

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 electron systems:  
Hubbard model

"Correlations"

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

Grammar: *either ... or*

Mathematics, natural sciences:

$$\langle AB \rangle \neq \langle A \rangle \langle B \rangle$$

e.g., densities:

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

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

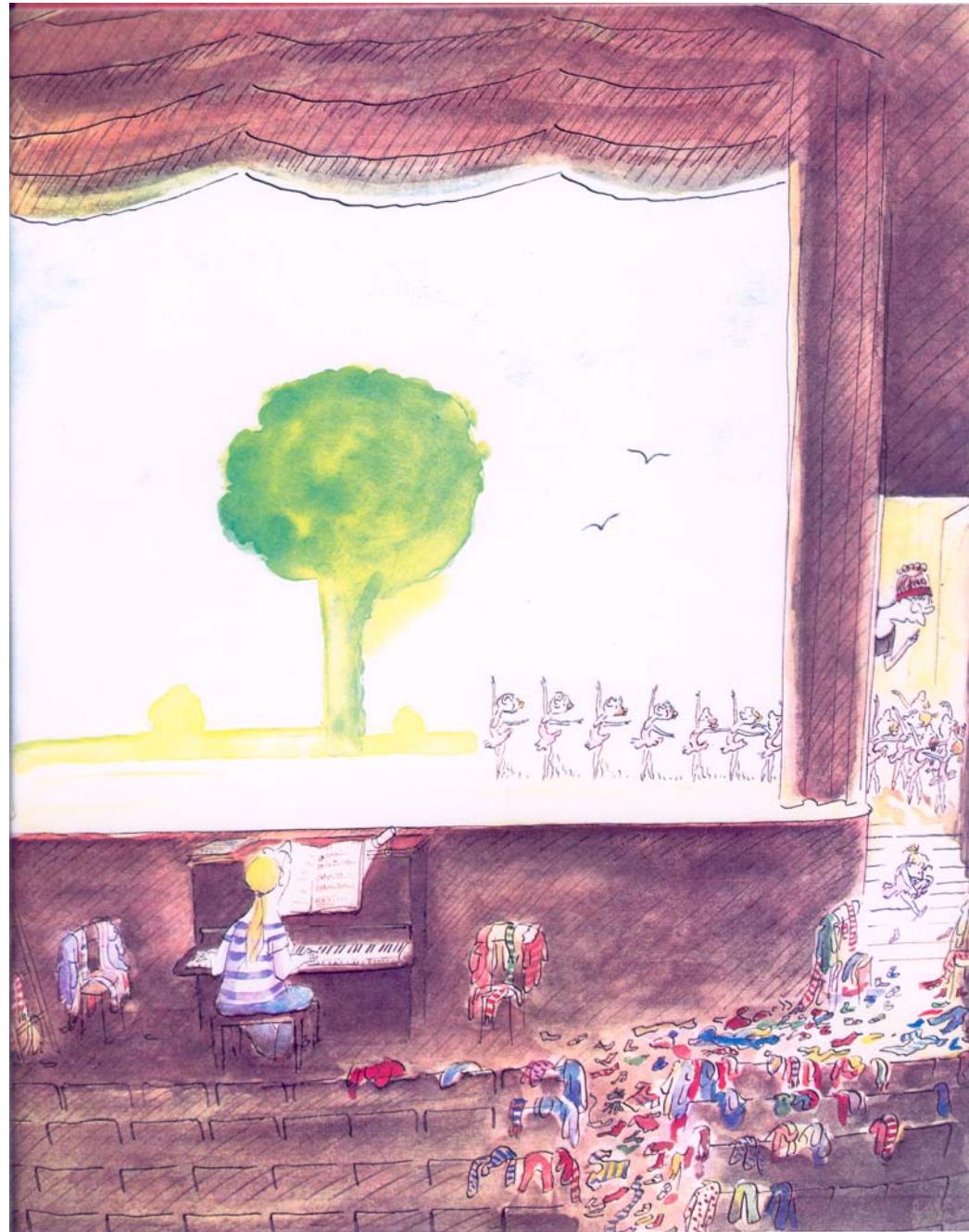
correlation  $\neq$  causality

## Short-range spatial correlations in everyday life



Time average insufficient

Correlations  
vs.  
long-range order



*(Sempe)*

# Electronic Correlations in the Periodic Table



# Periodic Table of the Elements

1 IA New Original	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 H 1.00794	2 He 4.002602	3 Li 6.941	4 Be 9.012182	5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797	11 Na 22.989770	12 Mg 24.3050	13 Al 26.981538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955912	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938045	26 Fe 55.845	27 Co 58.933195	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc 98	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.36	47 Ag 107.8682	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	57 to 71 Lanthanide series	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.96655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.98038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 to 103 Actinide series	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Uun (269)	111 Uuu (272)	112 Uub (277)	113 Uut (284)	114 Uuq (285)	115 Uuh (288)	116 Uuq (289)	117 Uue (289)	118 Uuo (293)

Partially filled d-orbitals

Atomic masses in parentheses are those of the most stable or common isotope.

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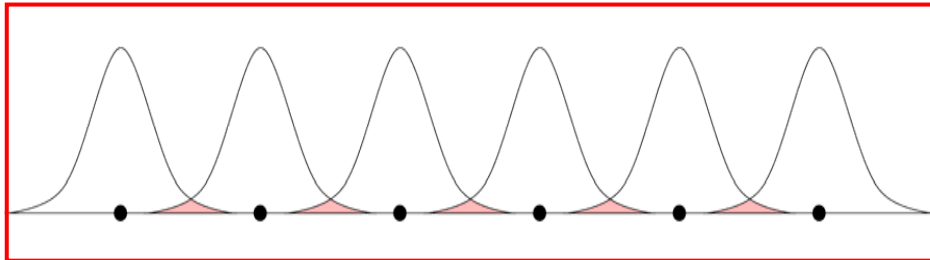
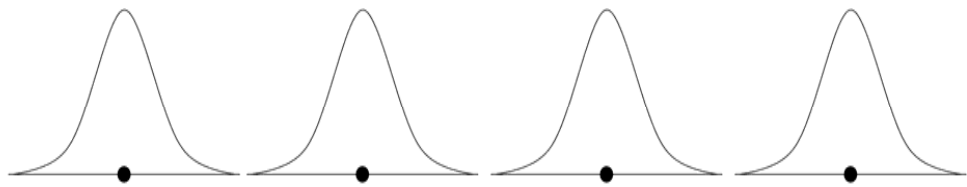
Note: The subgroup numbers 1-18 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 110-118 are the Latin equivalents of those numbers.

Partially filled f-orbitals

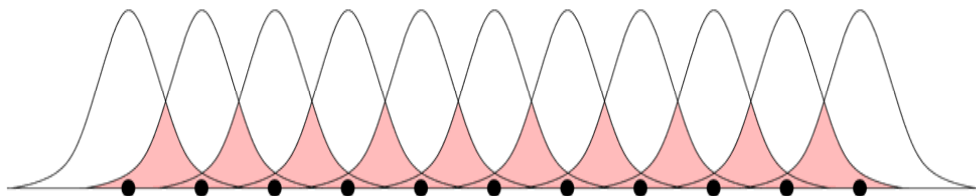
Narrow d, f-orbitals → strong electronic correlations



# Electronic Bands in Solids



overlap of wave functions:  
matrix element  $t$



Estimate strength of correlations:

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

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

Consequences?

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

Small  $W$ : Strong electronic correlations

Property	Energy levels	Representation	Example
Insulator	Atomic levels	Localized electrons $n_{i\sigma}$	Solid Ne NaCl
Correlated metal	Narrow bands	$n_{i\sigma} \leftrightarrow n_{\mathbf{k}\sigma}$	Transition + rare earth metals/oxides (Ni, $V_2O_3$ , Ce)
Simple metal	Broad bands	Extended waves $n_{\mathbf{k}\sigma}$	Na, Al

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19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955910	22 Ti Titanium 47.88	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938049	26 Fe Iron 55.845	27 Co Cobalt 58.933200	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 101.07	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.29
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 to 71 Lanthanide series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.078	79 Au Gold 196.96655	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98038	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
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Atomic masses in parentheses are those of the most stable or common isotope.

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Note: The subgroup numbers 1-18 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 110-118 are the Latin equivalents of those numbers.

