What does "Strong Correlation" mean?

What are strongly correlated systems?

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Themes in this talk

What does "Strong Correlation" mean?

Different meaning in different contexts!

What systems are here considered to be "strongly correlated"?

In such systems, which aspects of a Kohn-Sham calculation are:

Applicable if chosen appropriately.

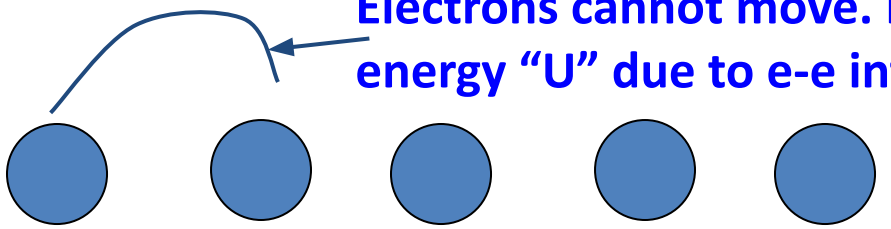
Not directly applicable at all - source of misconceptions

Informative - a starting point for improved calculations.

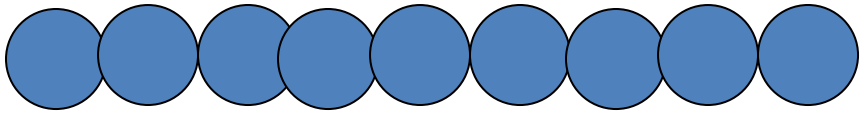
The question asked by Mott in the 1930's

What happens if you bring atoms together to form a solid?

Electrons cannot move. It costs energy "U" due to e-e interactions



At large distance, an atomic-like <u>insulator</u>



At close distance, forms bands

<u>Odd</u> number of electrons - MUST be a <u>metal</u> in band theory

Simplest picture of the "Mott metal-insulator transition

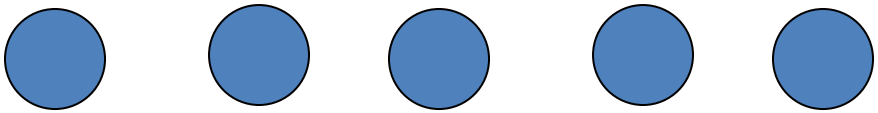
The question asked by Mott in the 1930's

What happens if you bring atoms together to form a solid?

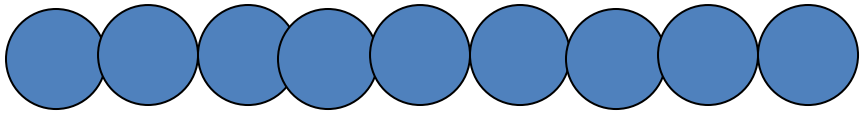
But there is an additional consideration

Electrons cannot move. It costs energy "U" due to e-e interactions

At large distance, an atomic-like insulator



At close distance, forms bands



For "closed shell" atoms (partially filled shell, i.e., s, p, d, f orbitals) (always an even number of electrons):

The system can merge smoothly to filled bands (insulator)

or

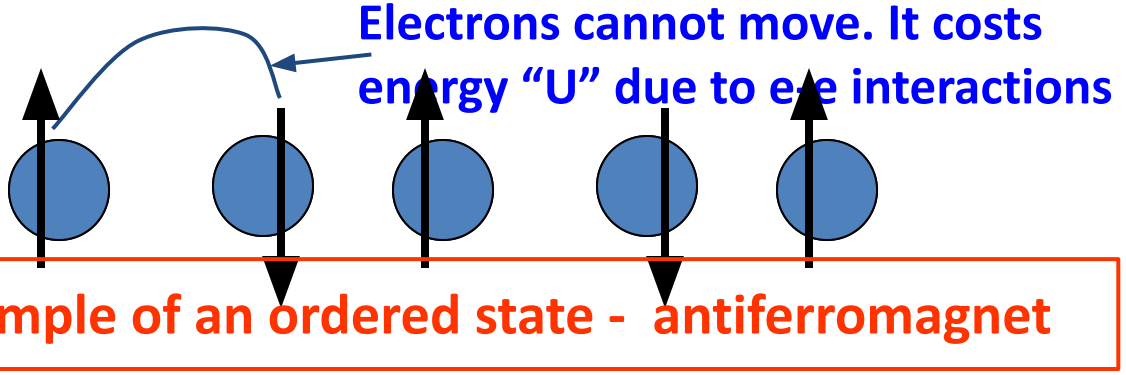
overlapping bands which may be metallic

The question asked by Mott in the 1930's

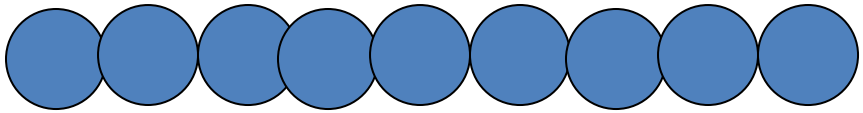
What happens if you bring atoms together to form a solid?

But there is an additional consideration

At large distance, an atomic-like insulator



At close distance, forms bands



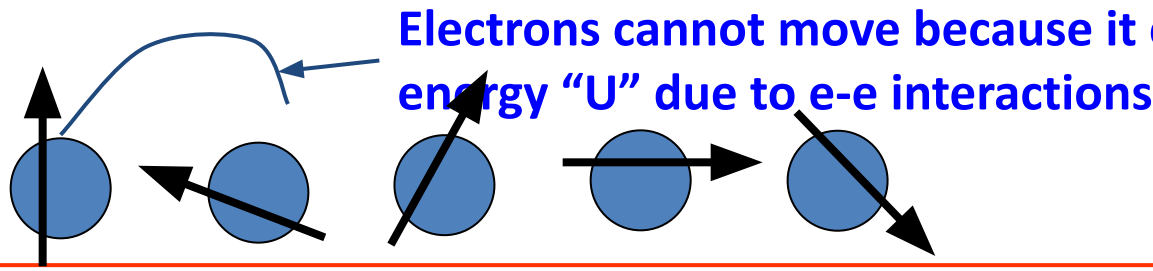
For "open shell" atoms (partially filled shell, i.e., s, p, d, f orbitals).
Hunds rule: lowest energy atomic state is maximum spin

The system at large distance is magnetic

The question asked by Mott in the 1930's

What happens if you bring atoms together to form a solid?

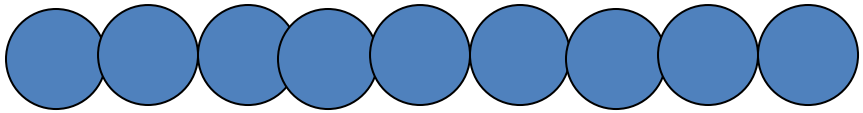
But there is an additional consideration



At large distance, an atomic-like insulator

Disordered moments no average magnetization

At close distance, forms bands



For "open shell" atoms (partially filled shell, i.e., s, p, p, f orbitals).
Hunds rule: lowest energy atomic state is maximum spin

The system at large distance is magnetic

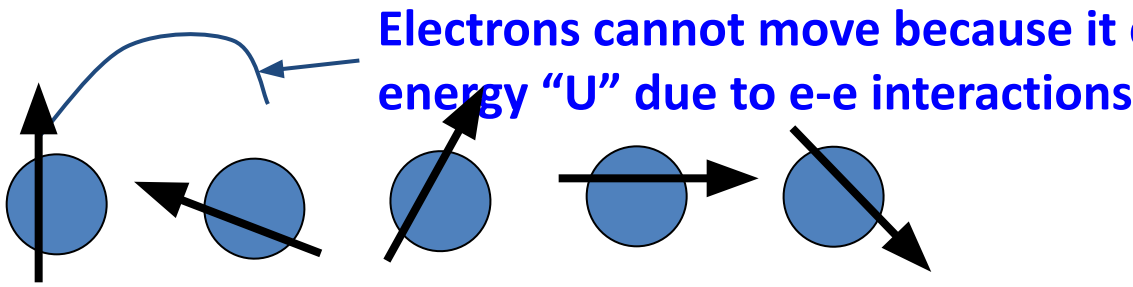
The energy gap depends on "local moments" not on order!

