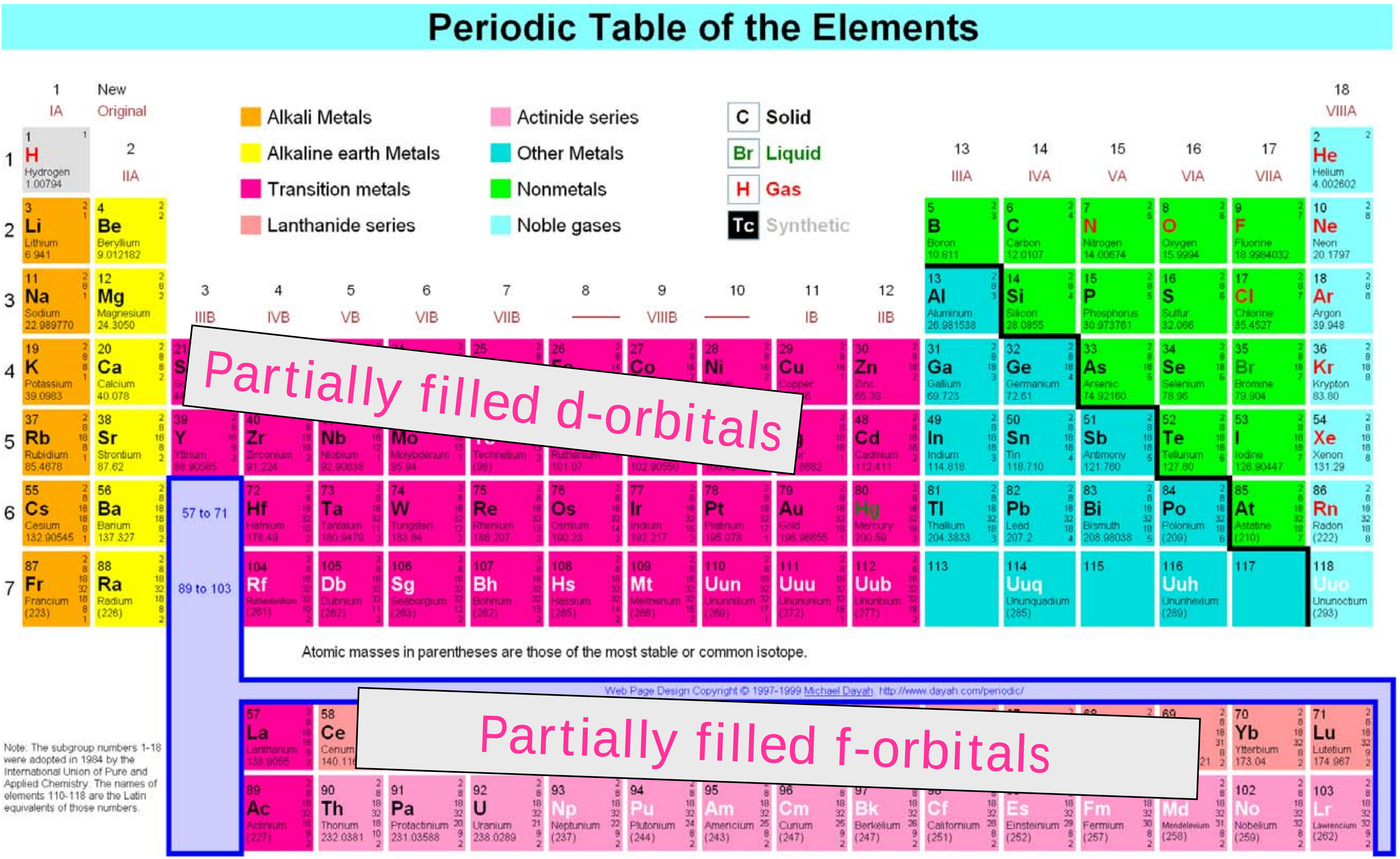
vs.

long-range order



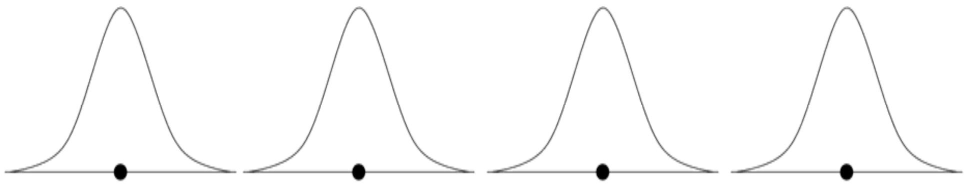
(*Sempe*)

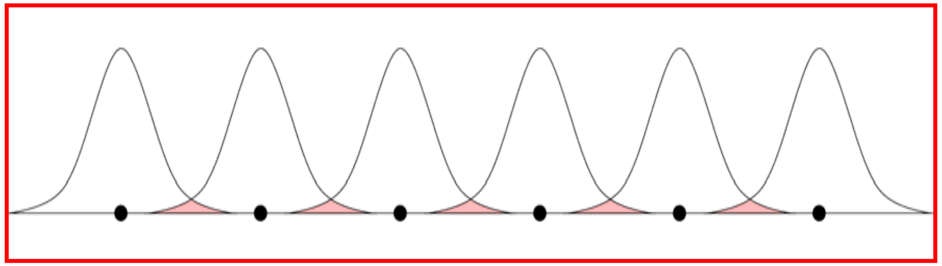
Electronic Correlations in the Periodic Table



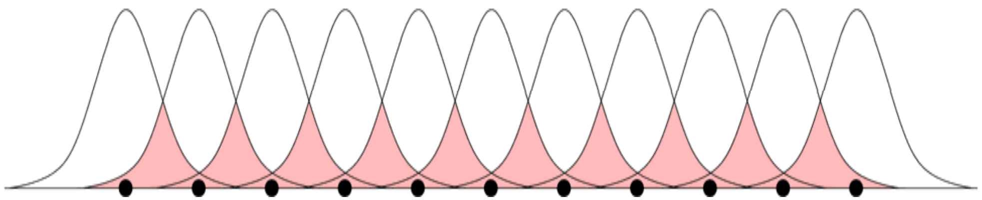
Narrow d,f-orbitals → strong electronic correlations

Electronic Bands in Solids





overlap of wave functions:
matrix element *t*



Property	Energy levels	Represen-tation	Example
Insula-tor	Atomic levels	Localized electrons $n_{\mathbf{i}\sigma}$	Solid Ne NaCl
Corre-lated metal	Narrow bands	$n_{\mathbf{i}\sigma} \leftrightarrow n_{\mathbf{k}\sigma}$	Tran-sition + rare earth metals/ oxides (Ni, V_2O_3, Ce)
Simple metal	Broad bands	Extended waves $n_{\mathbf{k}\sigma}$	Na, Al

Estimate strength of correlations:

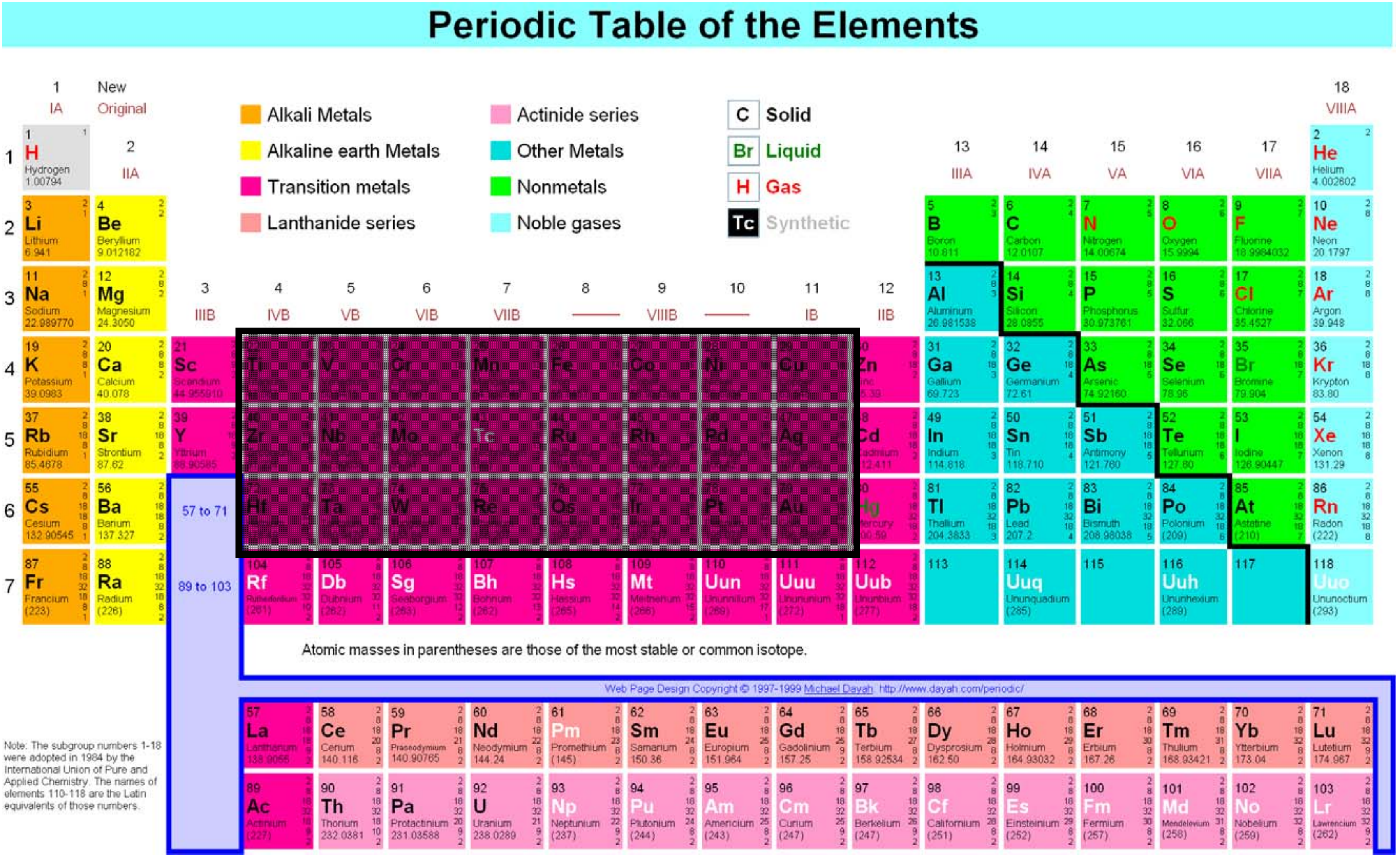
$$\frac{1}{\hbar}\left|\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}\right| = \mathrm{v}_{\mathbf{k}} = \frac{\text{lattice spacing: } a}{\text{average time spent on atom: } \tau} \sim \frac{1}{\hbar} aW$$

$$\Rightarrow \tau \sim \frac{\hbar}{W}$$

Consequences?