57 La Lanthanum 138.9055	58 Ce Cerium 140.116	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.26	69 Tm Thulium 168.93421	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
89 Ac Actinium (227)	90 Th Thorium 232.0381	91 Pa Protactinium 231.03588	92 U Uranium 238.0289	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)

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

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



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IA												IIA						VIIIA			
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3	Li											4	Be							10	Ne
11	Na											12	Mg							18	Ar
19	K											20	Ca							36	Kr
37	Rb											38	Sr							54	Xe
55	Cs											56	Ba							86	Rn
87	Fr											88	Ra							118	Og

Alkali Metals

Alkaline earth Metals

Transition metals

Lanthanide series

Actinide series

Other Metals

Nonmetals

Noble gases

C Solid

Br Liquid

H Gas

Tc Synthetic

Atomic masses in parentheses are those of the most stable or common isotope.

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57	La	58	Ce	59	Pr	60	Nd	61	Pm	62	Sm	63	Eu	64	Gd	65	Tb	66	Dy	67	Ho	68	Er	69	Tm	70	Yb	71	Lu
89	Ac	90	Th	91	Pa	92	U	93	Np	94	Pu	95	Am	96	Cm	97	Bk	98	Cf	99	Es	100	Fm	101	Md	102	No	103	Lr

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

# Electrons vs. Quasiparticles, Fermi liquid theory

# Electrons

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



Fermi-Dirac statistics

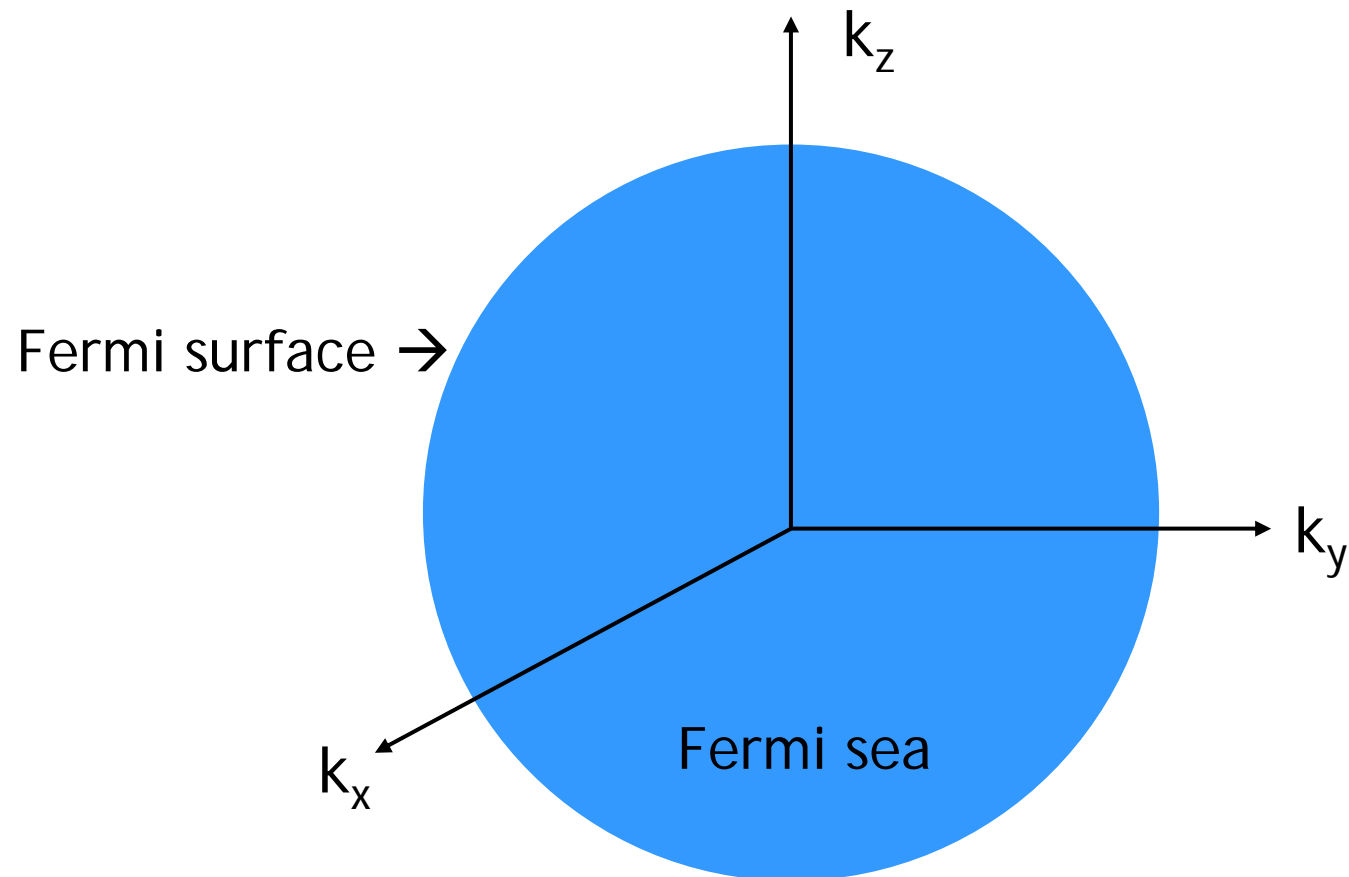


Pauli exclusion principle  
of many fermions

Fermi body/surface

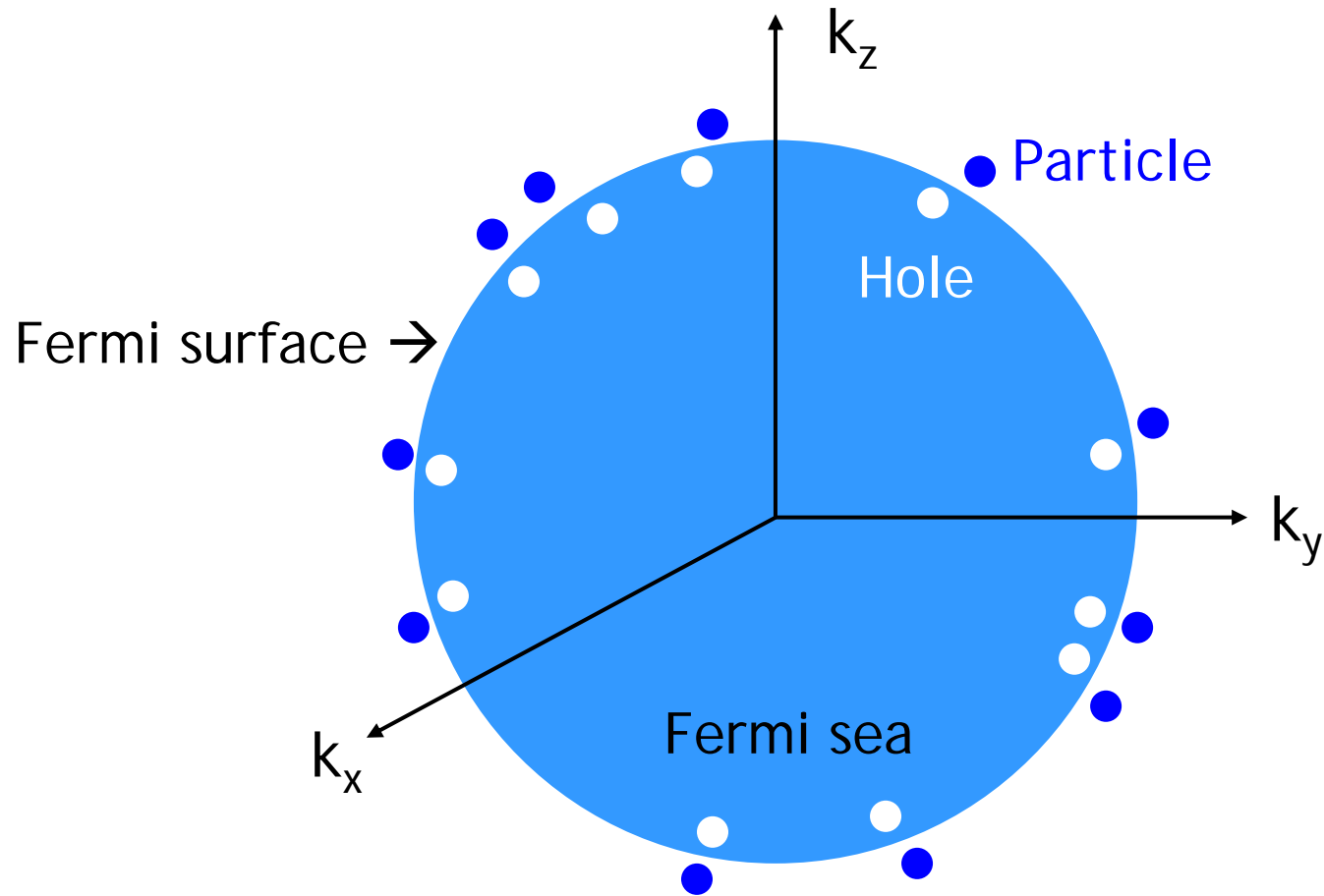
No such thing for bosons!

