

Kvantni materiali : od pasovne teorije do koreliranih elektronov

Jernej Mravlje

Gradivo za predavanja pri specialističnem seminarju: "Izbrane teme iz teoretične fizike"

V Ljubljani, Feb 2018.

Redneck perspective on strong correlations



- a working-class white person from the southern US, especially a politically reactionary one.



Left-wing radicals vs. conservative

From : <http://condensedconcepts.blogspot.si>

- **Left-wing:**



- emergence (Phil Anderson, Nobel '77)

Completely new conceptual structures and techniques are needed. We must go beyond Landau's mean-field theory and Fermi liquid theory: topological order, quasi-particles with fractional quantum numbers, AdS-CFT, quantum criticality, ...

To the barricades!

- **Right-wing**

- atomistic details (Walter Kohn, Nobel prize 98)

... we have the conservatives who believe that the key ingredients are atomistic detail, good density functionals, perturbation theory, mean-field theory, and the random-phase approximation.

New concepts and methods are not really needed. They have a good system [just like capitalism].

In particular, we don't need a revolution, just bigger computers!



To balance Rok's part I will discuss more the redneck part

- Density functional theory
- Dynamical mean-field theory
(a centrist thread - a bridge between left and right)
- The idea was also to bring the discussion in contact to recent research work ruthenates and on TaS_2 (next week)

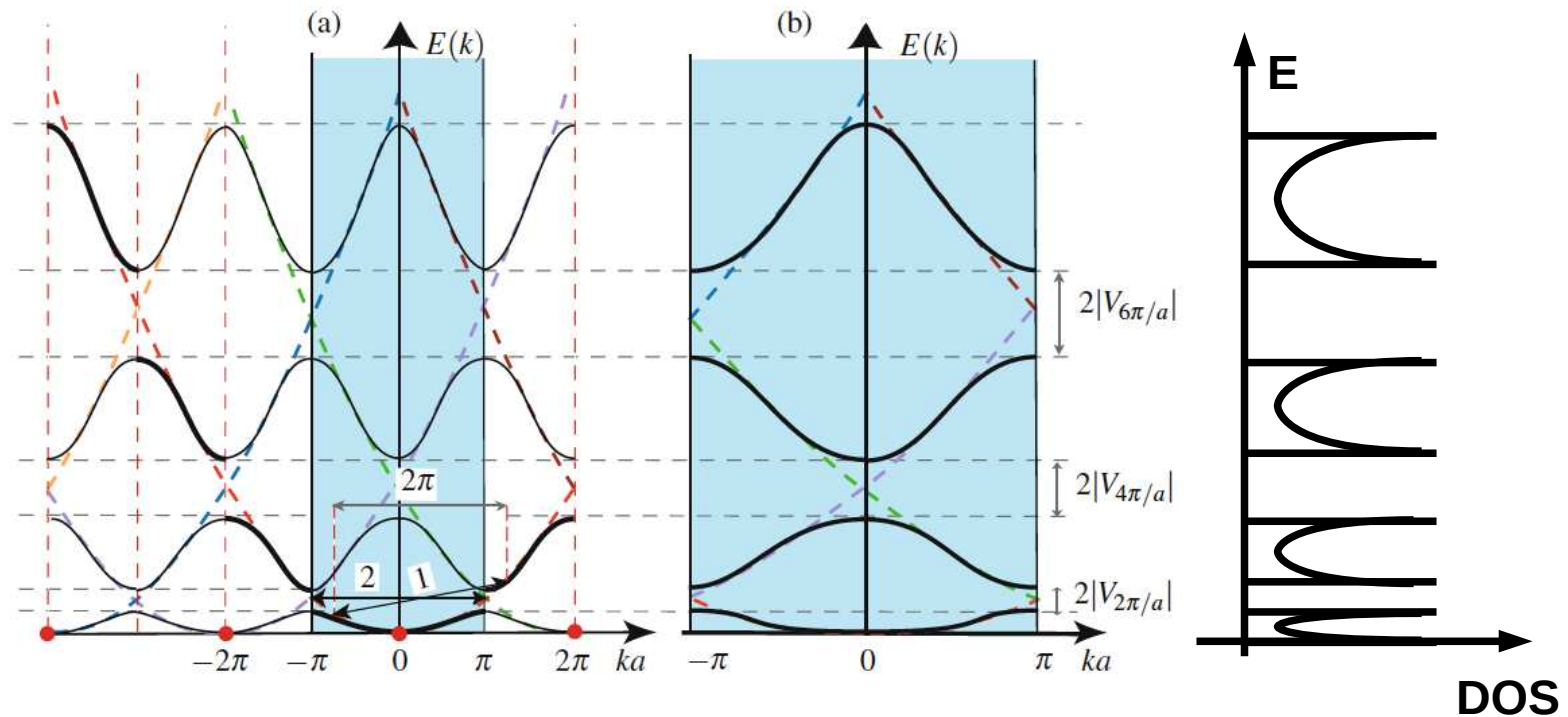
Some (10?) facts about SCES

(Initially, I wanted to make 10 – like 10 commandments from the bible. Then it was 7, like 7 things one should absolutely avoid on the first date. I ended up at only a few (tend to forget ...))

Fact 1: there is a thing called a DFT
and it describes the bandstructure of
many compounds well

Fact 1: there is a thing called DFT
and it describes the *bandstructure* of
many compounds *well*

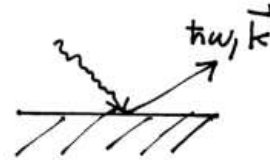
Bandstructure



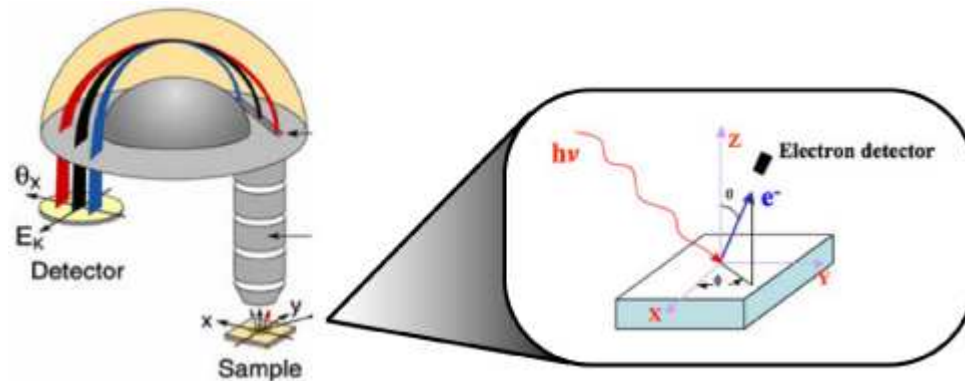
- k -resolved spectrum $A(k, E) = \sum_{kn} \delta[E - E_n(k)]$;
 $DOS = \sum_k \delta[E - E(k)]$. DOS determines many
 properties of solid state

Well: Fact 2: Several experimental techniques exist that allow quantitative comparison with theory

Measuring spectra PES, ARPES

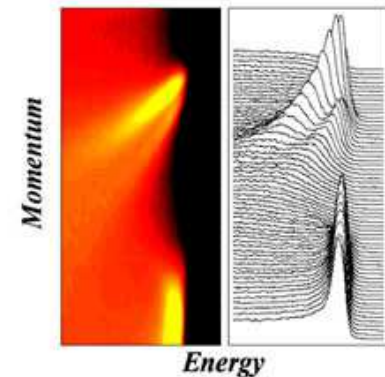
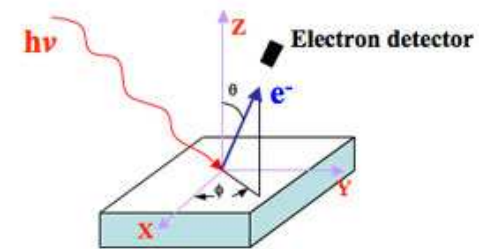
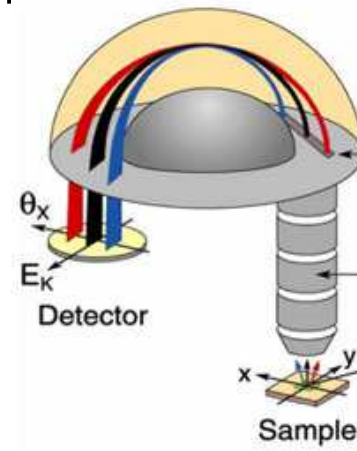


- Probes occupied one-electron states
 $I(\mathbf{k}, E) = f(E) A(\mathbf{k}, E)$
- PES : \mathbf{k} -integrated, probes DOS
- ARPES : \mathbf{k} -resolved, probes $A(\mathbf{k}, E)$



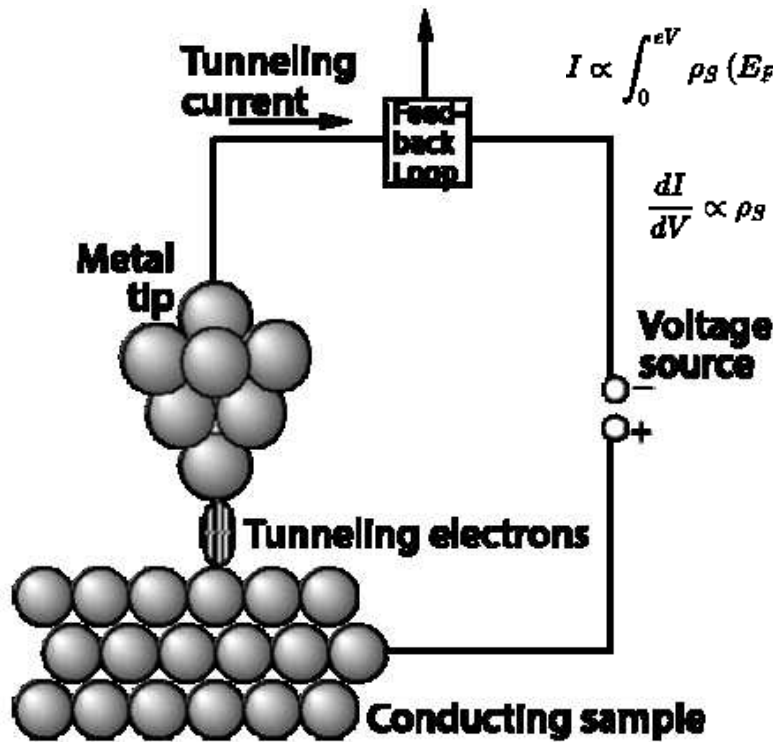
ARPES

- Probes occupied part of spectral function
- Energy resolution
10meV (synchrotron)
1meV(laser)



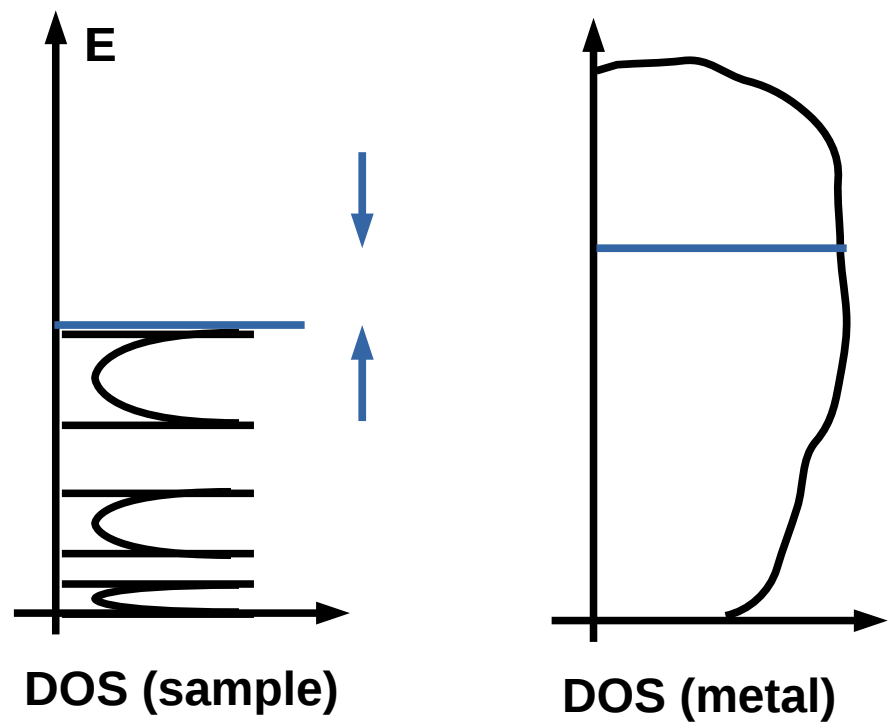
STS (measures ~DOS)

• STM :
$$I = \frac{4\pi e}{\hbar} \int_{-\infty}^{\infty} [f(E_F - eV + \epsilon) - f(E_F + \epsilon)] \rho_S(E_F - eV + \epsilon) \rho_T(E_F + \epsilon) |M_{\mu\nu}|^2 d\epsilon, \quad (1)$$



$$I \propto \int_0^{eV} \rho_S(E_F - eV + \epsilon) \rho_T(E_F + \epsilon) d\epsilon, \quad (3)$$

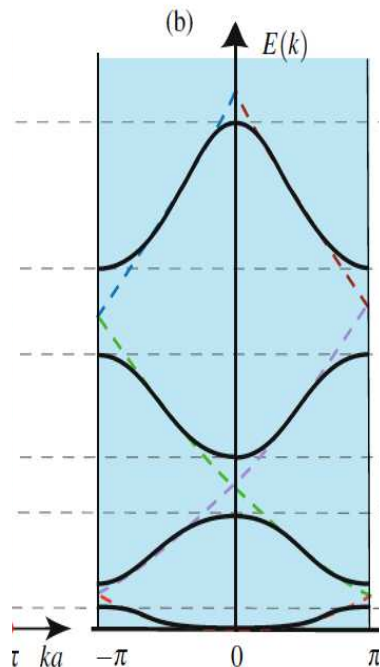
$$\frac{dI}{dV} \propto \rho_S(E_F - eV), \quad (4)$$



Optical conductivity

- Also gives information about DOS (more precisely, joint DOS)

$$\sigma(\Omega) = \sum_k \int d\omega v_k^2 A_k(\omega) A_k(\omega + \Omega) \frac{f(\omega) - f(\omega + \Omega)}{\Omega}$$



- Schroedinger equation for $\Psi(\vec{r}_1, \dots, \vec{r}_N)$

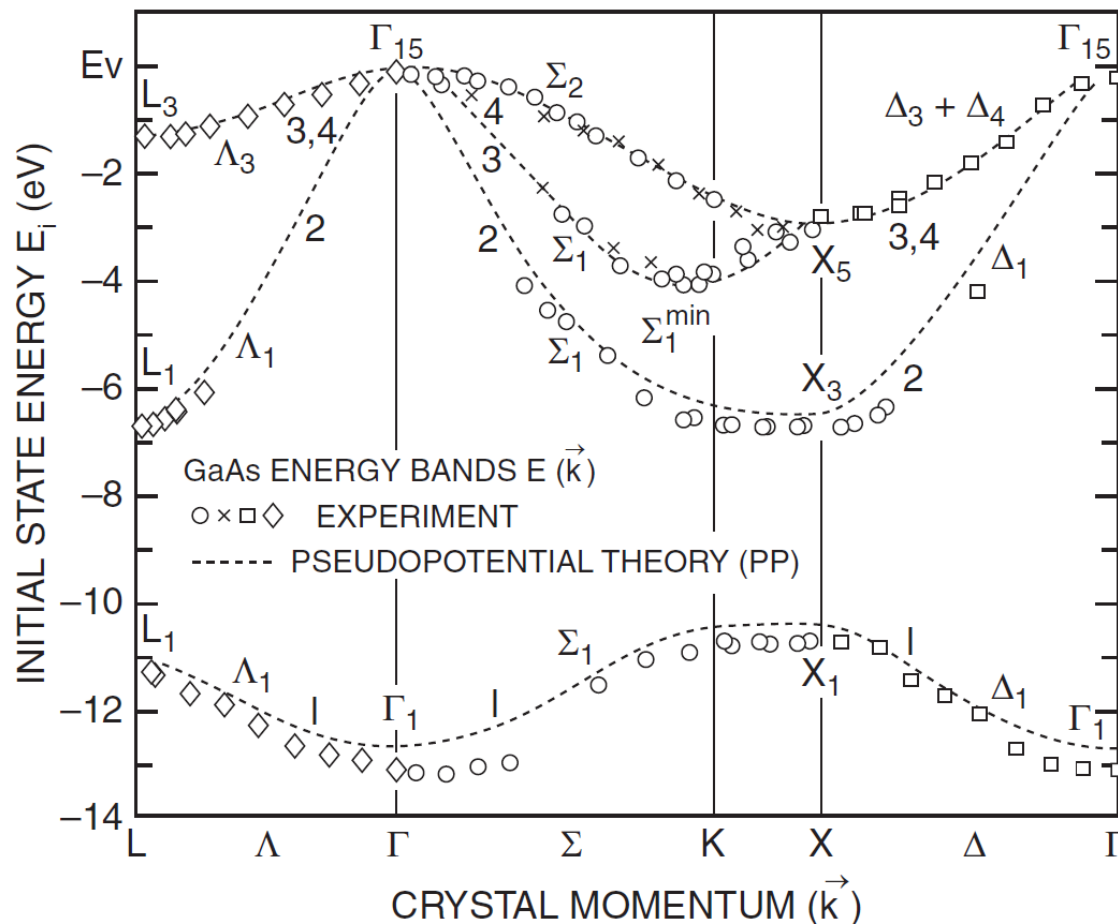
$$\hat{H}\Psi = [\hat{T} + \hat{V} + \hat{U}] \Psi = \left[\sum_i^N \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 \right) + \sum_i^N V(\vec{r}_i) + \sum_{i<j}^N U(\vec{r}_i, \vec{r}_j) \right] \Psi = E\Psi$$

$$n(\vec{r}) = N \int d^3r_2 \cdots \int d^3r_N \Psi^*(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N).$$

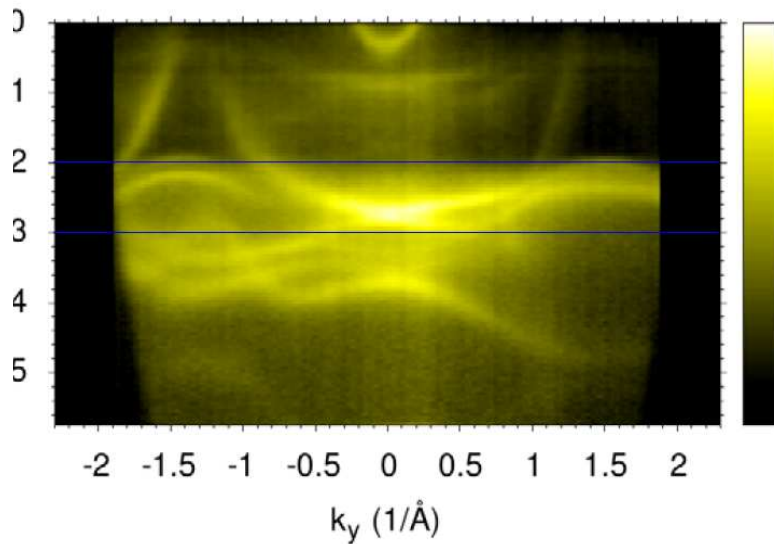
there is a bijective relation between $V(r)$, $n(r)$. $V(r)$ defines the ground state density. The relation can be inverted. There is a unique functional

$$\Psi_0 = \Psi[n_0]$$

Fact 1: there is a thing called DFT and it describes the bandstructure of many compounds well