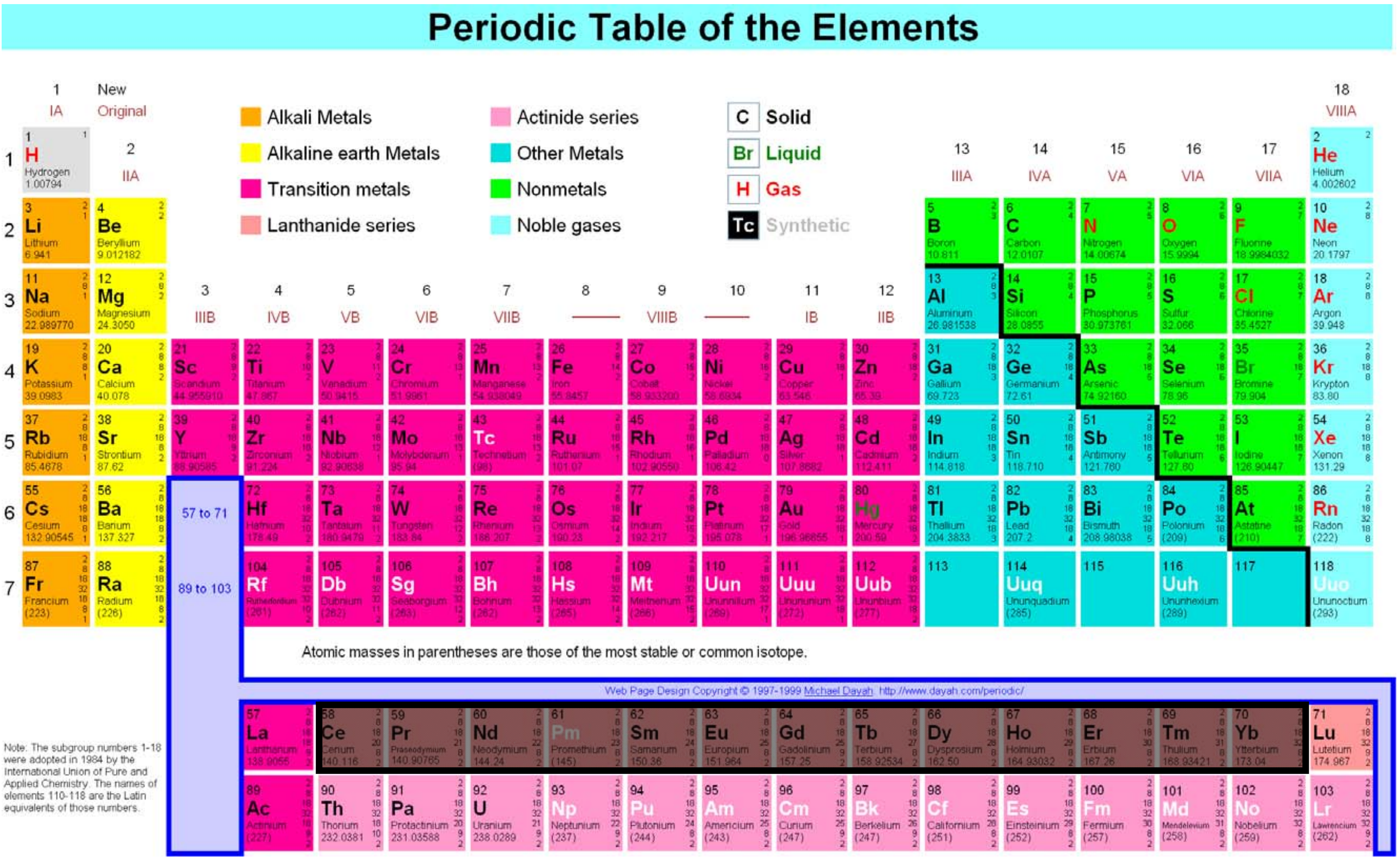
$$\left|\varepsilon_{\mathbf{k}}\right| \propto \text{band overlap } t \sim \text{band width } W$$

Small W: Strong electronic correlations

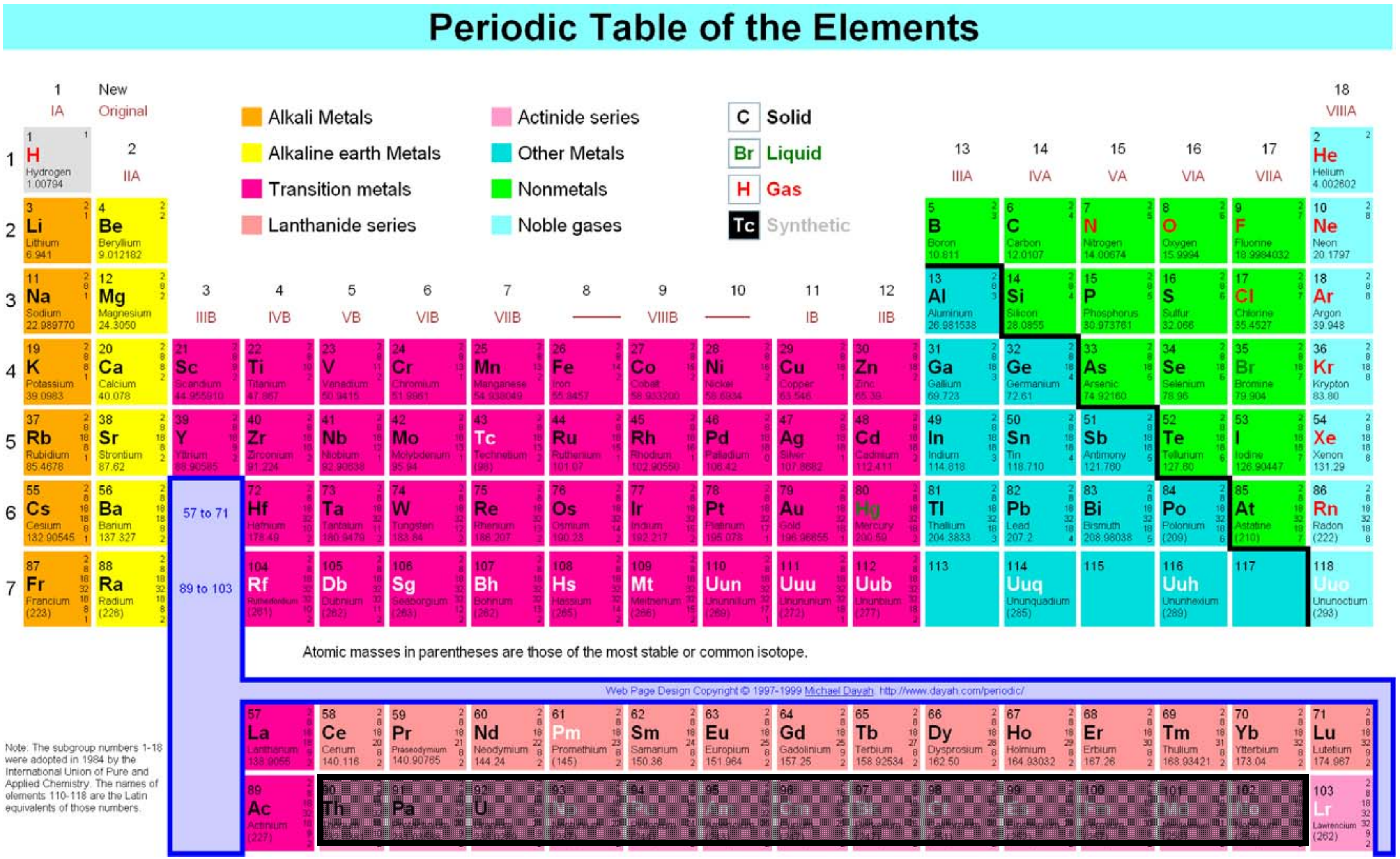


Transition metals: Spin, charge, orbital order; electron-lattice coupling, Mott-Hubbard metal-insulator transitions, high T_c, ...