# Fermi gas: Ground state





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



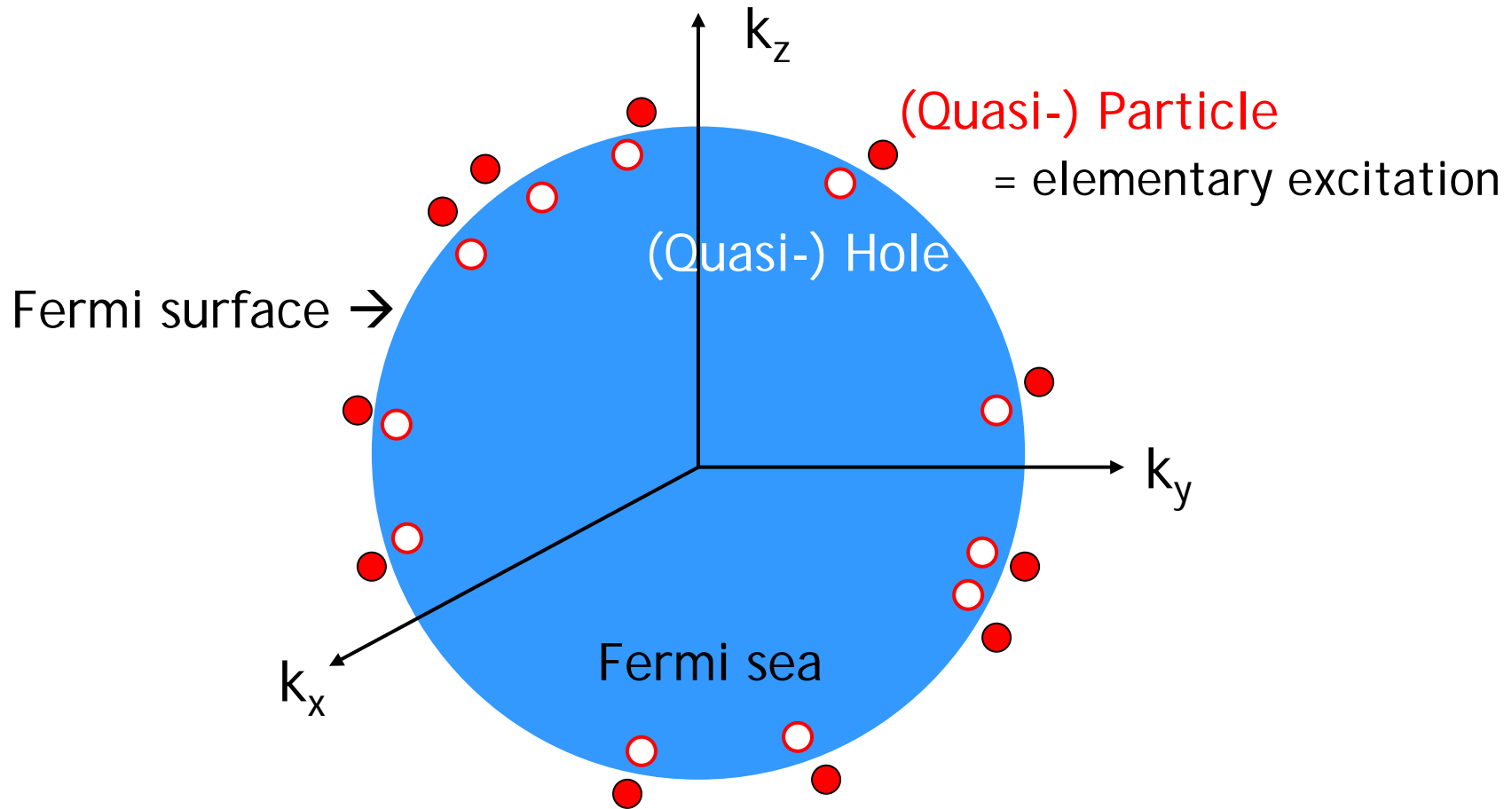
Exact  $k$ -states ("particles"): infinite life time

Switch on interaction adiabatically ( $d=3$ )

# Landau Fermi liquid

Landau (1956/58)

1-1 correspondence between k-states



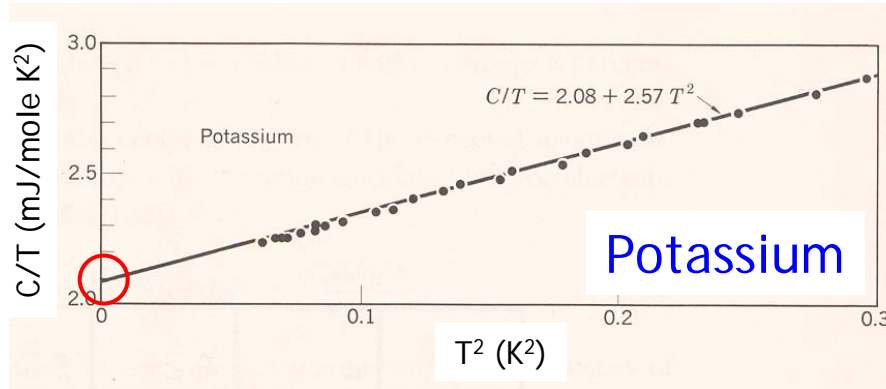
Well-defined k-states ("quasiparticles") with

- finite life time
- effective mass
- effective interaction

# Electronic Correlations in Solids: Examples

1.

## Simple metals

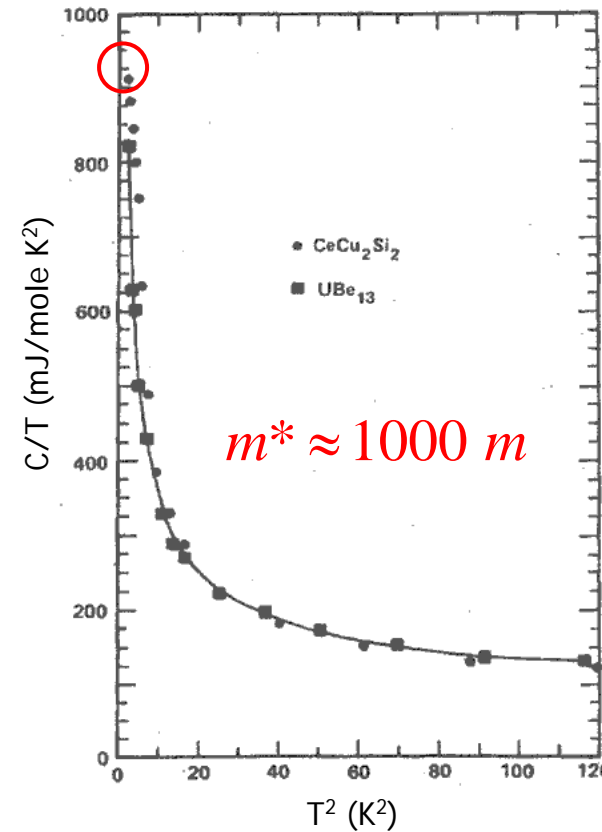


Consequence of elementary excitations (quasiparticles)

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

## "Heavy Fermions"

Steglich *et al.* (1979)



Stewart *et al.* (1983)

CeCu<sub>2</sub>Si<sub>2</sub>, UBe<sub>13</sub>:  
very heavy quasiparticles

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

2.

Magnetic impurity in a metallic host:  
The Kondo effect



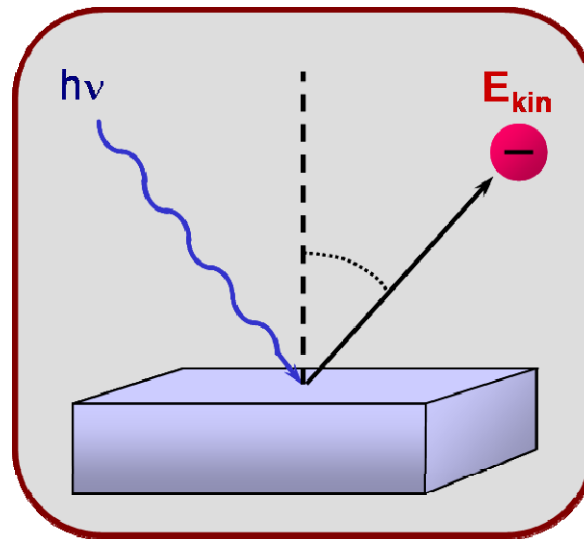
Ce

Explanation of the three peak structure?

