

ELECTRONIC STRUCTURE OF STRONGLY CORRELATED SYSTEMS

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AND CHEMISTRY

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- RESONANT (SOFT) X RAY SCATTERING

Some Historical Landmarks

- 1929-1931 Bloch Wilson theory of solids
- 1937 De Boer and Verwey (NiO-CoO breakdown of band theory)
- 1937 Peierls 3d electrons avoid each other (basically the Hubbard model)
- 1949 Mott Metal insulator transition
- 1950 Jonker, van Zanten, Zener - Pervoskites double exchange
- 1957 BCS theory of superconductivity
- 1958 Friedel Magnetic impurities in metals
- 1959 Anderson superexchange ($U \gg W$)
- 1962 Anderson model for magnetic impurities in metals
- 1964 Kondo theory of Kondo effect
- 1964 Hubbard model- Hohenberg Kohn DFT- Goodenough Transition metal compounds

Some historical landmarks

- 1965 Goodenough Kanamori Anderson rules for superexchange interactions
- 1968 Lieb and Wu exact solution of 1D Hubbard model
- 1972 Kugel Khomskii theory of orbital ordering and superexchange
- 1985 Van Klitzing quantum Hall effect
- 1985 ZSA classification scheme of transition metal compounds
- 1986 Bednorz and Muller High T_c superconductors
- 1988 Grunberg and Fert giant magneto resistance

Periodic Table of the Elements 2005

1 H 1.01																	18 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 15.99	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 25.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (270)	109 Mt (268)	110 Ds (281)	111 Rg (272)							



58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.97	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Strongly correlated materials

- Often 3d transition metal compounds
- Often Rare earth metals and compounds
- Some 4d and some actinides
- Some organic molecular systems C60, TCNQ salts
- Low density 2D electron gases Quantum and fractional quantum Hall effect
- Magnetic materials and impurities

Wide diversity of properties

Take for example only the transition metal oxides

- Metals: CrO_2 , Fe_3O_4 $T > 120\text{K}$
- Insulators: Cr_2O_3 , SrTiO_3 , CoO
- Semiconductors: Cu_2O
- Semiconductor –metal: VO_2 , V_2O_3 , Ti_4O_7
- Superconductors: $\text{La}(\text{Sr})_2\text{CuO}_4$, LiTiO_4 , LaFeAsO
- Piezo and Ferroelectric: BaTiO_3
- Multiferroics
- Catalysts: Fe, Co, Ni Oxides
- Ferro and Ferri magnets: CrO_2 , $\gamma\text{Fe}_2\text{O}_3$
- Antiferromagnets: $\alpha\text{Fe}_2\text{O}_3$, MnO , NiO ---