Transition metal oxides: direct view of d-electrons



Rare earth elements: Heavy fermion-, Kondo lattice-, RKKY-behavior,
unconventional superconductivity,
non-Fermi liquid behavior, volume anomalies



Actinides: Heavy fermion behavior, unconventional superconductivity, volume anomalies, strong spin-orbit coupling

Electrons vs. Quasiparticles, Fermi liquid theory

Electrons

Spin = $\frac{1}{2}\hbar$ Fermion

$\Downarrow$

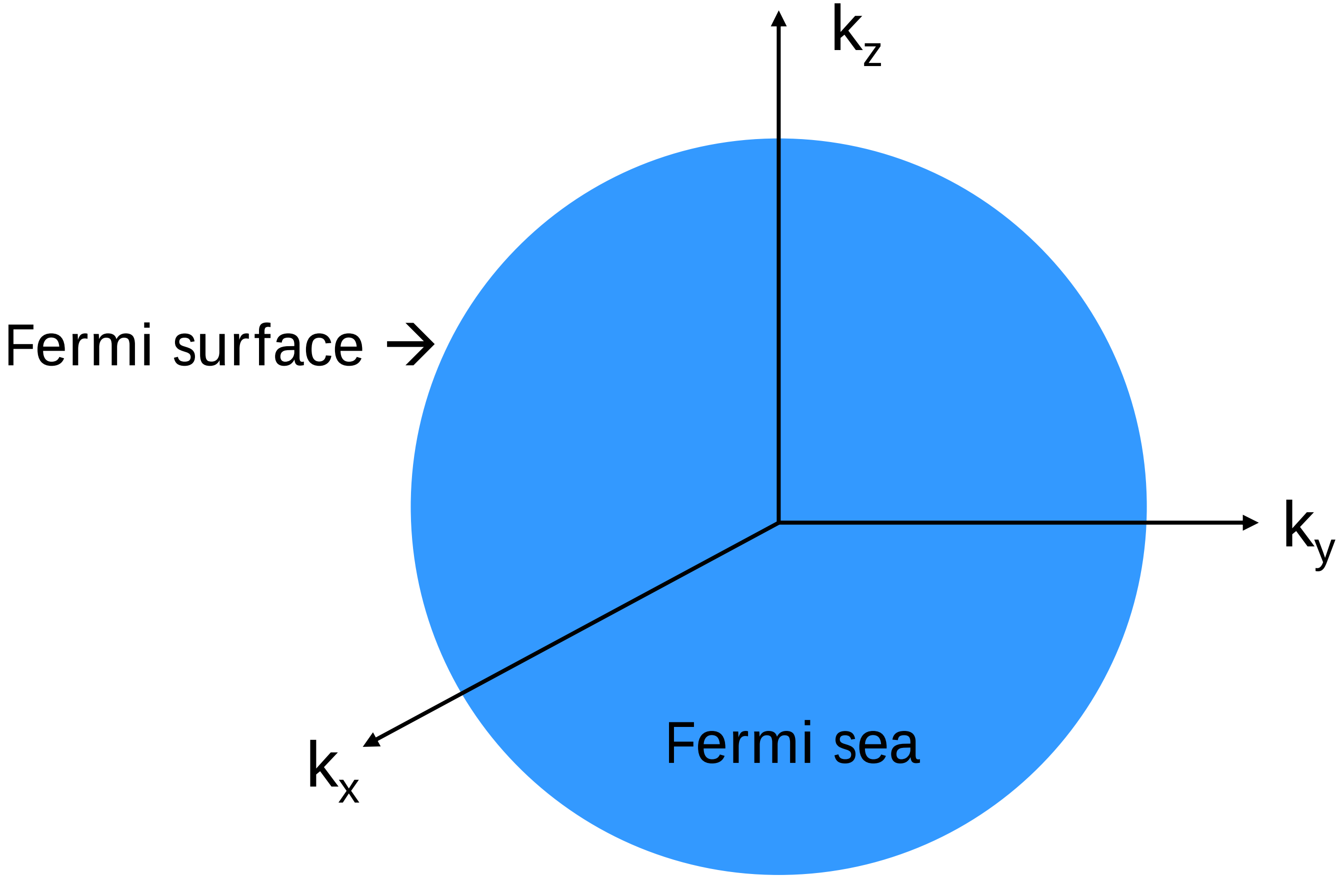
Fermi-Dirac statistics

$\Downarrow$ Pauli exclusion principle of many fermions

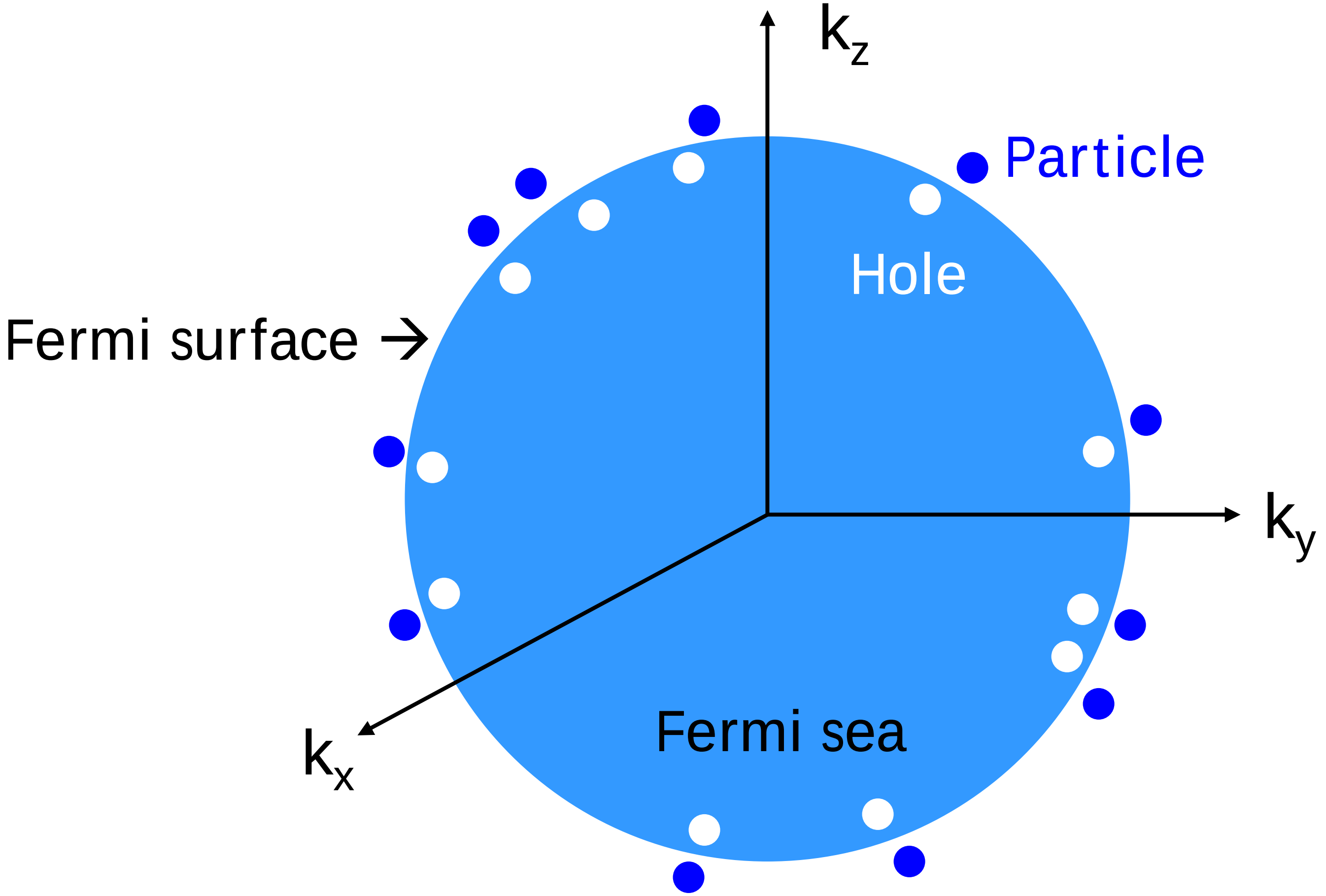
Fermi body/surface

No such thing for bosons!

Fermi gas: **Ground state**



Fermi gas: **Excited states (T>0)**



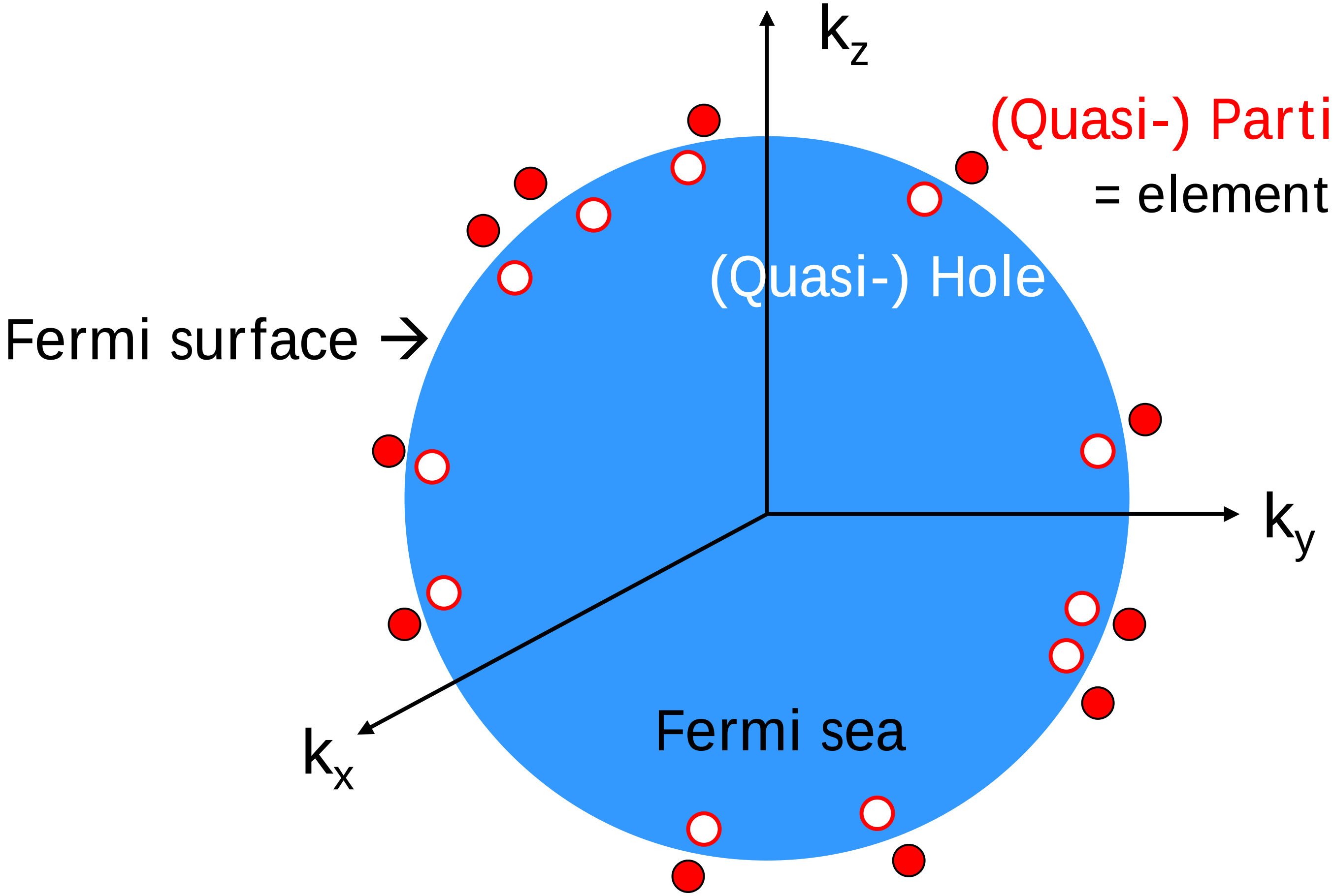
Exact **k**-states ("particles"): infinite life time