Excursion:

Detection of electronic correlations in solids by  
Photoemission spectroscopy

# 1. Photoemission Spectroscopy (PES)

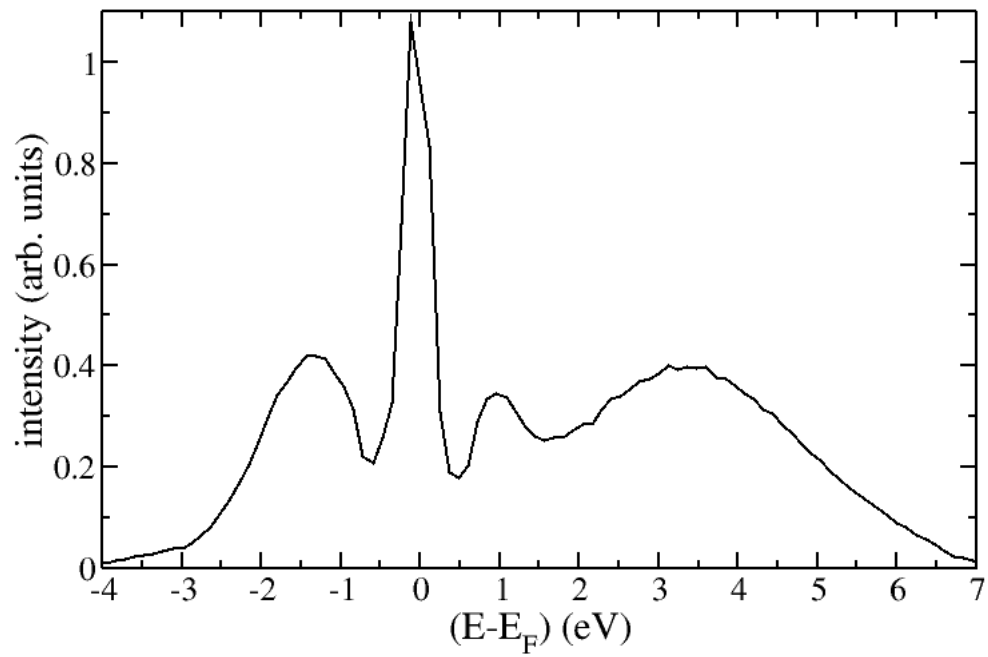


Angular Resolved PES = ARPES

Measures **occupied** states of electronic spectral function

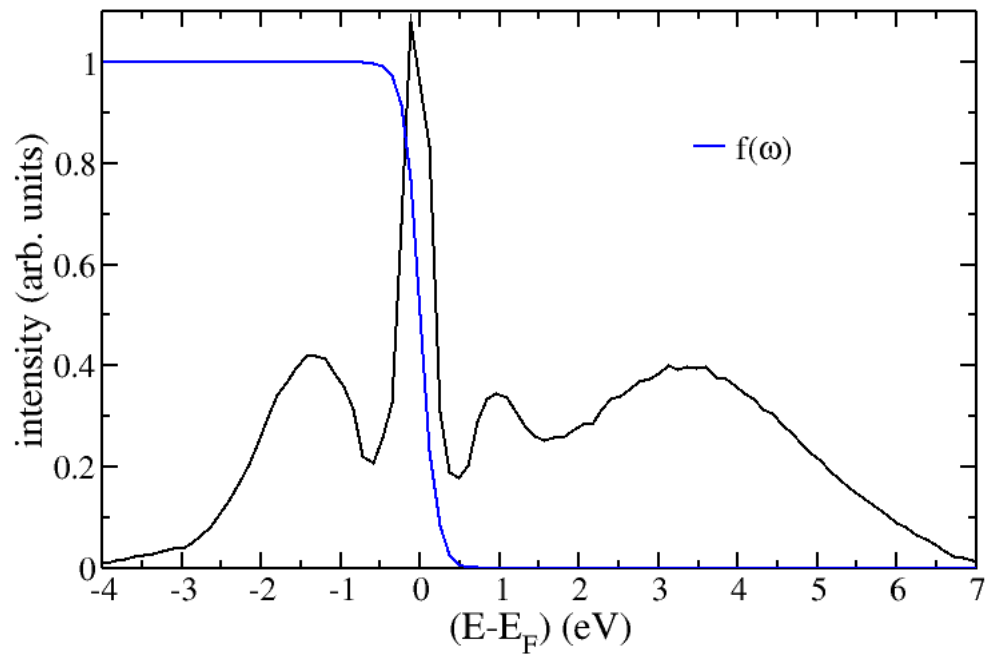


PES



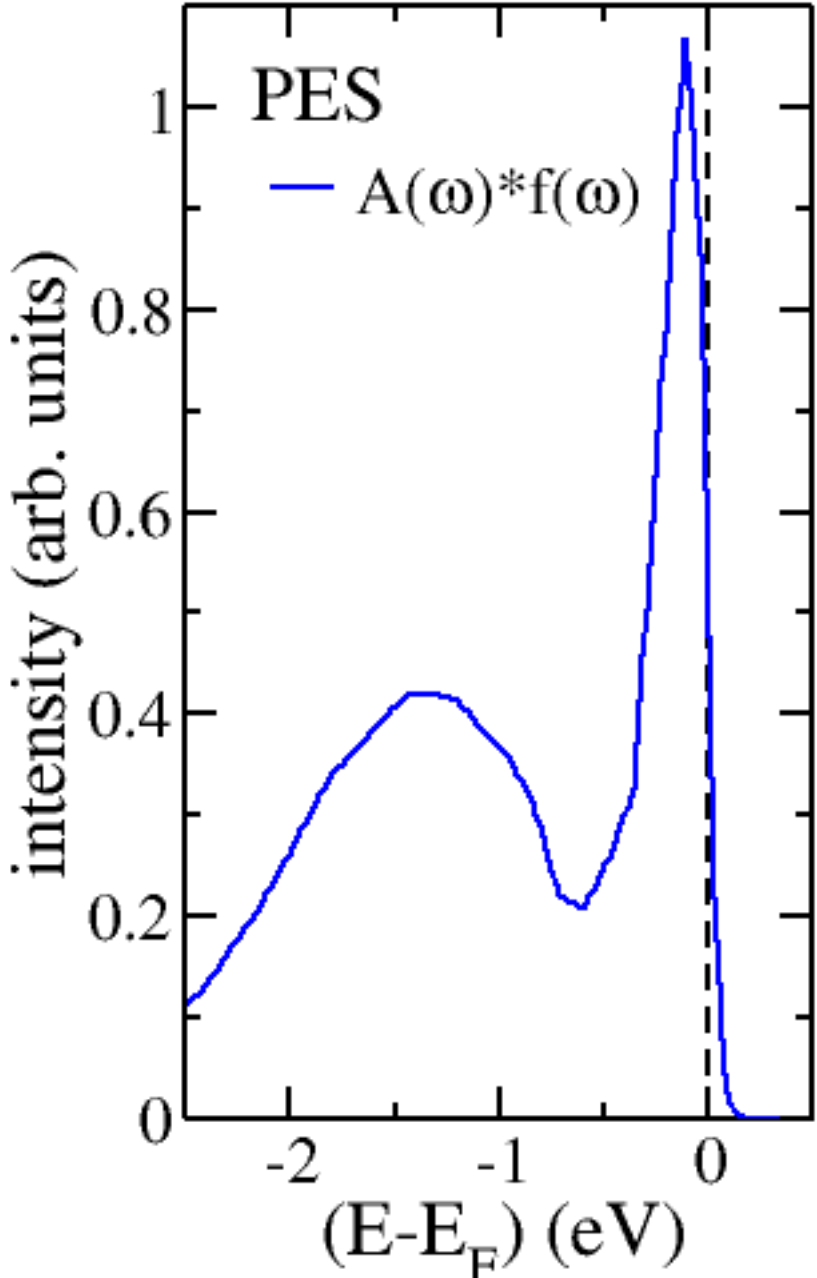
Ideal spectral function of a material