The question asked by Mott in the 1930's

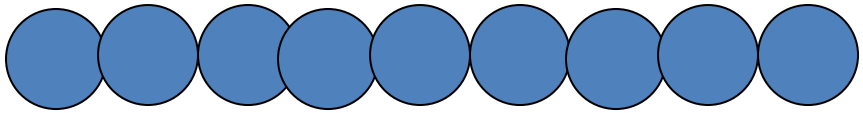
What happens if you bring atoms together to form a solid?

But there is an additional consideration

At large distance, an atomic-like insulator



At close distance, forms bands



For "open shell" atoms (partially filled shell, i.e., s, p, d, f orbitals).
Hunds rule: lowest energy atomic state is maximum spin

The most interesting "Mott transition" is from an magnetic insulator to a <u>?????</u>

Why do interesting "strongly correlated" properties emerge near the"Mott transition"

Low energy scales (almost always due to the local moments)

Large temperature dependence

Magnetism due to local moments

T_c ~ 1K – 1000 K sets scale for magnetism

Large effects of correlation

Low energy excitations 1K – 1000 K

Quantum fluctuations of the local moments

Compare this to

Typical scales for valence electronic excitations in non-magneic solids

~ 1 eV/k_b ~ 8,000 K

No strong T-dependence for T<< 8000K

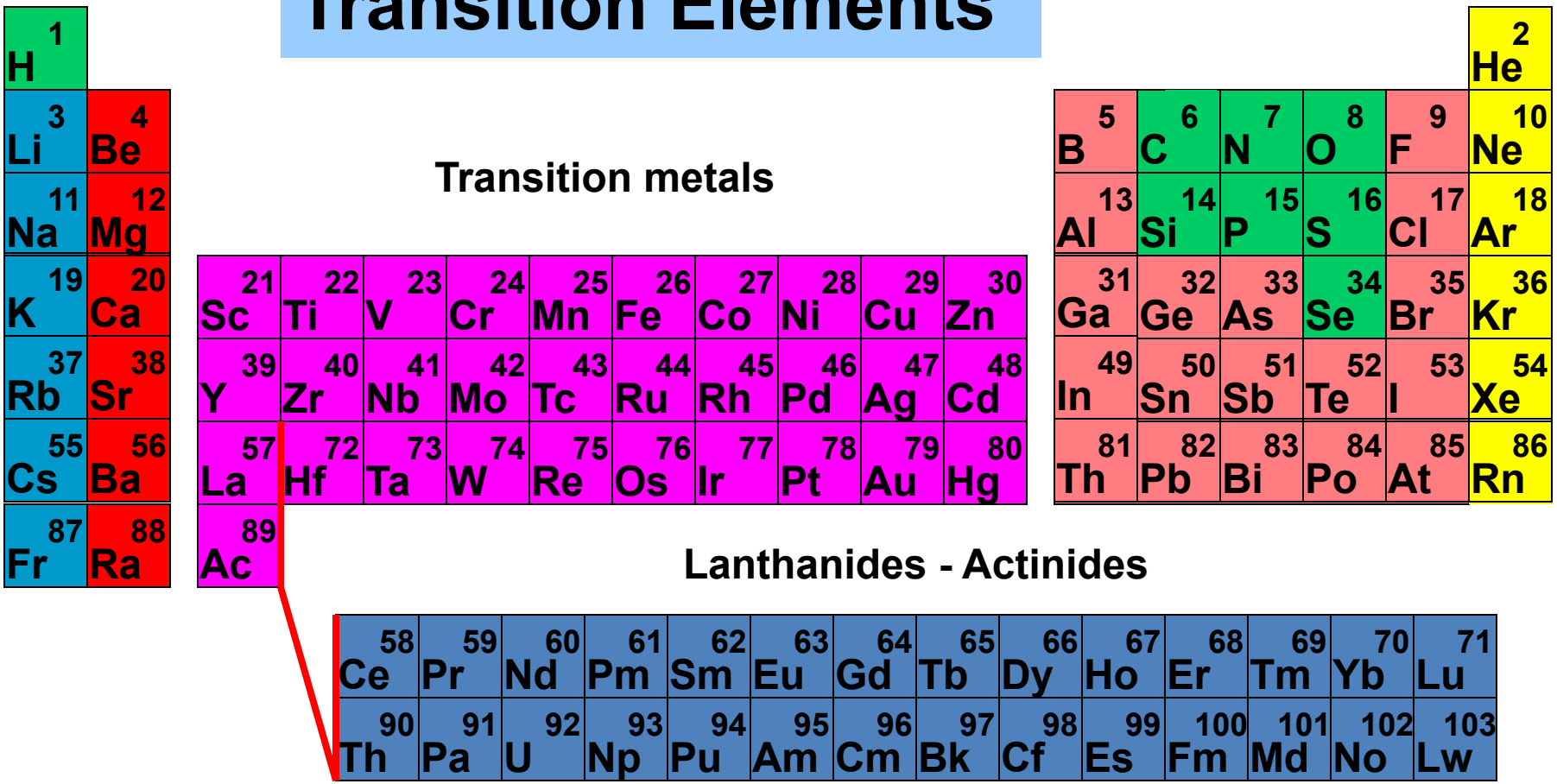
Examples: Si, NaCl, Cu, Na, ….

What materials have properties that causes them to be near the“Mott transition”

Materials containing atoms that retain features of open-shell atomic-like in the solid (i. local moments)

Transition Elements!