Switch on interaction adiabatically (d=3)

Landau Fermi liquid

Landau (1956/58)

1-1 correspondence between **k**-states

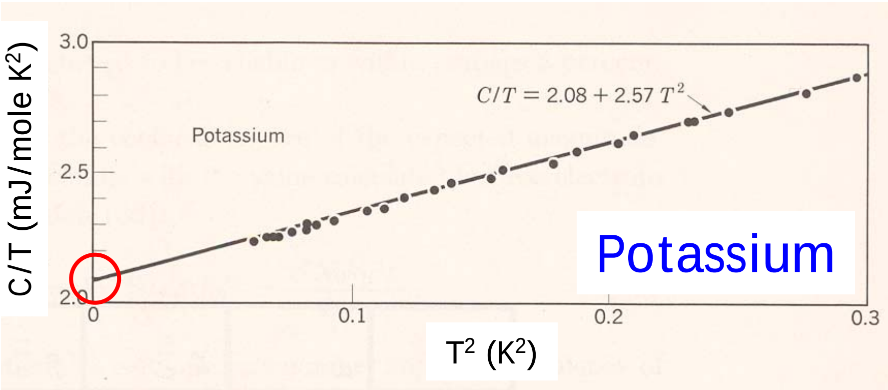


Well-defined **k**-states ("quasiparticles") with
- finite life time
- effective mass
- effective interaction

Electronic Correlations in Solids: Examples

1.

Simple metals

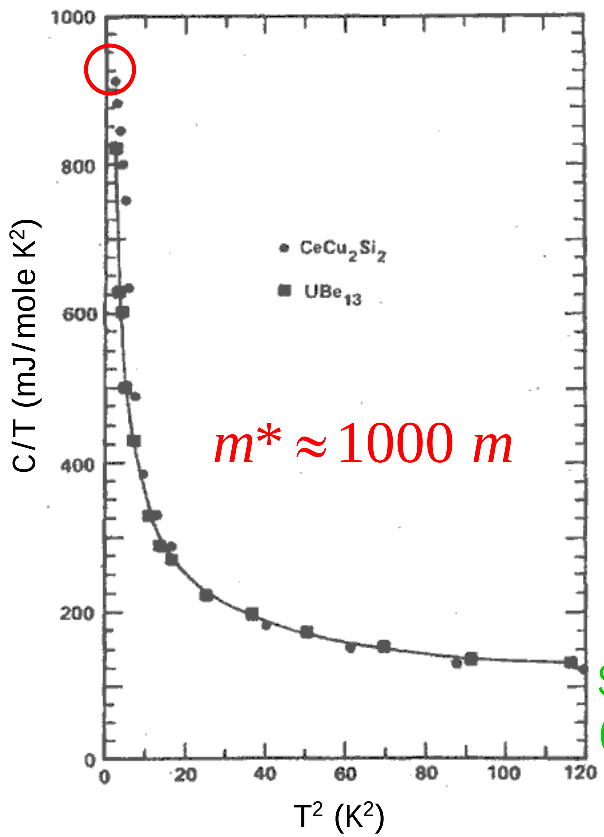


Consequence of elementary excitations (quasiparticles)

$$\lim_{T\to 0}\frac{c_V}{T}\approx\gamma_0 \Rightarrow m^*\approx m$$

"Heavy Fermions"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

$CeCu_2Si_2$, UBe_{13}:
very heavy quasiparticles

$$\lim_{T\to 0}\frac{c_V}{T}=\gamma\propto\frac{m^*}{m},\quad v_F=\frac{\hbar k_F}{m^*}$$

2.

Magnetic impurity in a metallic host: The Kondo effect

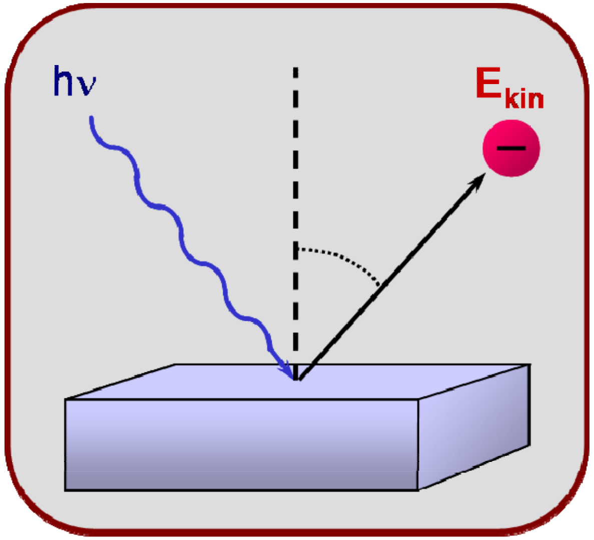
Ce

Explanation of the three peak structure?

Excursion:

Detection of electronic correlations in solids by Photoemission spectroscopy

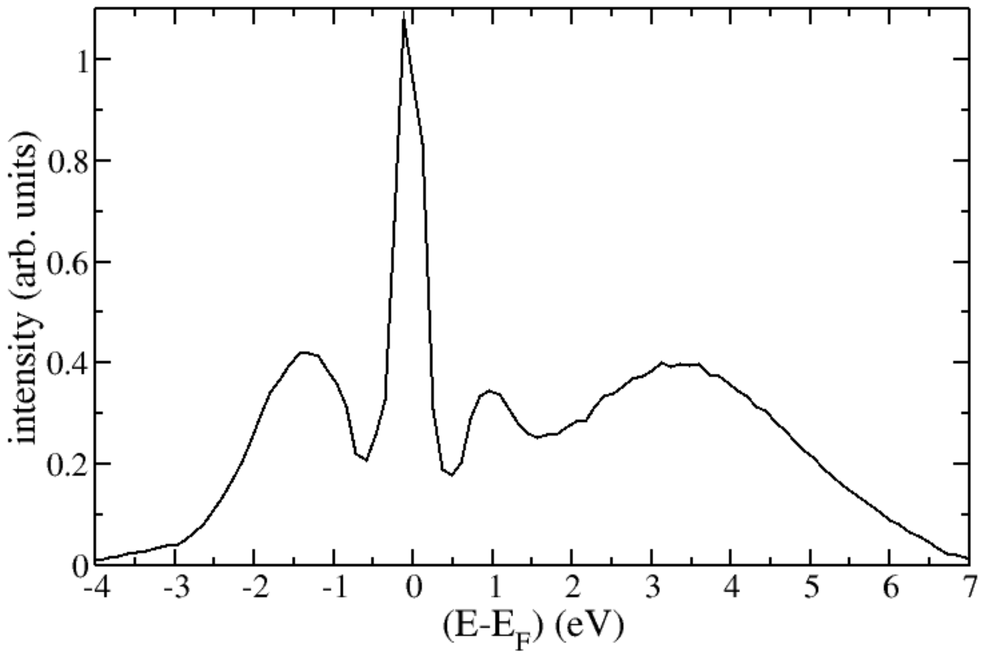
1. Photoemission Spectroscopy (PES)