# PES



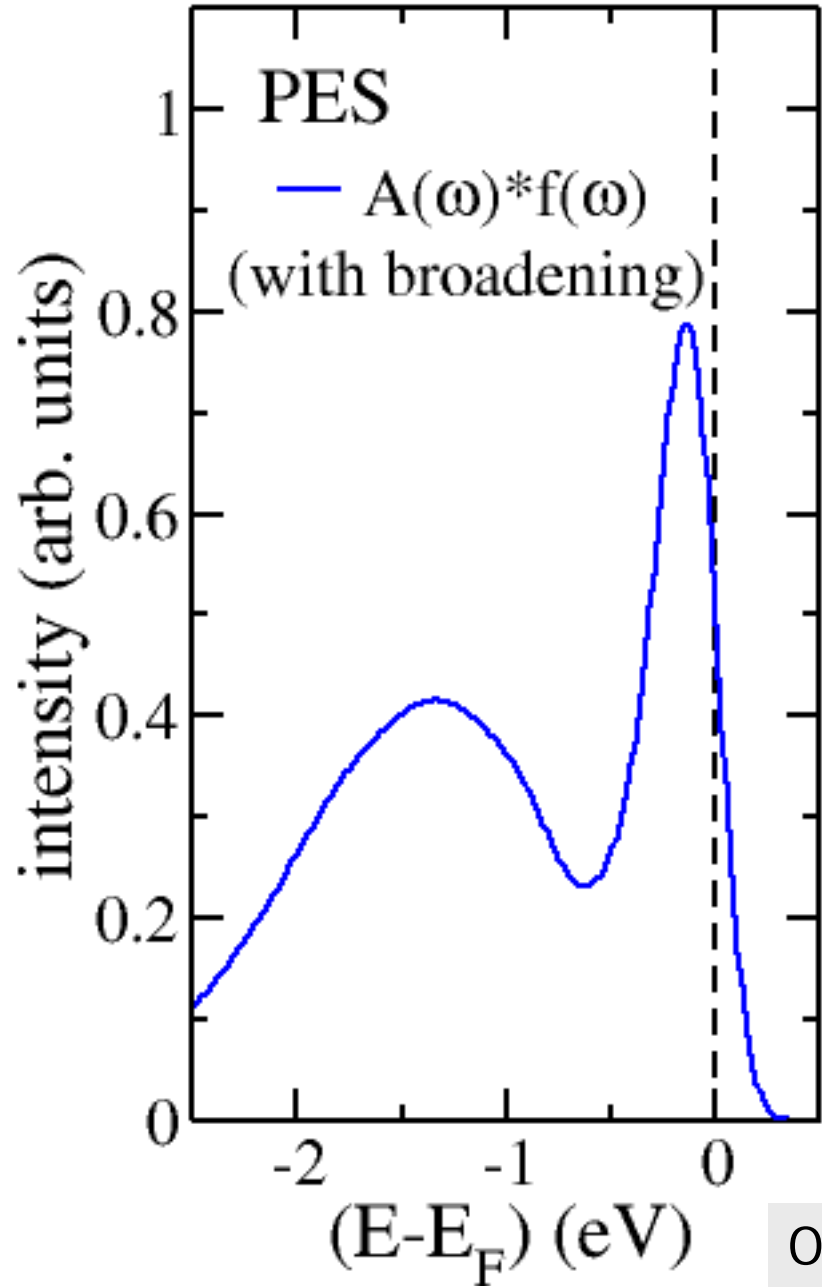
Ideal spectral function of a material

PES



Occupied states  
(ideal)

PES



Occupied states  
(measured)

Only two peaks visible

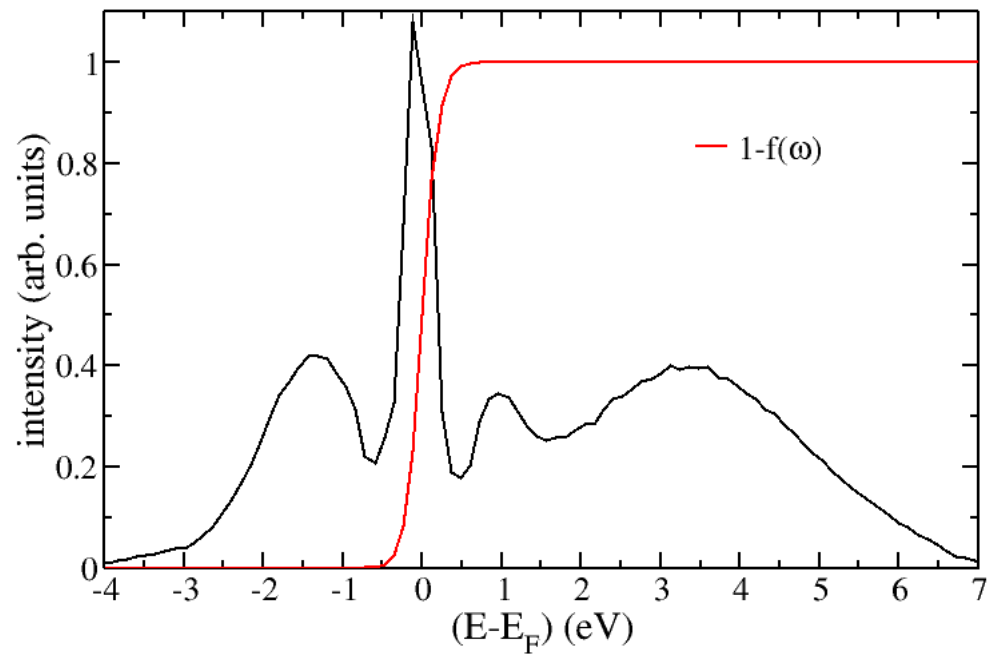
## 2. Inverse Photoemission Spectroscopy (IPES)

Measures **unoccupied** states of electronic spectral function

Information also available by:

