CONDENSED MATTER PHYSICS II
Physics 561, Fall 2005
University of Illinois

Prof. Richard M. Martin

Lecture 1: Introduction

Overview

Background Material – 2^{nd} quantization, Hartree-Fock, . . .

PART I: Elementary Excitations

PART II: Strongly Interacting Electron Systems

PART III: Quantum Phases of Matter:
Metals, Insulators, Superconductivity, Quantum Hall Effect, . . .

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Lecture 1: Introduction

Class Materials

Web Site for course: **http://w3.physics.uiuc.edu/~rmartin/561/**

Primary Text: ***Advanced Solid State Physics*** **by Philip Phillips**
Westview Press; 1st edition, 2002
Paperback: 416 pages, ISBN: 0813340144

Other references: **See list of books on reserve**

General Articles:

"More is Different", P. W. Anderson, *Science* 177:393-396, 1972
"A different Universe – Reinventing Physics from the Bottom Down"
R. B. Laughlin, Basic Books, New York, 2005.

Outline of Course I

- Background
    - Start from fundamental hamiltonian
    - Clear division –
        - Ground electronic state with low energy nuclear degrees of freedom
        - High energy electronic excitations
        - EXCEPT for interesting low energy electronic excitations
    - The Great Challenges –
        - Electron-electron interactions – phases formed by the electrons
        - Phases formed by the nuclei – crystals, liquids, liquid crystals, . . .

- "Elementary excitations" and Many-body perturbation theory
    - The best choice of excitations to treat as approximately independent
    - Basis for formulating many-body theory in terms of residual interactions
        - 2nd quantization
        - Correlation functions and Green's functions
    - Response functions - experiments
    - Particle addition/removal – quasiparticles – experiments
    - Key results of many-body perturbation methods
        - Fermi liquid theory
        - Quasiparticle "GW" calculations for excited states
        - Luttinger Theorem, . . .

Outline of Course II

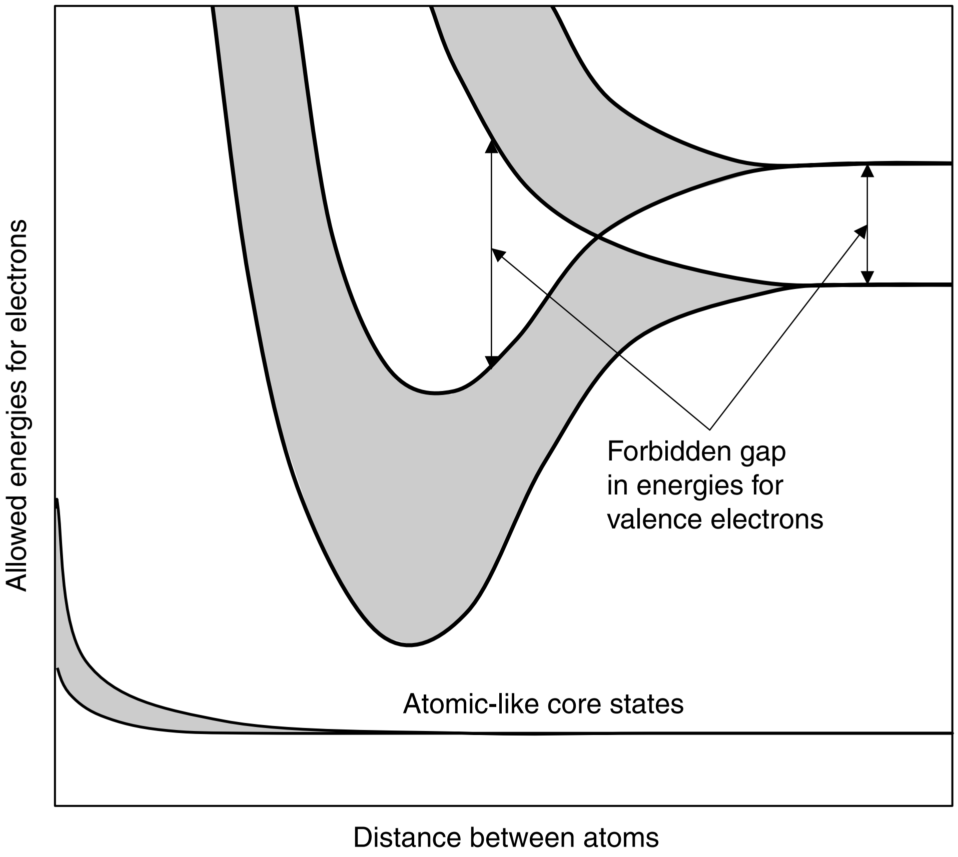
- Strongly Correlated Problems
    - Broken symmetry and order parameters
        - Magnetism, Metal-Insulator transitions, . . .
    - Models for strongly interacting systems – Anderson, Kondo, Hubbard, . . .
        - Solution of the impurity Anderson/Kondo models
    - Dynamical mean field theory
        - Example of Hubbard Model
        - Maps lattice model to an effective impurity Anderson model
        - Metal-insulator transition
    - Survey of Strongly interacting problems - Hi-Tc, . . .

- Quantum Phases of Matter:

  Metals, Insulators, Superconductivity, Quantum Hall Effect, . . .
    - Superconductivity - the paradigm for new phases of matter
        - Landau-Ginzberg theory – before BCS
    - Classification of states by topology of wavefunction
        - Bohm-Aharonov effect, Berry's phase, . . .
        - Metals, insulators, superconductors, . . .
    - Superconductivity – in more depth
    - Quantum Hall effect – fractional effect

The first decade of Quantum Mechanics

Understanding in terms of independent particles



Kimball, 1935

Formation of bonds and bands

Atoms, molecules, solids, …. Bloch Theorem

Metals, Insulators

The great challenge – Electron-Electron Interactions

Examples of Effects of Correlations Extended band-like vs. Localized atomic-like behavior of electrons in solids

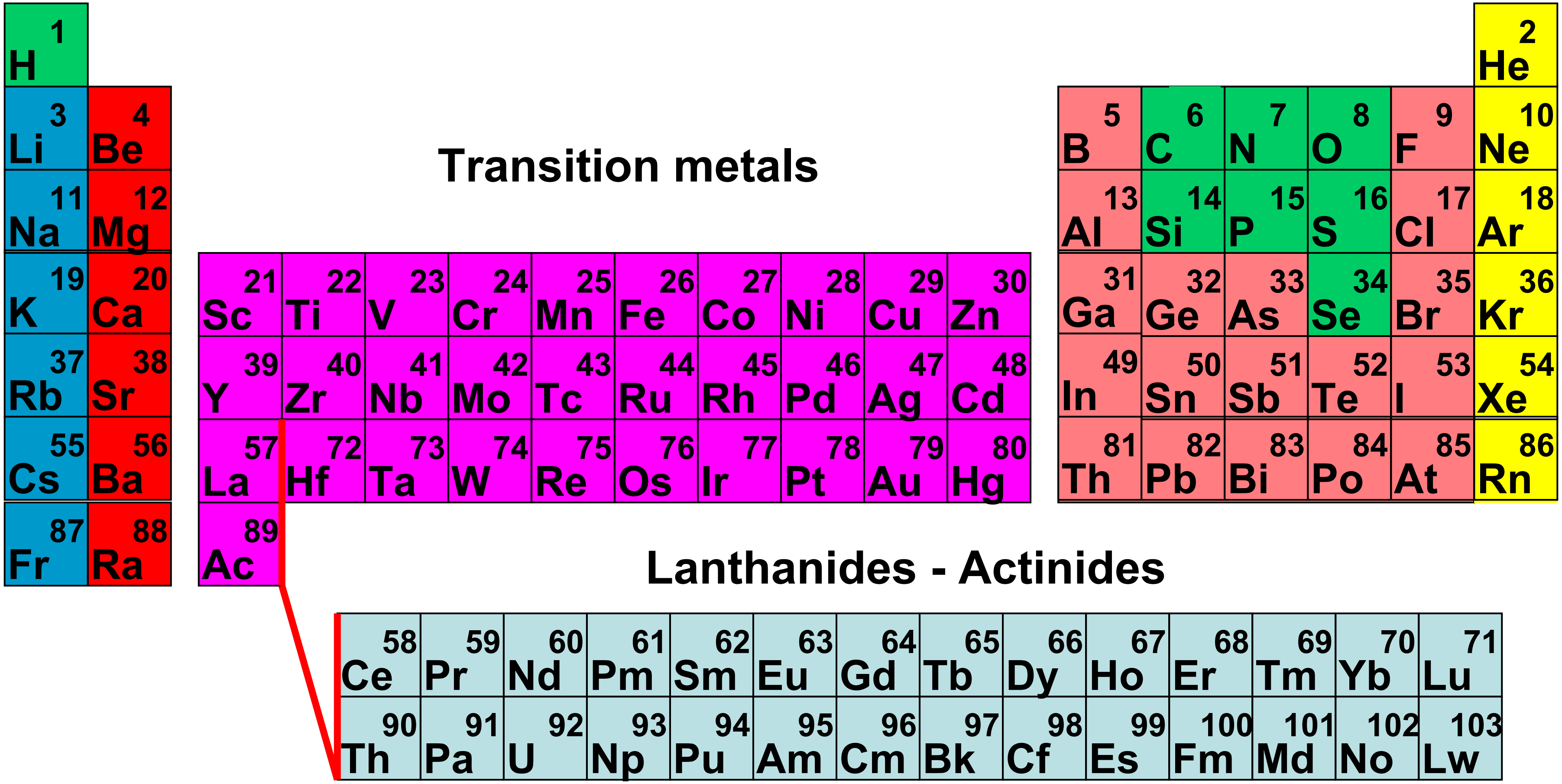
Delocalized states	Localized states
Nearly free electron bands	4f states
Alkali metals: Na, K, ...	Rare earths: Pr – Th

Intermediate cases

Semiconductors	Transition Metals
"Band Gap Problem"	Magnetism, Met-Ins Trans.