**Properties depend on composition and structure
in great detail**

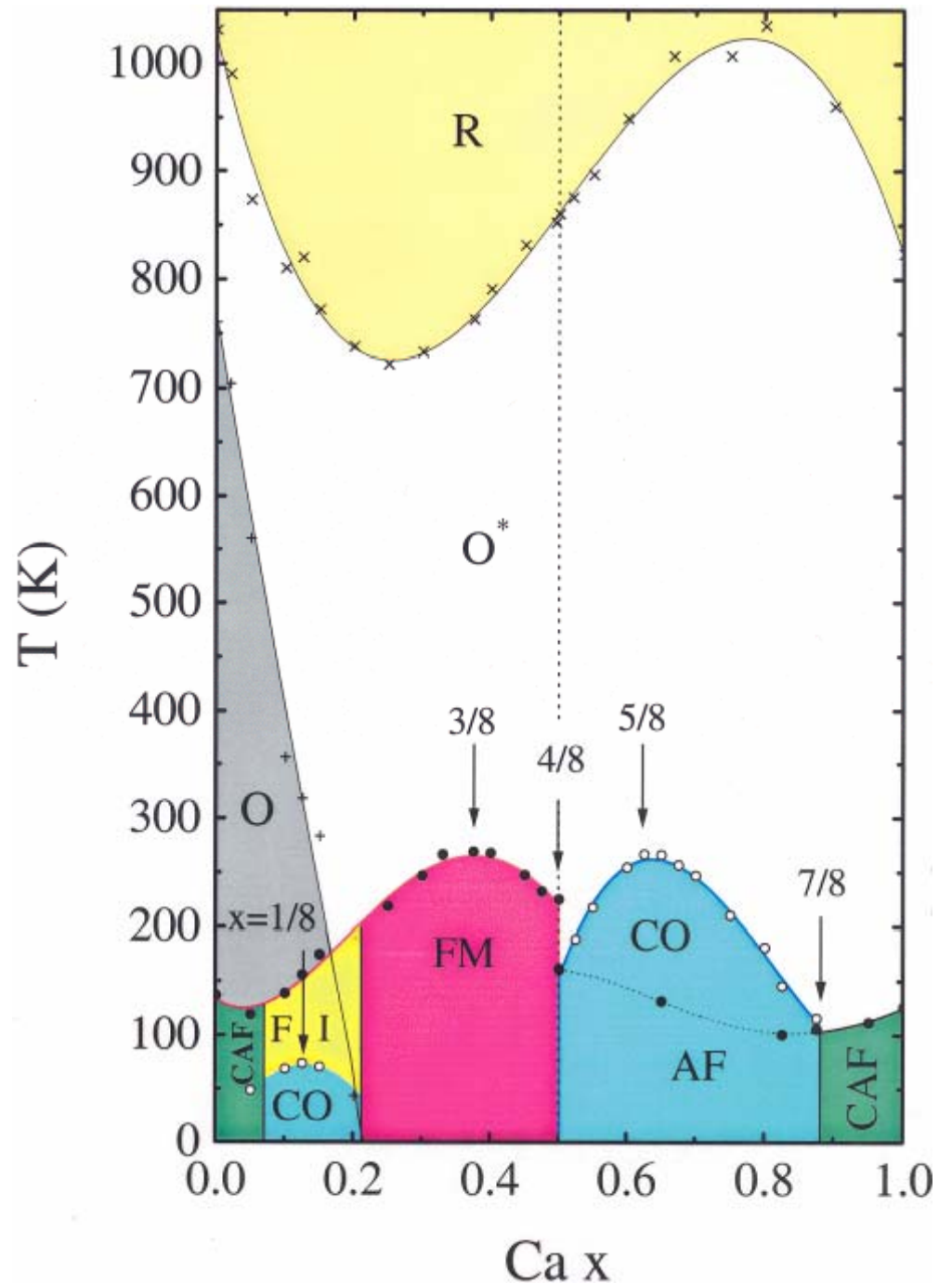
Phase Diagram of $La_{1-x}Ca_xMnO_3$

Uehara, Kim and Cheong

R: Rhombohedral

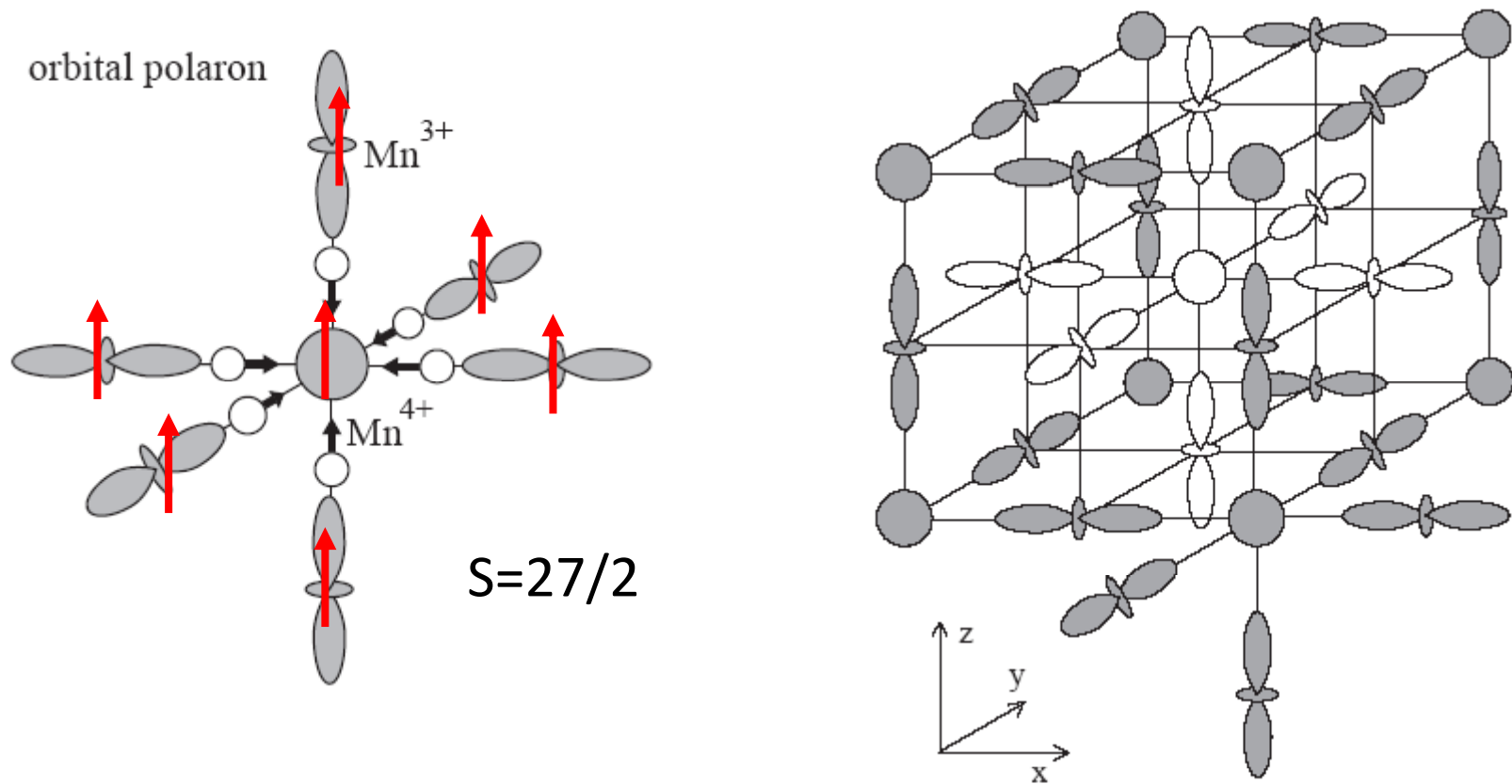
O: Orthorhombic
(Jahn-Teller distorted)

O*: Orthorhombic
(Octahedron rotated)



Model for Charge, Spin and Orbital Correlations in Manganites

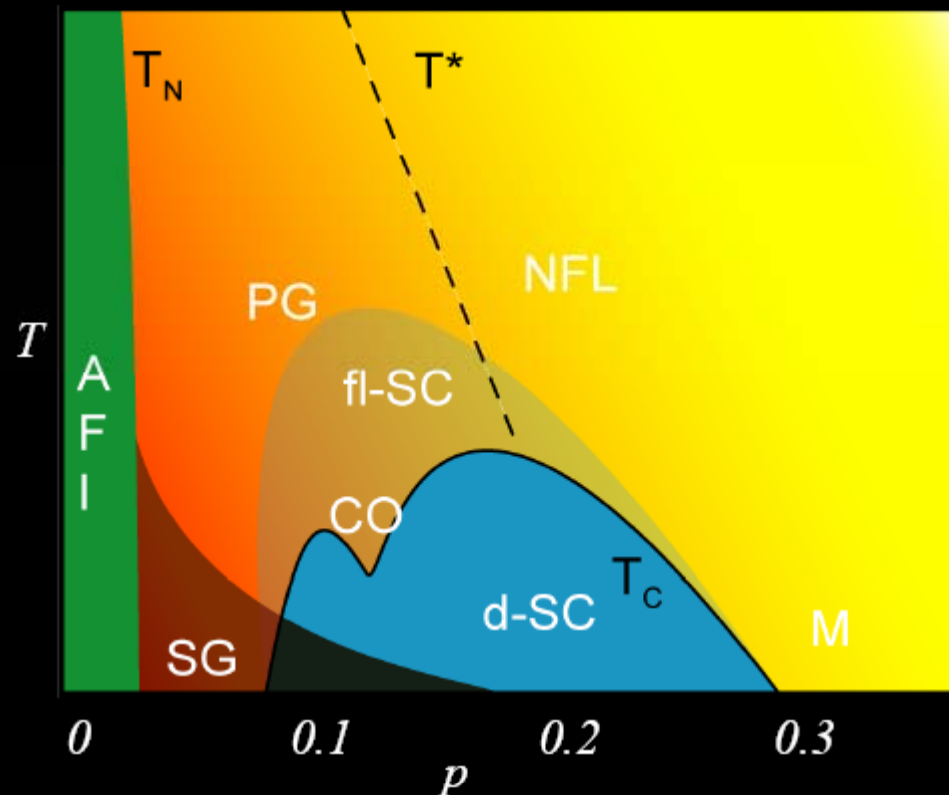
Mn⁴⁺, d³, S=3/2, No quadrupole; Mn³⁺, S=2, orbital degeneracy



Mizokawa et al (2001)