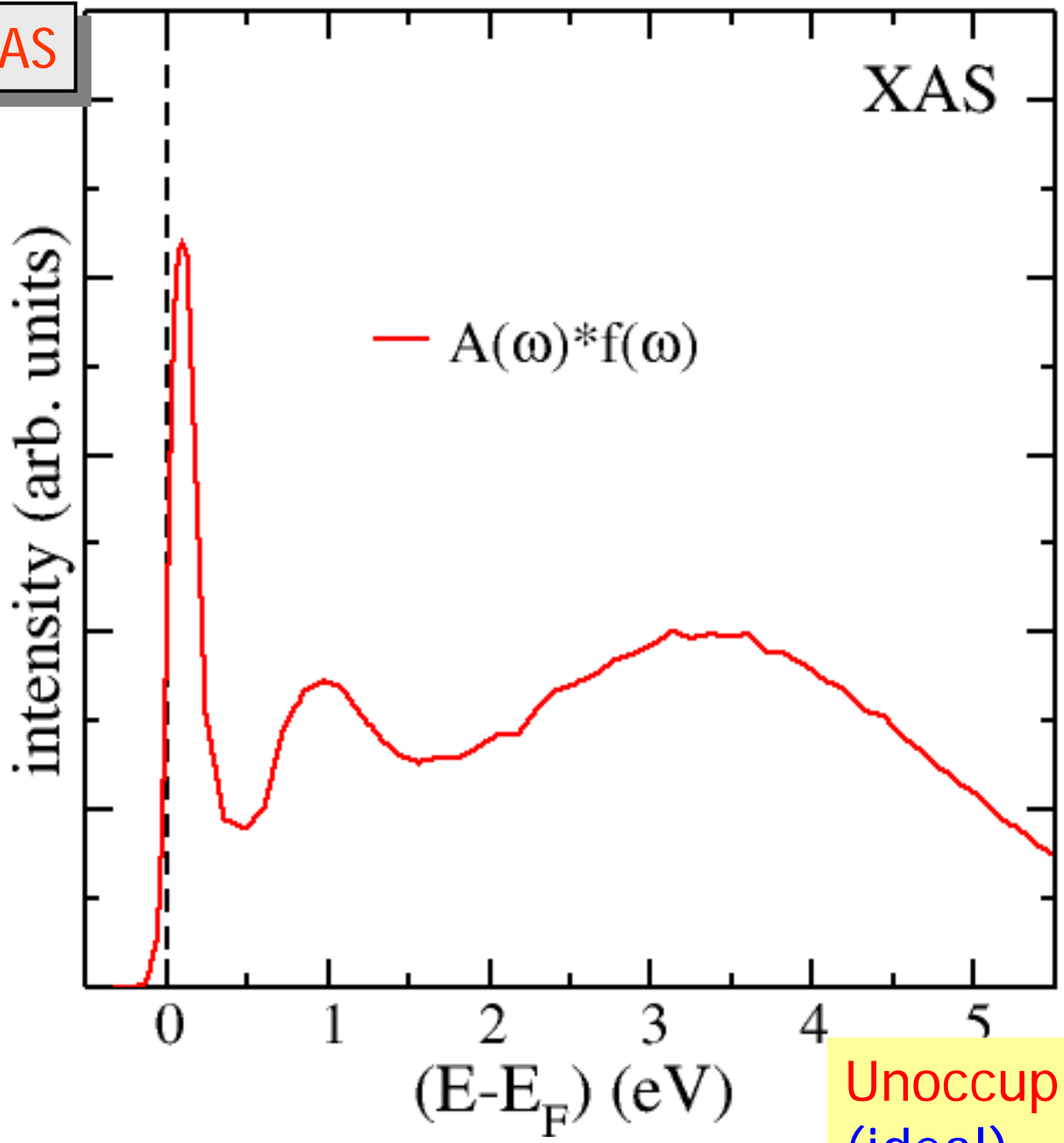
**X-ray Absorption Spectroscopy (XAS)**

# IPES/XAS



Ideal spectral function of a material

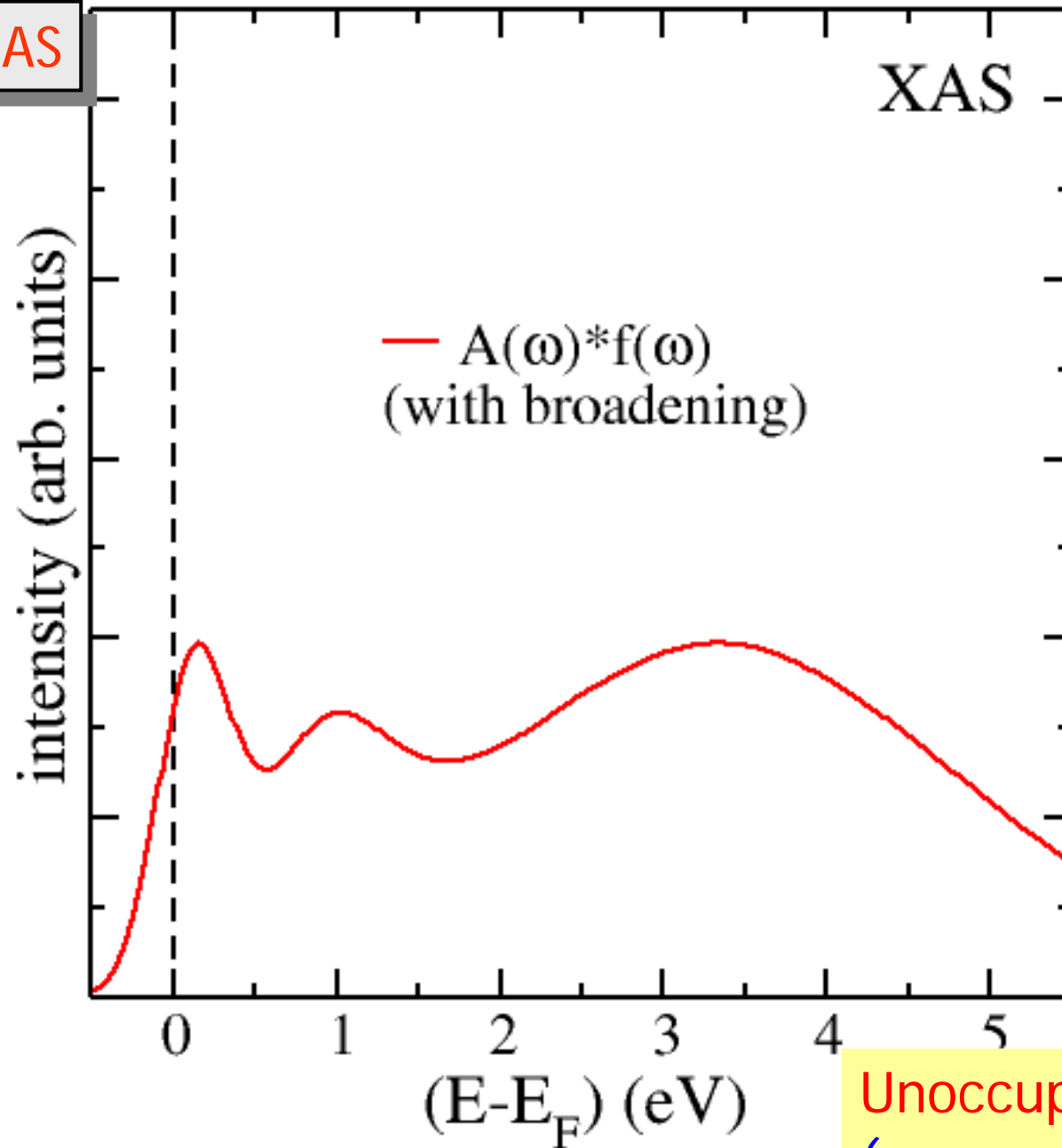
IPES/XAS



Unoccupied states  
(ideal)



IPES/XAS



Unoccupied states  
(measured)

3.

## Photoemission spectra of Ni: -6 eV satellite

Guillot, ..., Falicov (1977)

Not reproducible by  
Density Functional Theory/  
Local Density Approximation

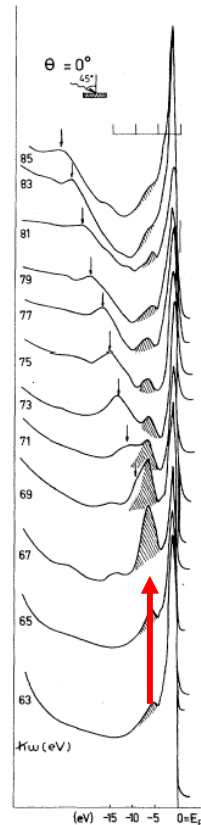
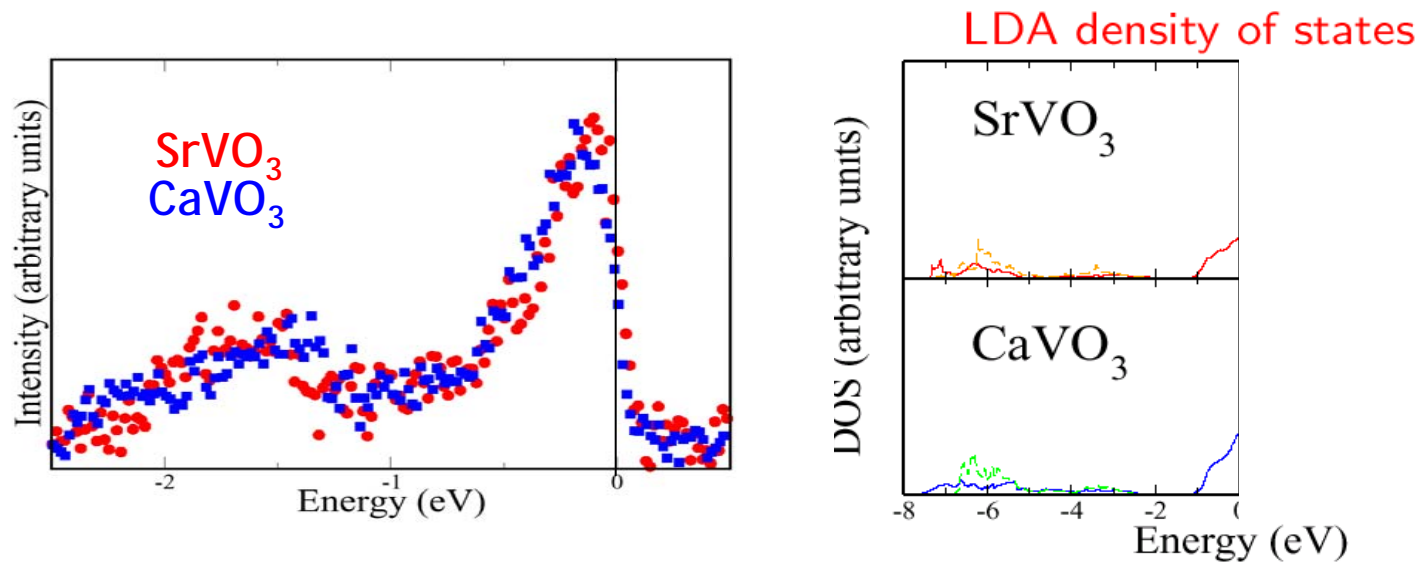


FIG. 1. Photoemission spectra of a clean Ni(100) surface for photon energy  $\hbar\omega$  between 63 and 85 eV. The peak *A* corresponds to the *d* bands; *B* (dashed area) is the structure located at 6 eV from the Fermi level. The arrows indicate the Auger transition.