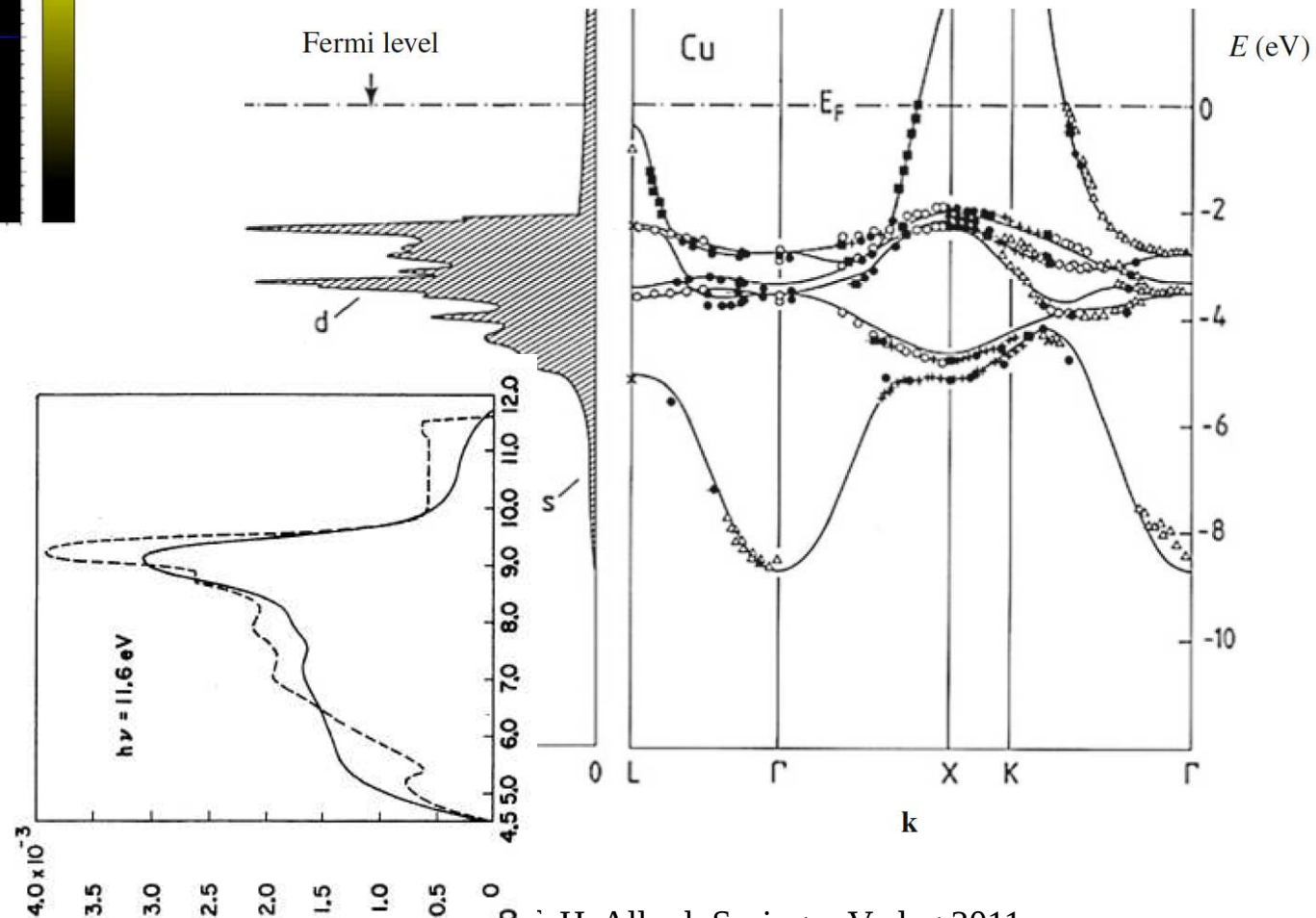


ARPES on Cu



New Journal of Physics **14** (2012) 043009

Symbols: peak of $I(k,E)$



- Sharp excitations over wide energy range
- Agrees with band theory

cf. H. Alloul, Springer-Verlag 2011:

Courths, R., Hüfner, S.: *Phys. Rep.* **112**, 55 (1984)

Eckardt, H., Fritsche, L., Noffke, J.: *J. Phys. F* **14**, 97 (1984)

This DFT looks quite neat. What is it? (blackboard)

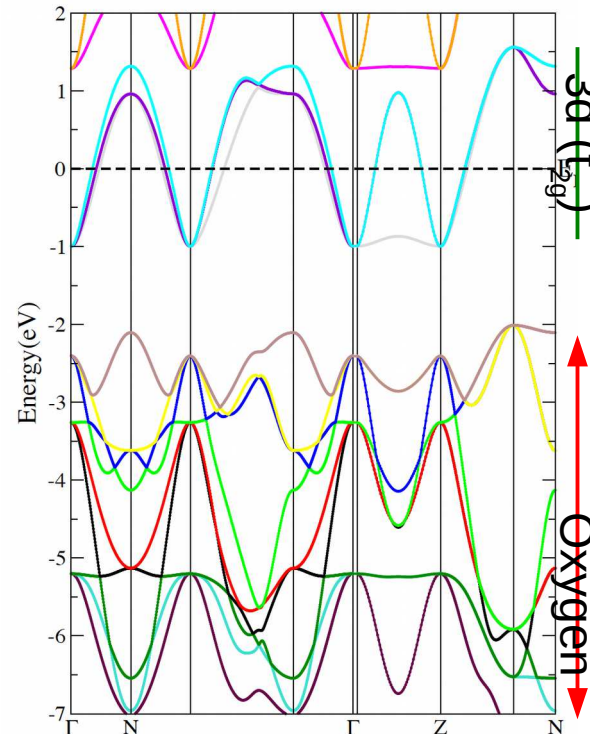
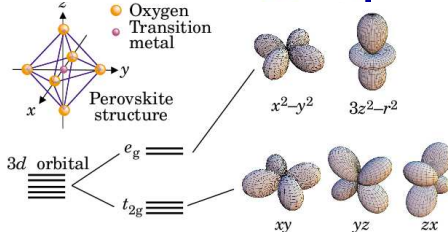
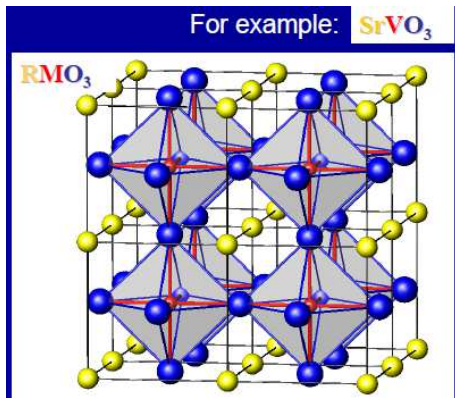
- Comments: information about exact energy of homogeneous electron gas is built in

- LDA is ab-initio technique: you put in coordinate of atoms and you get E (can investigate which structures are stable)
- It describes state in terms of auxiliary Kohn-Sham states
- Energies of these eigenstates for some reason are close to the experiments for several cases (noone really knows why)

- The energies also have meaning: take SrVO_3

Transition metal oxides; structure and band-structure

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----------------------------|----------------------------|-----------------------------|-------------------------------|---------------------------|----------------------------|------------------------------|----------------------------|------------------------------|----------------------------|------------------------------|---------------------------------|--------------------------------|-------------------------------|---------------------------------|-----------------------------|--------------------------------|-----------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|--------------------------------|---------------------------------|----------------------------|------------------------------|------------------------------|------------------------------|---------------------------|-------------------------------|---------------------------------|-------------------------------|-------------------------------|-------------------------------|------------------------------|--------------------------------|--------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|-------------------------------|--------------------------------|-------------------------------|----------------------------|---------------------------------|--------------------------------|------------------------------|-----------------------------|
| 1 H 1.008 Hydrogen | 2 He 4.003 Helium | 3 Li 6.941 Lithium | 4 Be 9.012 Beryllium | 5 B 10.811 Boron | 6 C 12.011 Carbon | 7 N 14.007 Nitrogen | 8 O 15.999 Oxygen | 9 F 18.998 Fluorine | 10 Ne 20.180 Neon | 11 Na 22.990 Sodium | 12 Mg 24.305 Magnesium | 13 Al 26.982 Aluminum | 14 Si 28.086 Silicon | 15 P 30.974 Phosphorus | 16 S 32.065 Sulfur | 17 Cl 35.453 Chlorine | 18 Ar 39.948 Argon | 19 K 39.098 Potassium | 20 Ca 40.078 Calcium | 21 Sc 44.956 Scandium | 22 Ti 47.88 Titanium | 23 V 50.942 Vanadium | 24 Cr 51.996 Chromium | 25 Mn 54.938 Manganese | 26 Fe 55.845 Iron | 27 Co 58.933 Cobalt | 28 Ni 58.693 Nickel | 29 Cu 63.546 Copper | 30 Zn 65.38 Zinc | 31 Ga 69.723 Gallium | 32 Ge 72.630 Germanium | 33 As 74.922 Arsenic | 34 Se 78.96 Selenium | 35 Br 79.904 Bromine | 36 Kr 83.80 Krypton | 37 Rb 85.468 Rubidium | 38 Sr 87.62 Strontium | 39 Y 88.906 Yttrium | 40 Zr 91.224 Zirconium | 41 Nb 92.906 Niobium | 42 Mo 95.94 Molybdenum | 43 Tc 98 Technetium | 44 Ru 101.07 Ruthenium | 45 Rh 101.07 Rhodium | 46 Pd 106.36 Palladium | 47 Ag 107.868 Silver | 48 Cd 112.411 Cadmium | 49 In 114.818 Indium | 50 Sn 118.710 Tin | 51 Sb 121.757 Antimony | 52 Te 127.6 Tellurium | 53 I 126.905 Iodine | 54 Xe 131.29 Xenon |
|-----------------------------|----------------------------|-----------------------------|-------------------------------|---------------------------|----------------------------|------------------------------|----------------------------|------------------------------|----------------------------|------------------------------|---------------------------------|--------------------------------|-------------------------------|---------------------------------|-----------------------------|--------------------------------|-----------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|--------------------------------|---------------------------------|----------------------------|------------------------------|------------------------------|------------------------------|---------------------------|-------------------------------|---------------------------------|-------------------------------|-------------------------------|-------------------------------|------------------------------|--------------------------------|--------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|-------------------------------|--------------------------------|-------------------------------|----------------------------|---------------------------------|--------------------------------|------------------------------|-----------------------------|



An observation

- Bands quite narrow (2eV) in contrast to Cu (~10eV)

Part 2

When LDA breaks down:

electronic correlations



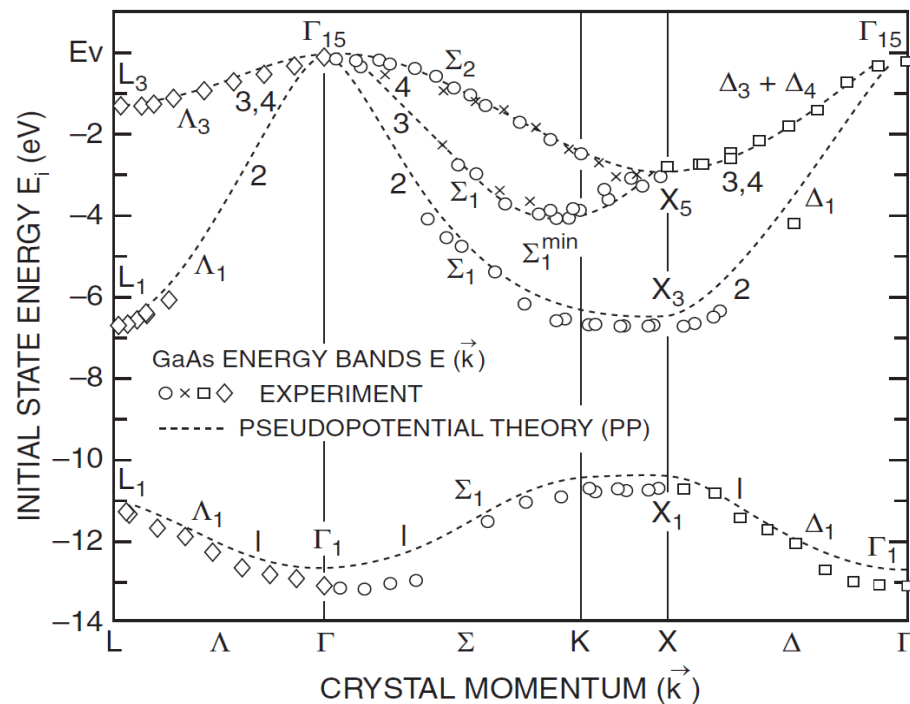
Redneck perspective on strong correlations (part 2)



From past week

Fact 1. there is a thing called DFT(LDA) and it describes the bandstructure of many compounds well

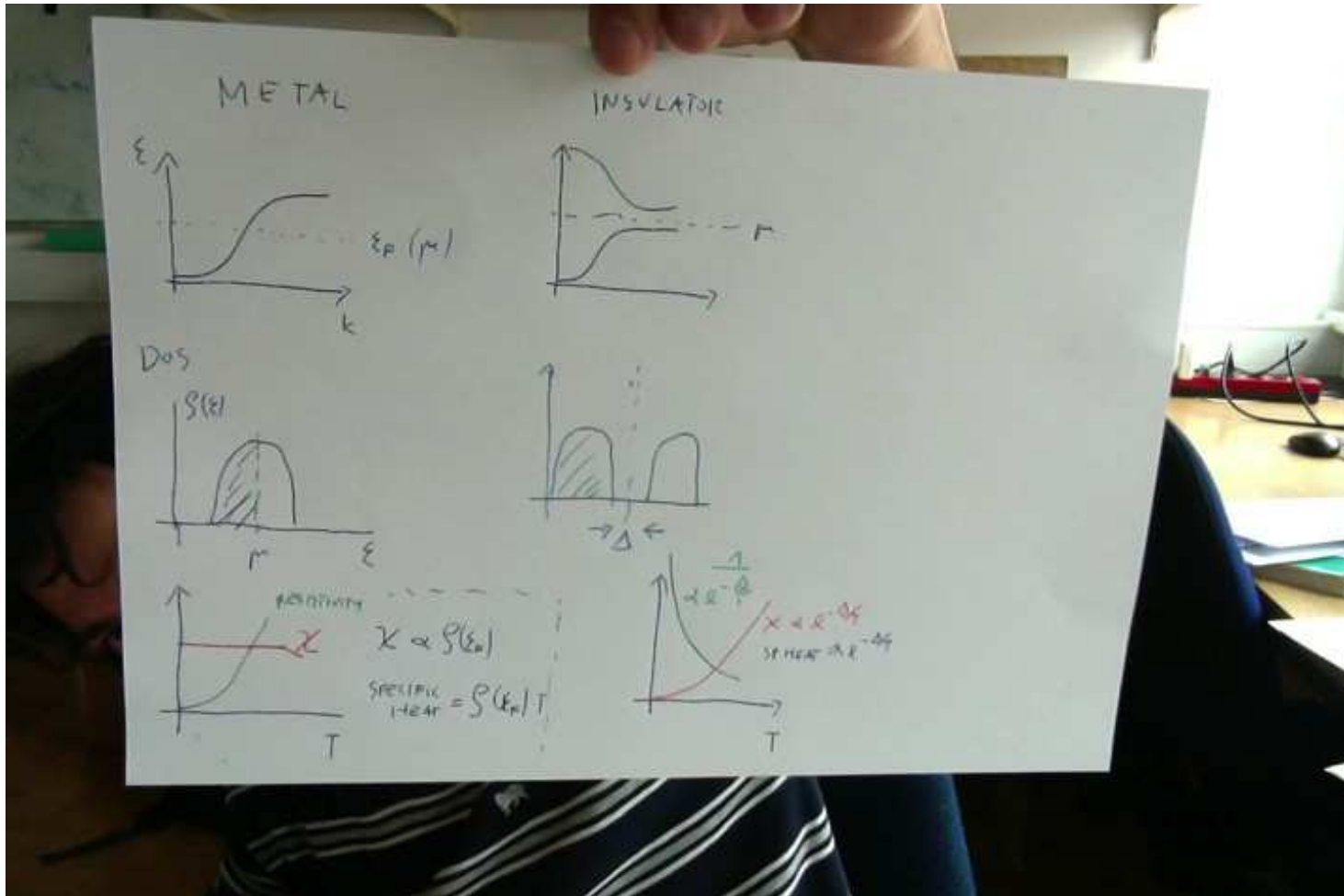
Fact 2. Several experimental techniques exist that allow quantitative comparison with theory



- LDA breaks down when interactions get strong
- Electronic correlations and Mott transition
- DMFT
- Sr_2RuO_4 : Correlated metal with low coherence scale due to Hund's rule coupling
- Spin-liquid behavior in TaS_2

Resistivity, magnetic susceptibility,
and specific heat : band-insulators
vs. metals

Resistivity, magnetic susceptibility, and specific heat : band-insulators vs. metals



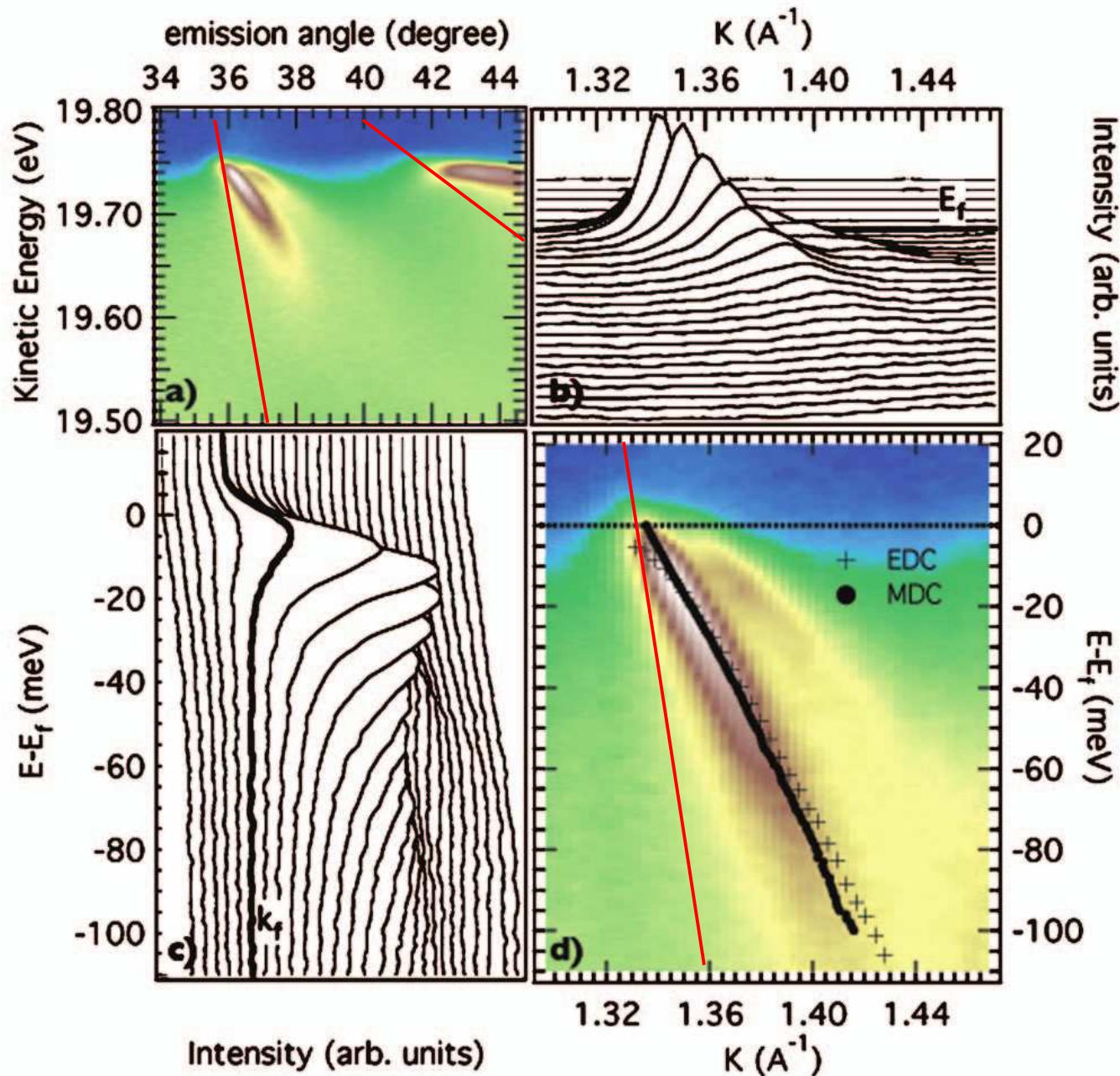
Note: band insulator needs even # of els. / band.