Angular Resolved PES = ARPES

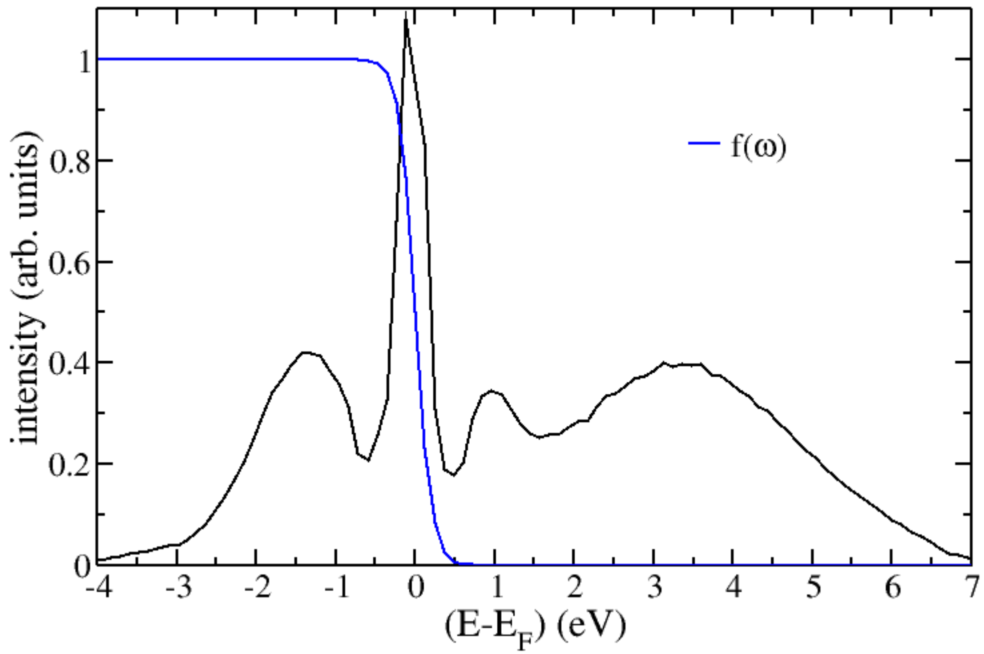
Measures occupied states of electronic spectral function

PES



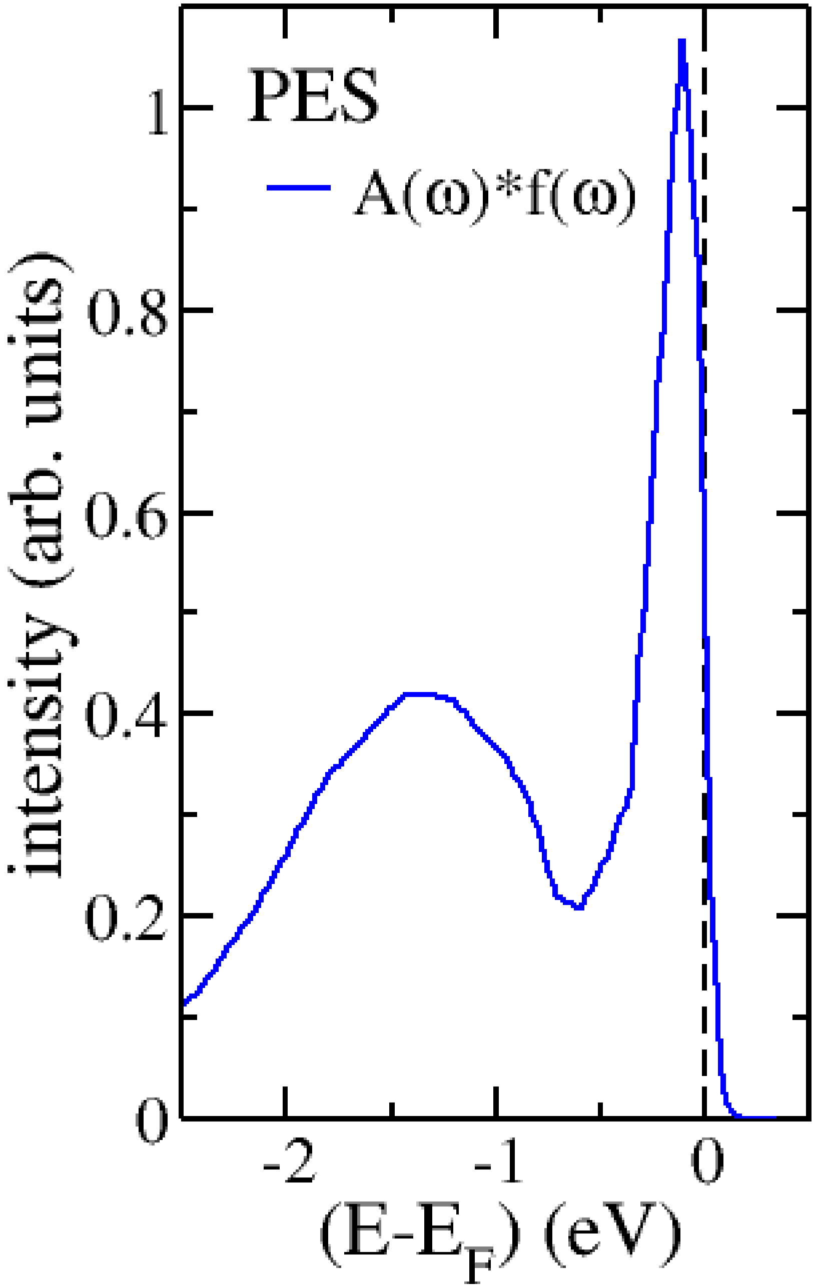
Ideal spectral function of a material

PES



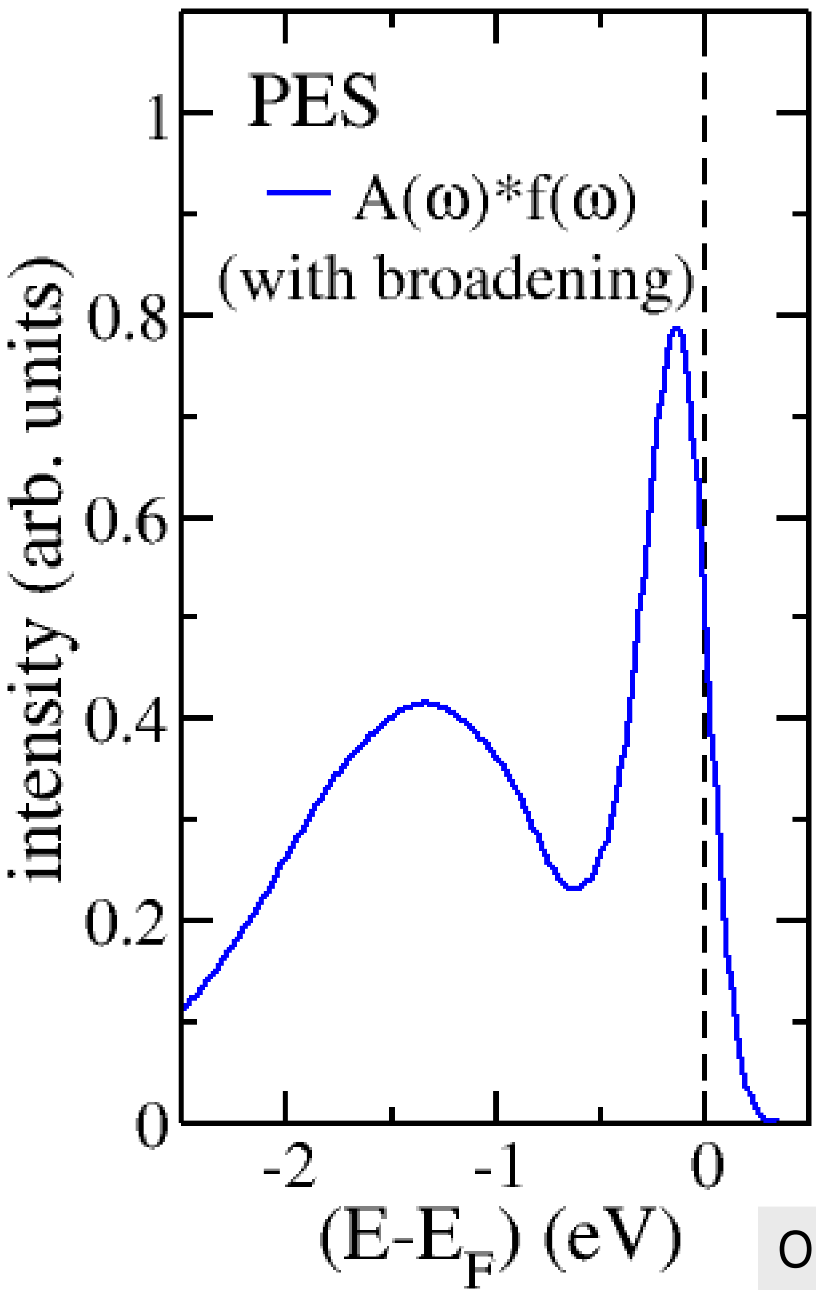
Ideal spectral function of a material

PES



Occupied states (ideal)

PES



Occupied states (measured)

Only two peaks visible

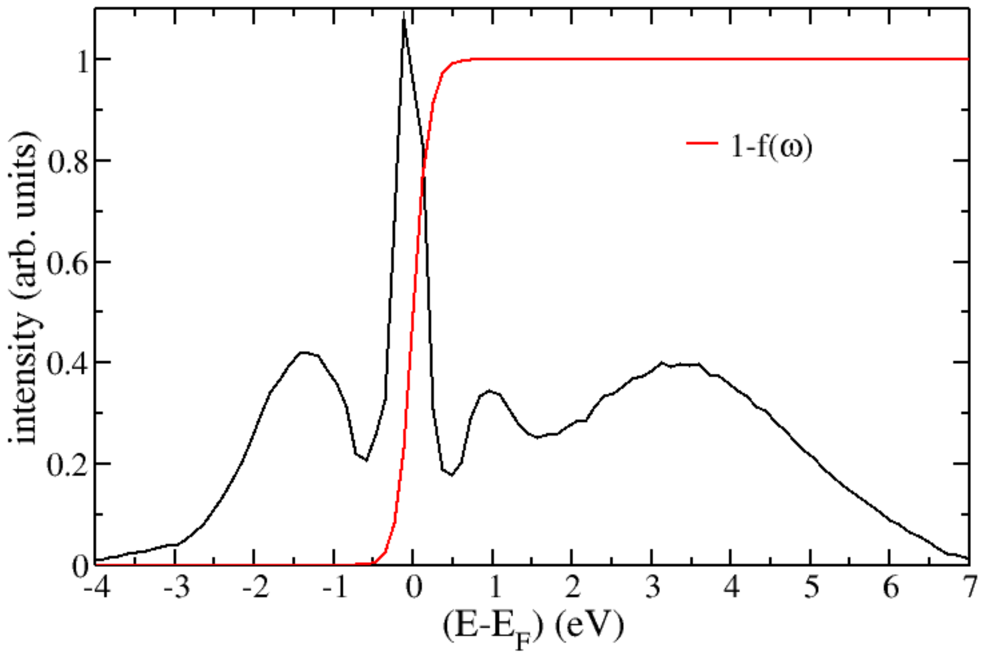
2. Inverse Photoemission Spectroscopy (IPES)