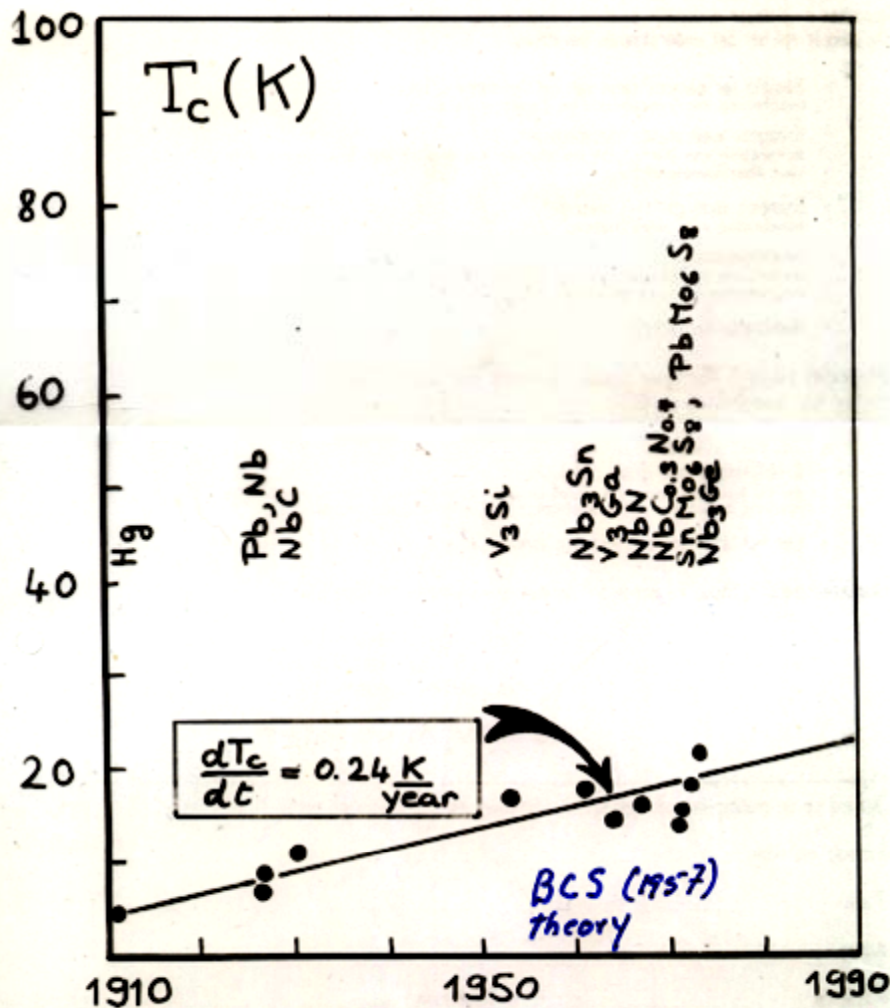
High T_c superconductor like $\text{La}_{2-p}\text{Sr}_p\text{CuO}_4$ phase diagram

Schematic phase diagram of hole-doped cuprates



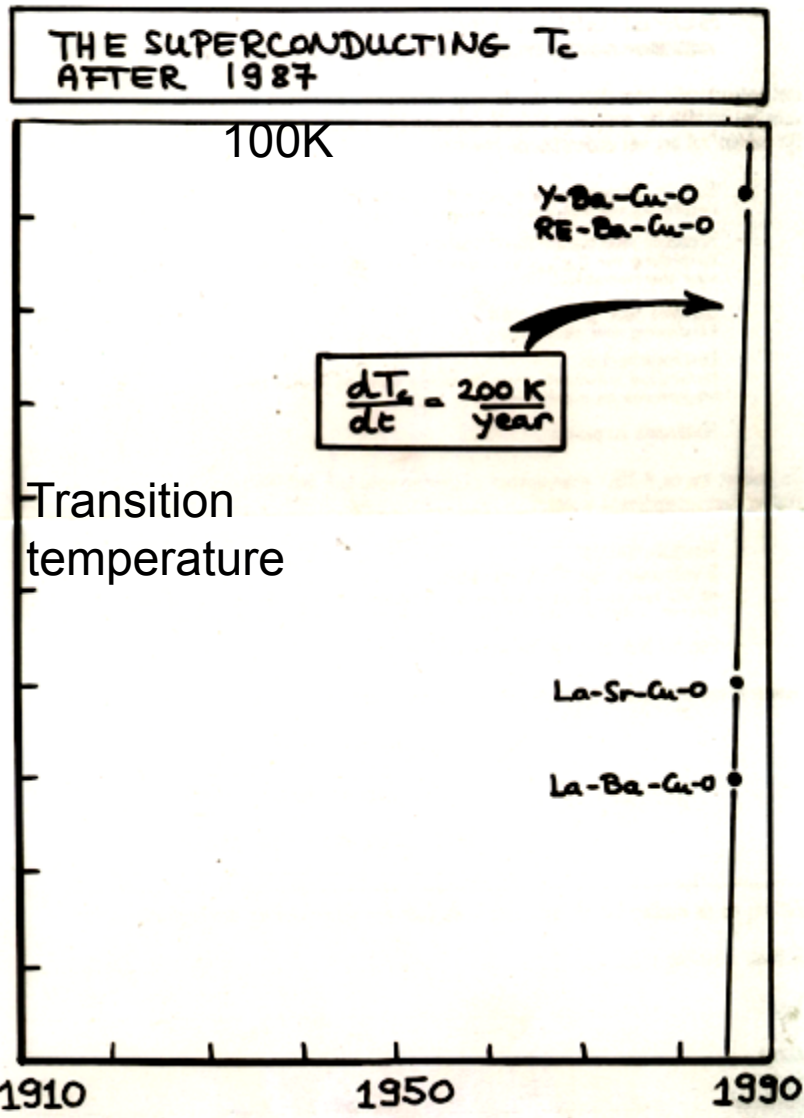
The many-body quantum state underpinning these phenomena (equivalent of Fermi Liquid for BCS) has not been identified.

THE SUPERCONDUCTING T_c
BEFORE 1986



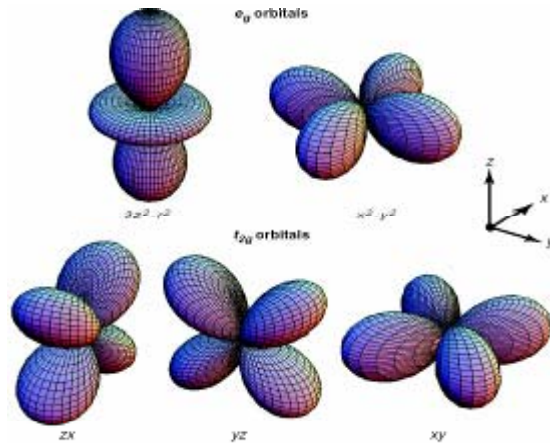
Thought to be BCS
electron phonon driven
 T_c Max ~ 35 K

Theory in 1957 -1961 led us
To believe to avoid magnetism
avoid oxides, start with
reasonable conductors

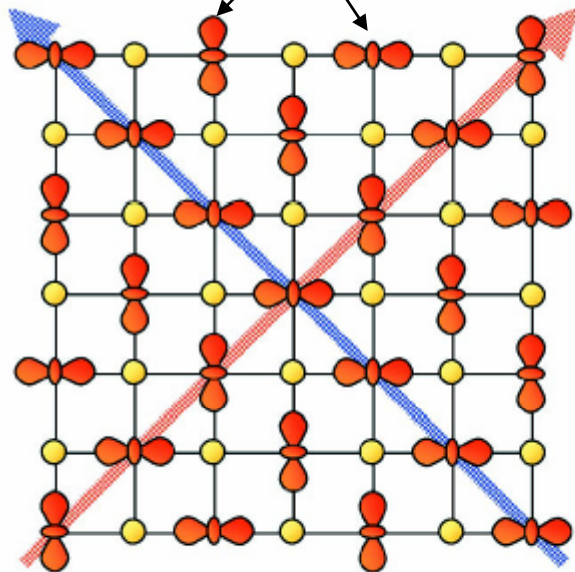


Contrary to conventional wisdom Bednorz and Muller in 1986 discovered much higher T_c 's in MAGNETIC OXIDES OF Cu.