Mott Metal-Insulator Transitions
    Hydrogen under pressure (not reached experimentally)
    NiO, CuO materials, . . .
Anderson/Kondo/Heavy Fermion Problems
    "Anomalous" Rare Earths, e.g., Ce
    Hi-Tc, ….
Lower Dimensions
    One-dimension – Luttinger Liquids
    2-d – (fractional) Quantum Hall Effect

Periodic Table



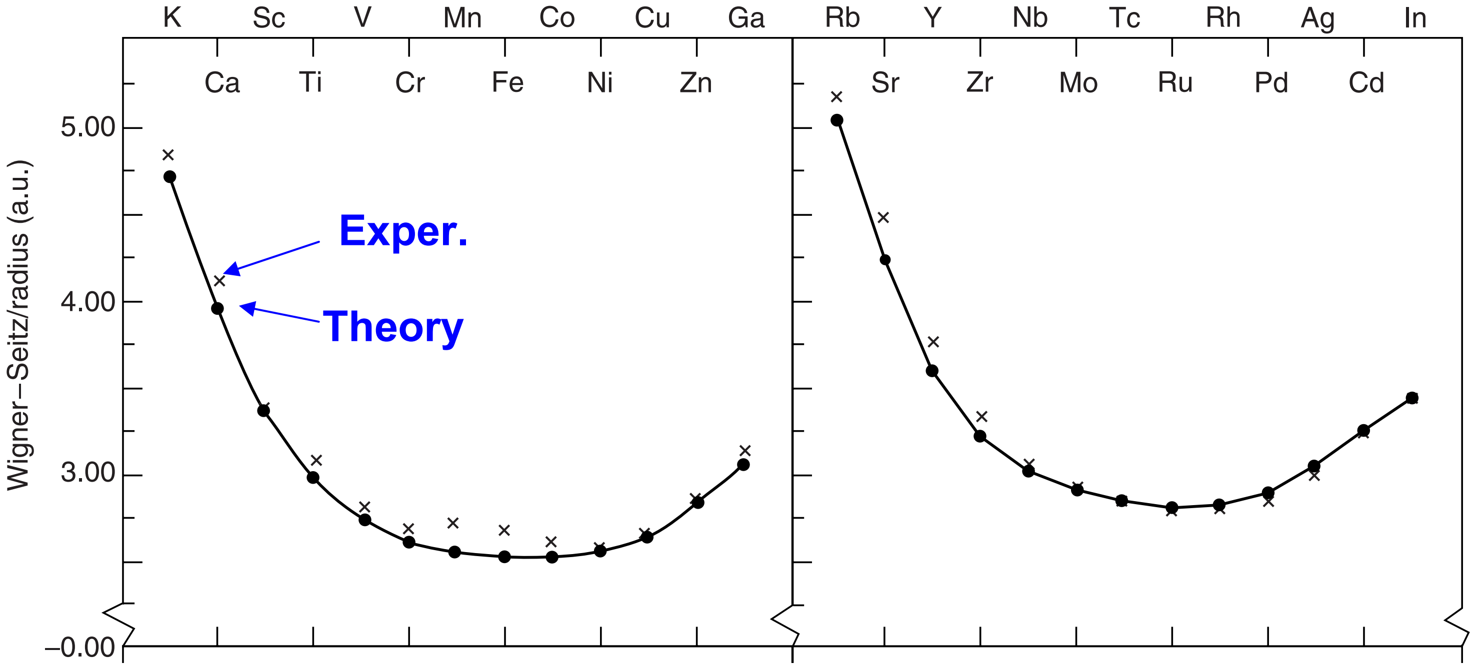
Transition metals

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Th	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac															

Lanthanides - Actinides

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
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 Lw

For Wide-band Systems
Effective Independent-Particle Methods
work well for some properties



Lattice constants of the 3d and 4d transition metals
Comparison of theory (no parameters) and experiment

Many comparable results for semiconductors, ionic crystals, . . .

Martin, Fig. 2.3

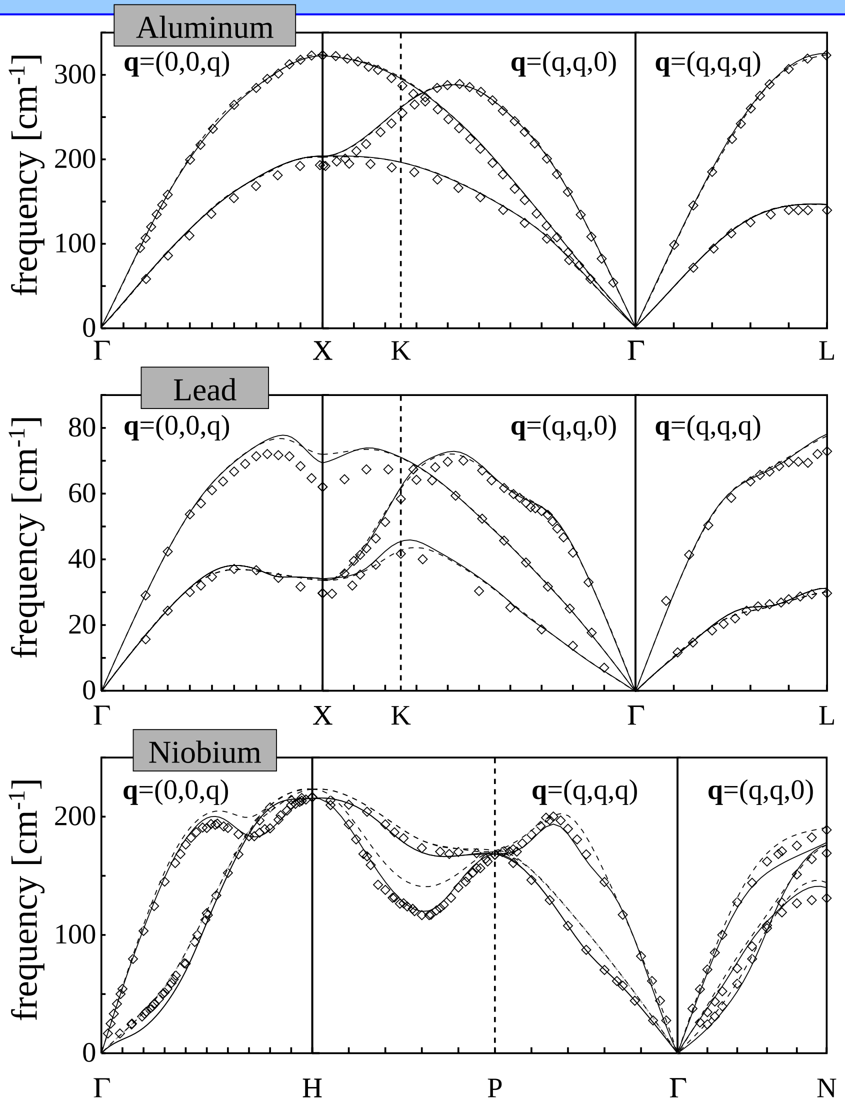
Calculation of phonon energies

Phonons

Comparison of theory and experiment

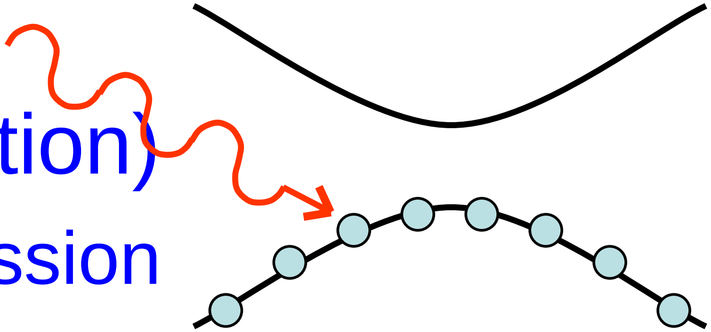
- Calculated from the response function – “Density functional perturbation theory”
- Now a widely-used tool in mean field density functional calculations

De Gironcoli, et al.