Breakdown of band picture: correlated metals and Mott insulators

Fact 3: strong Coulomb repulsion leads to a breakdown of band theory and occurrence of Mott insulator

- Partial breakdown: quasiparticles with large renormalizations compared to band-theory
- Complete breakdown: Mott insulator

Partial breakdown (Sr_2RuO_4)

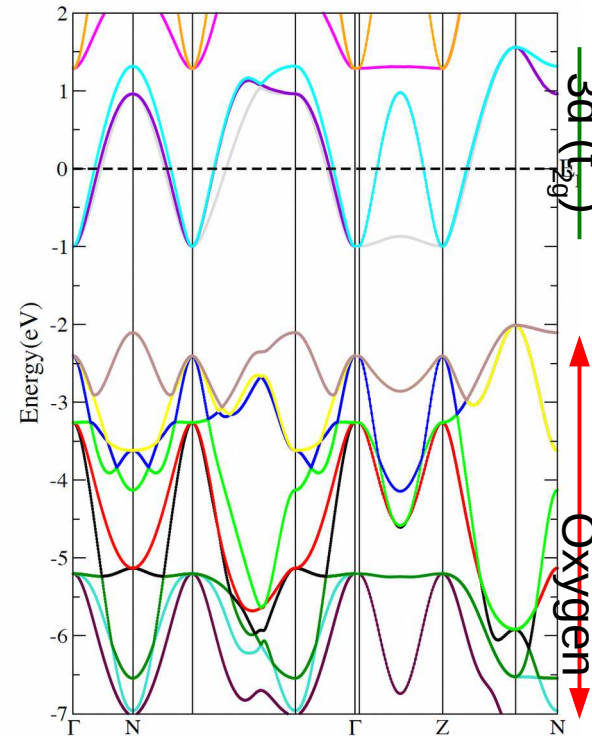
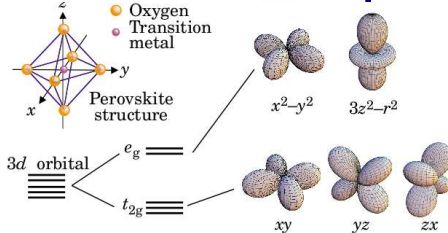
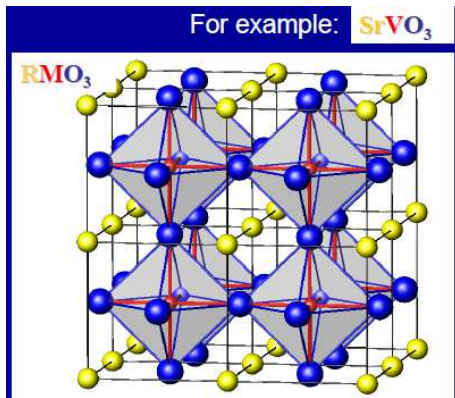


- Completely different picture.
- Coherent excitations only up to a 0.1eV
- Heavy quasiparticles ($E=k^2/2m$, dE/dk)

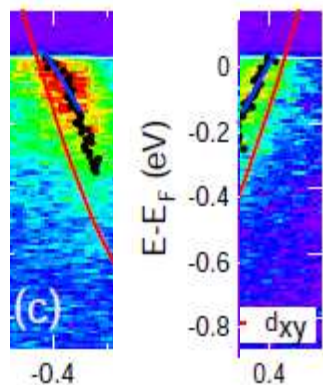
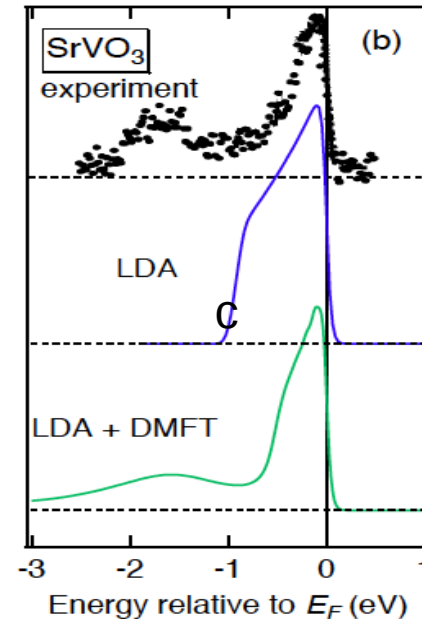
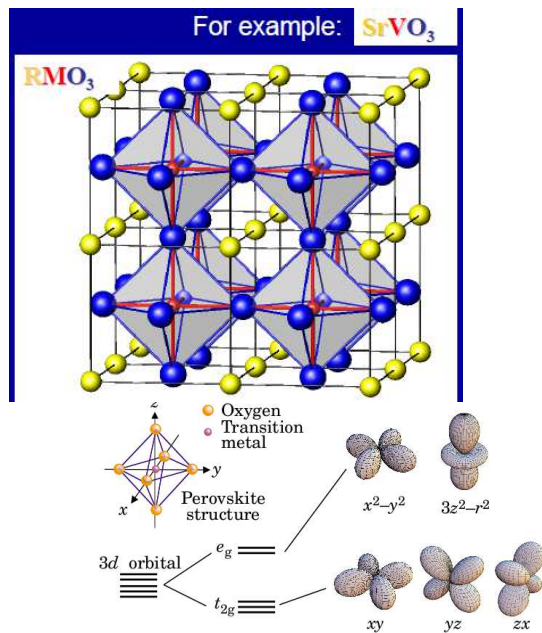
Red: band-theory
Strong renormalizations

Transition metal oxides; structure and band-structure

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----------------------------|----------------------------|-----------------------------|-------------------------------|---------------------------|----------------------------|------------------------------|----------------------------|------------------------------|----------------------------|------------------------------|---------------------------------|--------------------------------|-------------------------------|---------------------------------|-----------------------------|--------------------------------|-----------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|--------------------------------|---------------------------------|----------------------------|------------------------------|------------------------------|------------------------------|---------------------------|-------------------------------|---------------------------------|-------------------------------|-------------------------------|-------------------------------|------------------------------|--------------------------------|--------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|-------------------------------|------------------------------|---------------------------|--------------------------------|--------------------------------|-----------------------------|-----------------------------|
| 1 H 1.008 Hydrogen | 2 He 4.003 Helium | 3 Li 6.941 Lithium | 4 Be 9.012 Beryllium | 5 B 10.811 Boron | 6 C 12.011 Carbon | 7 N 14.007 Nitrogen | 8 O 15.999 Oxygen | 9 F 18.998 Fluorine | 10 Ne 20.180 Neon | 11 Na 22.990 Sodium | 12 Mg 24.305 Magnesium | 13 Al 26.982 Aluminum | 14 Si 28.086 Silicon | 15 P 30.974 Phosphorus | 16 S 32.065 Sulfur | 17 Cl 35.453 Chlorine | 18 Ar 39.948 Argon | 19 K 39.098 Potassium | 20 Ca 40.078 Calcium | 21 Sc 44.956 Scandium | 22 Ti 47.88 Titanium | 23 V 50.942 Vanadium | 24 Cr 51.996 Chromium | 25 Mn 54.938 Manganese | 26 Fe 55.845 Iron | 27 Co 58.933 Cobalt | 28 Ni 58.693 Nickel | 29 Cu 63.546 Copper | 30 Zn 65.38 Zinc | 31 Ga 69.723 Gallium | 32 Ge 72.630 Germanium | 33 As 74.922 Arsenic | 34 Se 78.96 Selenium | 35 Br 79.904 Bromine | 36 Kr 83.80 Krypton | 37 Rb 85.468 Rubidium | 38 Sr 87.62 Strontium | 39 Y 88.906 Yttrium | 40 Zr 91.224 Zirconium | 41 Nb 92.906 Niobium | 42 Mo 95.94 Molybdenum | 43 Tc 98 Technetium | 44 Ru 101.07 Ruthenium | 45 Rh 102.91 Rhodium | 46 Pd 106.42 Palladium | 47 Ag 107.87 Silver | 48 Cd 112.41 Cadmium | 49 In 114.82 Indium | 50 Sn 118.71 Tin | 51 Sb 121.76 Antimony | 52 Te 127.6 Tellurium | 53 I 126.90 Iodine | 54 Xe 131.29 Xenon |
|-----------------------------|----------------------------|-----------------------------|-------------------------------|---------------------------|----------------------------|------------------------------|----------------------------|------------------------------|----------------------------|------------------------------|---------------------------------|--------------------------------|-------------------------------|---------------------------------|-----------------------------|--------------------------------|-----------------------------|--------------------------------|-------------------------------|--------------------------------|-------------------------------|-------------------------------|--------------------------------|---------------------------------|----------------------------|------------------------------|------------------------------|------------------------------|---------------------------|-------------------------------|---------------------------------|-------------------------------|-------------------------------|-------------------------------|------------------------------|--------------------------------|--------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|---------------------------------|-------------------------------|---------------------------------|------------------------------|-------------------------------|------------------------------|---------------------------|--------------------------------|--------------------------------|-----------------------------|-----------------------------|

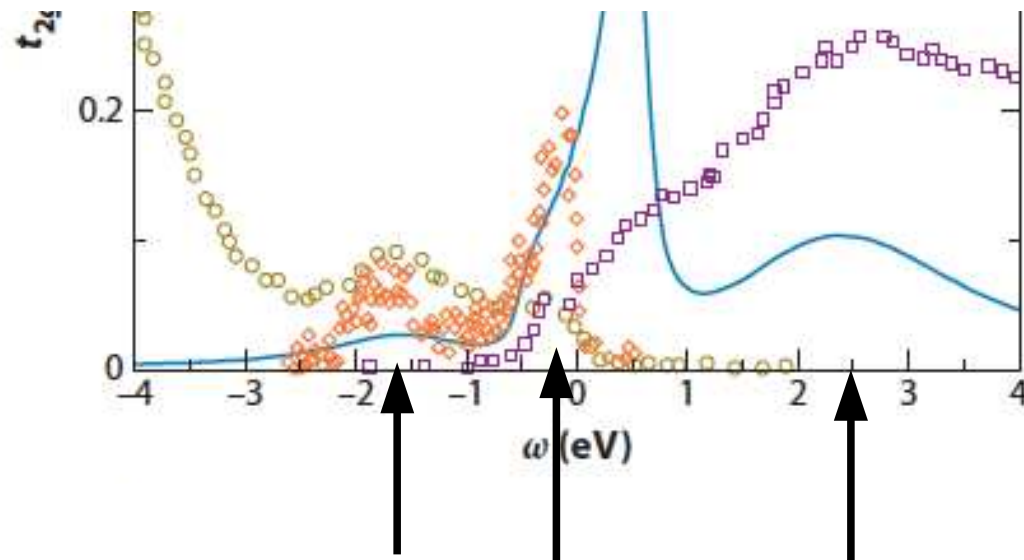
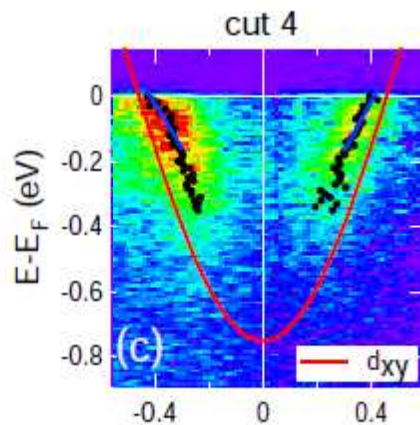
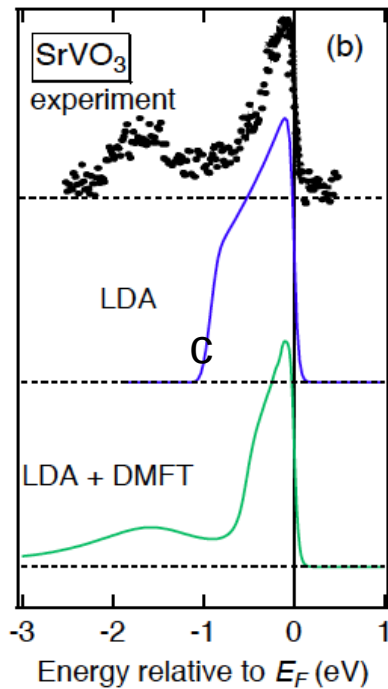


TMOs: structure and el. structure



- PES: satellites (not present in LDA)
- ARPES: coherent excitations only up to a 0.5eV
- Renormalization of slope (mass) by 2

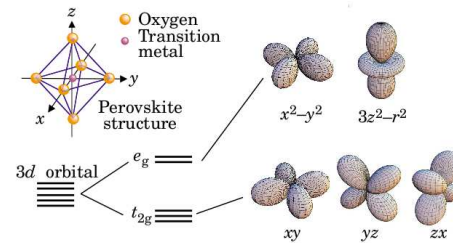
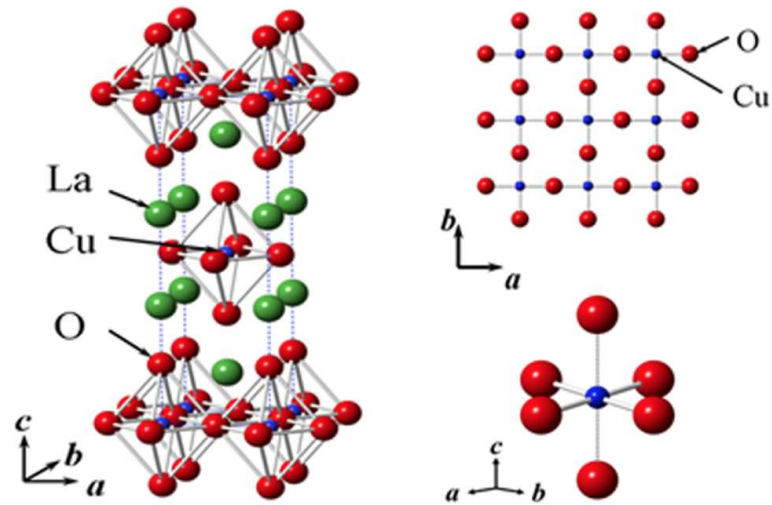
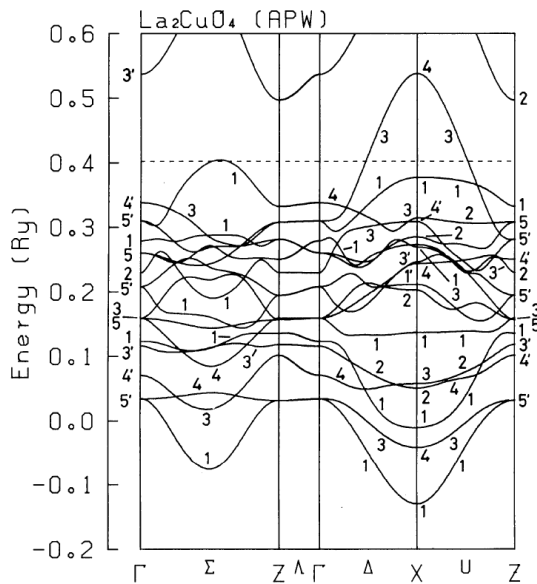
TMOs: photoemission



- PES: atomic satellites (not present in LDA)
- QP peak (narrowed by 2 from LDA)
- ARPES: coherent excitations only up to a 0.5 eV