Transition Elements

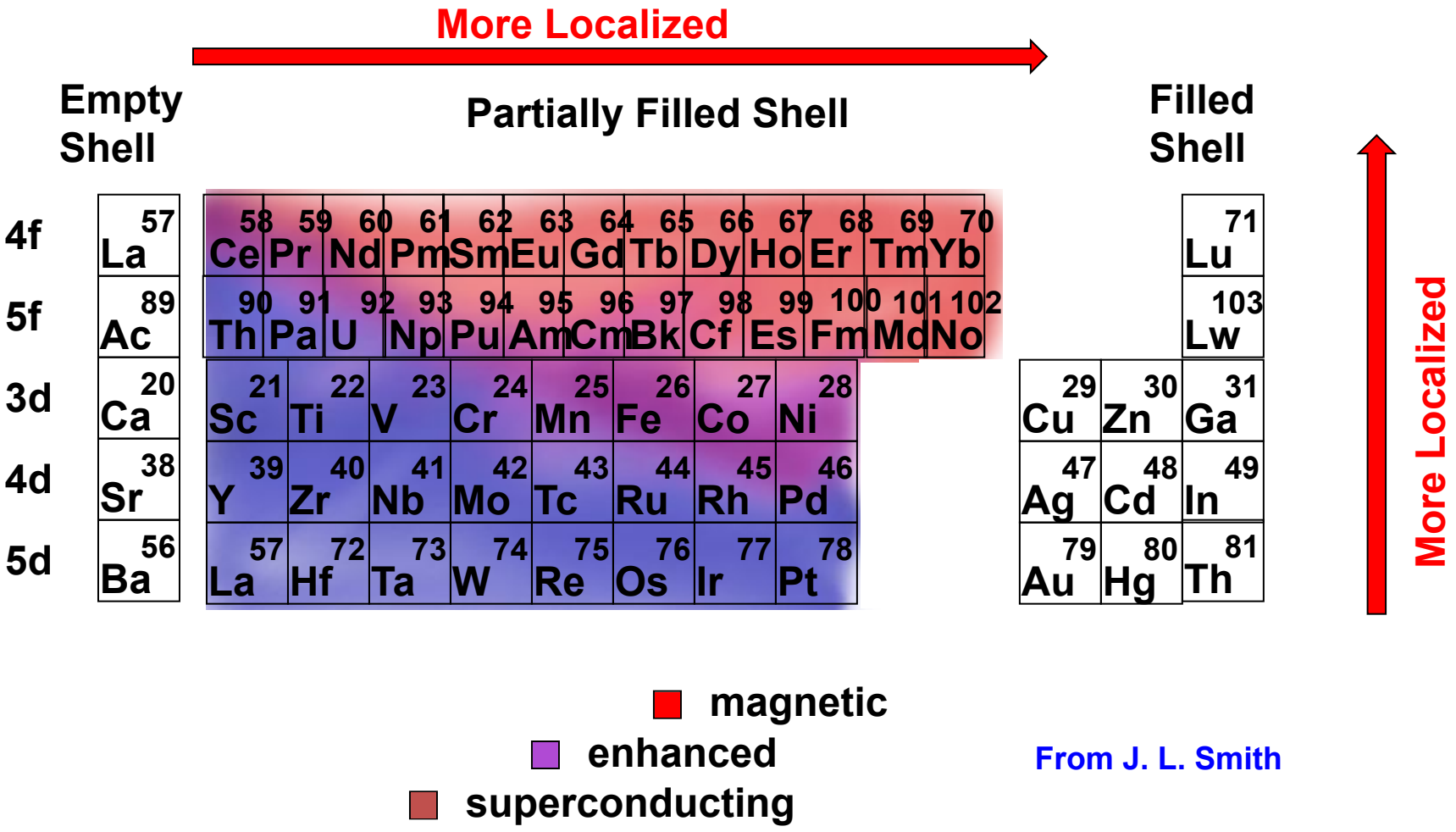


Localized d and f states – partially filled (open shell)

Strong interactions within d or f shell on each atom

Correlations with other atoms mainly by indirect coupling via the band-like states

Transition elements - rearranged



From J. L. Smith

Transition elements

localized states - notably 3d, 4f

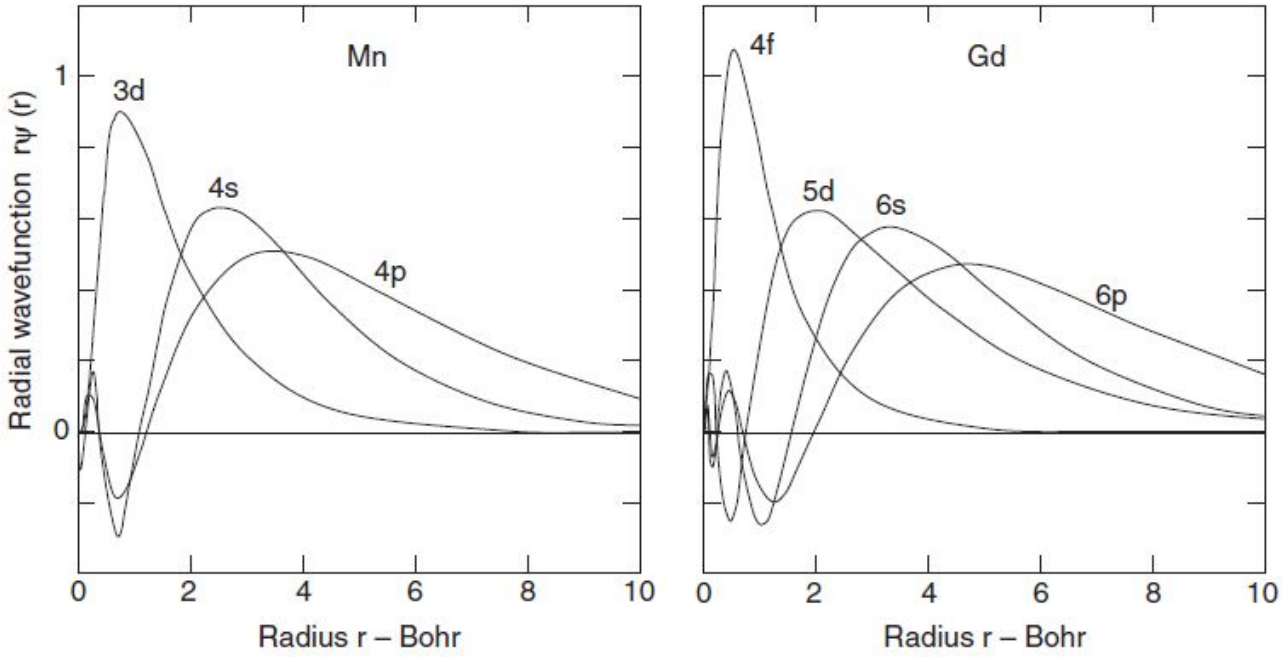
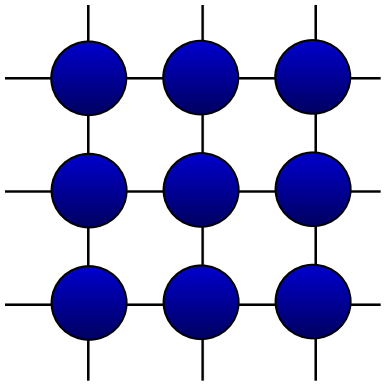


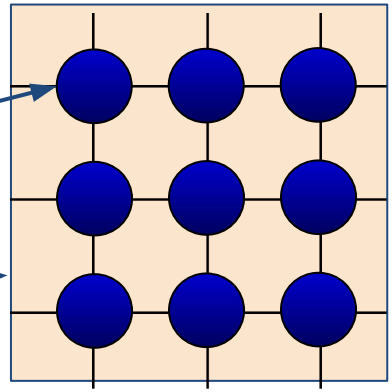
Figure 19.2. Radial wavefunctions $\phi_l(r) = r\psi_l(r)$ for Mn (left, similar to Fig. 10.1 in [1]) and Gd (right) generated by the Octopus website (code originally due to J. L. Martins). For Gd the $4f$ states are much more localized than the other valence states, so that they are almost unchanged in the solid. For Mn the $3d$ states are more localized than the $4s$ and $4p$ states, but not to the same degree as the $4f$ states of Gd or other lanthanides.

Schematic Picture

Solids with atoms that are intermediate between atomic-like and band-like character



Materials with some atoms that have localized atomic-like character coupled to other other band-like states



Transition Metals! Transition metal oxides! Certain Lanthanides!

Excamples of large effects of correlation and large temperature dependence

My list

Magnetism – spins are really electrons

T_c ~ 1K – 1000 K sets scale for magnetism

Metal – insulator transitions

Transition metal oxides

Kondo Effect -- magnetic impurities in metals

T_K can be ~ 10^{-3} K or 10^{+3} K

In each case there are also high energy scales – band widths – exchange energies – multiplet energies ……