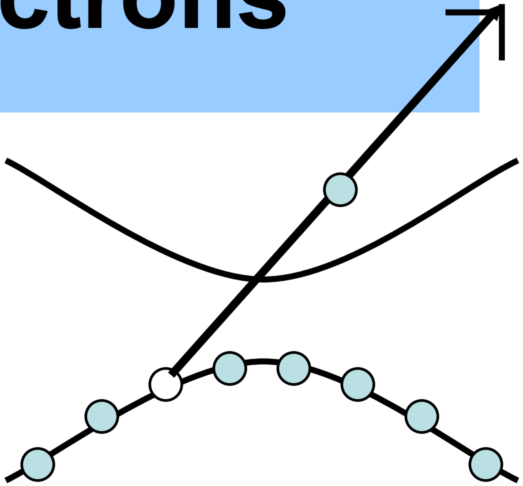
S. de Gironcoli, Phys.Rev B 51, 6773 (1995)

Excitations of the electrons



- Excitations
- Electron removal (addition)
  - Experiment - Photoemission
  - Theory – Quasiparticles
    “GW” Approximation
- Electron excitation
  - Experiment – Optical Properties
  - Theory – Excitons
    Bethe-Salpeter equation (BSE)

Excitations of the electrons



- Excitations
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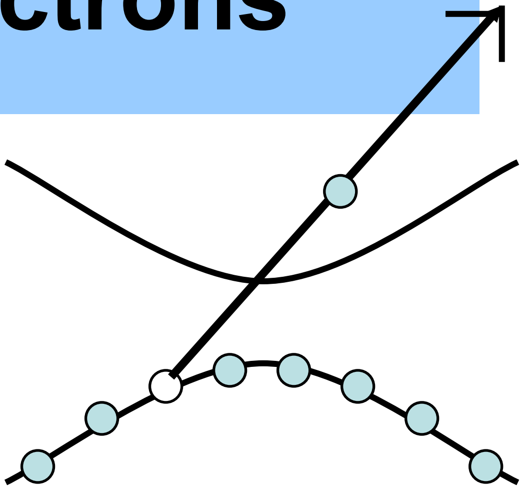
Excitations of the electrons



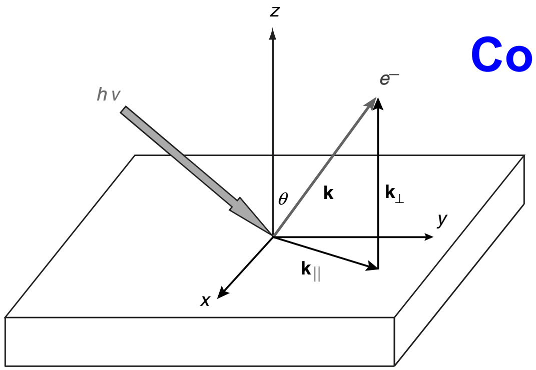
- **One-particle Green's function:**
  $G(x,x',t,t') =$
  $-i \langle N| T[\psi(r,t)\psi^+(r't')] |N\rangle$

- **Independent particles:**
  $G(r,r',t,t') = i \, \Sigma_{m\,occ} \varphi_m(r)\varphi_m(r') \, e^{-i\varepsilon_m(t-t')}$, $t < t'$
  $G(r,r',E) = \Sigma_m \, \varphi_m(r)\varphi_m(r') \, [\, E - \varepsilon_m \pm i\delta]^{-1}$
  or $G(E) = [\, E - H_0 \pm i\delta]^{-1}$

Self Energy due to interactions

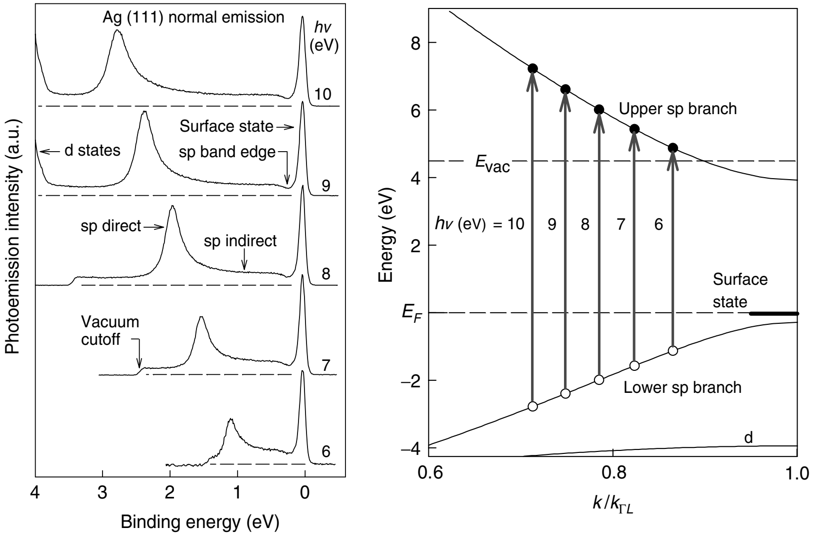
- Including Interactions
  $G(E) = [\, E - H_0 - \Sigma(E) \pm i\delta]^{-1}$

Powerful Experiment
Angle Resolved Photoemission (Inverse Photoemission) Reveals Electronic Removal (Addition) Spectra

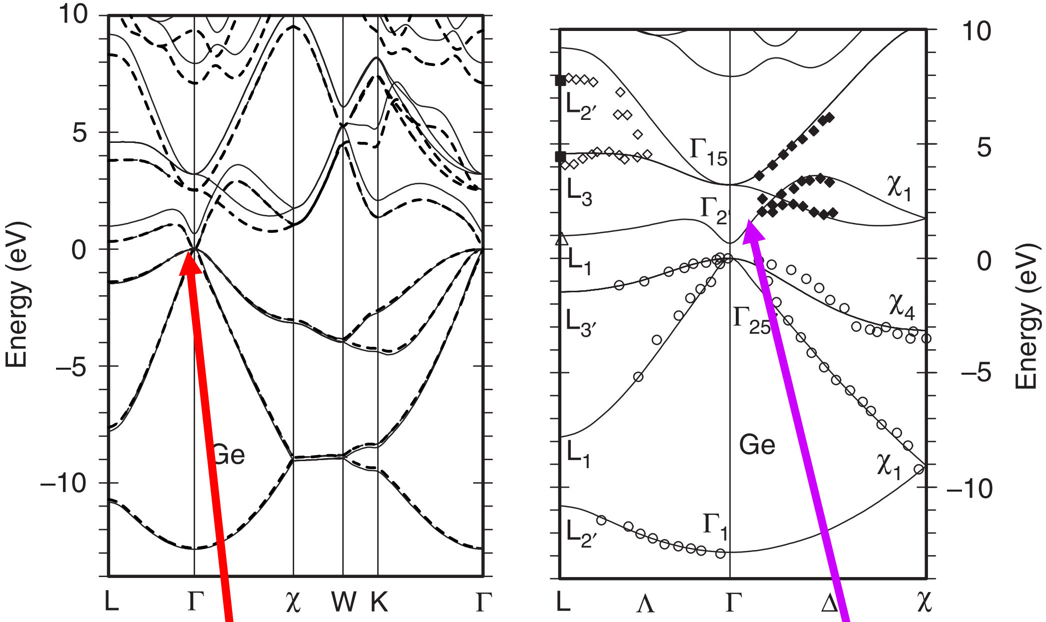


Comparison of theory (lines) and experiment (points)

Silver



Germanium



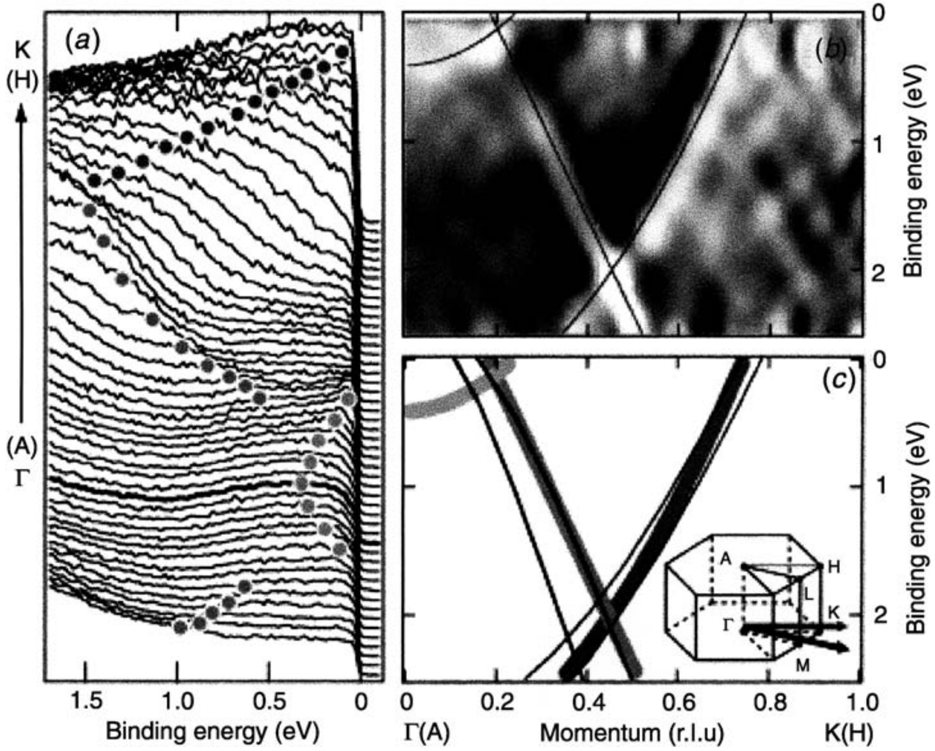
A metal in "LDA" calculations!

Improved many-Body Calculations

Martin, Figs. 2.22, 2.23, 2.25

Powerful Experiment Angle Resolved Photoemission (Inverse Photoemission) Reveals Electronic Removal (Addition) Spectra

Recent ARPES experiment on the superconductor MgB_2
Intensity plots show bands very close to those calculated using mean-field independent-particle methods



Martin, Fig. 2.30
From Domasicelli, et al.