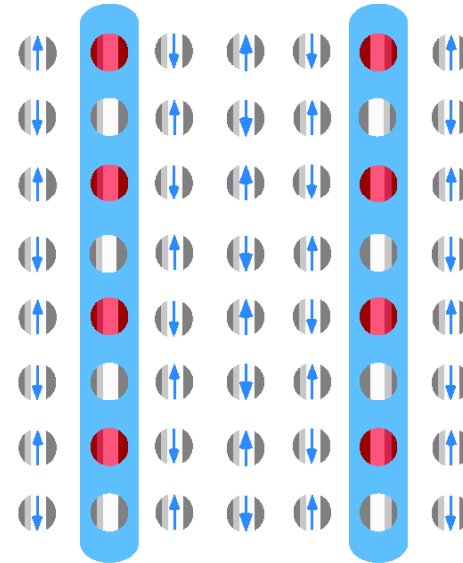
Ordering in strongly correlated systems



Quadrupole moment ordering



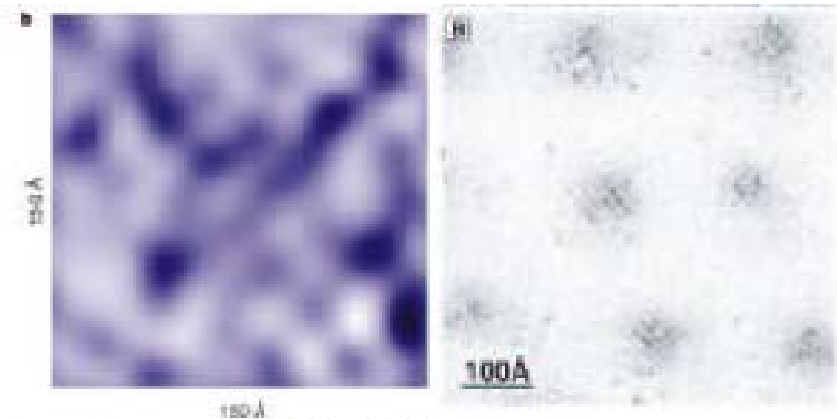
Stripes in Nd-LSCO



rivers of
Charge—
Antiferro/
Antiphase

$$\Delta Q < 0.5 e$$

Charge inhomogeneity in Bi2212



Pan, *Nature*, 413, 282 (2001);
Hoffman, *Science*, 295, 466 (2002)

$$\Delta Q \sim 0.1 e$$

Two extremes for atomic valence states in solids

extreme
Two Types of Valence states

Large overlap $R \sim d$ - Large dispersion $E(k)$
 $\psi_k \sim \frac{1}{\sqrt{N}} e^{ik \cdot r}$ (free electr.) \rightarrow s, p valence.

Little overlap - $R \ll d$ - Little dispersion
 $\psi_k \sim \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot R_i} \psi_0(r - R_i)$
 (tight binding) \Rightarrow Correlated.
 Atomic like \rightarrow 3d, 4f states

Coexistence-----Hybridization

Kondo, Mixed valent, Valence fluctuation, local moments, Semicond.-metal transitions, Heavy Fermions, High Tc's, Colossal magneto resistance, Spin trionics, orbitronics

Characteristics of solids with 2 extreme valence orbitals

$R \gg D$

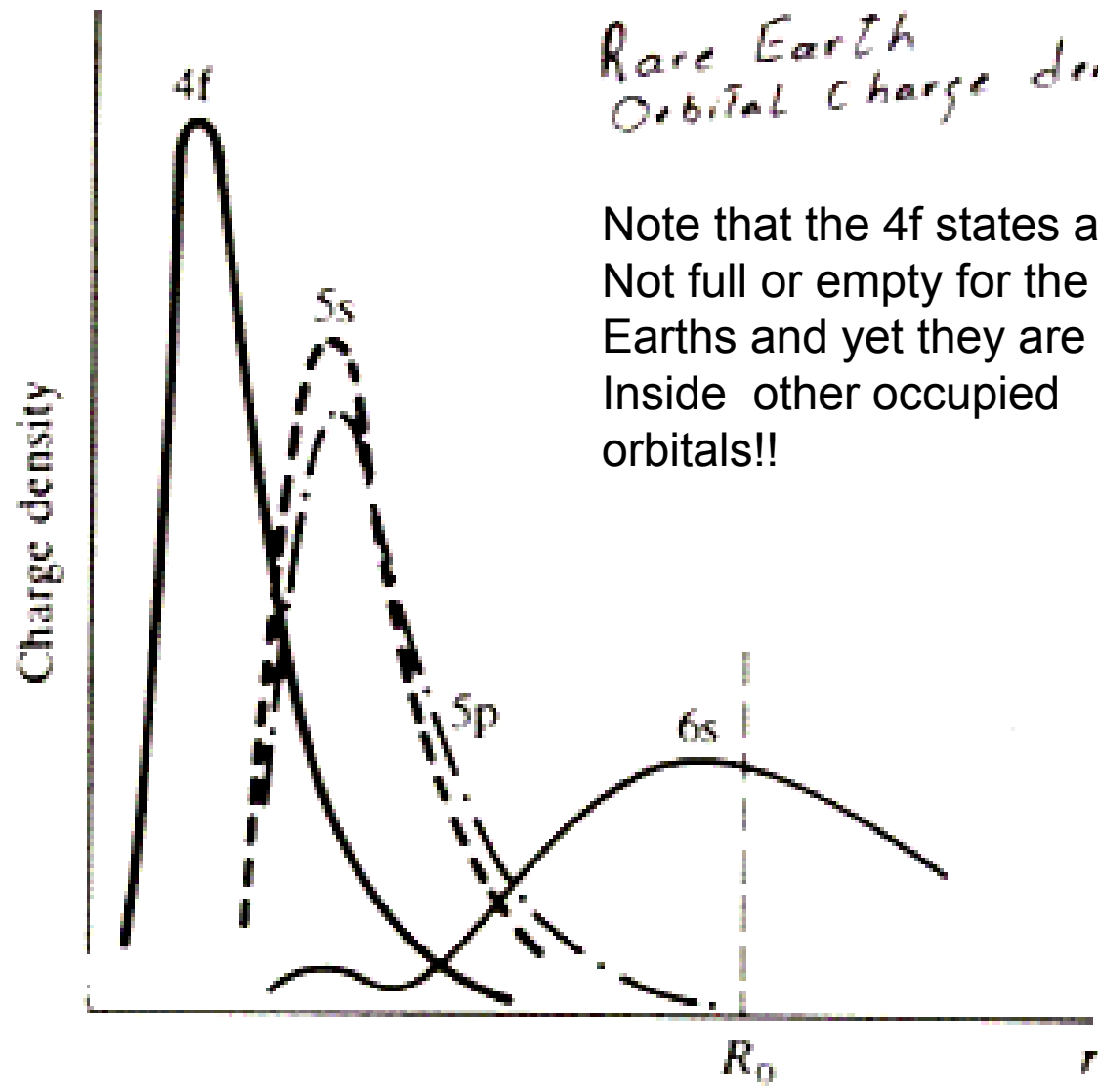
- electrons lose atomic identity
- Form broad bands
- Small electron electron interactions
- Low energy scale –charge fluctuations
- Non or weakly magnetic
- Examples Al, Mg, Zn, Si