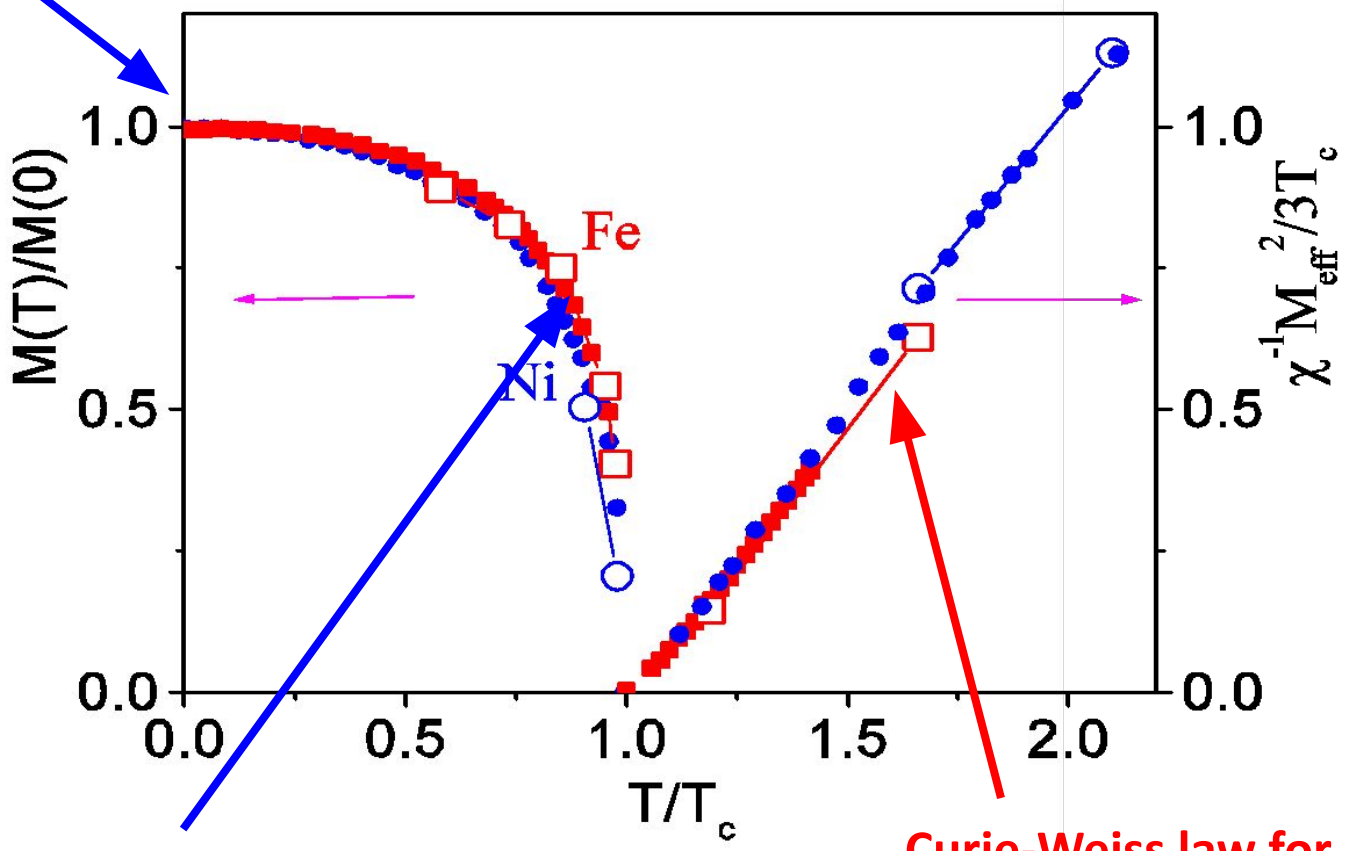
energy ~ eV ~ 10,000K

Must deal with more than one energy scale

Three examples

Magnetism in Fe, Ni

Magnetization at T=0
Given well by DFT



A T=0 DFT calculation does NOT apply!

Described roughly by model of local moments with thermal fluctuations

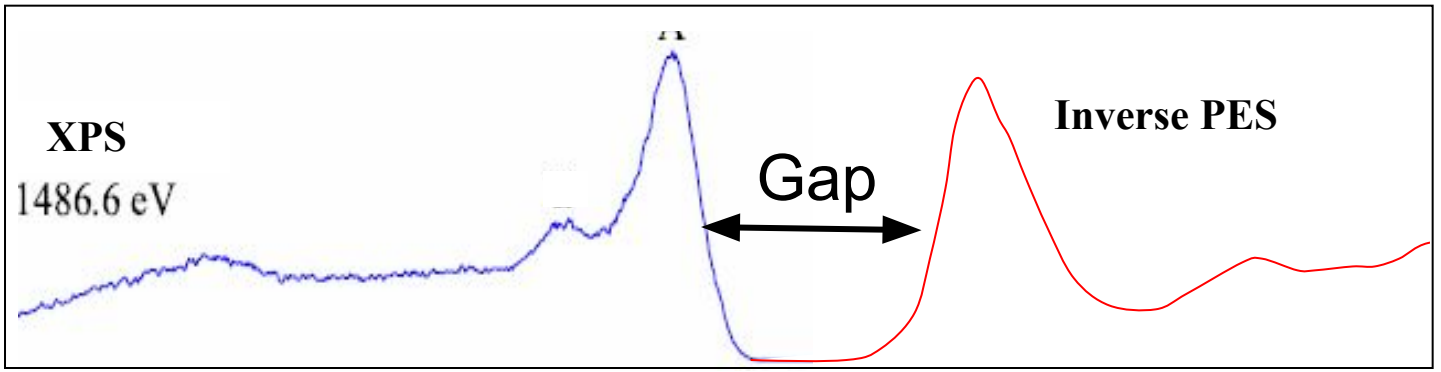
Curie-Weiss law for thermally disordered moments

$\chi \sim 1/(T - Tc)$ $\chi^{-1} \sim T - T_c$

The Original "Mott insulator" NiO

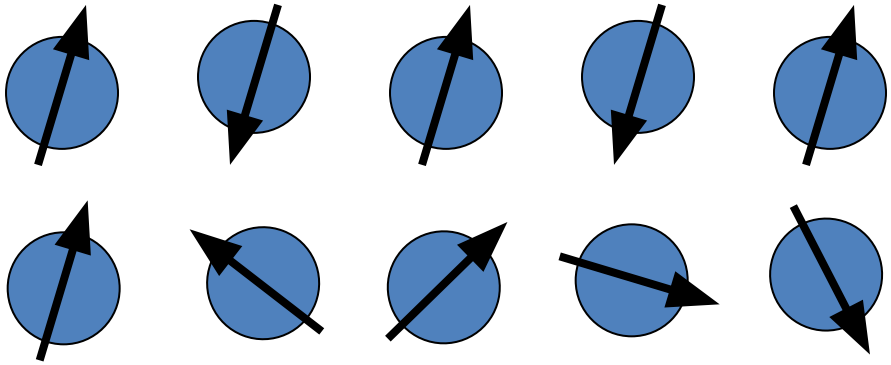
Would be a metal if there were no interactions

But it is an insulator!