Strongly Correlated Systems

Strong Correlation associated with:
- Localized electronic states
- Magnetism
- Anomalous enhanced behavior

Typical materials
- Transition metal compounds, rare earths, actinides
- 1-d, 2d systems – compounds, semiconductor devices

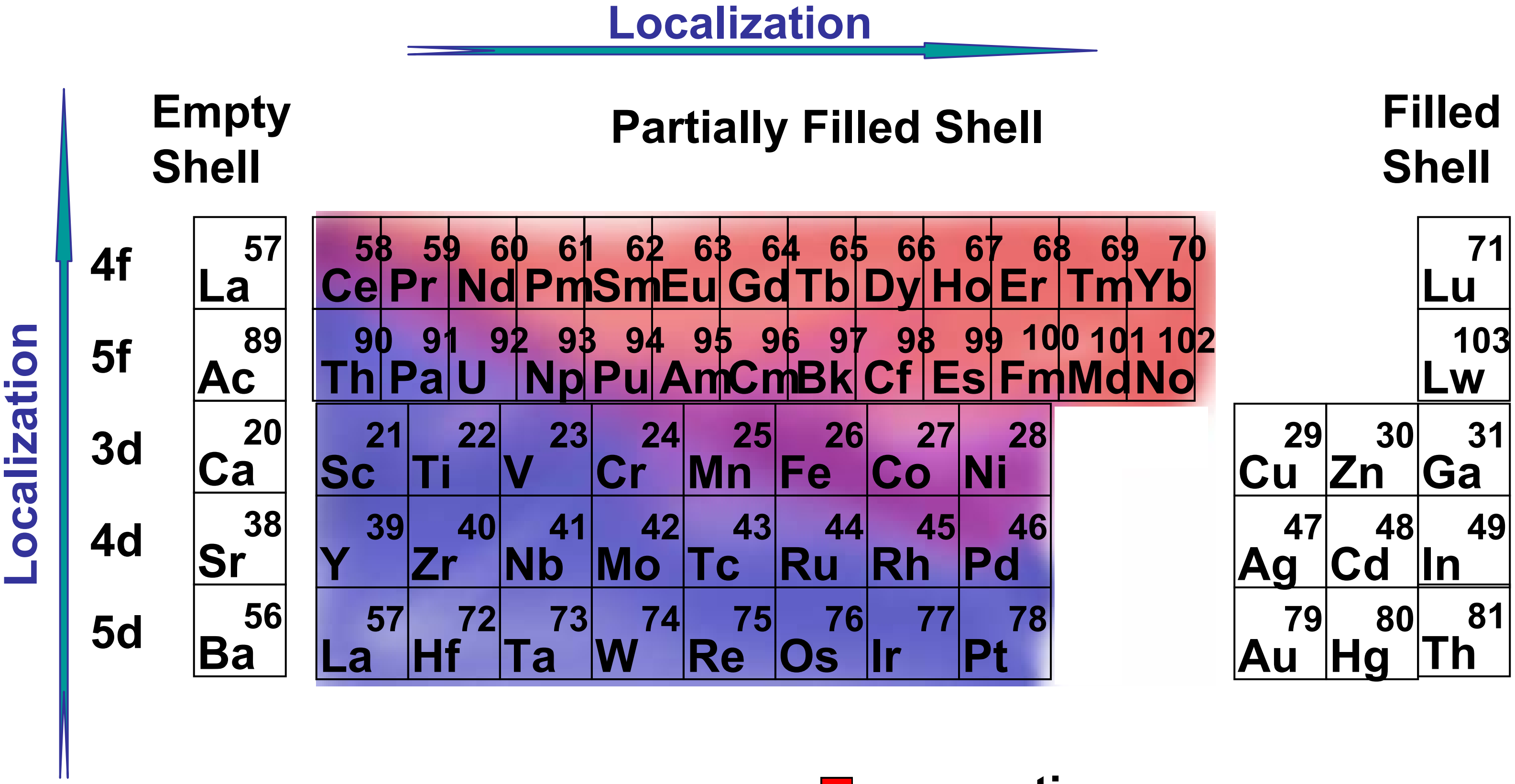
Mott Metal-Insulator Transitions
- Hydrogen under pressure (not reached experimentally)
- NiO, CuO materials, . . .

Anderson/Kondo/Heavy Fermion Problems
- "Anomalous" Rare Earths, e.g., Ce
- Hi-Tc, ….

Lower Dimensions
- One-dimension – Luttinger Liquids
- 2-d – (fractional) Quantum Hall Effect

Grand Challenges for many-body theory

Transition & Rare Earth Elements



Localization

	Empty Shell	Partially Filled Shell													Filled Shell		
4f	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
5f	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 Lw
3d	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni						29 Cu	30 Zn	31 Ga
4d	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd						47 Ag	48 Cd	49 In
5d	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt						79 Au	80 Hg	81 Th

Localization

🟥 magnetic

🟪 enhanced

🟦 superconducting

Taken from J. L. Smith

Examples of Strong Correlations

4f states   Lanthanide rare earths: Ce – Yb
Example of Tb (half-filled shell with 7 electrons – $4f^7$)

Electron removal   **Electron addition**

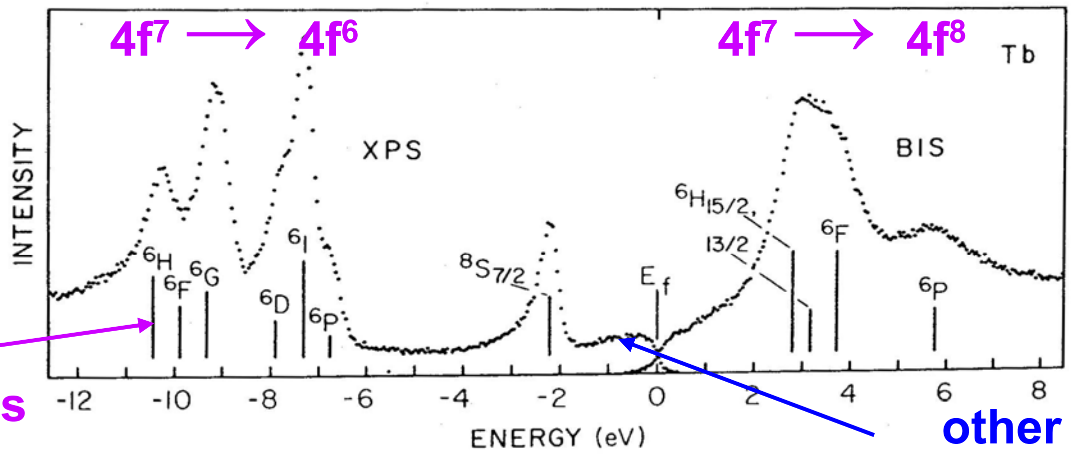


FIG. 1. 4*f* final states observed by XPS and BIS.

4f states – atomic energies

other states – form bands

For the 4f states, the energies to add or remove electrons are essentially the same as in an isolated atom – strong interactions on the atom lead to "multiplets" – different ways the same number of electrons on an atom can be arranged

Damascelli, et al., Rev. Mod. Phys. 75, 473 (2003)

Examples of Strong Correlations

4f states Lanthanide rare earths: Ce – Yb

Example of Tb (half-filled shell with 7 electrons – $4f^7$)