Measures unoccupied states of electronic spectral function

Information also available by:

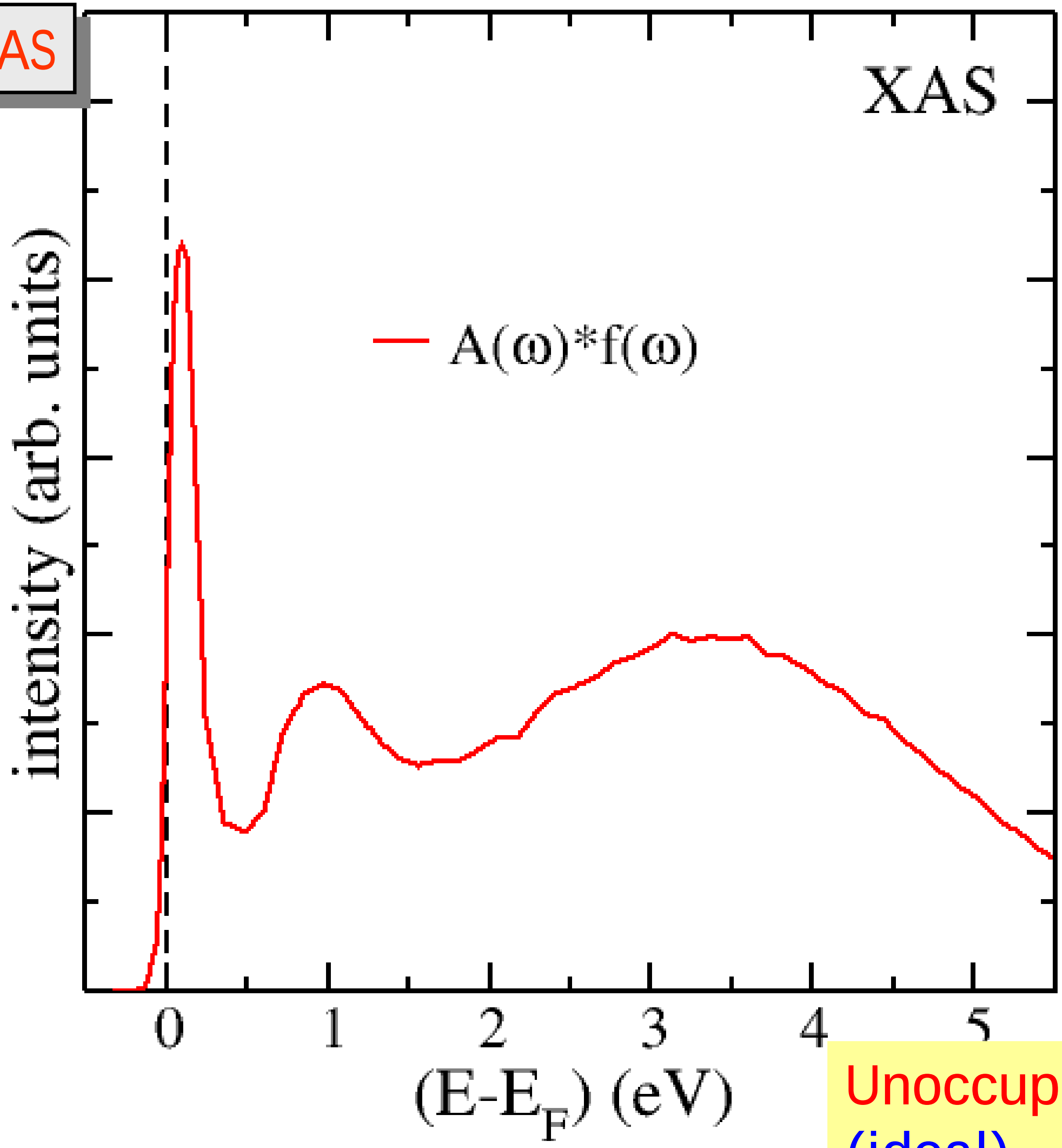
X-ray Absorption Spectroscopy (XAS)

IPES / XAS



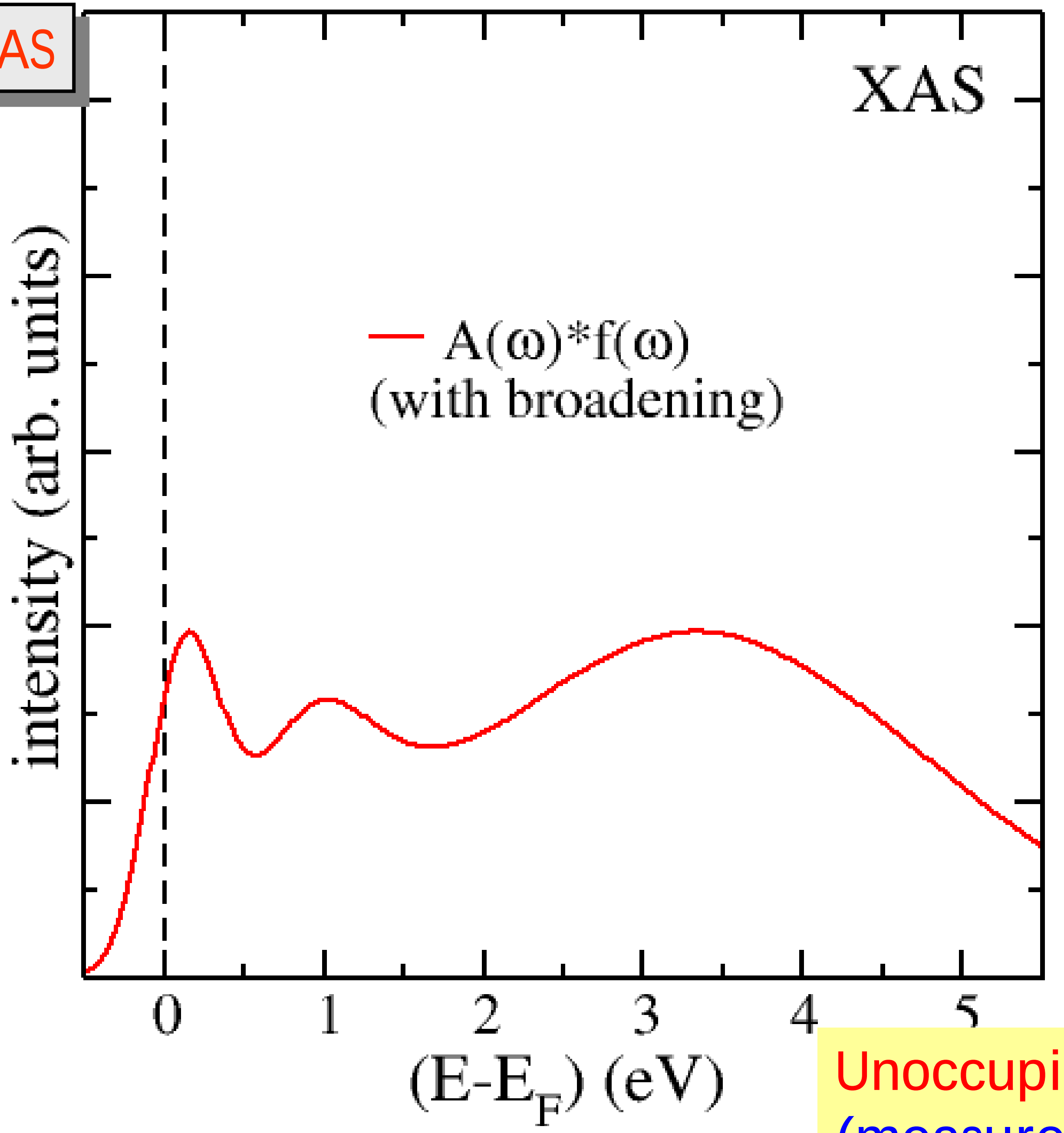
Ideal spectral function of a material

IPES / XAS



Unoccupied states
(ideal)

IPES / XAS



Unoccupied states
(measured)

3.

Photoemission spectra of Ni: -6 eV satellite

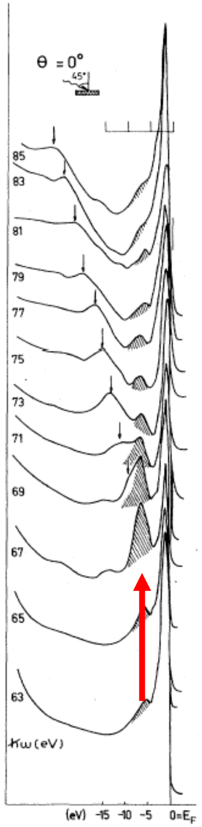


FIG. 1. Photoemission spectra of a clean Ni(100) surface for photon energy $\hbar\omega$ between 63 and 85 eV. The peak A corresponds to the d bands; B (dashed area) is the structure located at 6 eV from the Fermi level. The arrows indicate the Auger transition.