Explanation of the -6 eV satellite?

4.

## Photoemission spectra of $(\text{Sr}, \text{Ca})\text{VO}_3$

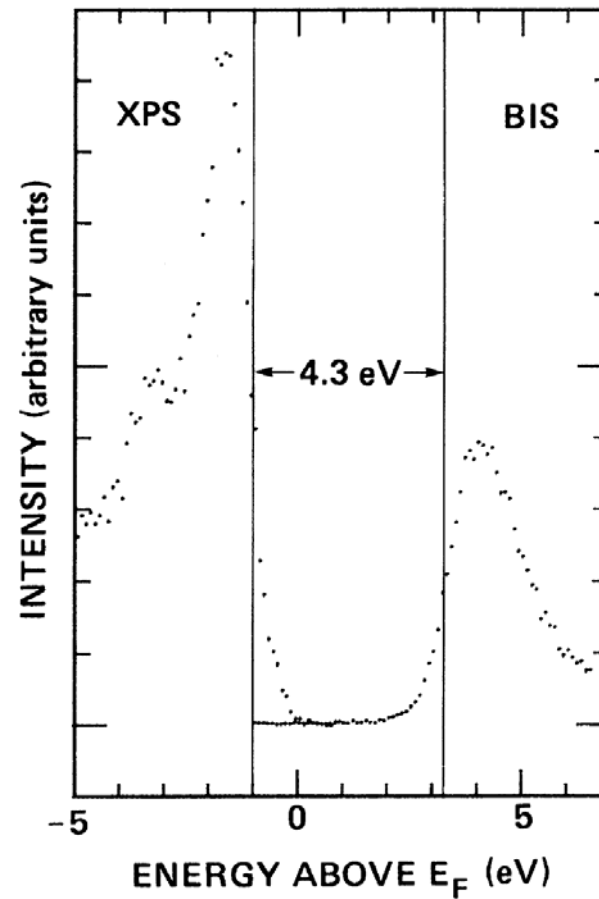


Osaka - Augsburg - Ekaterinburg collaboration: Sekiyama *et al.*, 2004

Reason for shift of spectral weight?

5.

## Photoemission spectra of NiO

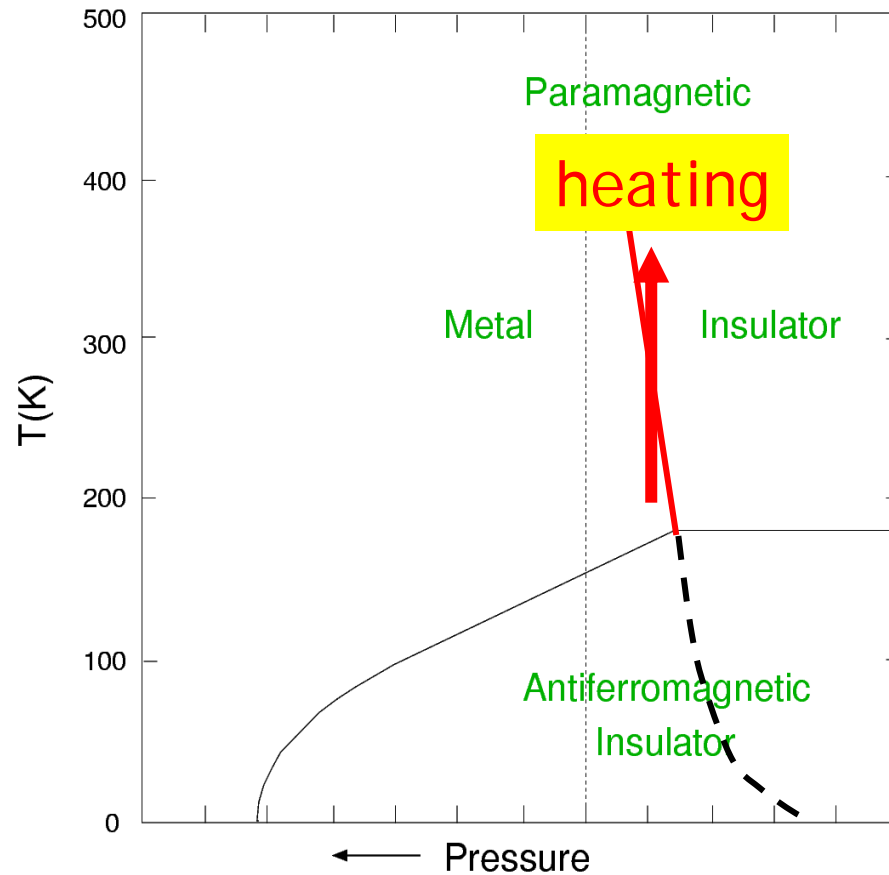


Sawatzky, Allen (1984)

Origin of gap  
(antiferromagnetism)?

6.

## Metal-insulator transition in $V_2O_3$



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

- PI  $\longleftrightarrow$  PM: 1. order transition without lattice symmetry change
- Anomalous slope of  $P(T)$   
→ *Pomeranchuk effect* in  $^3\text{He}$

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

} Large susceptibilities

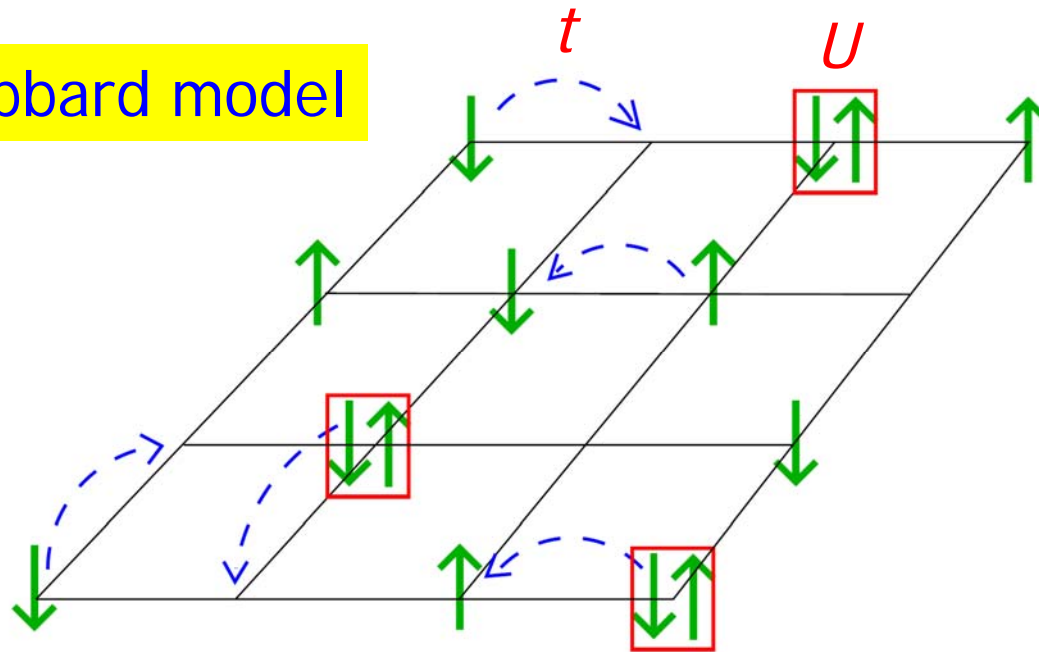
with

Technological applications:

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

# Model approaches to correlated electrons

# Hubbard model

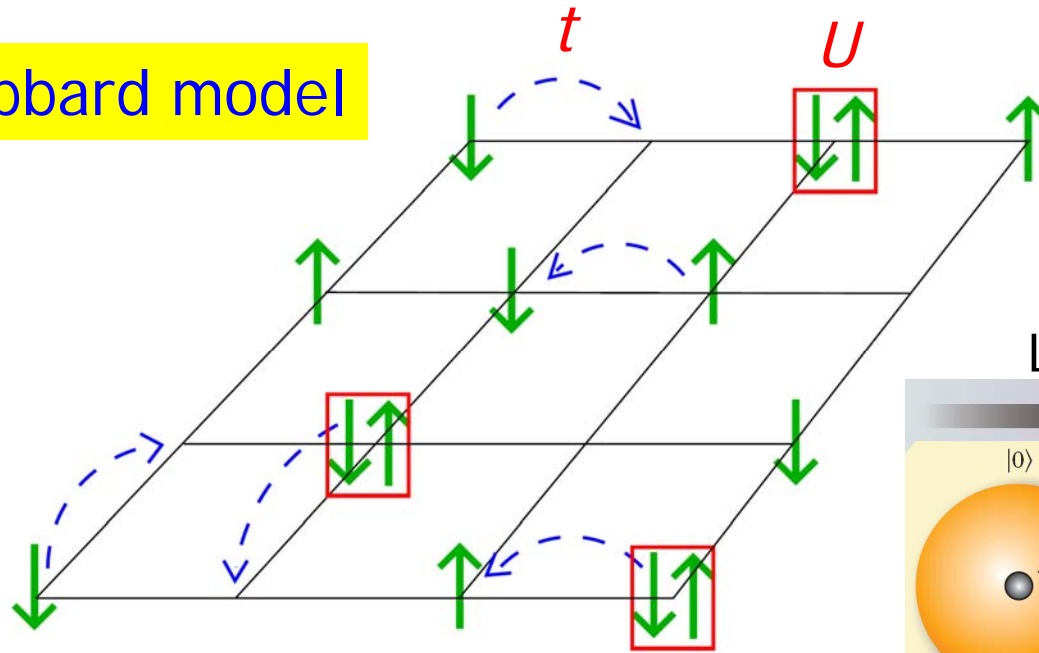


Gutzwiller, 1963  
Hubbard, 1963  
Kanamori, 1963

→ Microscopic theory  
of ferromagnetism?

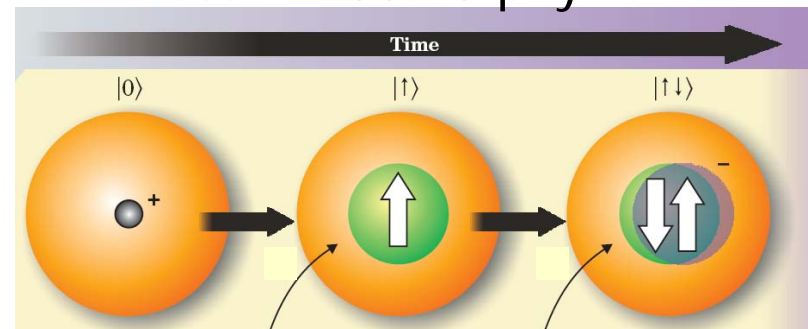


# Hubbard model



Gutzwiller, 1963  
 Hubbard, 1963  
 Kanamori, 1963

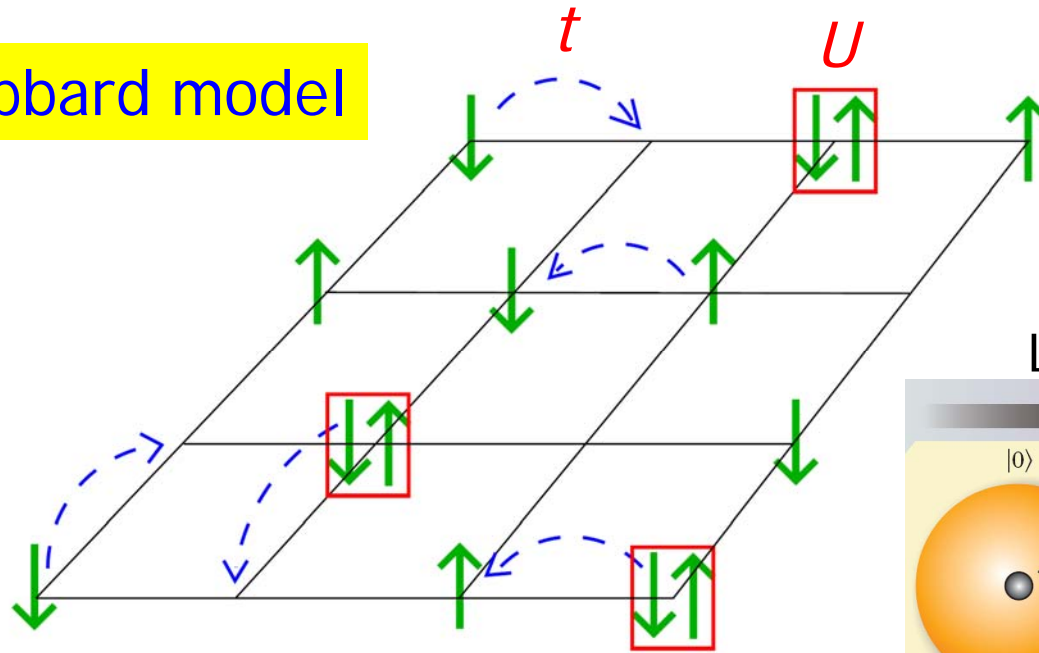
Local Hubbard physics:



time

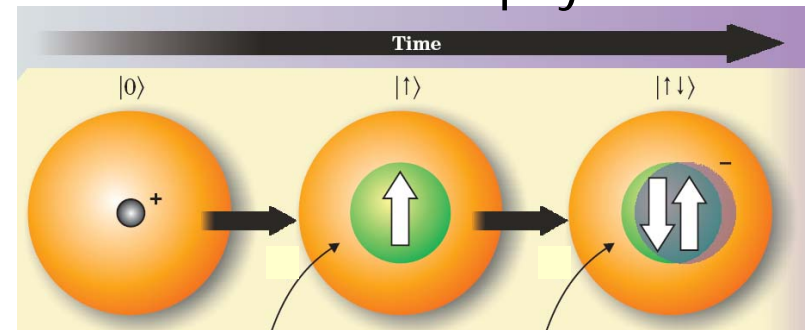
$$\begin{aligned}
 H &= \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \\
 &= -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}
 \end{aligned}$$

# Hubbard model



Gutzwiller, 1963  
Hubbard, 1963  
Kanamori, 1963

Local Hubbard physics:



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

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

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

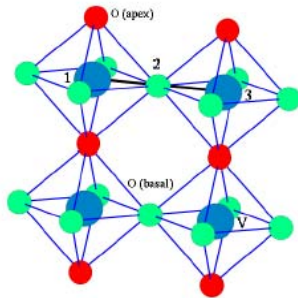
Correlation phenomena:  
Metal-insulator transition  
Ferromagnetisms, ...

Hartree-(Fock)  
mean-field theory  
generally insufficient

# Beyond models: How to include material-specific details?

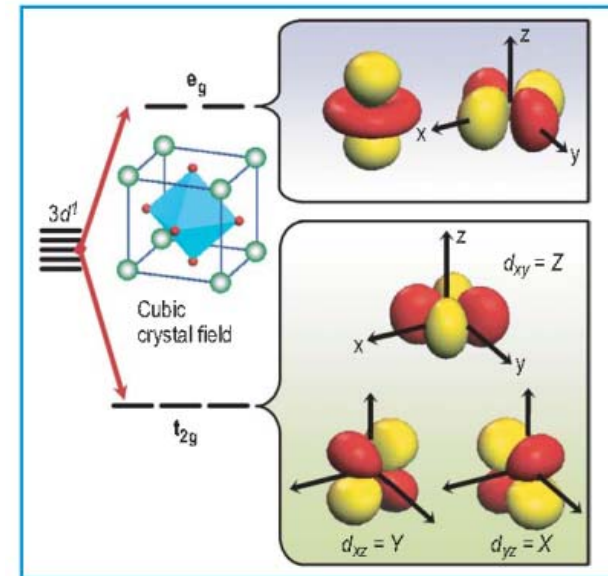
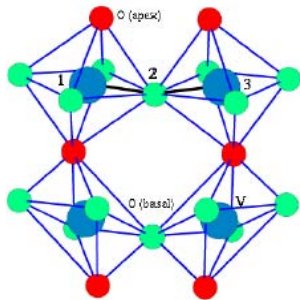
## Crystal structure

$\text{SrVO}_3$ :  $\angle 123 = 180^\circ$

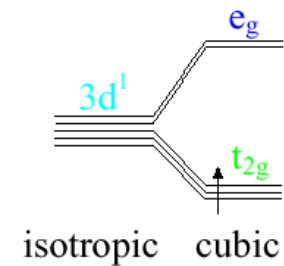


orthorhombic distortion

$\text{CaVO}_3$ :  $\angle 123 \approx 162^\circ$



## Band scheme



# WANTED

Reliable, comprehensive  
approximation scheme  
for  
correlated electron  
models and materials  
for  
arbitrary input parameters

→ Dynamical Mean-Field Theory