Lowest energy to add an electron in a 4f state

n ⟶ n - 1

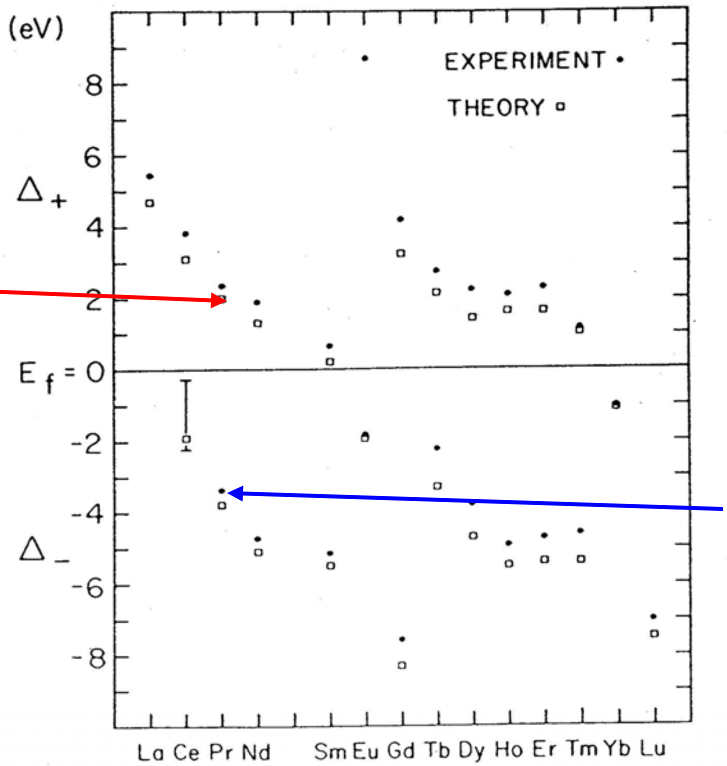


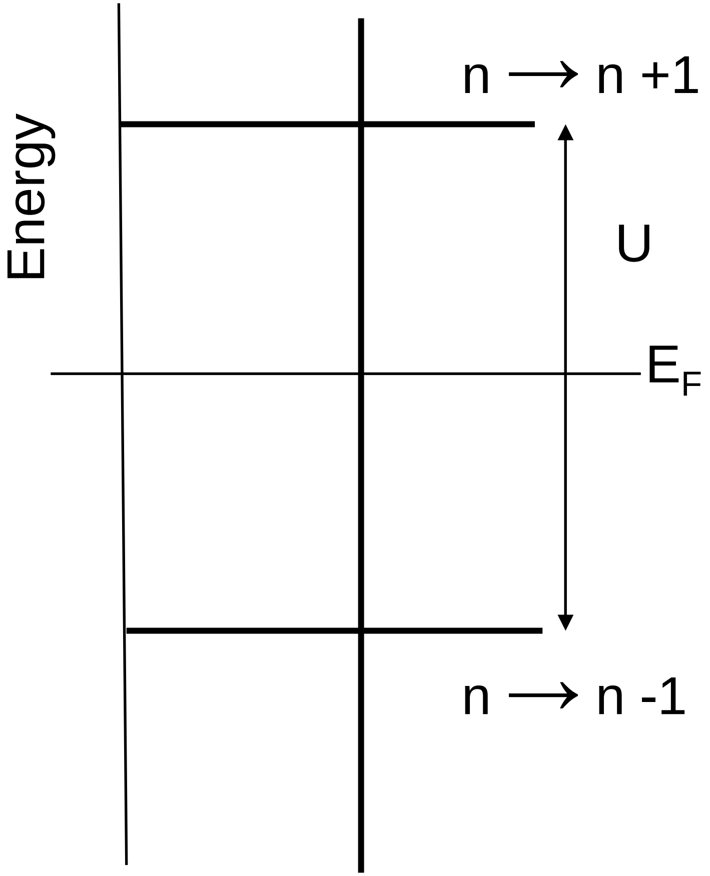
FIG. 2. Comparison of experimental and theoretical (Refs. 11 and 12) values of Δ_- and Δ_+. The experimental Δ_- value for Ce lies within the error bar.

Lowest energy to remove an electron from a 4f state

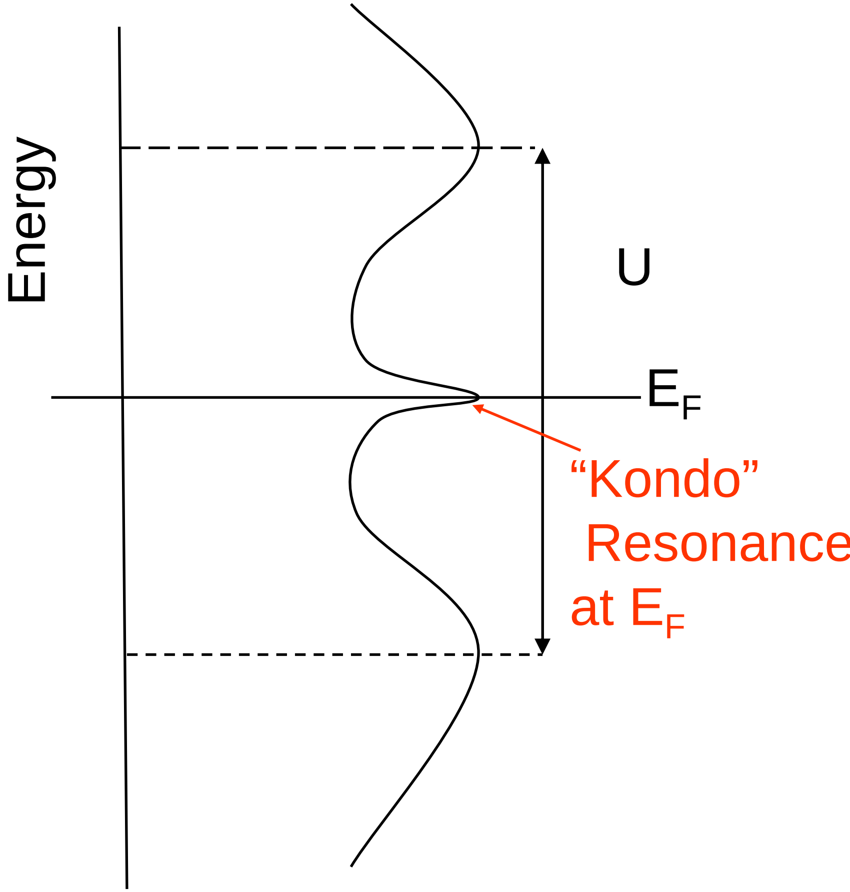
n ⟶ n - 1

Kondo/Anderson Problem

- **Impurity problem – also generalized to lattice**
  - Density of states



Decoupled

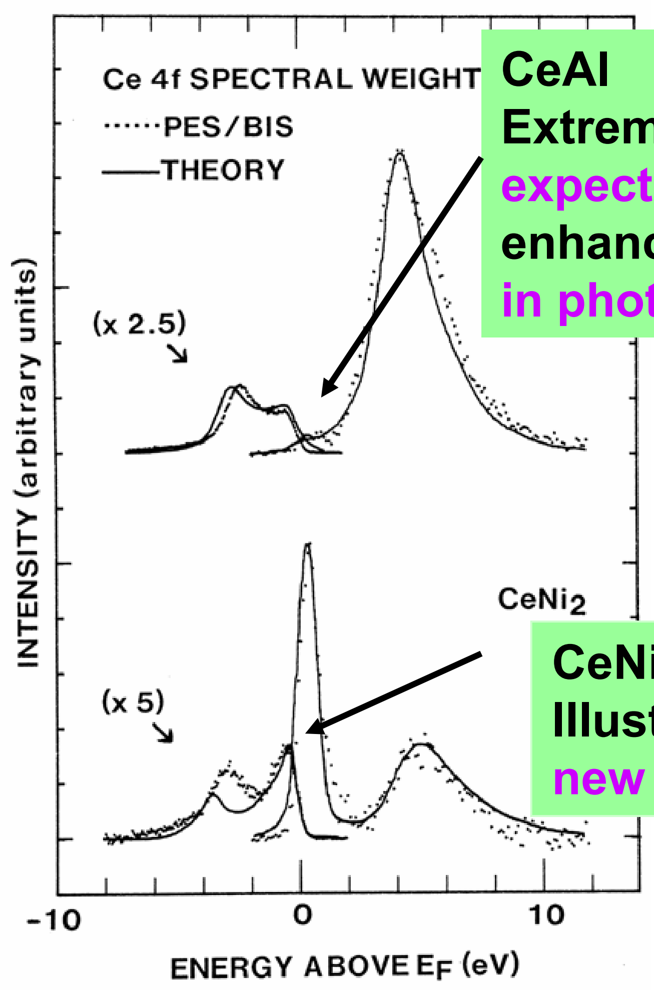


Coupled

Example of Extreme Enhancements - Ce

Ce

J. W. Allen and Coworkers



CeAl (“heavy fermion material”)
Extremely large specific heat (1000 times larger than expected on simple arguments !) shows there is a large enhancement due to correlation – but almost no weight in photoemission at Fermi energy !

The 4f state is degenerate - interaction with the metallic band electrons lifts degeneracy and forms correlated many-body state

CeNi$_2$
Illustrates the “many-body” peak at Fermi energy - new energy scale due to correlation