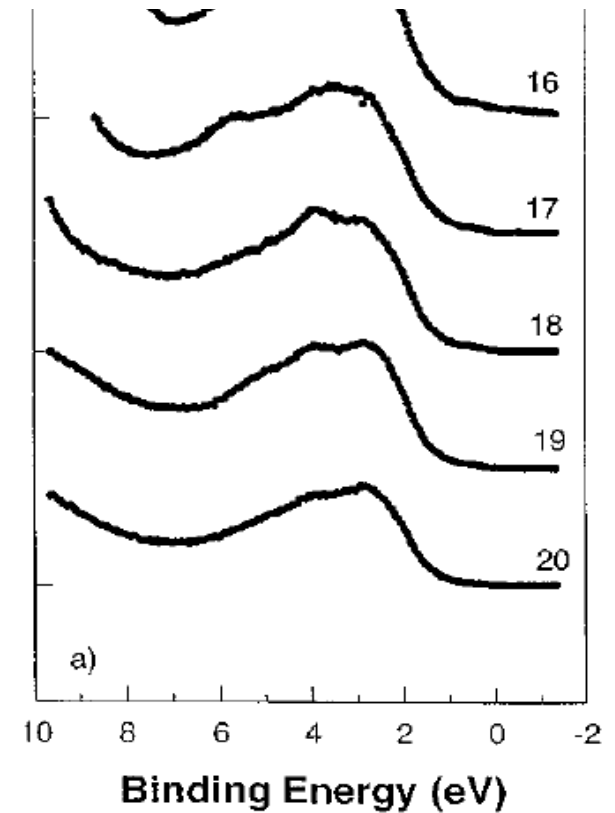
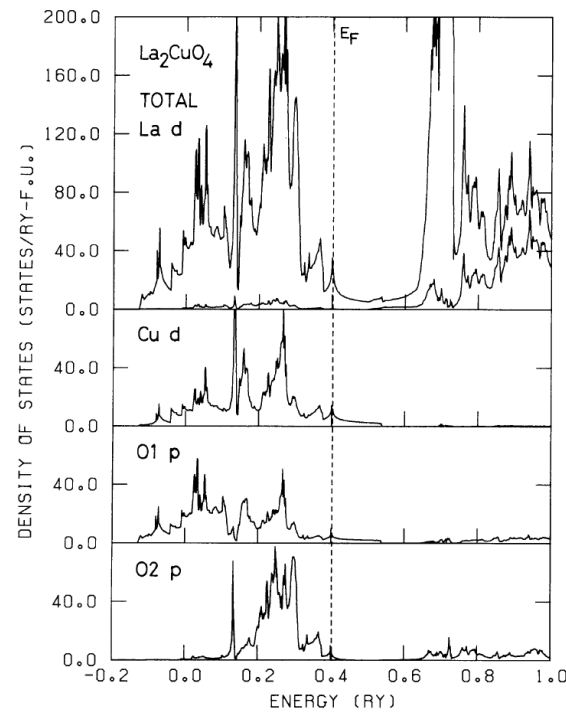
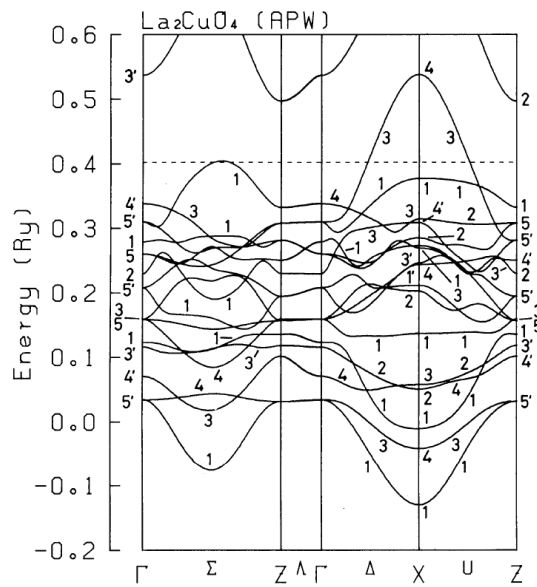
La₂CuO₄

- 9 els in Cu 3d orbitals: 1 hole in x^2-y^2

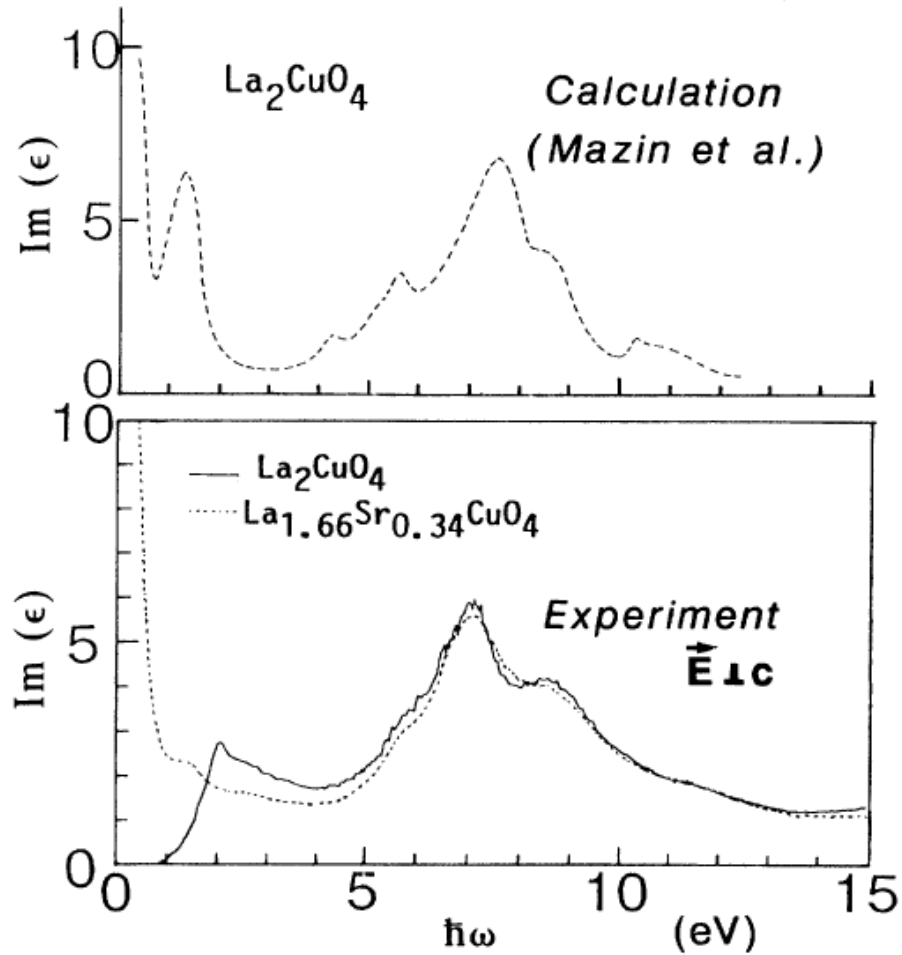


Mott transition: La_2CuO_4 is (Mott) insulator

- PES shows a 2eV gap instead of a metal



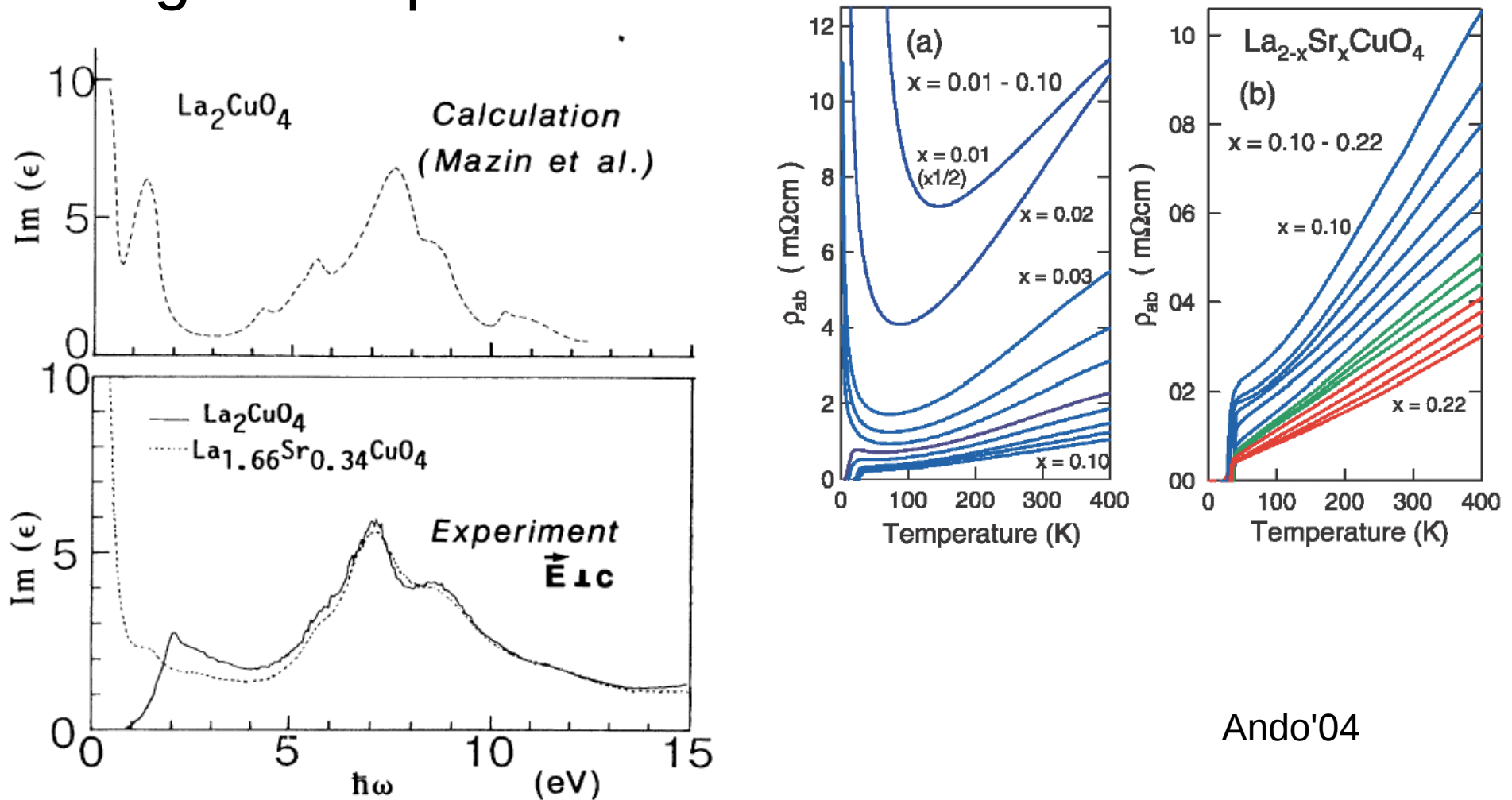
Optical conductivity also shows gap



Notice overall LDA describes result well, only low energy spectral weight is missing

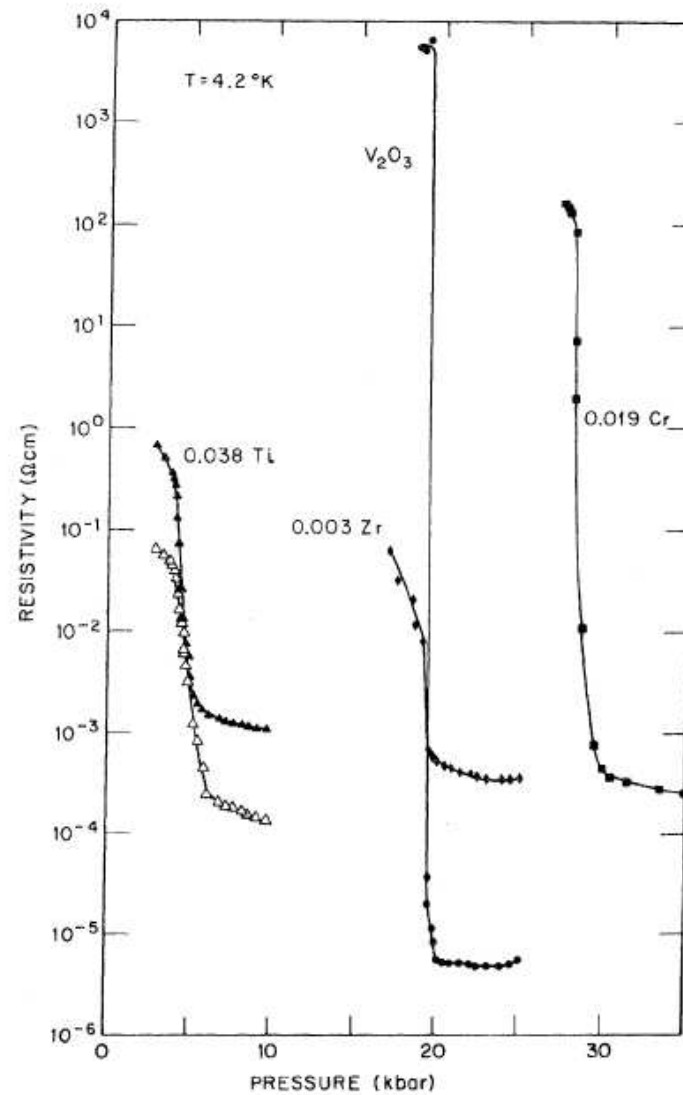
On doping, metallicity is restored; filling controlled Mott transition

- (Actually, more than that : doped LSCO is a high T_c superconductor!)



Ando'04

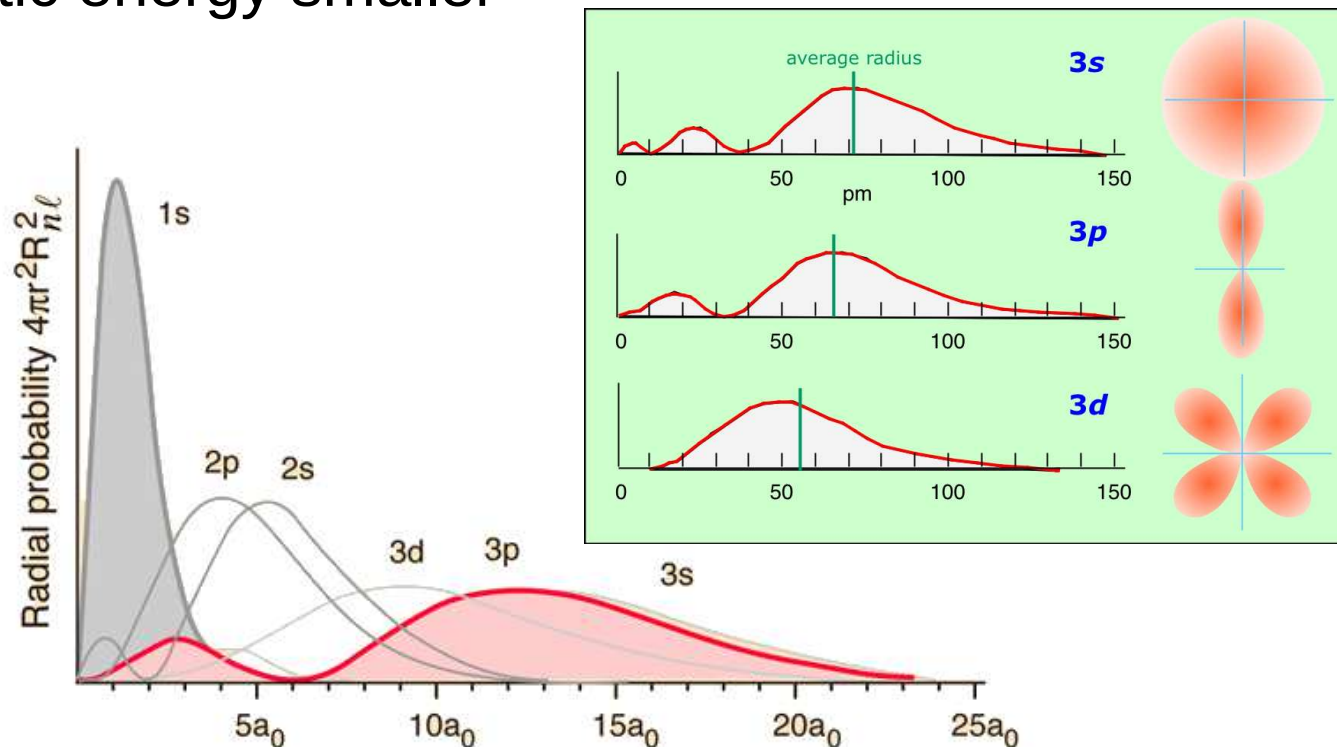
Band-width controlled driven Mott transition



Fact 4: orbitals matter!

Why 3d special?

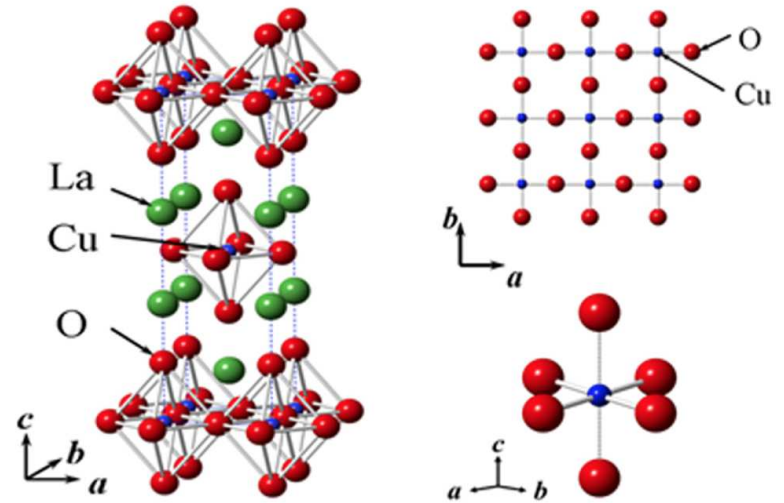
- 3d orbitals don't have nodes, reach further into core
- -> charge is screened less
- -> kinetic energy smaller



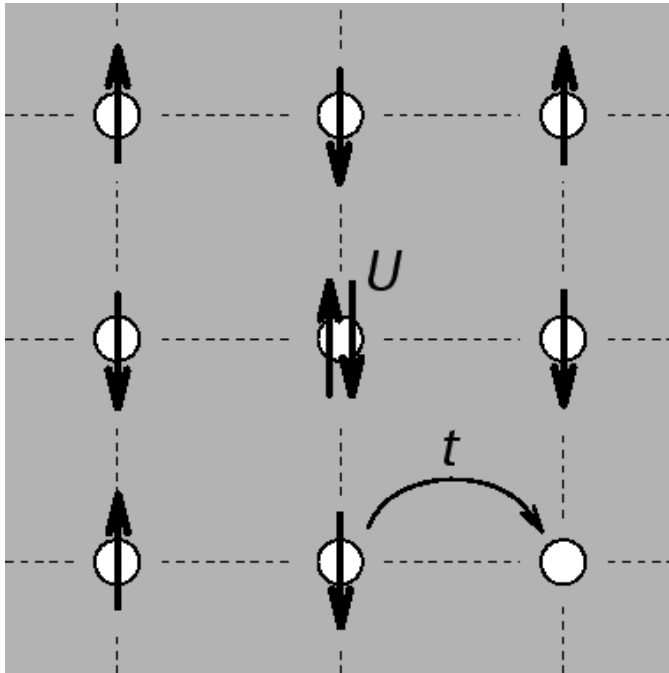
Values of interaction can also be calculated

- Atomic U_{at} (3d orbitals) $\sim e^2/4\pi\epsilon_0 r \sim 15 \text{ eV}$
- In oxides screened to $U \sim 5 \text{ eV}$
- 4d orbitals $\sim 2.5 \text{ eV}$; 5d orbitals 1.5 eV

- One has an insulating state in a half-filled band
- Mott insulator
- Hubbard model: take band of x^2-y^2 orbitals and supplement it by Hubbard repulsion U
- LDA bands as a starting point for many body calculations