$R \ll D$

- Valence Electrons remain atomic
- Narrow bands
- Large electron electron interactions (on site)
- Low energy scale-spin fluctuations
- Magnetic (Hunds' rule)
- Gd, CuO, SmCo₃

Many solids have coexisting $R \gg D$ and $R \ll D$ valence orbitals i.e. rare earth 4f and 5d, CuO Cu 3d and O 2p, Heavy Fermions, Kondo, High T_{c,s}, met-insul. transitions

Special place for transition metal and rare earths



Atoms in a periodic array in solids

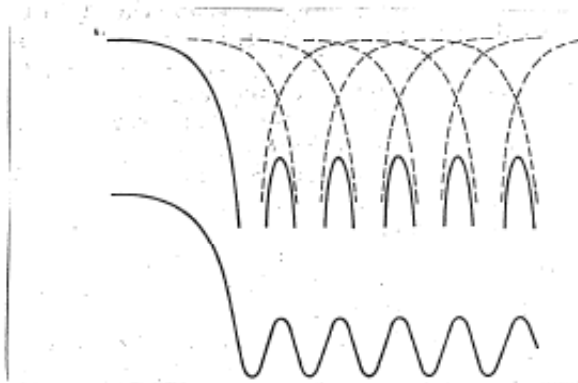
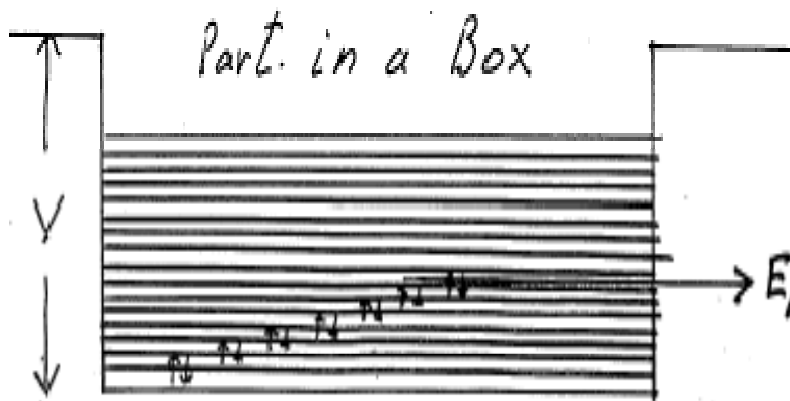


Fig. 5-1. The electrostatic potential through a line of atoms in a crystal and parallel to such a line.



We are interested in the potential Produced by the nuclei and the inner electrons on the outermost “Valence” electrons

$$\phi_k(r) = \frac{1}{\sqrt{\Omega}} e^{ik \cdot r}$$

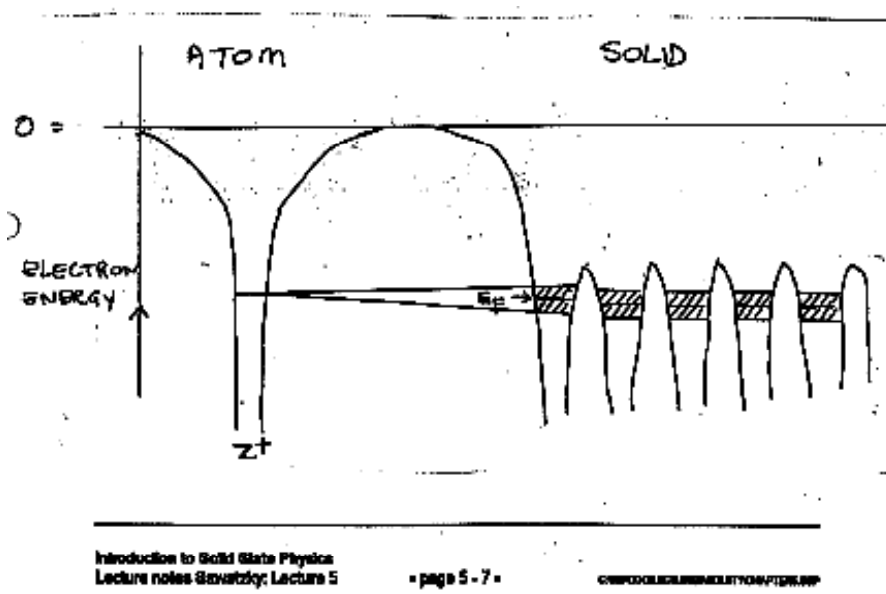
$$E_k = \frac{\hbar^2 |k|^2}{2m}$$

$K=2\pi/\text{wave length}$

E_f is the Fermi level up to which Each k state is filled with 2 electrons

ALSO BORING ONLY METALS !!

More atomic like states for atoms in solids with large inter-atomic spacing compared to orbital radius



Electrons can quantum mechanically Tunnel from atom to atom forming again Waves and bands but now the Bands are finite in width. If such a band is full (2 electrons per atom for S orbitals the material will be an insulator Because of a forbidden gap to the next band of states INSULATOR OR SEMICONDUCTOR

**Still rather boring since we have no magnetism systems
With and odd number of electrons per atom would all
be metallic**

Surely a lattice of H atoms separated
by say 1 cm would not behave like a
metal

What have we forgotten ?

The electron electron repulsive
interaction

Why are 3d and 4f orbitals special

- Lowest principle q.n. for that l value
- Large centrifugal barrier $l=2,3$
- Small radial extent, no radial nodes
orthogonal to all other core orbitals via
angular nodes
- High kinetic energy (angular nodes)
- Relativistic effects
- Look like core orb. But have high energy and
form open shells like valence orb.