Kondo Effect in for Ce Impurities
“Kondo Lattice” for Ce compounds

Ce – volume collapse – spin fluctuations

Low volume non-magnetic α-phase of Ce

High volume magnetic γ-phase of Ce

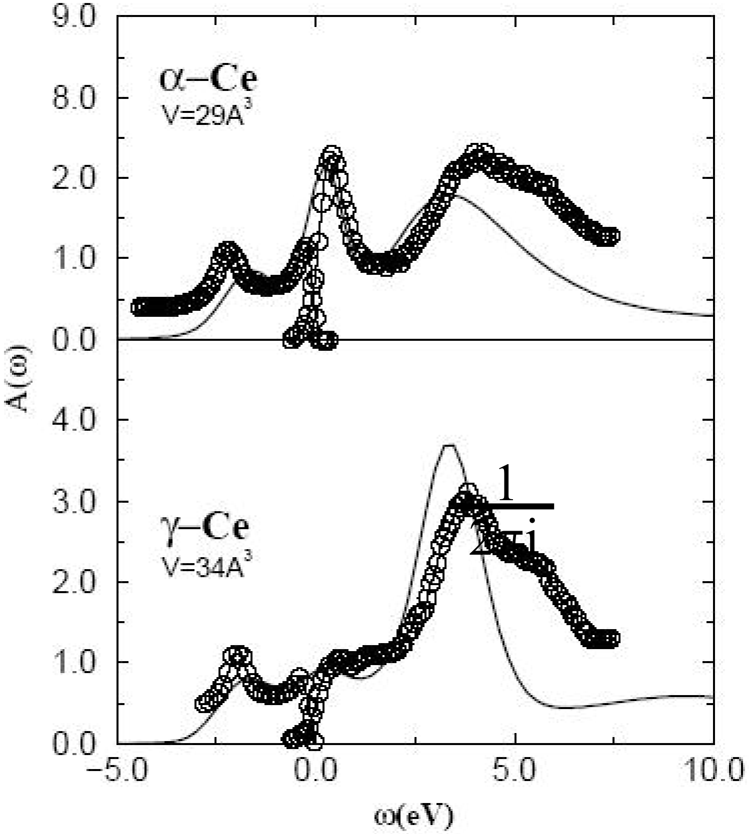
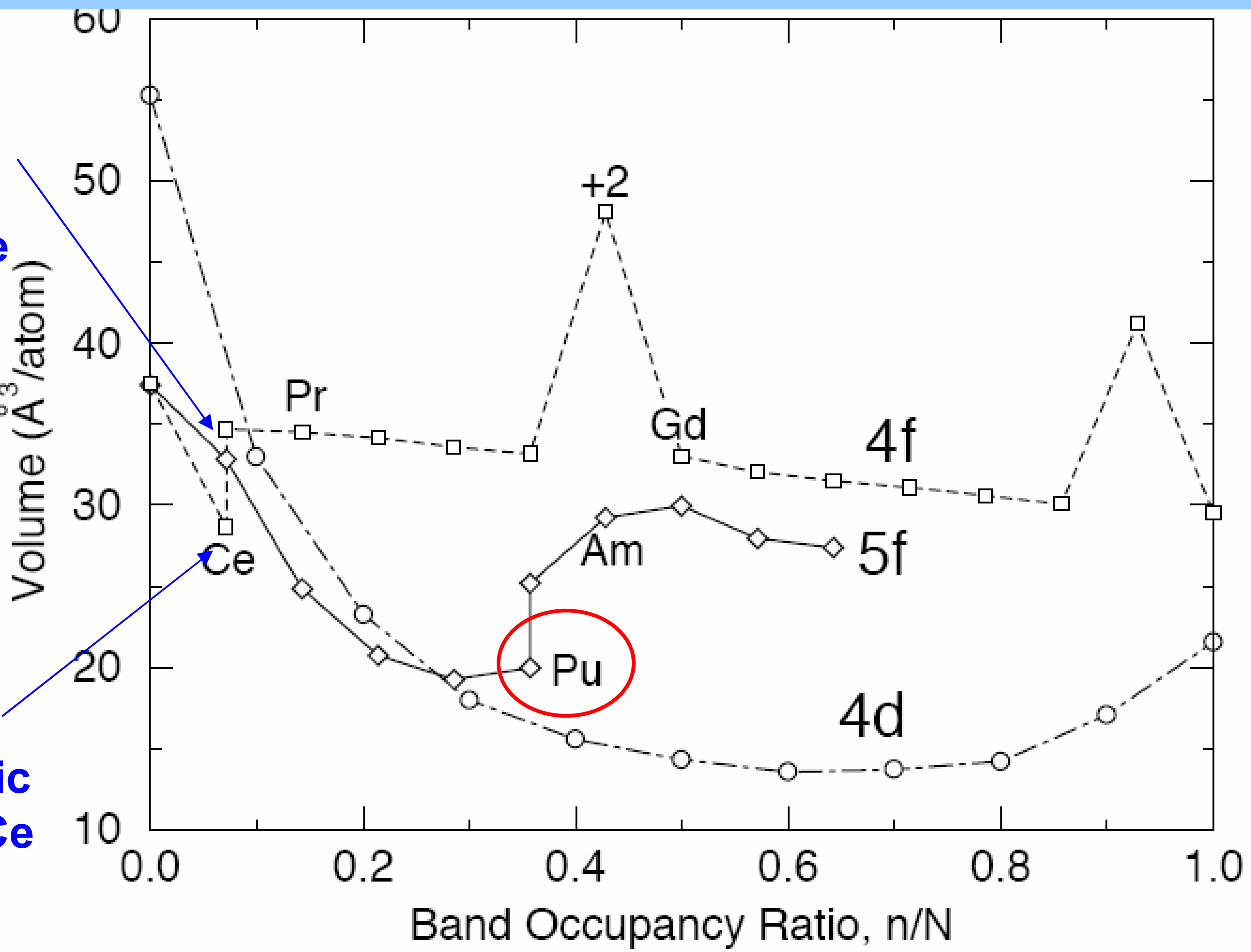


Figure 17: Comparison between combined photoemission[110] and BIS[111] experimental (circles) and theoretical LDA+DMFT(QMC) total spectra (solid line) for α- (upper part) and γ-Ce (lower part) at $T = 580\,\mathrm{K}$. The experimental and theoretical spectra were normalized and the theoretical curve was broadened with resolution width of 0.4 eV [reproduced from Ref. 61].

Photoemission by J. W. Allen, et al.

Held, Scalletar, McMahan

Ce – volume collapse – spin fluctuations



High volume magnetic γ-phase of Ce

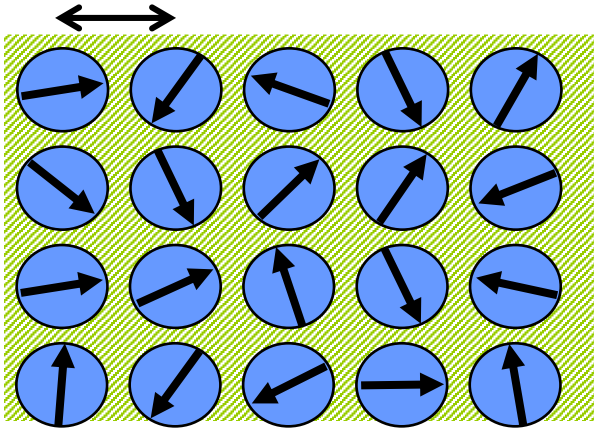
Low volume non-magnetic α-phase of Ce

15% volume change – same fcc structure –
Non-magnetic α phase to magnetic γ phase

From A. K. McMahan

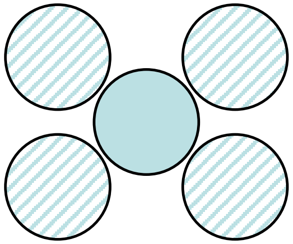
Hubbard Model

- **Lattice of sites**
  - Localized state on every site
  - Two electrons interact on same site
  - Partially filled band
  - Metal if interactions vanish
  - Expected to be an insulator (Mott insulator)) if interactions are very strong



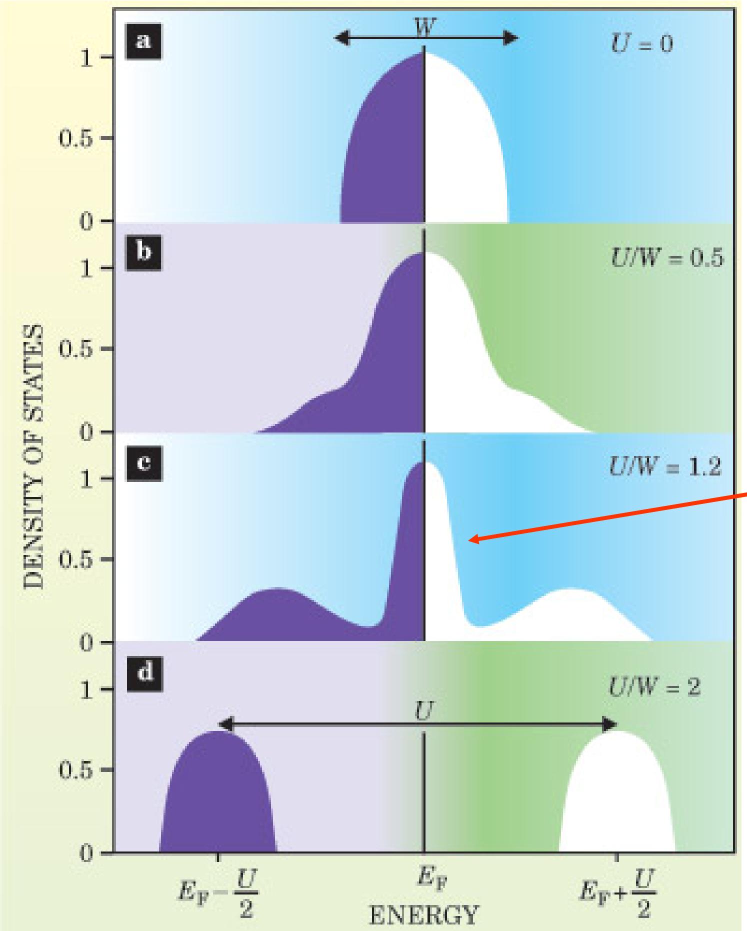
- **What happens in intermediate case?**
  - Phase transition?
    Order?
    . . .