Actually an antiferromagnetic insulator at low T

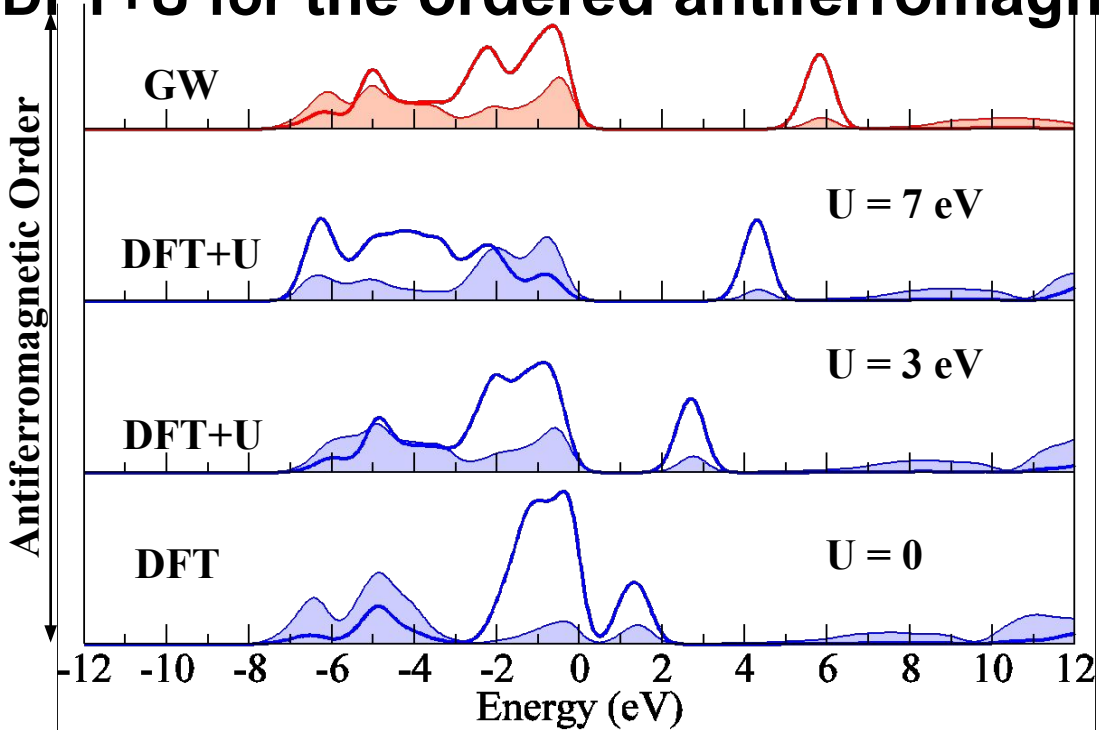
No average spin for T>Tc



Spectrum hardly changes at T>Tc – still a gap!

The Original "Mott insulator" NiO

Gap given well by GW and reasonably byDFT+U for the ordered antiferromagnet



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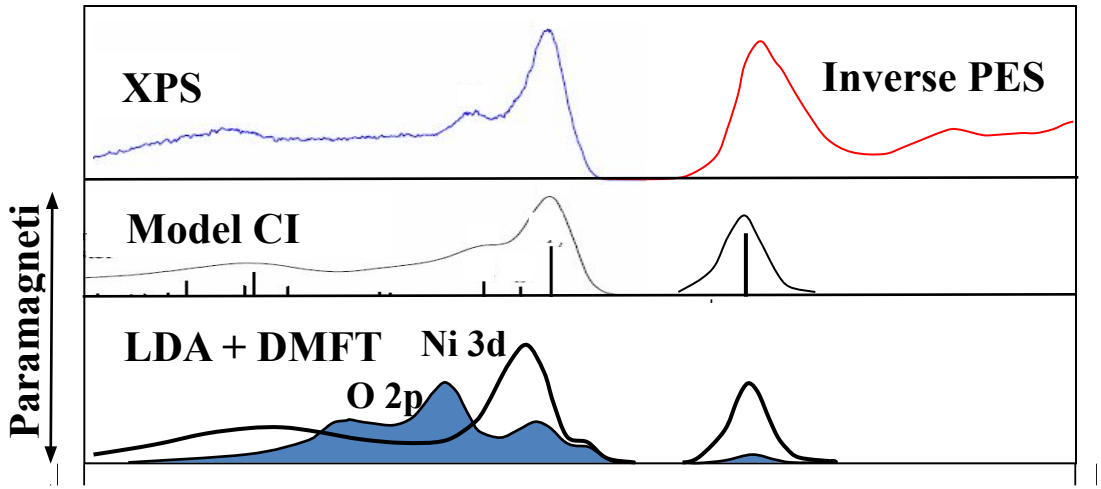
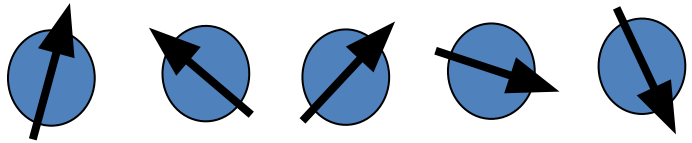


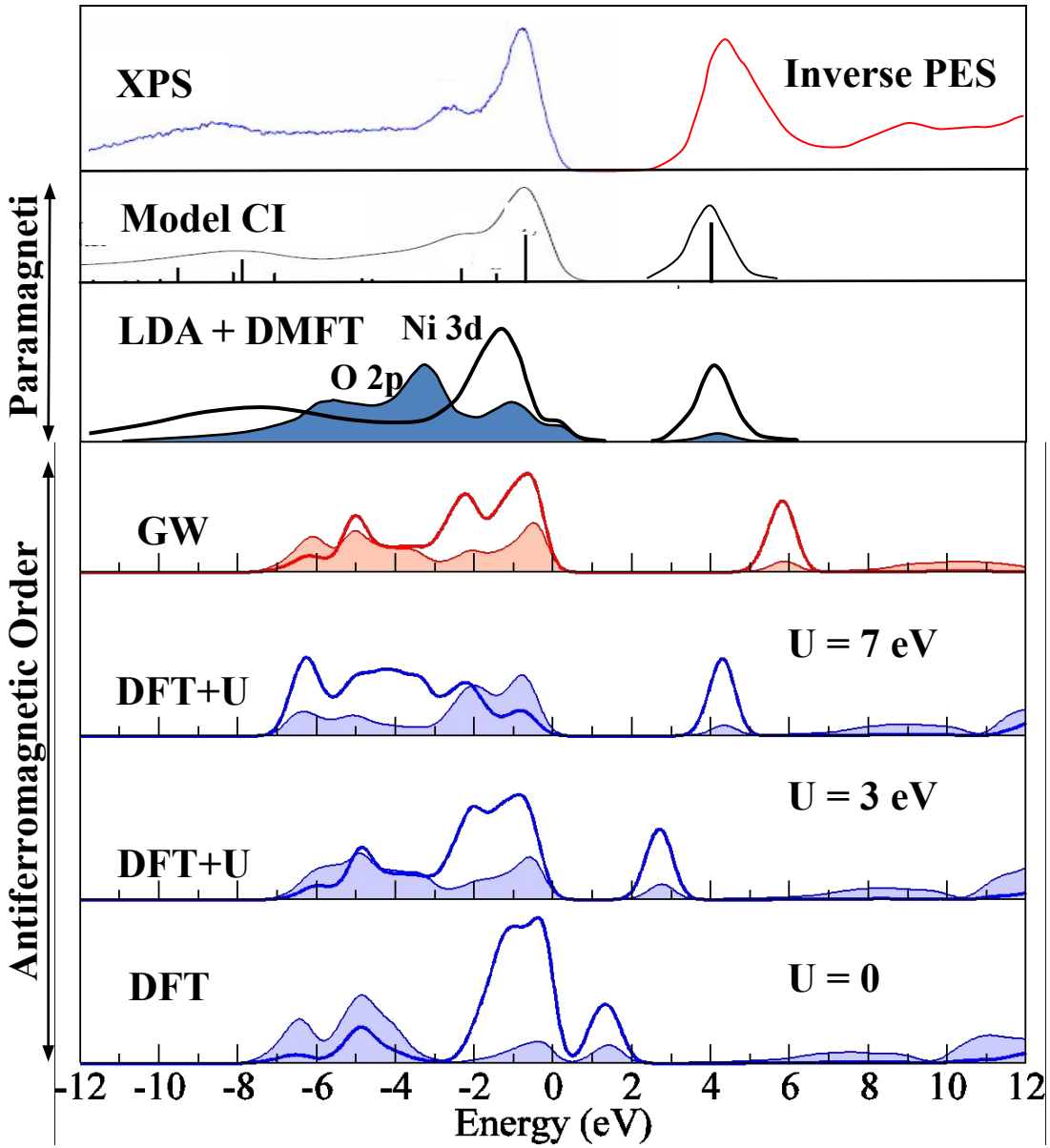


$T>T_c$ gap described by DMFT

Also $T<T_c$ (but not actually done yet)

T=0 DFT and GW do NOT apply!