A bit more about 3d & 4f

Atomic - hydrogenic $E_n^0 = \frac{mZ^2e^4}{2\hbar^2 n^2}$
 n = principle q. n

l comes in relativistic effects

$$E = \sqrt{p^2c^2 + m^2c^4} \approx mc^2 + \frac{p^2}{2m} - \frac{1}{8} \frac{(p^2)^2}{m^3c^2}$$

$\underbrace{\hspace{10em}}_{\text{mass velocity}}$

$$\Delta E = -\frac{1}{2ma^2} \left((E_n^0)^2 + 2E_n^0 Z e^2 \left\langle \frac{1}{r} \right\rangle + Z^2 e^4 \left\langle \frac{1}{r^2} \right\rangle \right)$$

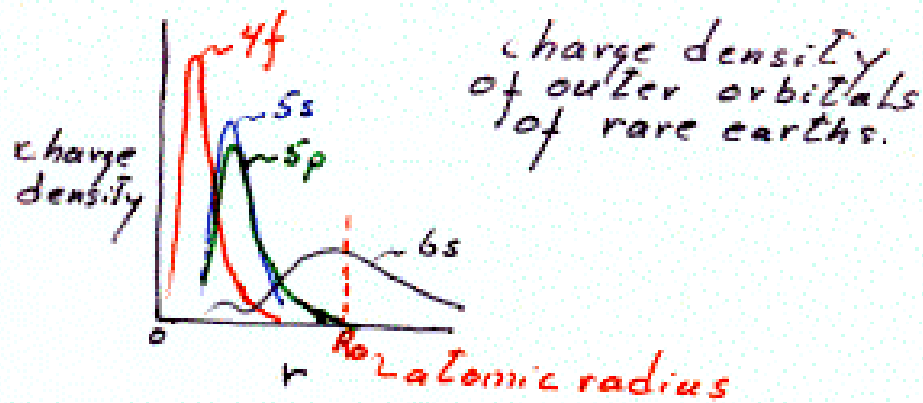
$$\left\langle \frac{1}{r} \right\rangle \text{ independent of } l = \frac{Z}{a_0 n^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{nl} = \frac{Z^2}{a_0^2 n^3 (l+1/2)} \quad a_0 = \text{Bohr radius}$$

$$\Delta E_{rel} = \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{l+1/2} - \frac{3}{4} \right) E_n^0 \left[\left(\alpha^2 \frac{e^2}{\hbar c} \right) \right]$$

For 3d (Cu) 3s energy ~ 120 eV
3p " ~ 70 eV
3d " ~ 10 eV

E_{rel} can be larger than E_{msl}
if we include larger Coulomb repulsion



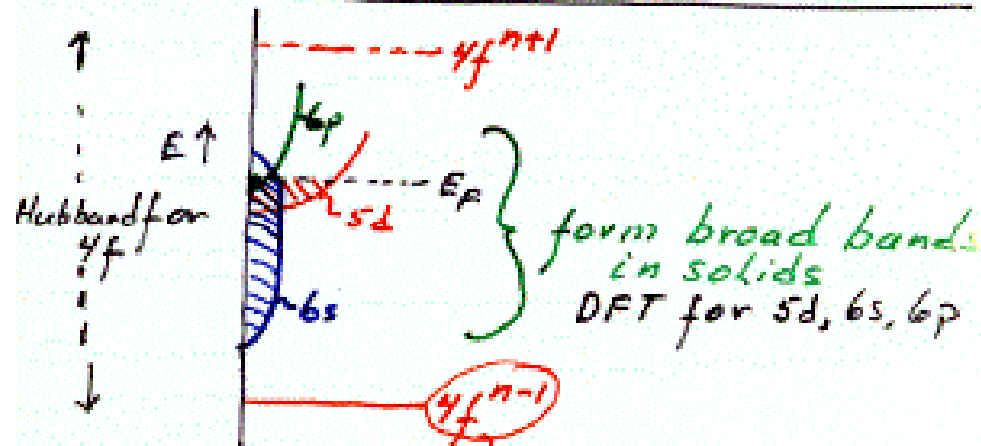
Elemental configuration



< 14 (open) but atomic

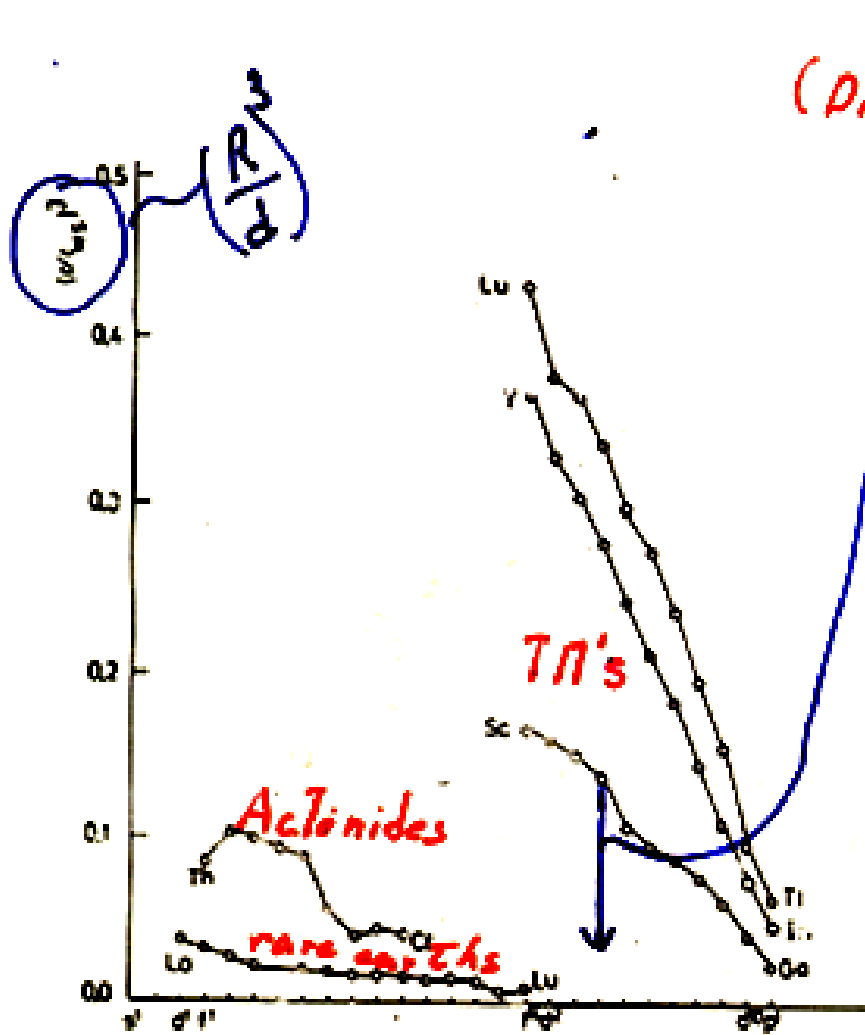
We will see later how to model this

Hubbard
For 4f



not full and not empty but well below E_F

Plot of the orbital volume /Wigner sites volume of the elemental solid for rare Earth 4f's, actinide 5f's, transition metal 3d's,4d'sand 5d's