Dynamical Mean Field Theory - DMFT – Map problem onto Self-consistent Anderson Impurity Model



- Spectrum of Green’s function on central site $G(E) = [\, E - H_0 - \Sigma(E) \pm i\delta]^{-1}$ consistent with neighbors

- Solve impurity problem using various many-body methods



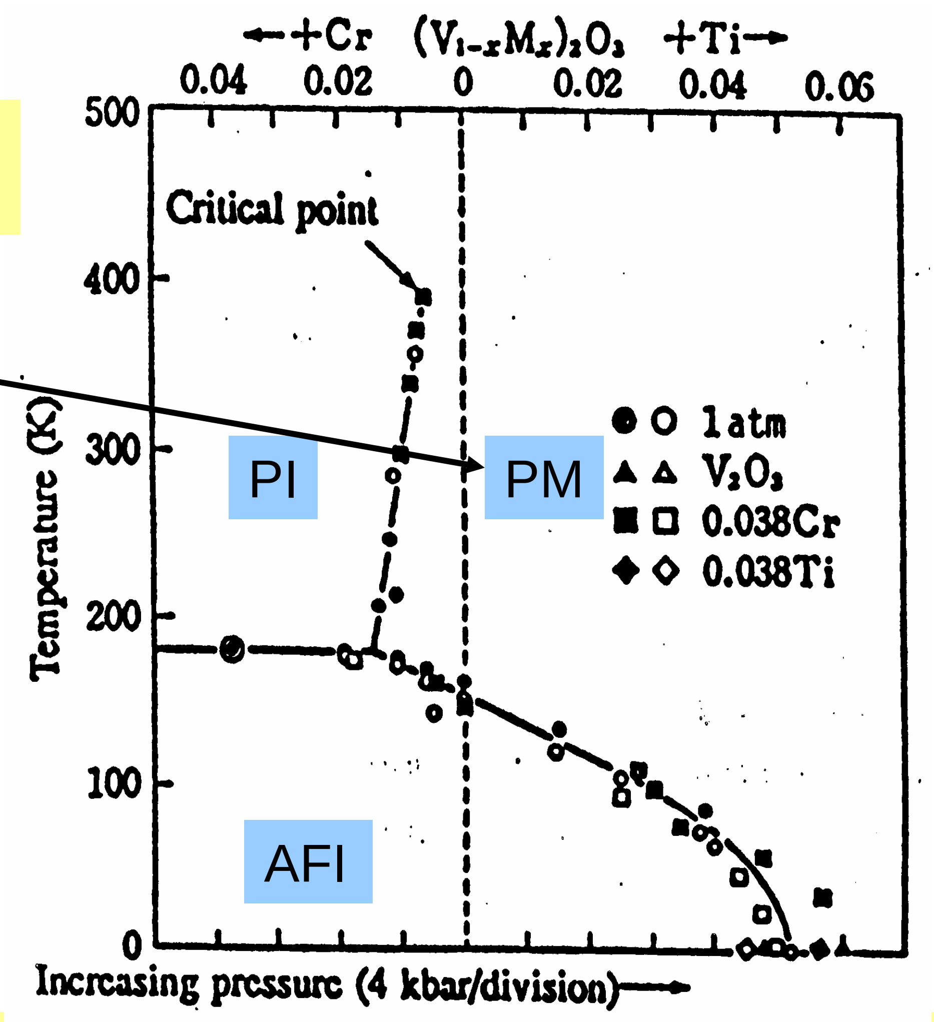
New many-body energy scale

Kotliar and Vollardt, Physics Today 2004

Paradigm example: $(V_{1-x}M_x)_2O_3$ (M=Cr, Ti)

McWhan, Rice et al.
PRL ’69, PRB ‘73

PI ⇔ PM
interpreted
as Mott transition of
1-band
Hubbard model



$2e^-$/ V^{3+} ion
3 orbitals/ion
4 ions/cell

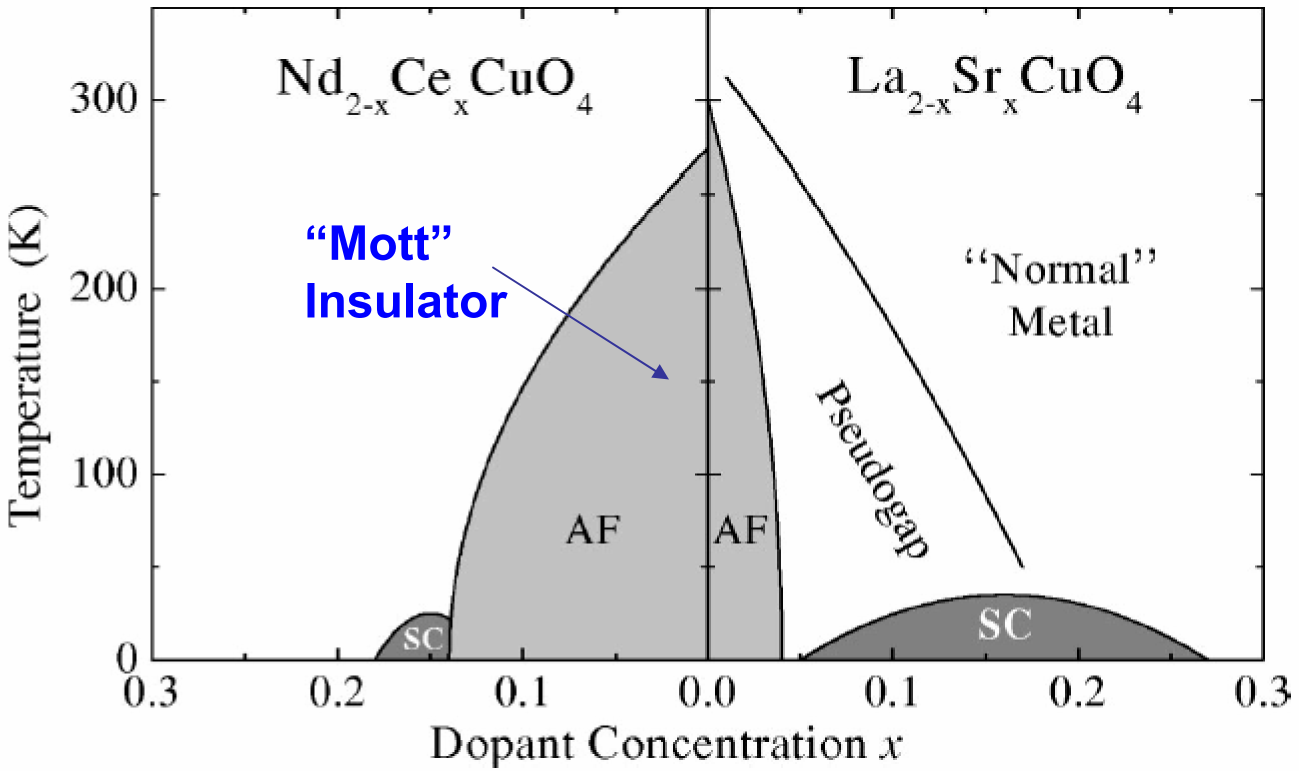
more
complex
than
1-band
Hubbard

Importance of realism: Ezhov et al, PRL ’99, Park et al, PRB ’00

⇒ Motivation for LDA + DMFT calculations (Held et al, PRL ’01)

From J. Allen

Phase Diagram – Hi-Tc materials



"Mott" Insulator

FIG. 1. Phase diagram of n- and p-type superconductors, showing superconductivity (SC), antiferromagnetic (AF), pseudogap, and normal-metal regions.