Hubbard model

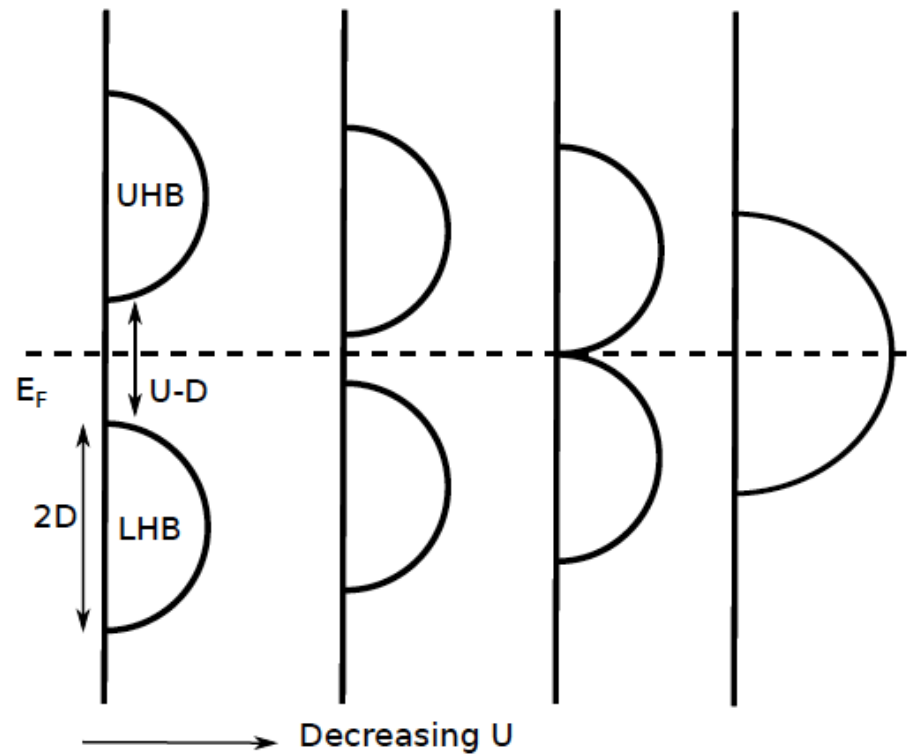


$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}$$

Mott picture of the Mott transition

- (atomic : blackboard)

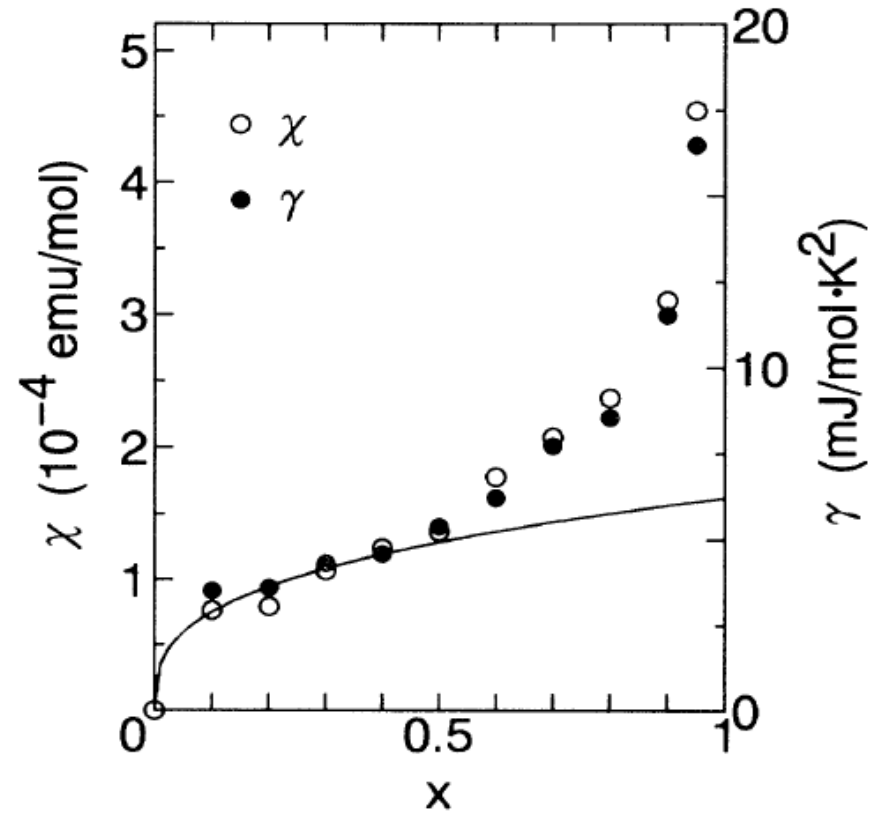
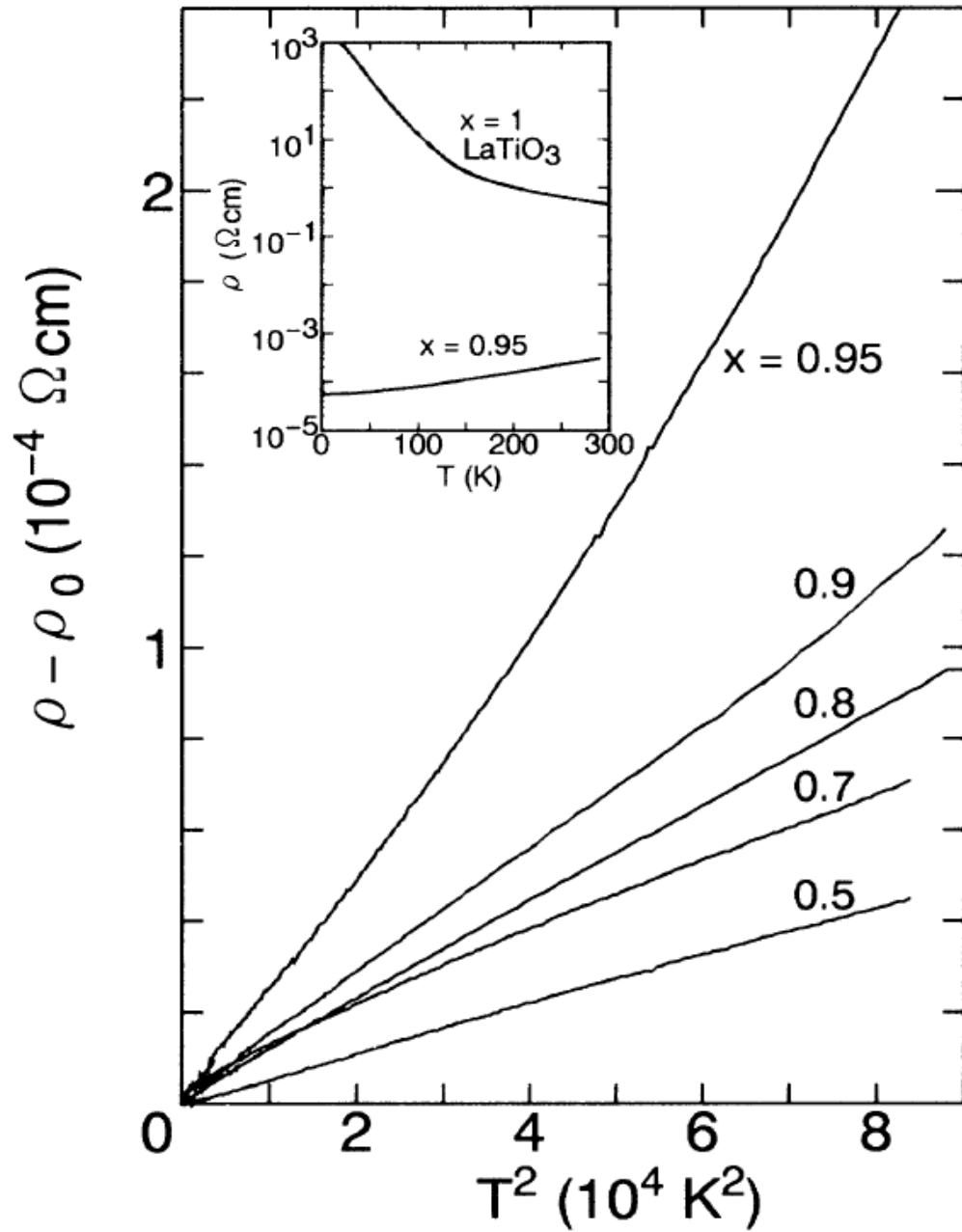


Fact 5 : Mott insulators are magnets

- localized electrons/site = spin
- Spins are coupled by exchange interaction -> Heisenberg model and magnetism
- Magnetic susceptibility rises as one cools down and magnetism arises

- Mott picture: adiabatic continuity with an insulator, but not with a metal:
- Does not described correctly doped Mott insulator

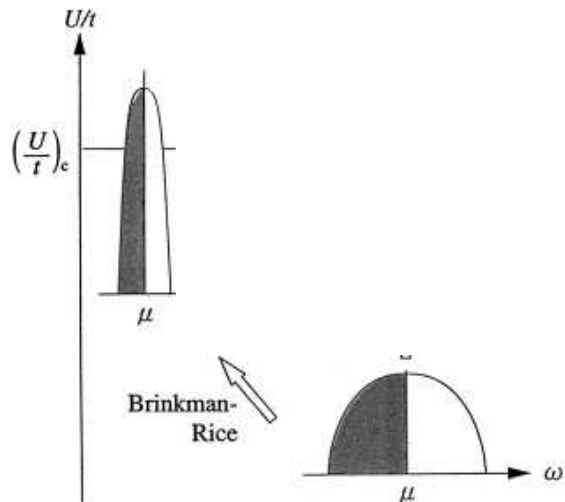
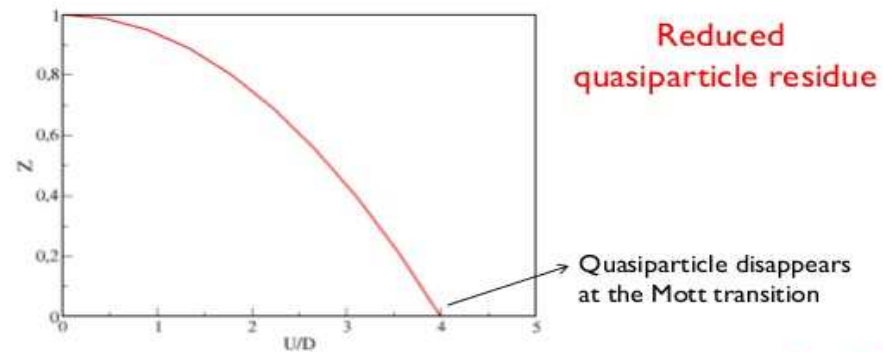
$\text{Sr}_{1-x}\text{La}_x\text{TiO}_3$



Brinkman-Rice picture

- Solving Hubbard model with a variational ansatz

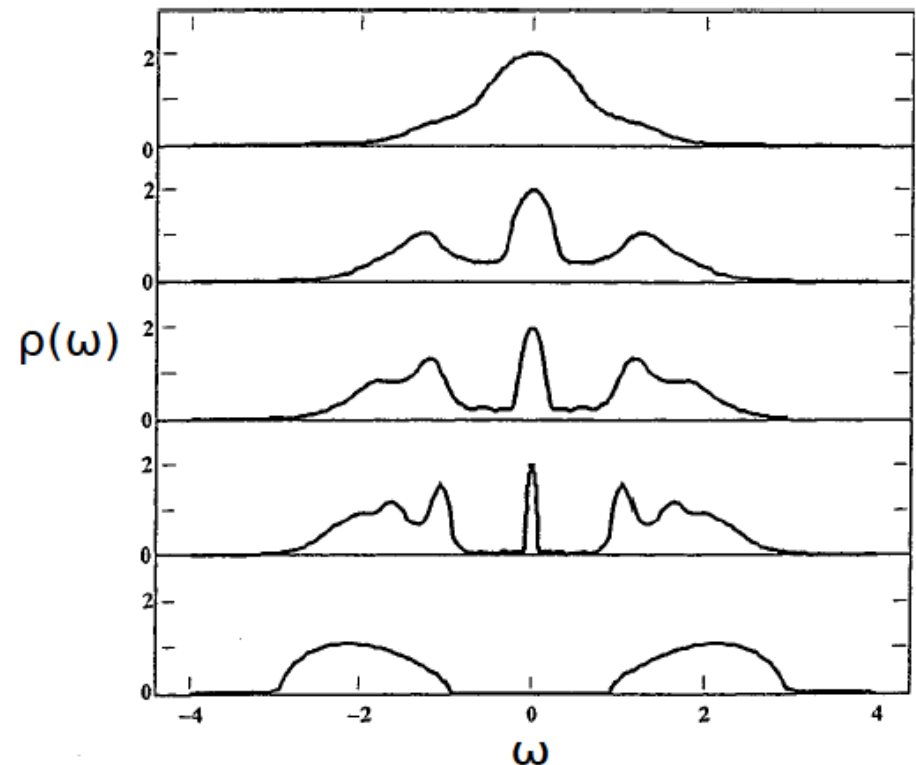
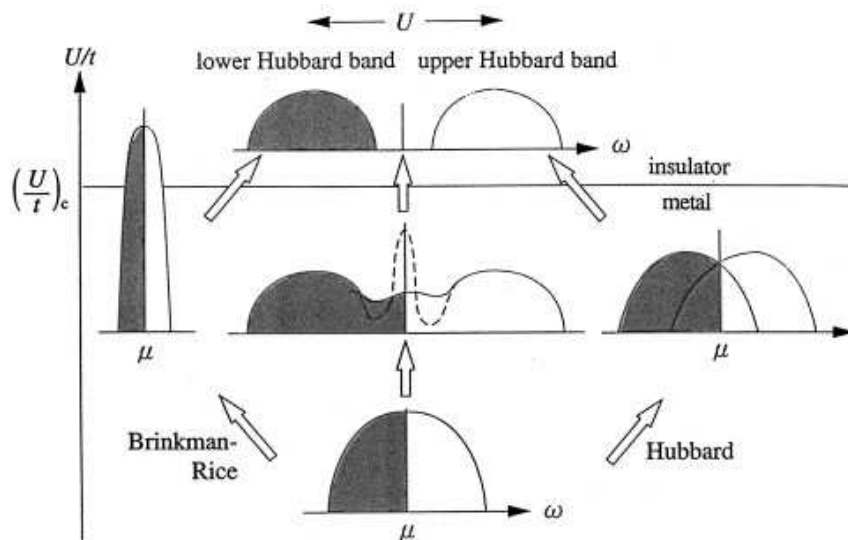
$$\begin{aligned}
 |\Psi_G\rangle &= g^{\hat{D}} |\text{FG}\rangle \\
 &= \prod_{R_i} [1 - (1 - g)\hat{D}_i] |\text{FG}\rangle,
 \end{aligned}$$



Doping driven: $Z \sim \delta$

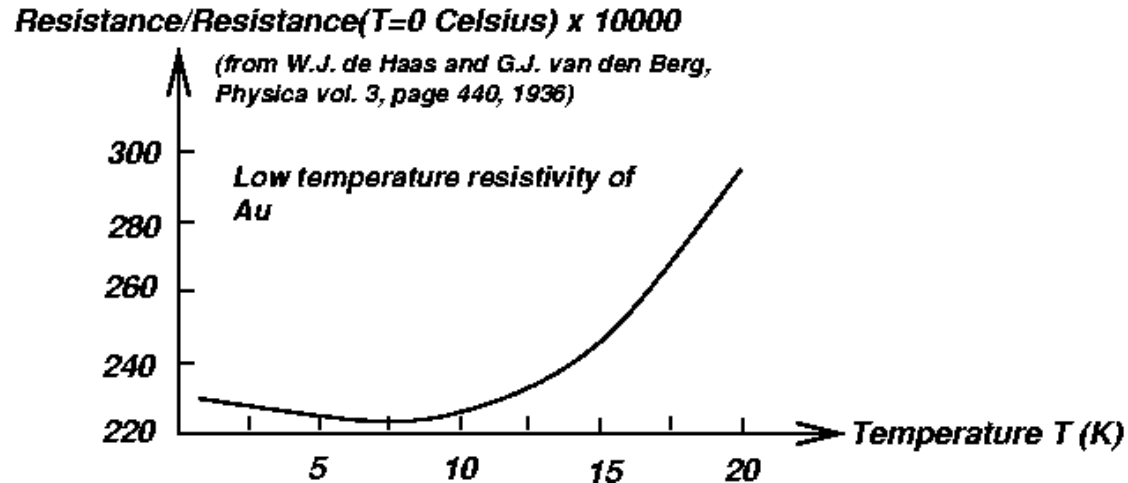
Fact 6: DOS of correlated metal consists of quasiparticle peak and Hubbard bands

- Mott transition: on metallic side adiabatic continuity with a noninteracting gas (with reduced bandwidth by Z), on insulating with an atom.