In compounds the ratio will be strongly reduced because the Element is "diluted" by other components

Van der Marel et al PRB

Band Structure approach vs atomic

Band structure

- Delocalized Bloch states
- Fill up states with electrons starting from the lowest energy
- No correlation in the wave function describing the system of many electrons
- Atomic physics is there only on a mean field like level
- Single Slater determinant states

Atomic

- Local atomic coulomb and exchange integrals are central
- Hunds rules for the Ground state -Maximize total spin-
Maximize total angular momentum-total angular momentum $J = L - S$ for $< 1/2$ filled shell , $J = L + S$ for $> 1/2$ filled shell
- Mostly magnetic ground states

Magnetism

(11)

No long range order

Band theory

Atomic

each k state empty
or doubly occupied $T=0$

Hunds rule
results in a
local moment

$$\chi(T) = \text{Const}$$

$$\vec{M} = \mu_B^2 D(\epsilon_F) \vec{B}$$

$\mu_B =$ Bohr magneton

$$\chi(T) = \frac{C}{T}$$

$$M = \frac{C B}{T}$$

still a problem is

$$C = \frac{N S(S+1) g^2 \mu_B^2}{3 k_B}$$

$\chi(T)$ for $T > T_c$ 3d TIT compounds.

Hunds rules

1) Maximize S

2) Maximize L

3) $J = L - S$ $< 1/2$ filled
 $= L + S$ $> 1/2$ filled

Atomic theory leads to magnetism

$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ ($\text{Cu}^{2+} 3d^9$ $S=1/2$ high spin)

GdCl₃ ($4f^7$ $S=7/2$)

Simplest approach to electronic structure –band theory

-free electron –constant potential- no atoms-

$$\Psi_k = \frac{1}{\sqrt{N}} \exp^{ik \cdot r}$$

- tight binding - full atomic potential

$$\Psi_k = \frac{1}{\sqrt{N}} \sum_i \exp^{ik \cdot R_i} (\Theta(r - R_i))$$

Hohenberg Kohn theorem

Each local external one particle potential corresponds to exactly one ground state density

$$n_{GS}^{(r)} \Rightarrow \hat{V}_{ext} \Rightarrow \hat{H} \Rightarrow |\Psi_{GS}(n_{GS})\rangle \Rightarrow O(n_{GS})$$
$$\langle \bar{\Psi}(n_{GS}) | \hat{O} | \Psi(n_{GS}) \rangle$$

Ground state expectation values (such as E) depend uniquely on $n_{GS}^{(r)}$

See www.physics.ohio-state.edu/~aullbur/bdf22.html

Ab initio Approach Density Functional theory

- Local Density Approximation

NATO ASI Series E. K. U. Gross @ R. M. Dreier
editors D. F. Theory Springer

Series B: Physics Vol. 337 (1995)

page 1 → Paper by W. Kohn

Phys. Rev. 136B, 864 (1964)

190A, 1133 (1964)

Jones and Gunnarsson
Rev. Mod. Phys. 61, 689 (1989)

We can get the exact ground state
energy and electron density by
following →

$$\left(\frac{-\hbar^2 \nabla^2}{2m} + v_{\text{eff}}(r) \right) \psi_j(r) = \epsilon_j \psi_j(r)$$

$$n(r) = \sum_{j=1}^N |\psi_j(r)|^2$$

$$v_{\text{eff}}(r) = \cancel{v(r)} + \int \frac{n(r')}{|r-r'|} dr' + v_{\text{xc}}(r)$$

↪ nonlocal pot.

$$v_{\text{xc}}(r) = \frac{\delta E_{\text{xc}}(n(r))}{\delta n(r)}$$

$$E_0 = \sum_i^N \epsilon_i - \int dr^3 n(r) \left[\frac{1}{2} V_H + v_{\text{xc}} \right] + E_{\text{xc}}(n)$$

Band theory - DF

$$\Psi = \frac{1}{\sqrt{n!}} |\phi_{k_1} \dots \phi_{k_n}| \quad (\text{Slater det.})$$

ϕ_{k_i} are one electron Bloch states

No correlation in Ψ but in \mathcal{H}_{eff}

$$\left[-\frac{1}{2} \nabla^2 + W(r) + V_H(r) + V_{KC}(r) \right] \phi_i(r) = \epsilon_i \phi_i(r)$$

2 one particle problems

$$V_H = \int d^3r' V(r-r') \rho(r')$$

$$V_{KC} = f(\rho(r)) \quad \rho(r) = \sum_{i=1}^n |\phi_i(r)|^2$$

$$\mathcal{L} \rightarrow \frac{dE_{KC}(\rho)}{d\rho}$$

exchange-correlation potential

Hohenberg Kohn

exact for $E_g \rightarrow \rho$ (ground state)

ϕ_i & ϵ_i have no physical meaning!!
math. functions to get E & ρ .

Single Slater det. Of
One electron Bloch
States. No correlation
In the wave function

Recall that the ground
State has few properties
It is the excited states that
Determine the response to
External perturbations such
as fields.

Ψ^{DF} also has no physical significance

E_g is exact $\phi_g(r)$ is exact but

$$\mathcal{H}_{\text{exact}} \Psi^{DF} \neq E_g \Psi^{DF}$$
$$\mathcal{H}_{\text{exact}} = \sum_{i=1}^n \left[-\frac{1}{2} \nabla_i^2 + W(r_i) + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \right]$$

→ nuclear + core electrons

in $\bar{\Psi}_g$ ϕ_i have k as good g.n.
($\mathcal{H}_{\text{eff}}^{DF}$ has transl. symm.)

$$\mathcal{H}_{\text{eff}}^{DF} \bar{\Psi}_g = E_g \bar{\Psi}_g$$

the terms $\frac{e^2}{|r_i - r_j|}$ will always have
matrix elements scattering

$k_L, k_L' \rightarrow k_L'', k_L'''$ i.e. from below to above k_L

e.g. $\phi_k = \frac{1}{\sqrt{N}} \sum_i \phi(r - R_i) e^{ik \cdot R_i}$ [tight binding]

For ~~$R \ll d$~~ $R \ll d < \left| \frac{e^2}{|r_i - r_j|} \right|$ will

dominate for two electrons on one
site. $\langle \star | 1 \rangle = U$

$$\langle \bar{\Psi} | \mathcal{H}_{int} | \bar{\Psi}'_{\substack{k_1 \rightarrow k_1' \\ k_2 \rightarrow k_2'}} \rangle = \frac{1}{N} U \delta(k_1 + k_2 - k_1' - k_2')$$

$\rightarrow 0$ for $N \rightarrow \infty$

Small if $U \ll W$ or E_F so only few electrons are involved

For $U \gg W$ must sum over all other electrons $\rightarrow \frac{n}{N} U$ or for $n \sim N \rightarrow U$

\therefore off diagonal matrix elements are large $\bar{\Psi}^{OF}$ is not an eig. fund.