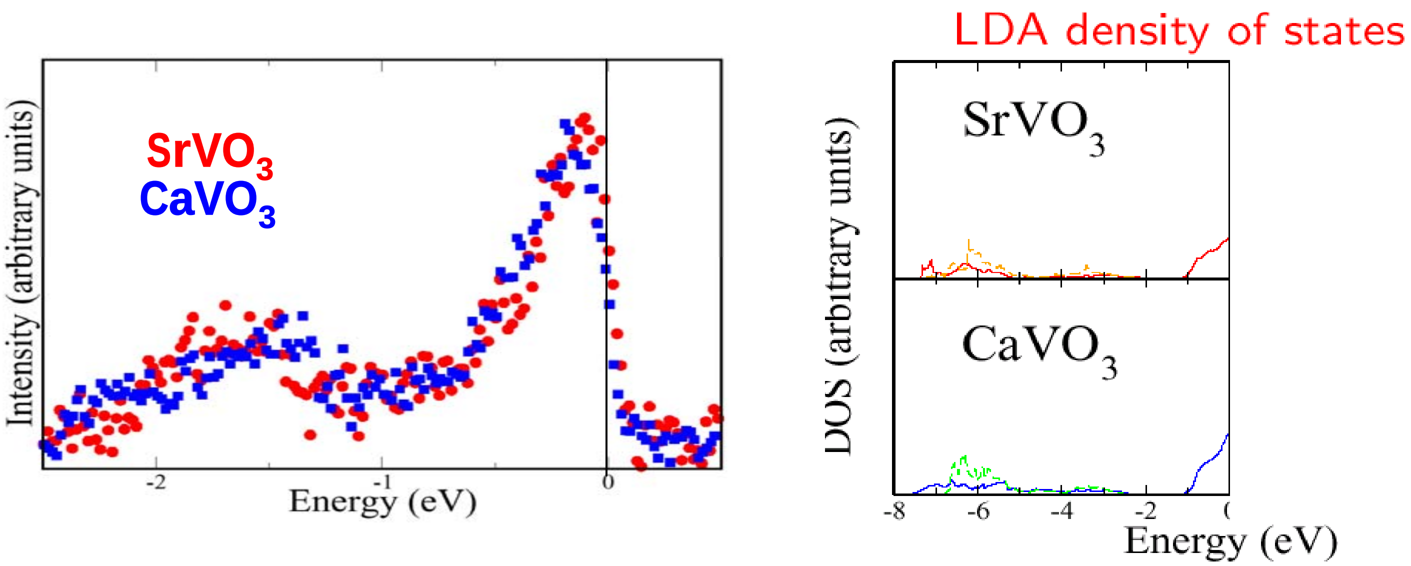
Guillot,..., Falicov (1977)

Not reproducible by
Density Functional Theory/
Local Density Approximation

Explanation of the -6 eV satellite?

4.

Photoemission spectra of (Sr,Ca)VO_3

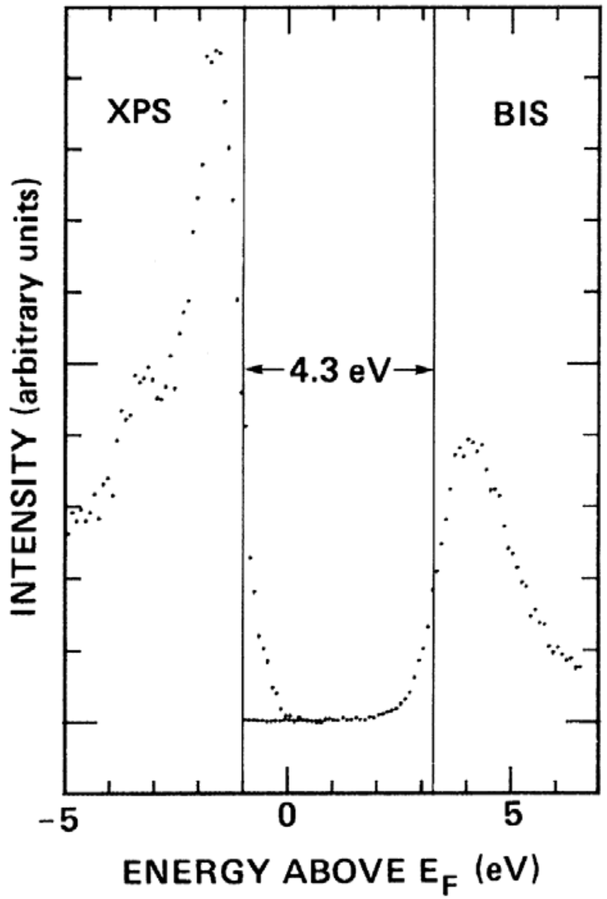


Osaka – Augsburg – Ekaterinburg collaboration: Sekiyama *et al.*, 2004

Reason for shift of spectral weight?

5.

Photoemission spectra of NiO

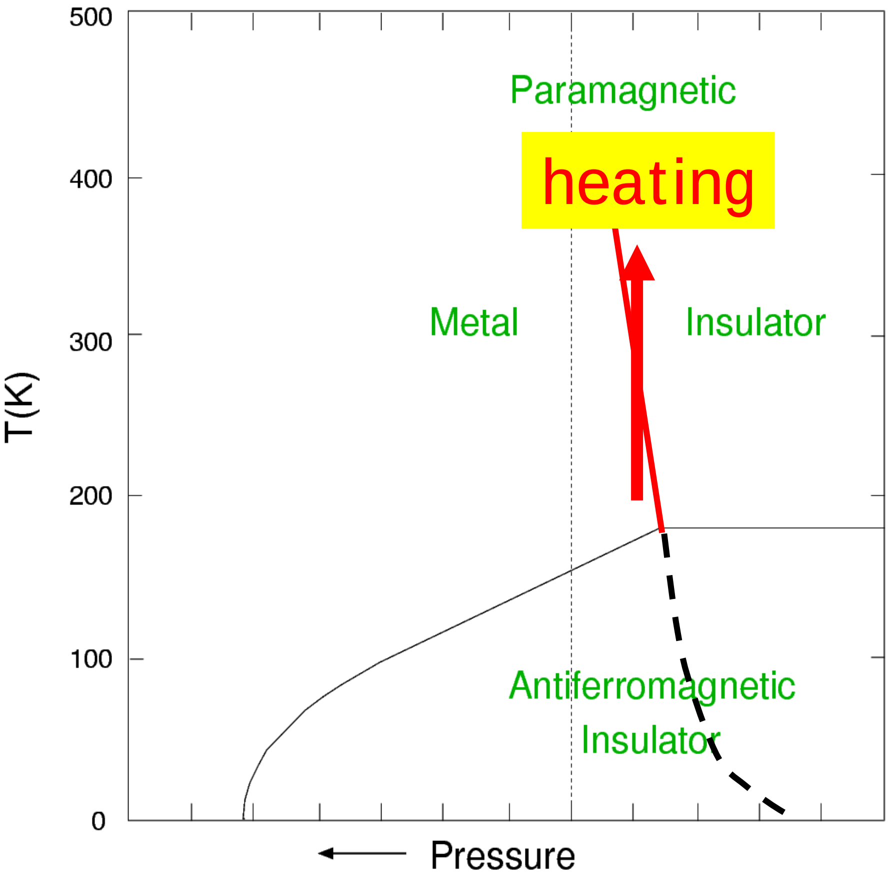


Sawatzky, Allen (1984)

Origin of gap (antiferromagnetism)?

6.

Metal-insulator transition in V_2O_3



Rice, McWhan (1970);
McWhan, Menth, Remeika,
Brinkman, Rice (1973)

- PI ⟷ PM: 1. order transition without lattice symmetry change

- Anomalous slope of P(T)

  → *Pomeranchuk effect* in ^{3}He

Microscopic explanation?

Correlated electron materials

Fascinating topics for fundamental research

- large resistivity changes
- huge volume changes
- high T_c superconductivity
- strong thermoelectric response
- colossal magnetoresistance
- gigantic non-linear optical effects

$\Big\}$ Large susceptibilities

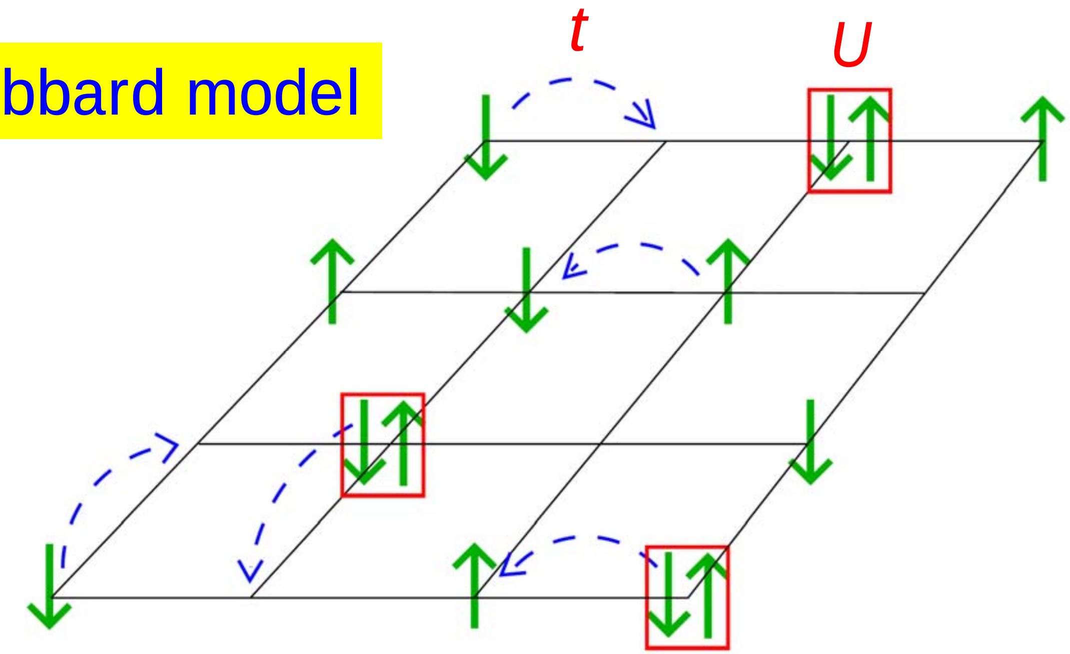
with

Technological applications:

- sensors, switches
- magnetic storage
- refrigerators
- functional materials, …

Model approaches to correlated electrons

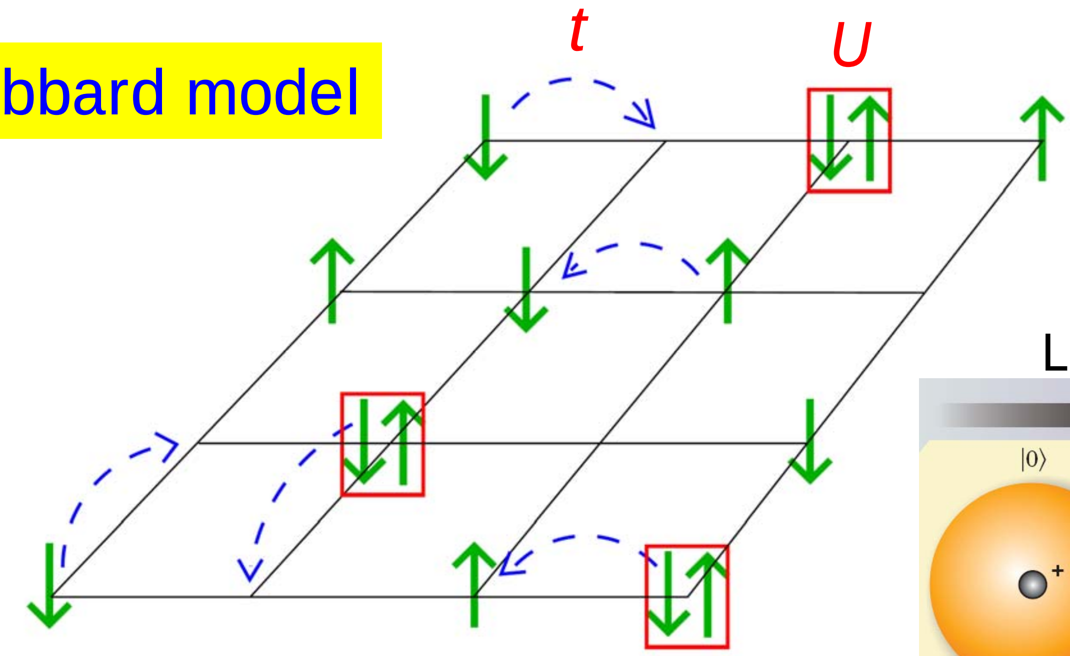
Hubbard model



Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

→Microscopic theory of ferromagnetism?

Hubbard model

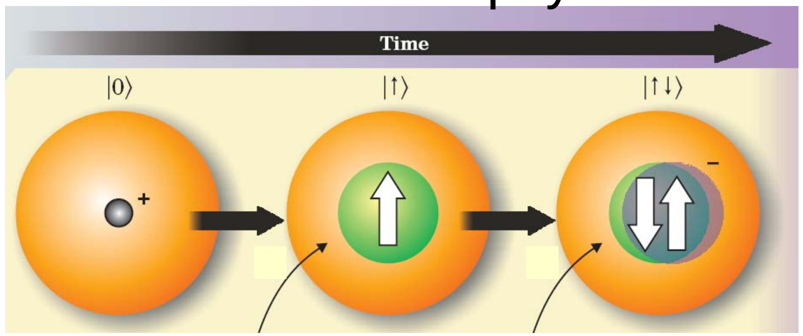


$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$= -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

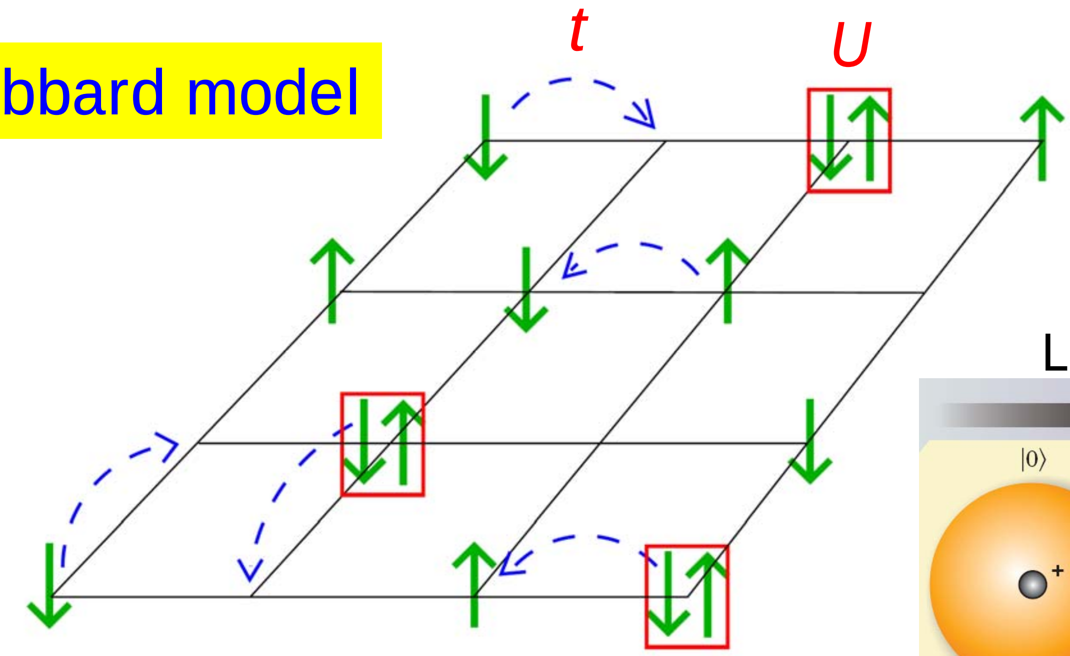
Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

Local Hubbard physics:



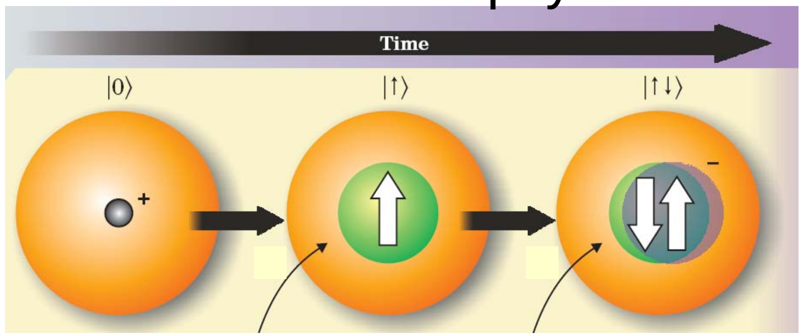
time

Hubbard model



Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

Local Hubbard physics:



$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$= -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$\boxed{\left\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \right\rangle \neq \left\langle n_{\mathbf{i}\uparrow} \right\rangle \left\langle n_{\mathbf{i}\downarrow} \right\rangle}$$

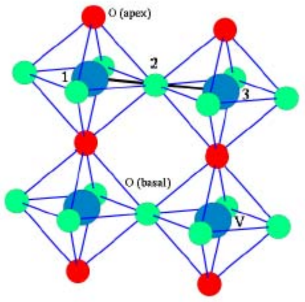
Correlation phenomena:
Metal-insulator transition
Ferromagnetisms,...

Hartree-(Fock)
mean-field theory
generally insufficient

Beyond models: How to include material-specific details?

Crystal structure

$SrVO_3$: $\angle 123 = 180°$

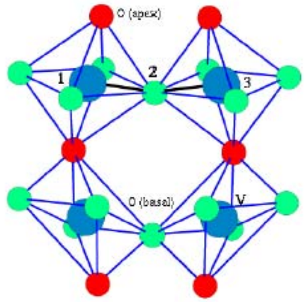


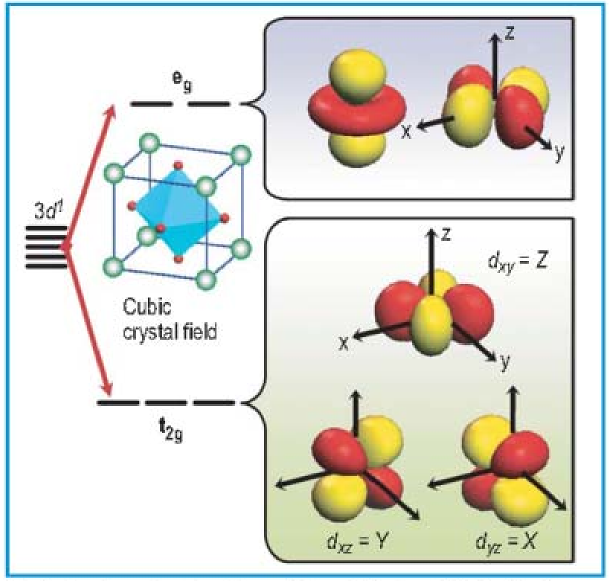
$\Downarrow$

orthorhombic distortion

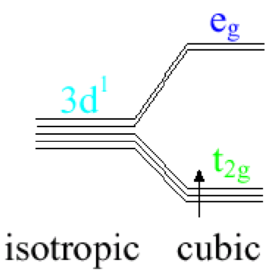
$\Downarrow$

$CaVO_3$: $\angle 123 \approx 162°$





Band scheme



→ Dynamical Mean-Field Theory