DMFT

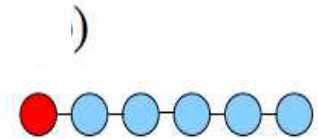
Kondo effect



Resistivity minimum:
associated to presence
of magnetic impurities

RG picture of Kondo: infrared slavery (like quarks)

- Anderson model \rightarrow Kondo model \rightarrow Kondo effect



$$H = \sum_k \epsilon_k n_k + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger d_\sigma + h.c. \right) + \epsilon n + U n_\uparrow n_\downarrow$$

$$H_{\text{Kondo}} = \sum_k \epsilon_k n_k + J \mathbf{S} \cdot \mathbf{s}$$

$$J(D') = \frac{J}{1/2 + J\rho \log(D'/D)}$$

$$T_K \sim D e^{-\frac{1}{2J\rho}}$$

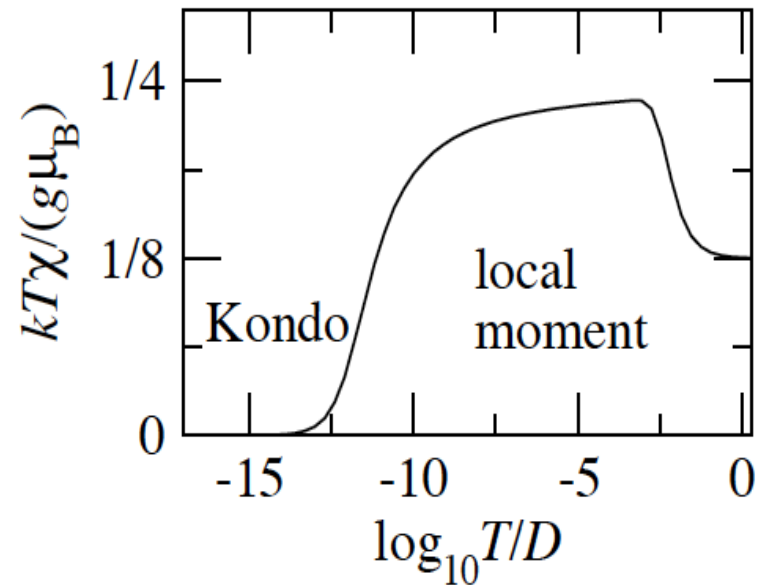
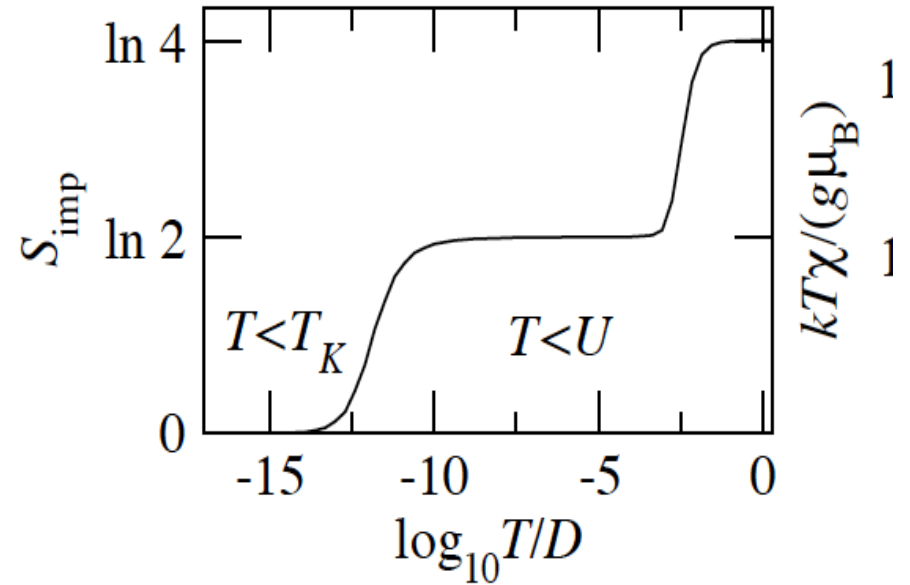
NRG results

$$H = \sum_k \epsilon_k n_k + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger d_\sigma + h.c. \right) + \epsilon n + U n_\uparrow n_\downarrow$$

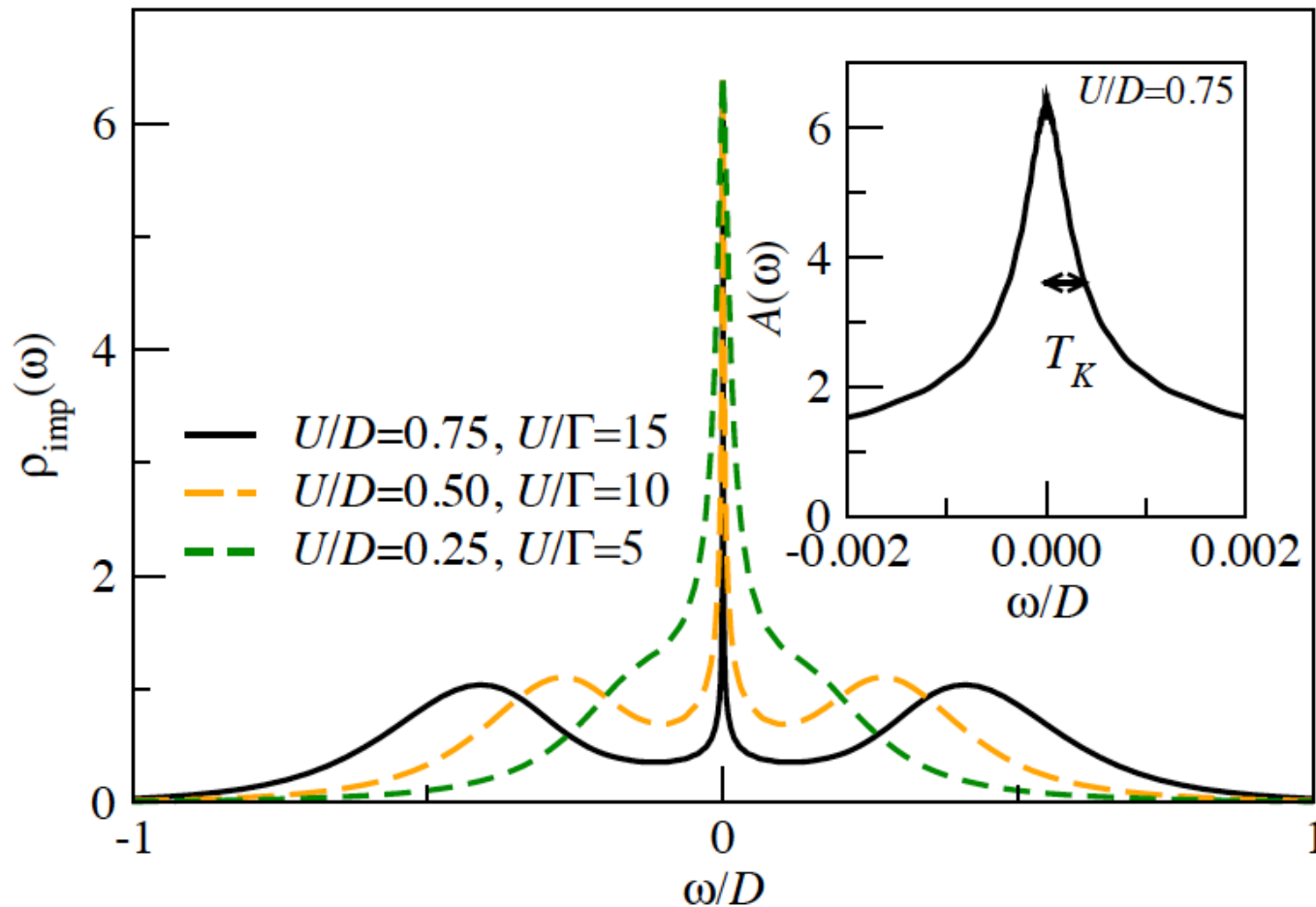
$$H_{\text{Kondo}} = \sum_k \epsilon_k n_k + J \mathbf{S} \cdot \mathbf{s}$$

$$J(D') = \frac{J}{1/2 + J\rho \log(D'/D)}$$

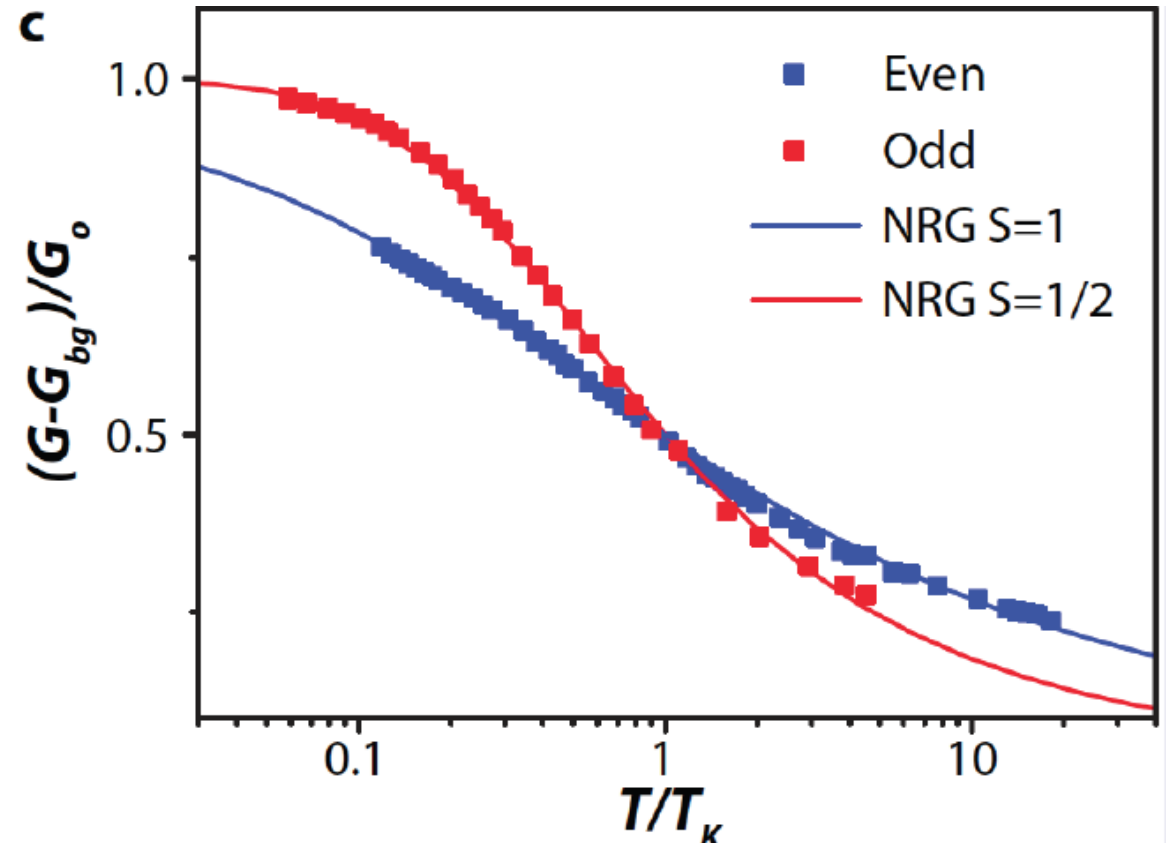
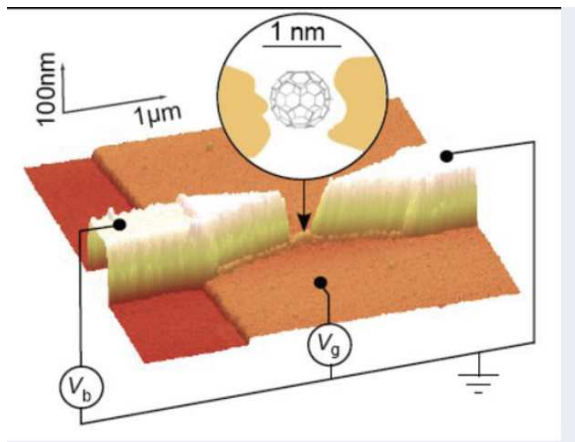
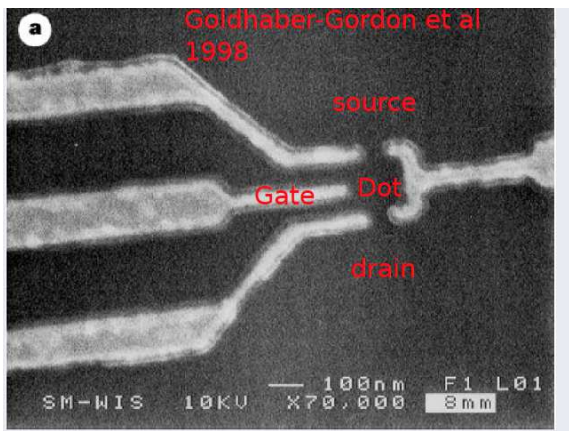
$$T_K \sim D e^{-\frac{1}{2J\rho}}$$

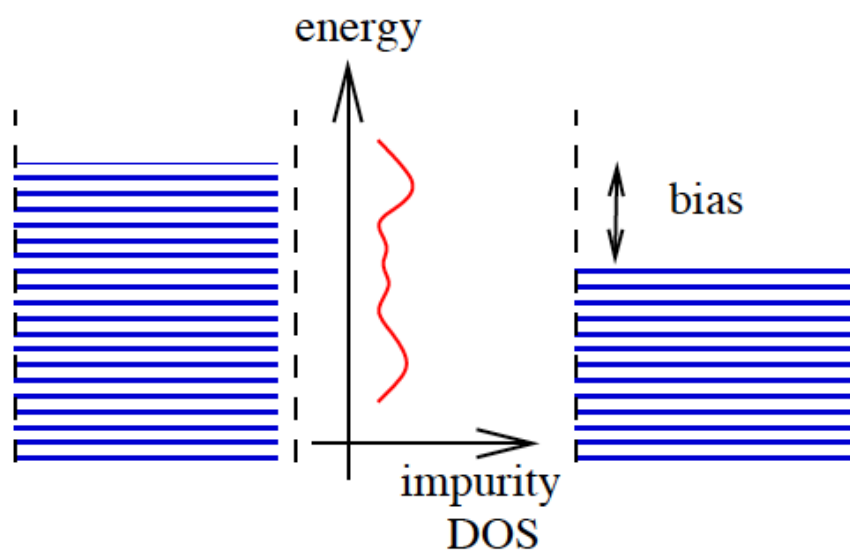
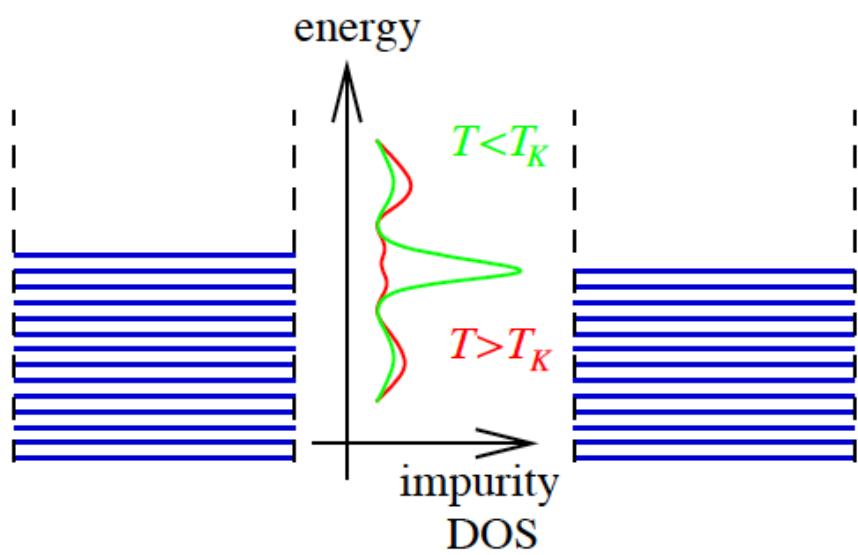
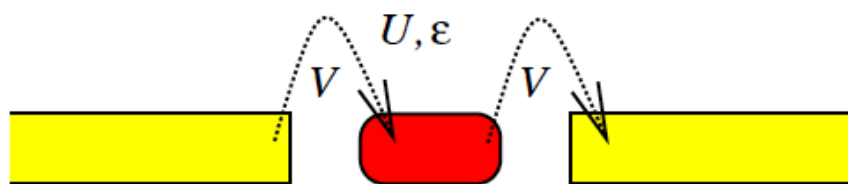


Spectral function of Anderson model

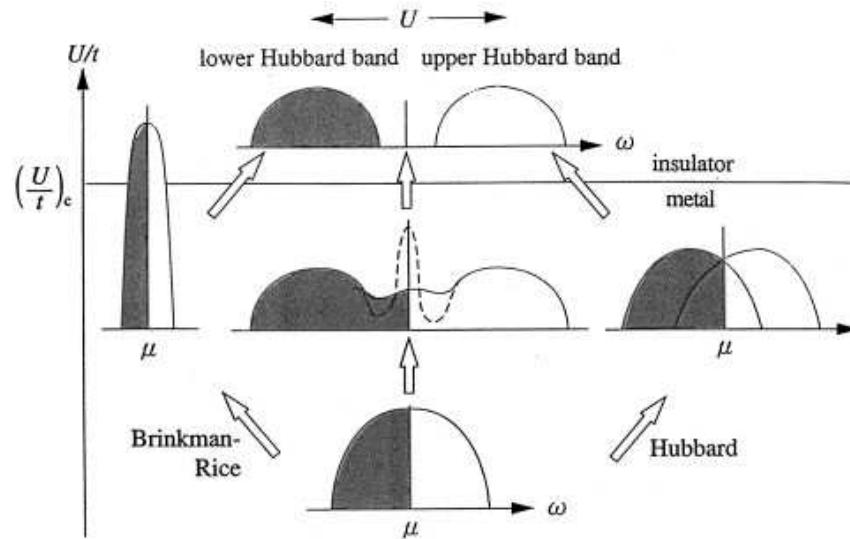


- Good numerics to calculate, tests in quantum dots and transmission through molecules

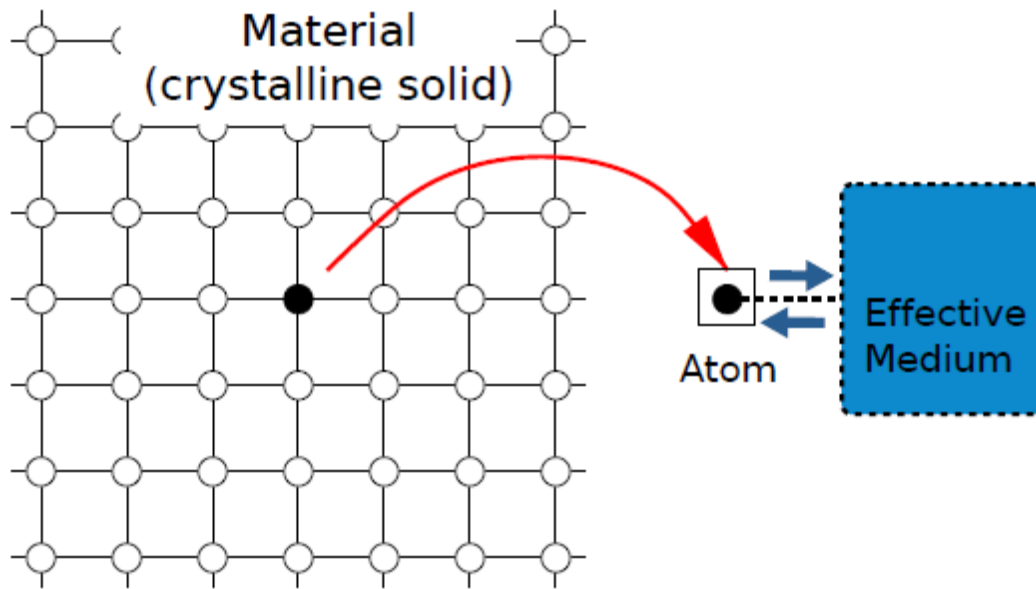




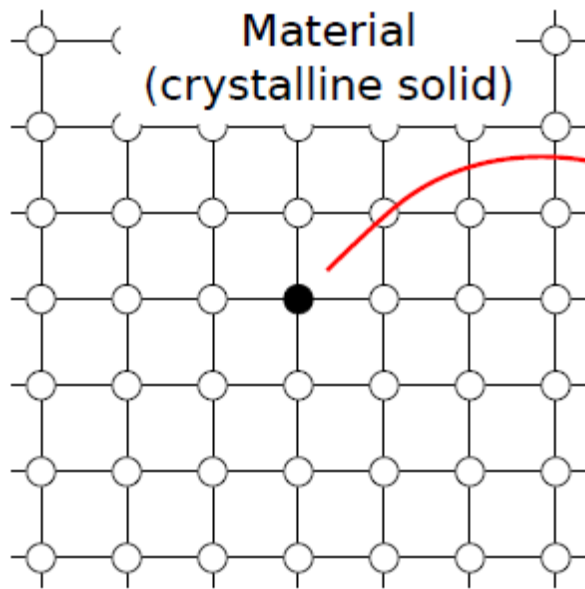
Back to bulk



Dynamical mean-field theory (DMFT)