For $R \ll d$ $1/2$ filled s band if we neglect W (Transl. symm.)

$$\bar{\Psi}_A = \frac{1}{\sqrt{n!}} | \phi_1 \phi_2 \dots \phi_n |$$

one electr./atom

also has the correct symmetry

off diag. matrix elements involve W

So for $U \gg W$ $\bar{\Psi}_A$ is a better starting point. (Note $E_A = E_{OF}$ $E_A = E_{OF}$ if $V_{kc} \approx -U$)

the one electron wave fcn. in Ψ_A is not a Bloch state



Broken Symmetry

↳ Quantum Chemistry

$s=1/2$ per atom $\chi(r) \sim \frac{c}{r}$

$$\bar{\Psi}_{\text{exact}} = a [\uparrow \uparrow \downarrow \uparrow \downarrow \uparrow] + b [\uparrow - \uparrow \uparrow \downarrow \uparrow] + \dots$$

$$\text{with } b \sim \frac{\langle \phi_i | U | \phi_{ii} \rangle}{U}$$

= Configuration Interaction

In DF all correlation effects in \mathcal{H}_{eff}
Correct \rightarrow correlation should be in $\bar{\Psi}$

Wave fcn. \rightarrow Must in total be periodic

Consider Band integer filling!

For Wide bands -

starting point $\bar{\Psi} = \frac{1}{\sqrt{N!}} |\psi_{k_1} \psi_{k_2} \dots \psi_{k_N}|$

- Single Slater Det. of one electron Bloch states

- Total wave is also periodic

- Both one electron ^(k) and total (K) momenta are good quantum no's.

For Narrow Bands - Localized moments

starting point - $\bar{\Psi}$ = product of atomic wave fcn

- Each atom has n electrons
(Stay at home principle)

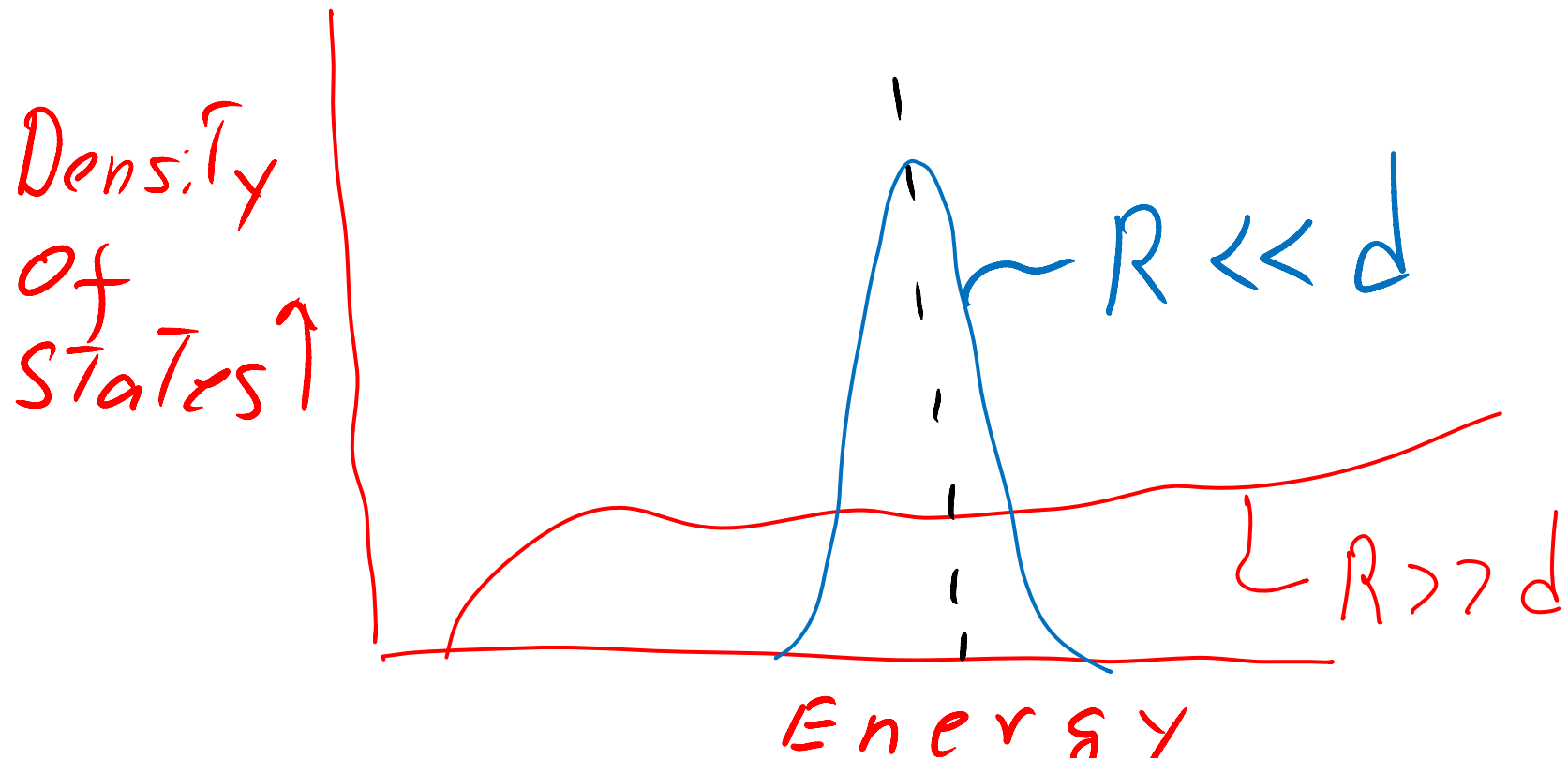
- fluctuation in this is not allowed

- Physics described by periodic array of atoms with only magnetic [No charge] degrees of freedom

General band theory result for $R \ll d$ together with $R \gg d$ states

For open shell bands $R \ll d$
 $R \ll d$ so bands are narrow

open therefore must be at E_f



Huge successes of DFT

- Obtain the correct ground state crystal structure and quite accurate lattice parameters for a large diversity of systems
- Obtain the correct magnetic structure for a large diversity of materials
- First principles method to calculate electron phonon coupling by introducing lattice distortions and obtaining the new ground state energy
- Extremely important role in also correlated electron systems for the determination of parameters to be used in many body Hamiltonian approaches.