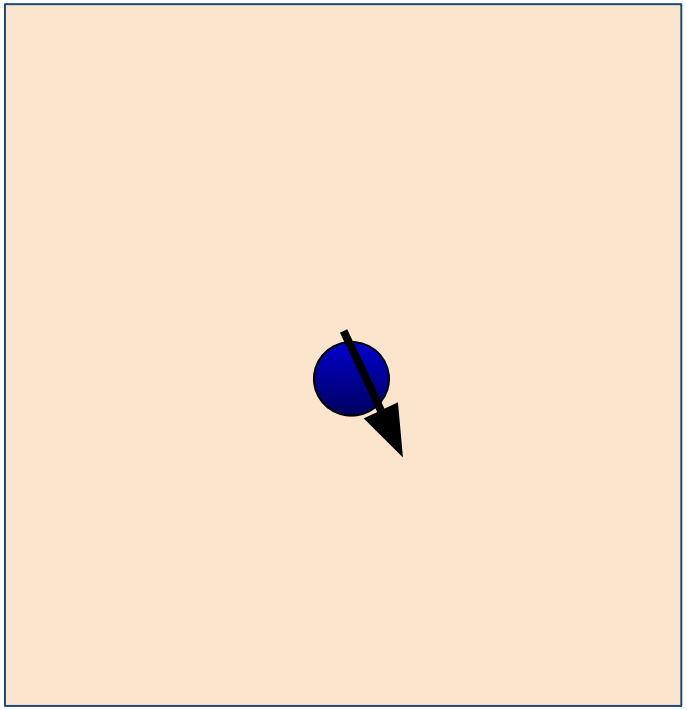
The Original "Mott insulator" NiO



Combining the methods

Kondo Effect - Anderson Impurity Model

Impurity with local moment in non-magnetic metal, e.g., Cu



Low energy scale due to moment fluctuation if local moment is weakly couple to surrounding metal

Exact solution

Strongly coupled no matter how weak!

Strongly correlated!

Kondo Effect - Anderson Impurity Model

Impurity with local moment in non-magnetic metal, e.g., Cu

Spectra

Narrow peak at Fermi energy

Three peak spectrum

"Hubbard side bands"

Non-interacting

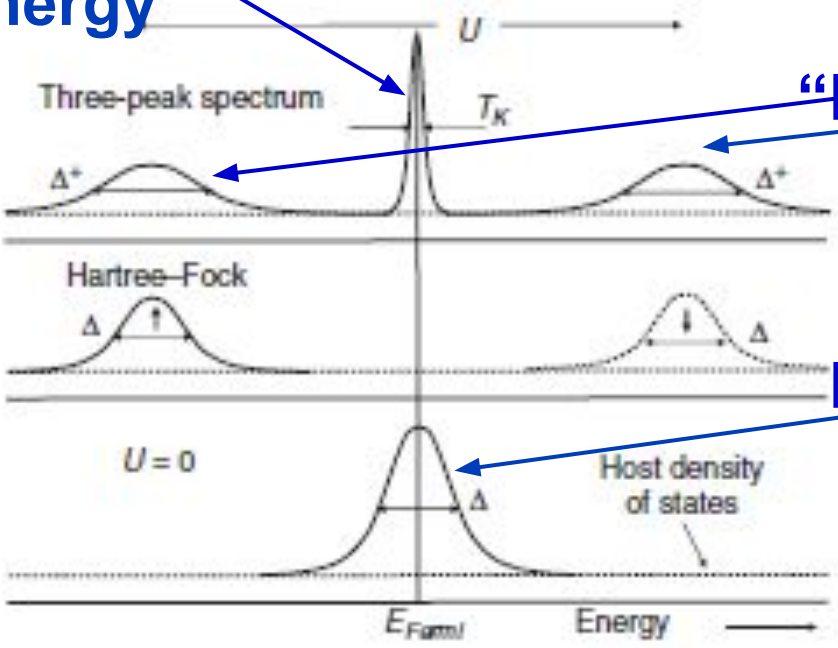
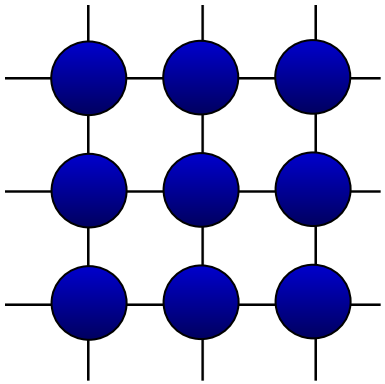


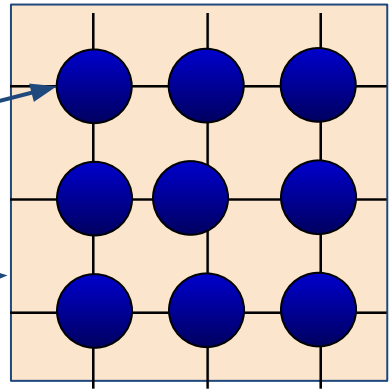
Figure 3.4. Schematic illustration of the spectrum (the sum of ↑ or ↓ spins) for the symmetric spin-1/2 AIM. (Bottom) The non-interacting case with $U = 0$ with a half-filled lorentzian resonant level with width Δ at the Fermi energy. (Middle) The unrestricted Hartree–Fock spectrum for U large enough to give a broken-symmetry magnetic solution with ↑ occupied and ↓ empty. (Top) The full spectrum with the characteristic three-peak structure, a narrow Kondo peak of width T_K at the Fermi energy, and two atomic-like peaks at energies split by $\approx U$. The width of the peaks denoted Δ^+ is greater than Δ, as discussed in the text.

Lattice of atoms with local moments

Solids with atoms that are intermediate between atomic-like and band-like character

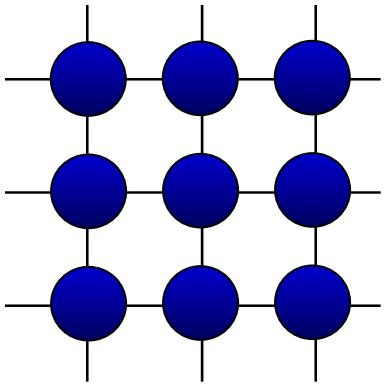


Materials with some atoms that have localized atomic-like character coupled to other other band-like states



Transition Metals! Transition metal oxides! Certain Lanthanides!

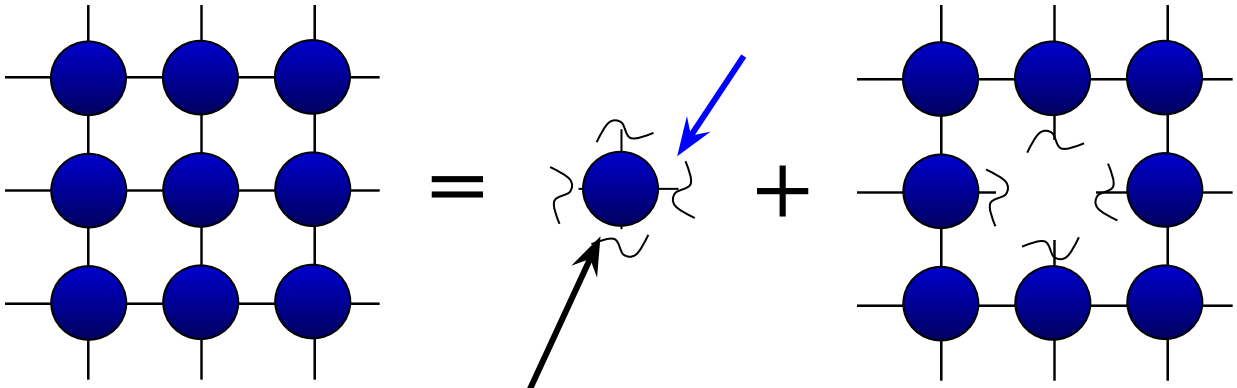
Dynamical Mean Field Theory (DMFT)



Keep ALL independent particle terms

Approximate Correlation between sites
(simplest case - no intersite correlation)

Keep (ALL) correlation on each site
(in principle exact)



Bath due to the rest of the system
treated as independent particles
Self-consistent Anderson Impurity model

Conclusions

What does "Strong Correlation" mean?