Dynamical mean-field theory (DMFT)



$$S = \int_0^\beta d\tau \left[\sum_{i\sigma} c_{i\sigma}^*(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) c_{i\sigma}(\tau) + \sum_{ij\sigma} t_{ij} c_{i\sigma}^*(\tau) c_{j\sigma}(\tau) + \sum_i U c_{i\uparrow}^*(\tau) c_{i\uparrow}(\tau) c_{i\downarrow}^*(\tau) c_{i\downarrow}(\tau) \right]$$

$$S_{\text{loc}} = - \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_\sigma c_\sigma^*(\tau_1) \mathcal{G}_\sigma^{-1}(\tau_1 - \tau_2) c_\sigma(\tau_2) + U \int_0^\beta d\tau c_\uparrow^*(\tau) c_\uparrow(\tau) c_\downarrow^*(\tau) c_\downarrow(\tau)$$

In limit of large d , self energy becomes local (independent of k)

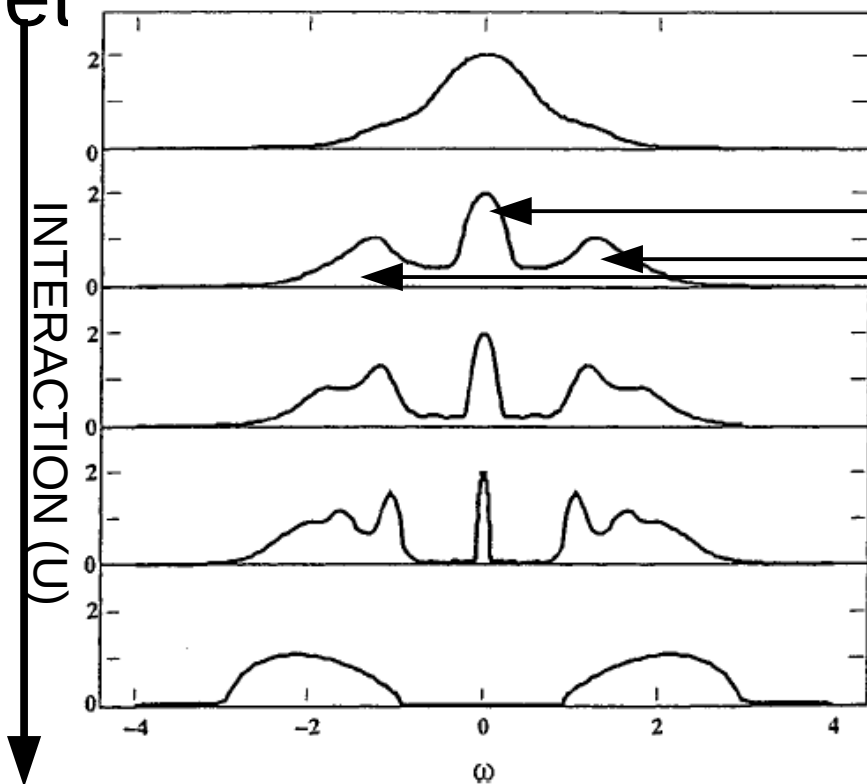
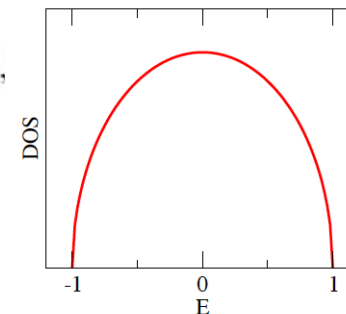
$$G_{\mathbf{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + \mu - \Sigma_\sigma(i\omega_n)}$$

DMFT results

- single orbital Hubbard model
- Metal-insulator transition

$$\mathcal{H}_t = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}),$$

$$\mathcal{H}_U = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}),$$

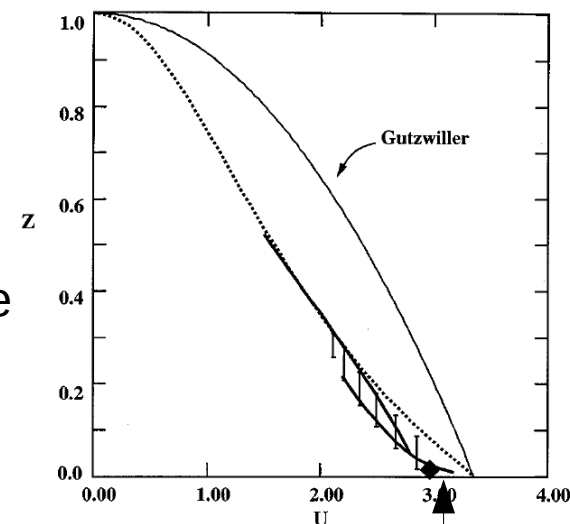


BAND-like

Quasiparticle band (weight Z)

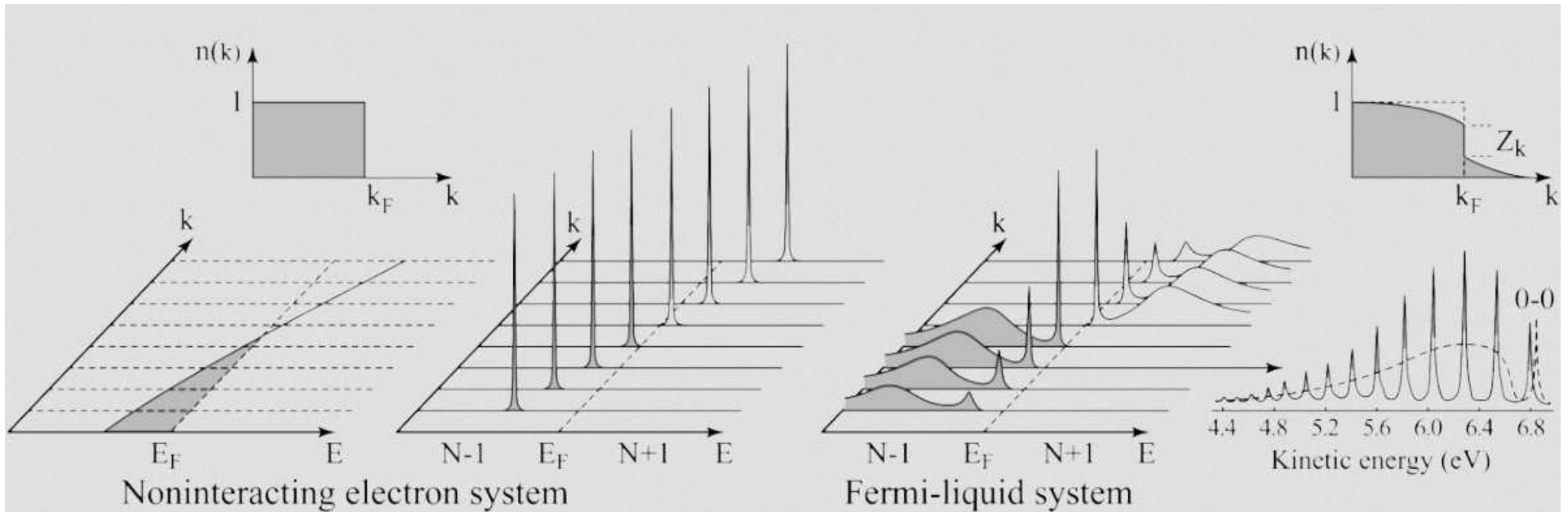
Atomic satellites (weight 1-Z)

ATOMIC-like



U_c

ARPES

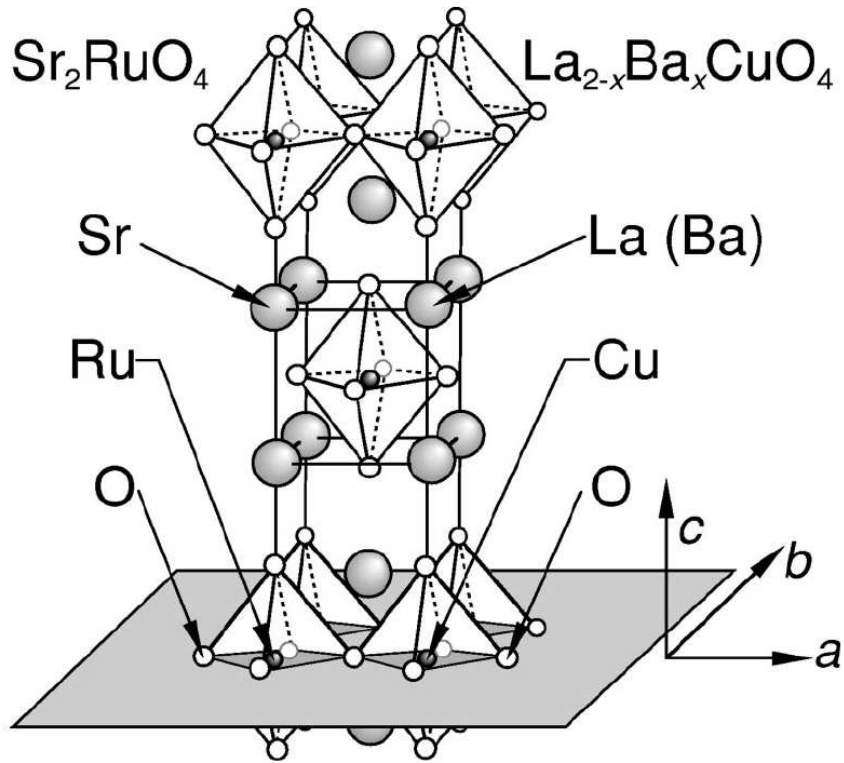


LDA+DMFT

- Take LDA bands
- Describe interactions with DMFT (subtracting mean-free part included in LDA).



Sr_2RuO_4 properties



p-wave supercond.

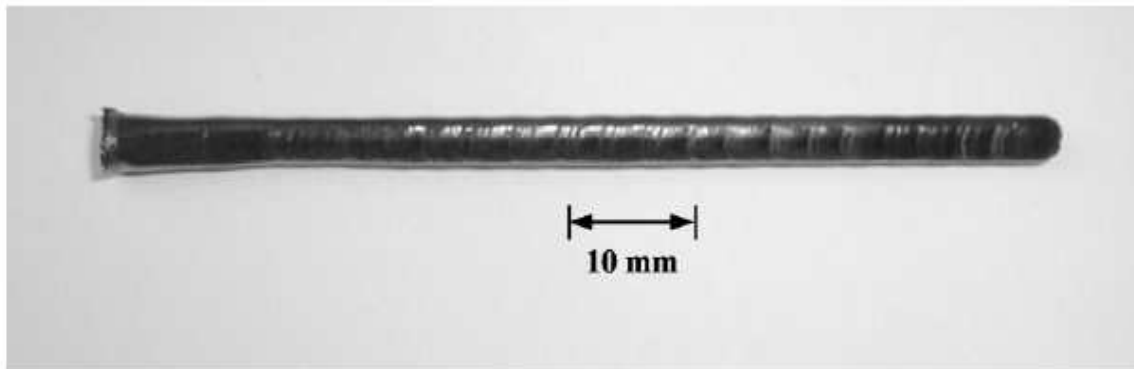
$T_c \sim 2\text{K}$

Maeno et al., Nature'94

Rice and Sigrist,
J.Phys.CM'95

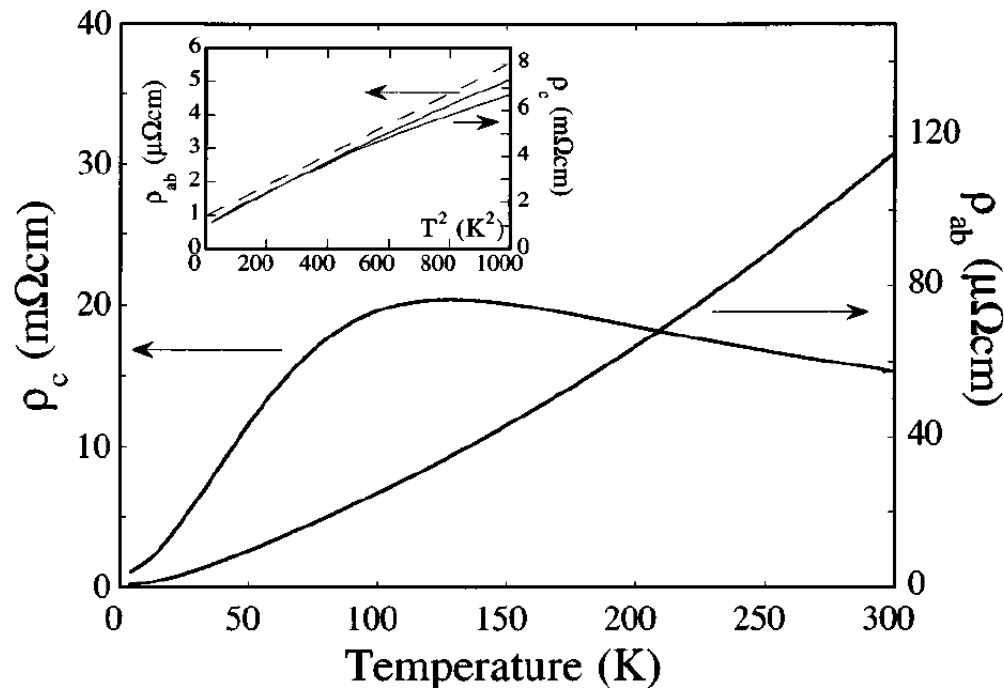
Correlated metal: Fermi
liquid, ($m^*/m \sim 4$)

4 el. in Ru t_{2g} orbitals

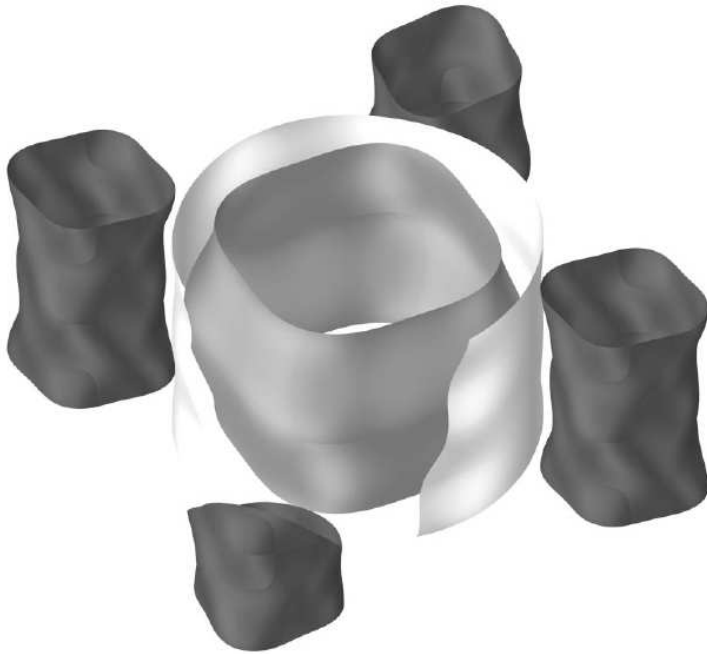


Fermi liquid behavior below 20K

Fact 7: In Fermi liquids $\rho \sim T^2$

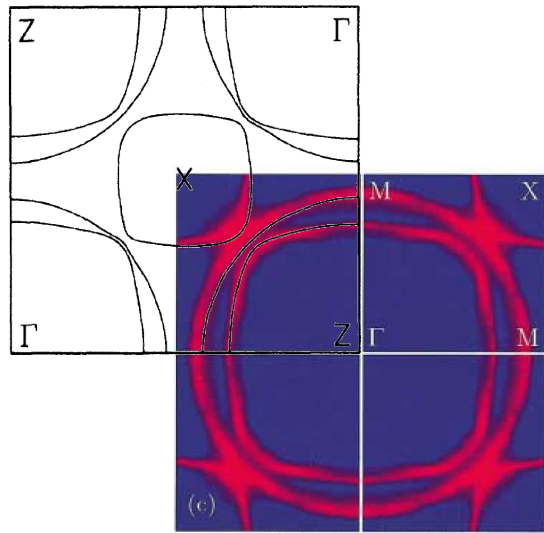


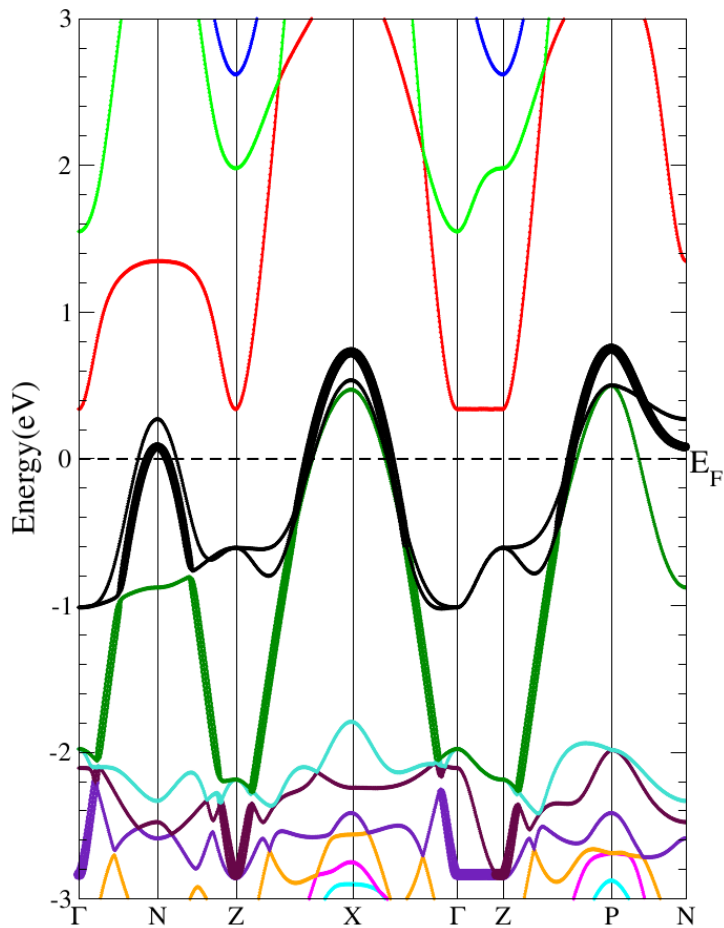
Fermi surfaces



Sr_2RuO_4 : el. structure

LDA and experiments give very similar Fermi surfaces. Shape can be understood (blackboard)





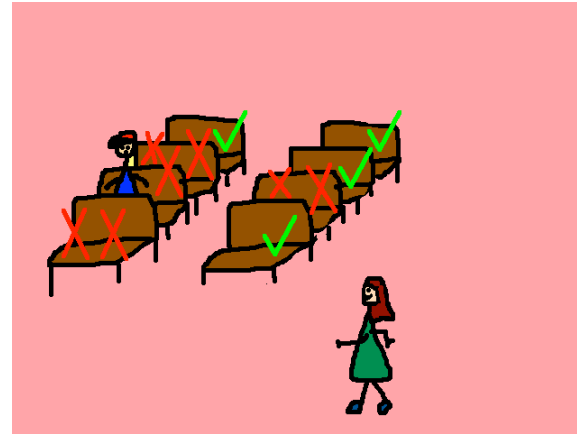
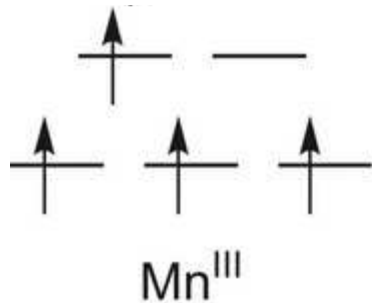
Strong renormalization.
 ~ 4

Band-width 3eV,
 $U \sim 2.5\text{eV}$.