Damascelli RMP 75, 473

Fermi Surfacem – measured by ARPES

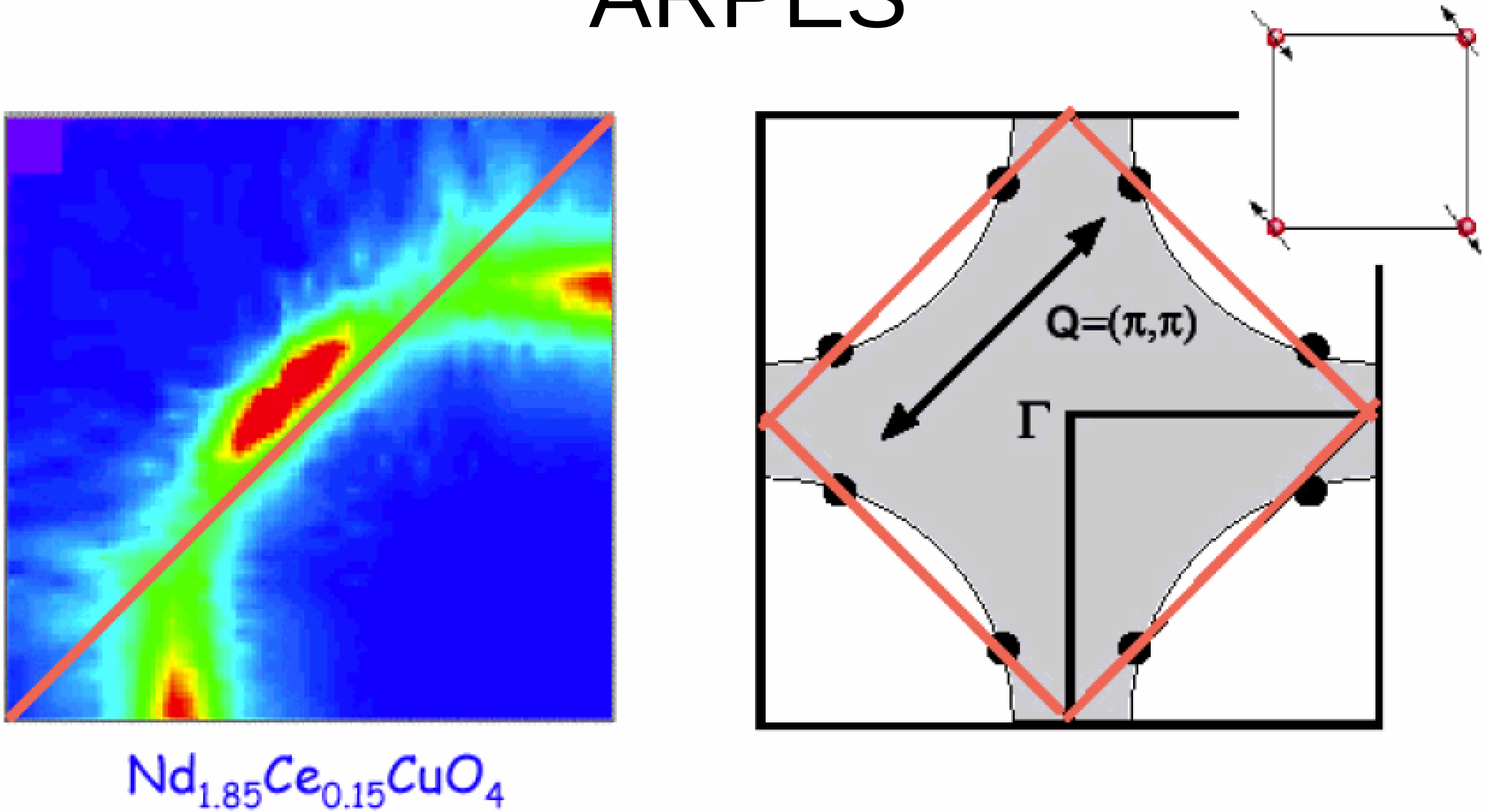
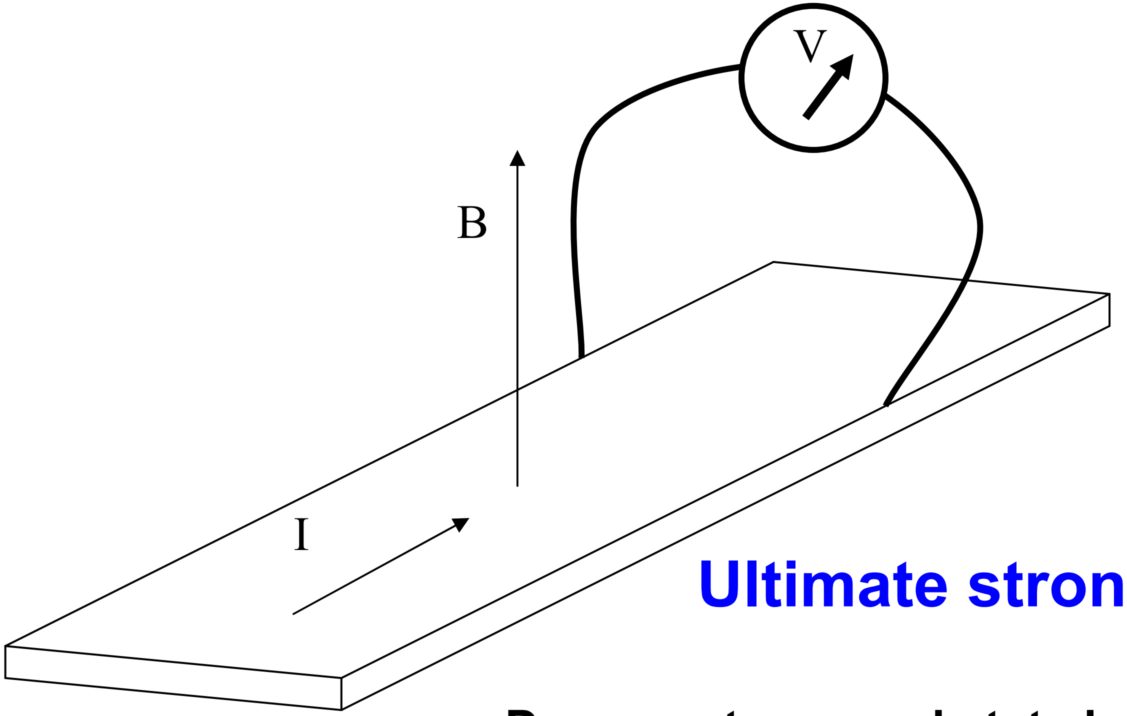


Fig. 13, pdf version of Z. X. Shen review, Angle-Resolved Photoemission Spectroscopy Studies of Curpate Superconductors, http://arxiv.org/ftp/cond-mat/papers/0305/0305576.pdf
Similar to RMP, Fig. 44 - Shows “hot spots” due to AF correlations

Quantum Hall Effect



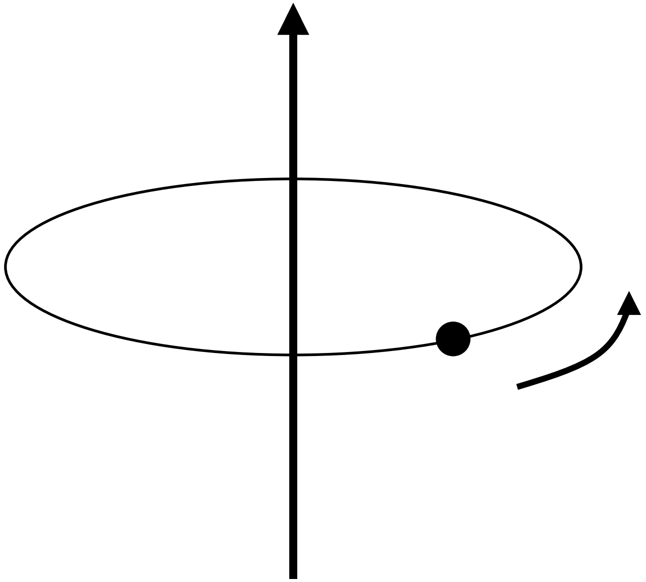
Ultimate strong interactions!

Degenerate ground state in the absence of interactions
No dispersion – no kinetic energy

Interactions qualitatively change the nature of the ground state for fractional filling of the Landau levels – breaks degeneracy – opens a gap

Fractional statistics, . . .

Geometric Phases in Quantum Mechanics

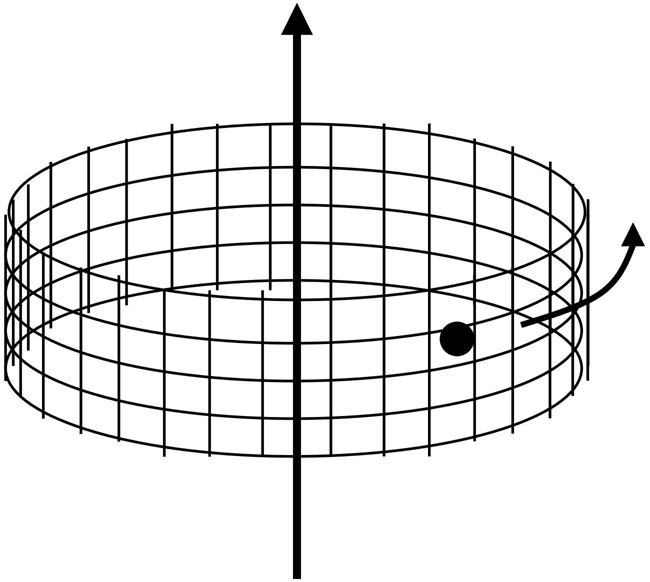


- Example – Aharonov-Bohm Effect:
- Transport a charge around the magnetic flux

$$H = \tfrac{1}{2}(p)^2 \Rightarrow \tfrac{1}{2}(p - (e/c)A)^2$$

- Berry Phase $= \gamma = (q/\hbar)\int A \cdot dr = q\Phi/(\hbar c)$ (modulo 2π)

Geometric Phases in Quantum Mechanics



- Torus boundary conditions on crystal
- Transport a charge around the supercell

$$H_{\mathbf{k}} = \tfrac{1}{2}(p + k)^2 \Rightarrow \tfrac{1}{2}(p + k - (e/c)A)^2 = \tfrac{1}{2}(p + k + \Delta k)^2$$

- Shift in k equivalent to gauge field
- Used by Kohn (1964) to distinguish insulators, metals, . . .

Unification of famous concepts in physics

- Significance of Electromagnetic Potentials in the Quantum Theory,
  Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959)
- Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions,
  J. M. Luttinger, Phys. Rev. 119, 1153 (1960).
- Two soluble models of an antiferromagnetic chain,
  E. H. Lieb, T. Schultz, and D. J. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961).
- Theory of the Insulating State,
  W. Kohn, Phys. Rev. 133, A171 (1963).
- Quantized Hall conductivity in two dimensions,
  R. B. Laughlin, Phys. Rev. 23, 5632 (1981).
- Theory of polarization of crystalline solids,
  R. D. King–Smith and D. Vanderbilt, Phys. Rev. B 47, 1651-1654 (1993).
- Electron Localization in the Insulating State,
  R. Resta and S. Sorella, Phys. Rev. Lett. 82, 373 (1999).
- Quantum Mechanical Position Operator and Localization in Extended System,
  A. Aligia and G. Ortiz, Phys. Rev. Lett. 82, 2560 (1999).

- Flux quanta, Fractional Statistics, degenerate ground states, Z phases, . . .

Questions
and partial answers – topics of current research

What is the Kondo effect? Anderson impurity model?

Well understood now – exact solutions -
new energy scale - model for other problems

What is a Kondo lattice? Anderson lattice model?

NO exact solutions
Do spins contribute to the Fermi surface?

What is the difference between a metal and an insulator?

What aspect(s) of the ground state wavefunction
are different for a metal vs and insulator?

Is a metal-insulator transition a phase transition?

Is there an order parameter?
Is it possible to have a metal insulator transition
without a change of symmetry – Mott transition?
What is a Resonating Valence Bond (RVB) state?

Questions
and partial answers – topics of current research

Is the Fermi surface well-defined in a many-body system?
  What is the evidence?
  The Luttinger theorem on the Fermi Surface –
    Original proof (Green's ftns) – recent topological proof

One dimension
  Bosonization?

What is a topological transition?
  Is it a phase transition?

What is a Berry's phase?
  Relation to metals, insulators, fractional statistics, . . .

Superconductivity and the quantum Hall effect

Evidence for unusual behavior in Hi-Tc materials -
  What is a pseudogap? Evidence?