Different meaning in different contexts!

What systems are here considered to be "strongly correlated"?

Systems with low energy excitations, large T dependence
Anderson Impurities, Heavy Fermions

Some antiferromagnets, ferromagnets

In such systems, which aspects of a Kohn-Sham calculation are:

Applicable if chosen appropriately.

Ordered States, e.g., Antiferromagnet,
ferromagnet at T=0

Not directly applicable at all - source of misconceptions

Disordered momenta at non-zero T

Informative - a starting point for improved calculations.

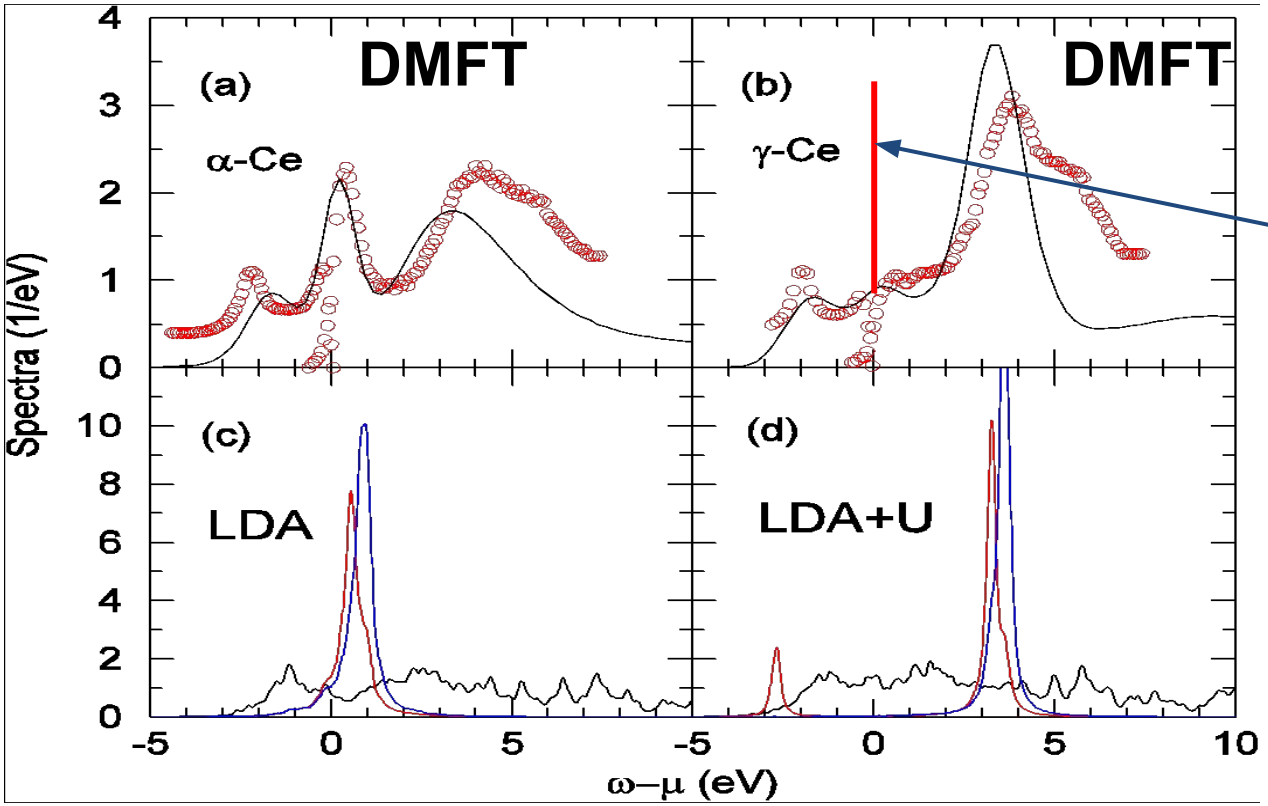
Model parameters for calculations like DMFT

EXTRAS

Lattice of atoms with local moments weekly coupled to other band-like states

Ce - 4f states coupled to band-like s, p, d states

Strongly coupled **Weakly coupled**

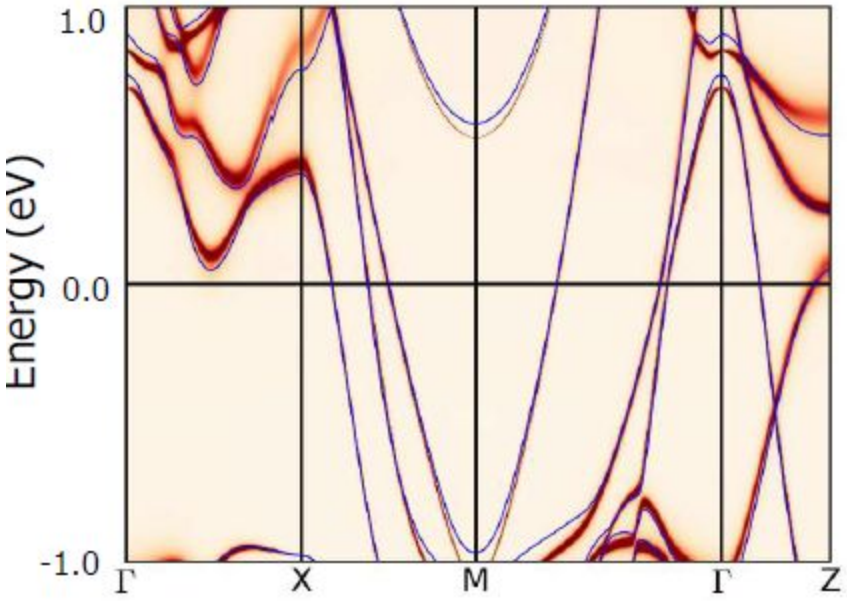


Narrow peal

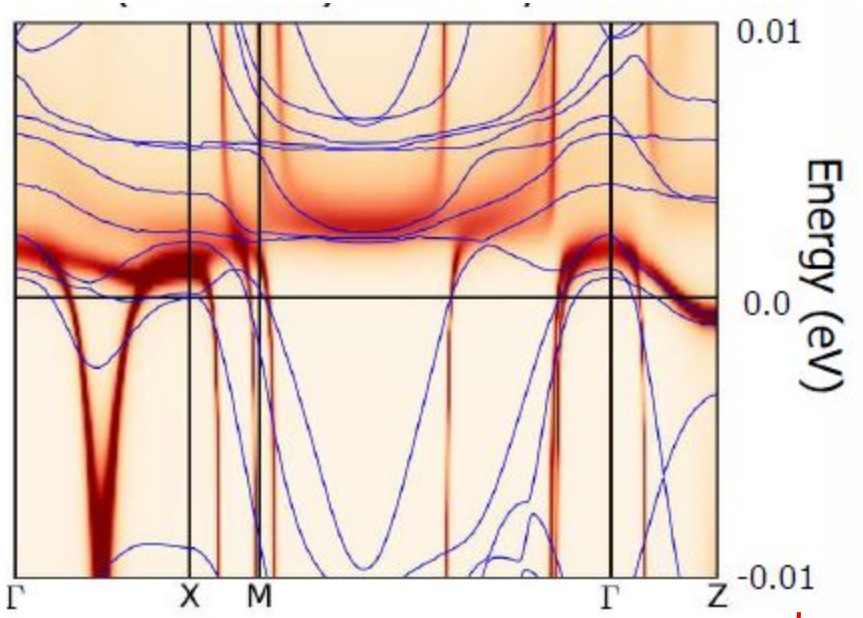
DFT+DMFT -- CeIrIn5

Heavy Fermion Material

T = 300 K



T = 10 K



Almost the same as DFT
with 4f-states removed

Similar to DFT
including 4-f states
Scaled by 1/100 !

Single-site, CTMC solver

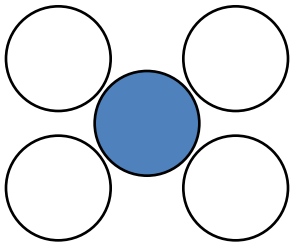
Choi, H. C., Min, B. I., Shim, J. H., Haule, K. and Kotliar, G. (2011). Temperature-dependent fermi surface evolution in heavy fermion ceirin5. *Cond-Mat* ***2011, arXiv:1105.2402v1.***

DMFT

(Map problem to Self-consistent Anderson Impurity Model)

Same U as in DFT + U

Solve for atom embedded in average field due to neighbors

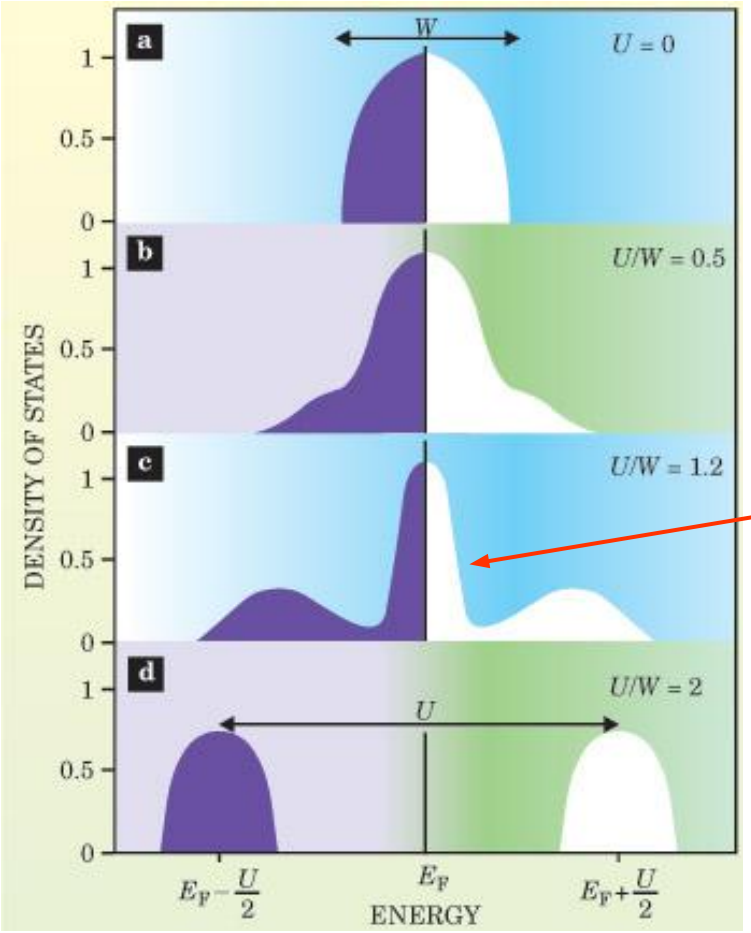


- **Spectrum of Green's function on central site**

  $G(E) = [\, E - H_0 - \Sigma(E) \pm i\delta]^{-1}$

  consistent with neighbors

- **Solve by Monte Carlo, . . .**



New energy scale

Kotliar and Vollardt, Physics Today 2004

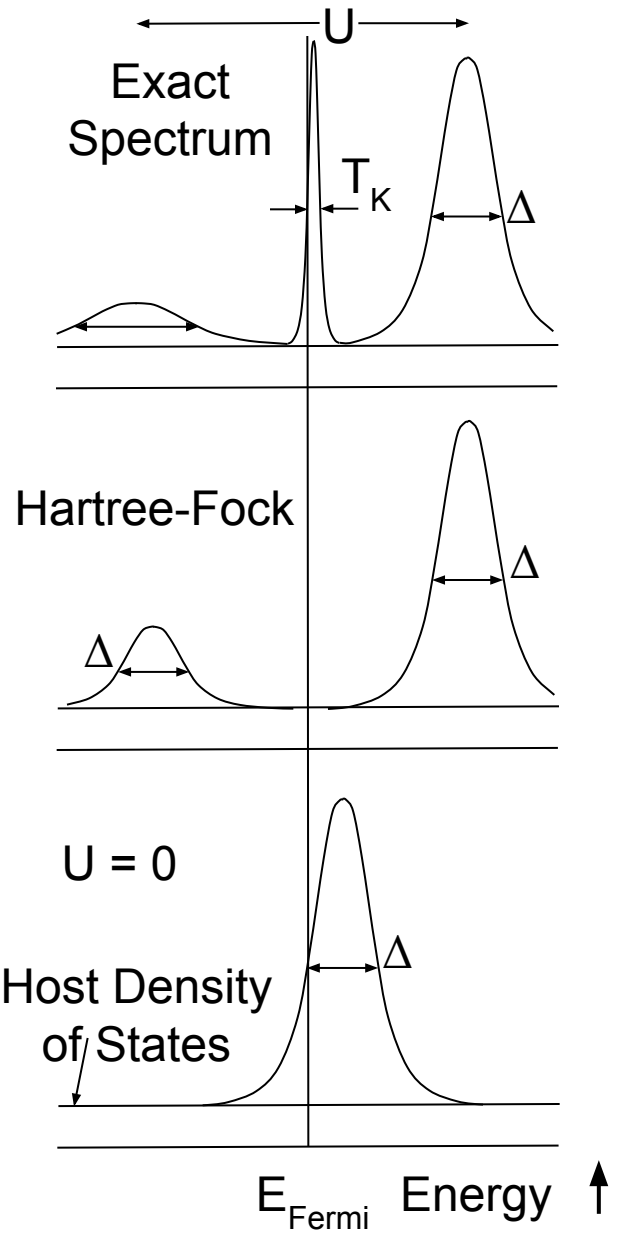
DMFT

"Three-Peak" Spectrum of the Anderson Impurity Model

Two high energy peaks for adding and subtracting electrons from the atomic-like states --- separated by U

A central "Kondo" peak
– always at the Fermi energy
Width ~ T_{Kondo}

A many-body energy scale
– signature that there is interesting behavior as a function of T



Relation of the methods

- **DFT - Kohn-Sham – potential $V_{KS}(r) = V_{Hartree}(r) + V_{xc}(r)$**
  - Static $V_{xc}[n(r)]$ - functional of the density n(r)
- **GW – dynamic self energy $\Sigma(r,r',E)$**
  - Calculate with perturbation theory
  - Often start with DFT (or extensions of DFT)
  - Green's function $G(r,r',E) = [G_0^{-1} - \Sigma]^{-1}$
- **DMFT – local dynamical $\Sigma(r,r,E)$ and G(r,r,E)**
  - **Philosophy very close to Kohn-Sham!**
    - Local site embedded in a mean-field medium is an "auxiliary system"
    - The difference is that this is a dynamical interacting auxiliary system
    - Result – dynamical self-energy instead of static Kohn-Sham potential
  - **Treats local on-site correlations more accurately**
  - **Relates directly to Kondo and Anderson Models**

When is Temperature Important

Nuclei vibration energy - ion motion

Typical scales for phonons in solids
~ 0.01 to 0.1 eV/k_b ~ 80 to 800 K

For many materials with electronic energy scales ~ 1eV, nuclei move with Born-Oppenheimer approximation with electrons in their ground state
The material melts before the electrons change much!

Examples: Si, NaCl, Cu, Na, ….

When is temperature important for the electronic properties?