(SrVO_3 had
 renormalization 2, but
 $U \sim 5\text{eV}$)

Going multi-orbital: new ingredient: Hund's rule coupling

- “Bus seat rule”



- Maximize 1st spin, 2nd orbital momentum, 3rd

$$U = \int d\mathbf{r}d\mathbf{r}' |\phi_m(\mathbf{r})|^2 V_c(\mathbf{r}, \mathbf{r}') |\phi_m(\mathbf{r}')|^2,$$

$$U' = \int d\mathbf{r}d\mathbf{r}' |\phi_m(\mathbf{r})|^2 V_c(\mathbf{r}, \mathbf{r}') |\phi_{m'}(\mathbf{r}')|^2, \text{ and}$$

$$J = \int d\mathbf{r}d\mathbf{r}' \phi_m(\mathbf{r}) \phi_{m'}(\mathbf{r}) V_c(\mathbf{r}, \mathbf{r}') \phi_m(\mathbf{r}') \phi_{m'}(\mathbf{r}').$$

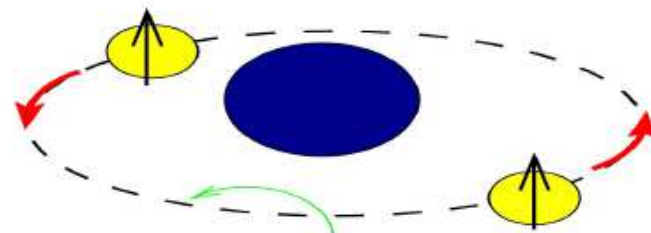
$$H_K = U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} + U' \sum_{m \neq m'} \hat{n}_{m\uparrow} \hat{n}_{m'\downarrow} + (U' - J) \sum_{m < m', \sigma} \hat{n}_{m\sigma} \hat{n}_{m'\sigma} +$$

$$-J \sum_{m \neq m'} d_{m\uparrow}^\dagger d_{m\downarrow} d_{m'\downarrow}^\dagger d_{m'\uparrow} + J \sum_{m \neq m'} d_{m\uparrow}^\dagger d_{m\downarrow}^\dagger d_{m'\downarrow} d_{m'\uparrow}.$$

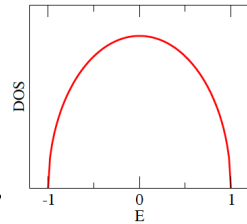
$$V_c = \frac{1}{|\mathbf{r} - \mathbf{r}'|}$$

exchange

$$H_{t_{2g}} = (U - 3J) \frac{\hat{N}(\hat{N} - 1)}{2} - 2J\vec{S}^2 - \frac{J}{2}\vec{L}^2.$$



DMFT results: 3orbital Kanamori model

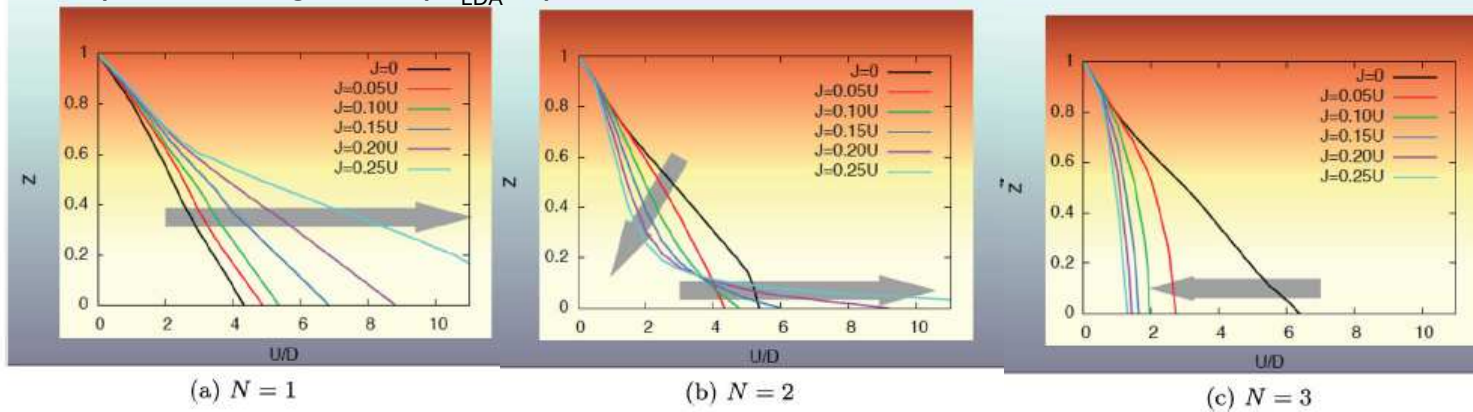


$$H_{t_{2g}} = (U - 3J) \frac{\hat{N}(\hat{N} - 1)}{2} - 2J\vec{S}^2 - \frac{J}{2}L^2$$

- $H = H_{\text{band}} + H_{\text{atom}}$

- Large and filling-dependent effects of J!

Quasiparticle weight $Z \sim (m_{\text{LDA}}/m)$:



- 1. shift of U_c 2. additional effect on correlations

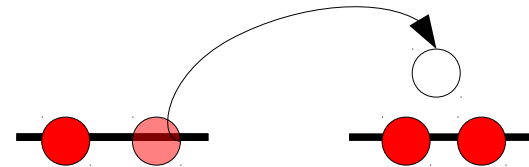
- At $N=2$, correlated state (a “Hund's metal”) far from Mott insulator (for physical values of J)

Why? : Two effects of J

1st modified atomic charge gap

- Effective interaction

$$U_{\text{eff}} = E(N+1) + E(N-1) - 2E(N)$$

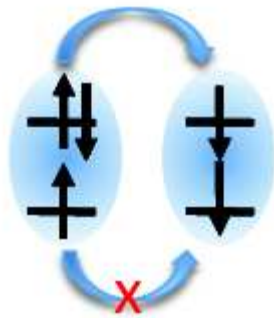


- $U - 3J$ away from half-filling (U_{eff} **diminished** by J)
- $U + (M-1)J$ at half filling (U_{eff} **increased** by J)
- Slater all d-states Hamiltonian (# of orbs. $M=5$)

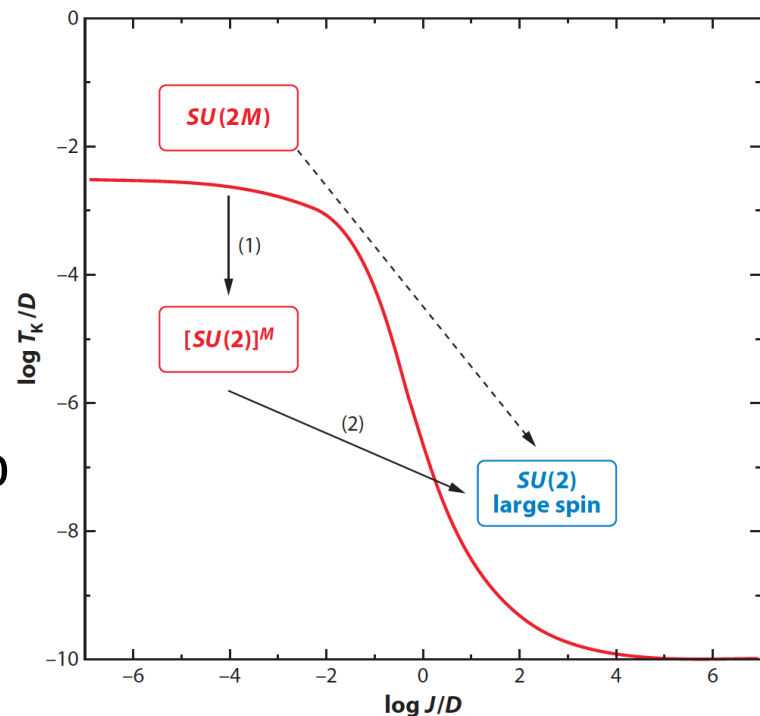
| Effective Coulomb interaction U_{eff} for Hund's rule ground-state | | | | | |
|---|---|-----------------|--------------|---------------------|----------|
| | Full Hamiltonian | Simple | Kanamori | Kanamori mean field | |
| d^1 | $F^0 - \frac{8}{49}F^2 - \frac{9}{441}F^4$ | $U_0 - J_H - C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^2 | $F^0 + \frac{1}{49}F^2 - \frac{54}{441}F^4$ | $U_0 - J_H + C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^3 | $F^0 + \frac{1}{49}F^2 - \frac{54}{441}F^4$ | $U_0 - J_H + C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^4 | $F^0 - \frac{8}{49}F^2 - \frac{9}{441}F^4$ | $U_0 - J_H - C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^5 | $F^0 + \frac{14}{49}F^2 + \frac{126}{441}F^4$ | $U_0 + 4J_H$ | $U_0 + 4J_H$ | $U + 4J$ | $U + 4J$ |
| d^6 | $F^0 - \frac{8}{49}F^2 - \frac{9}{441}F^4$ | $U_0 - J_H - C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^7 | $F^0 + \frac{1}{49}F^2 - \frac{54}{441}F^4$ | $U_0 - J_H + C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^8 | $F^0 + \frac{1}{49}F^2 - \frac{54}{441}F^4$ | $U_0 - J_H + C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |
| d^9 | $F^0 - \frac{8}{49}F^2 - \frac{9}{441}F^4$ | $U_0 - J_H - C$ | $U_0 - J_H$ | $U' - J$ | $U' - J$ |

2nd effect: J suppresses tunneling

- J lowers atomic degeneracy, blocks orbital fluctuations, hence prohibits some of the hopping
- Example: Create a charge excitation in half-filled two orbital problem. J allows it to move only in one of two possible ways.



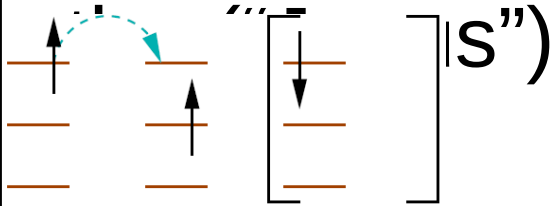
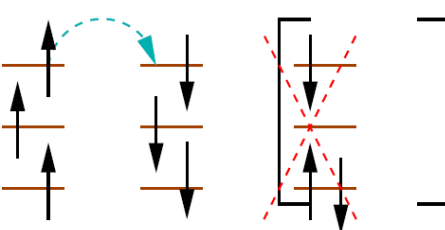
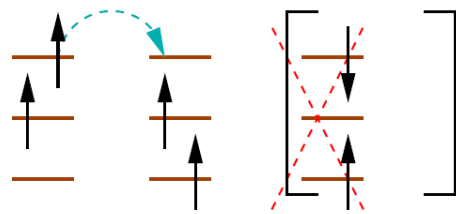
- Suppression of tunneling \rightarrow Kondo temperature known for a long time in Kondo problem



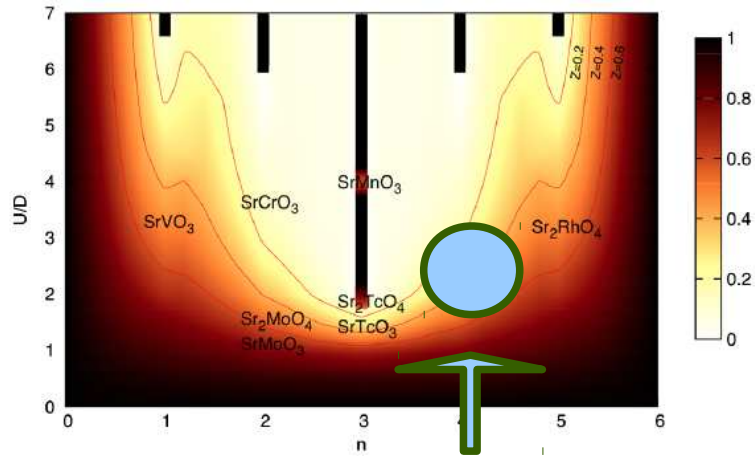
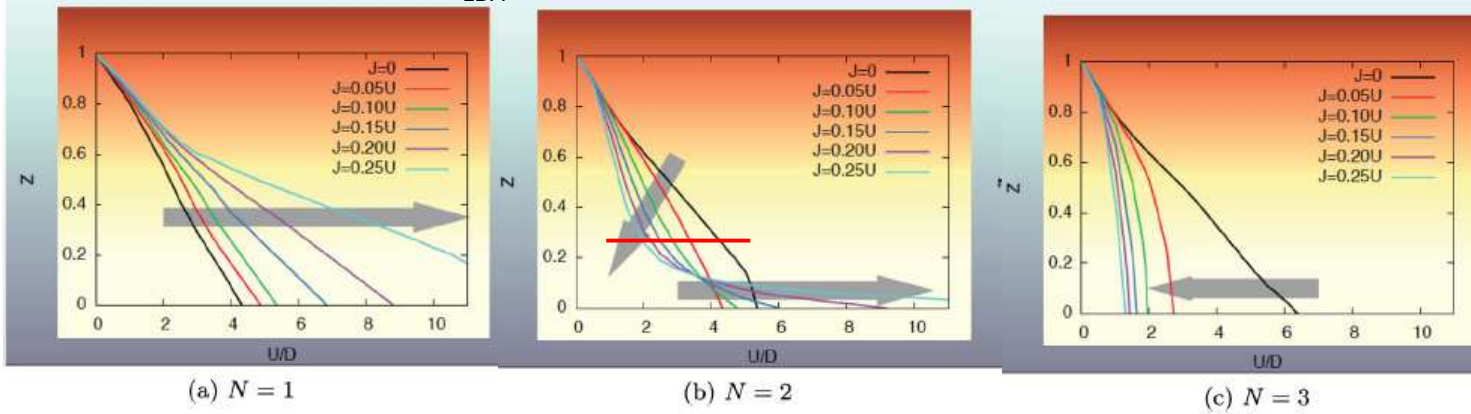
Yanase et al, J.Phys.Soc.Jpn. '97

(Schrieffer 1967, Okada, Yosida 1973, Jayaprakash et al, 1981, Nevidomskiy-Coleman 2009).

A localized perspective

| | single occ. | half-filled | |
|-------------------|---|--|---|
| atomic deg. |  <p>6 (unchanged by J)</p> |  <p>20 (supp → 4 by J)</p> |  <p>15 (supp → 9 by J)</p> |
| E of charge excit | diminished | increased | diminished |
| drives | metallic | insulating | incoherent metallic |

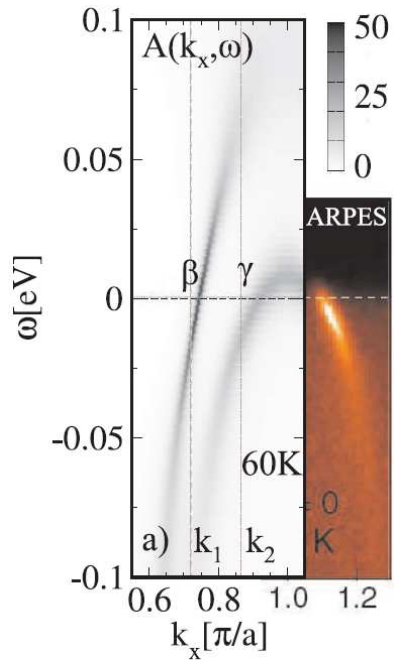
Quasiparticle weight $Z \sim (m_{LDA}/m)$:



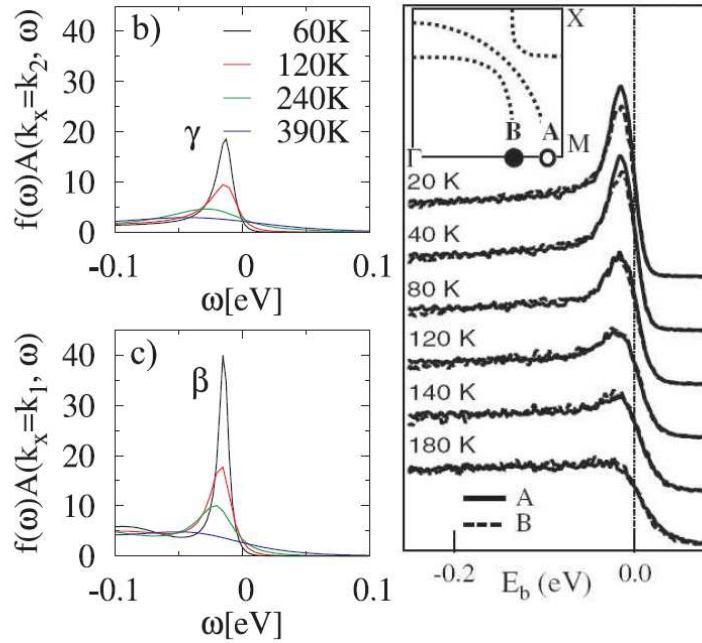
Correlated state, far from Mott, ruthenates and pnictides.

Coherence-incoherence crossover in Sr_2RuO_4

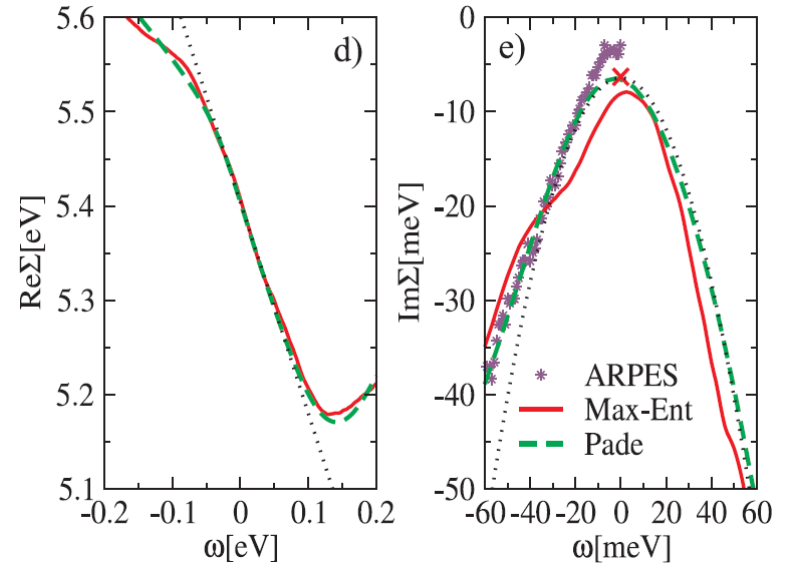
ARPES



Shen et al., PRL'07



Wang et al., PRL'04

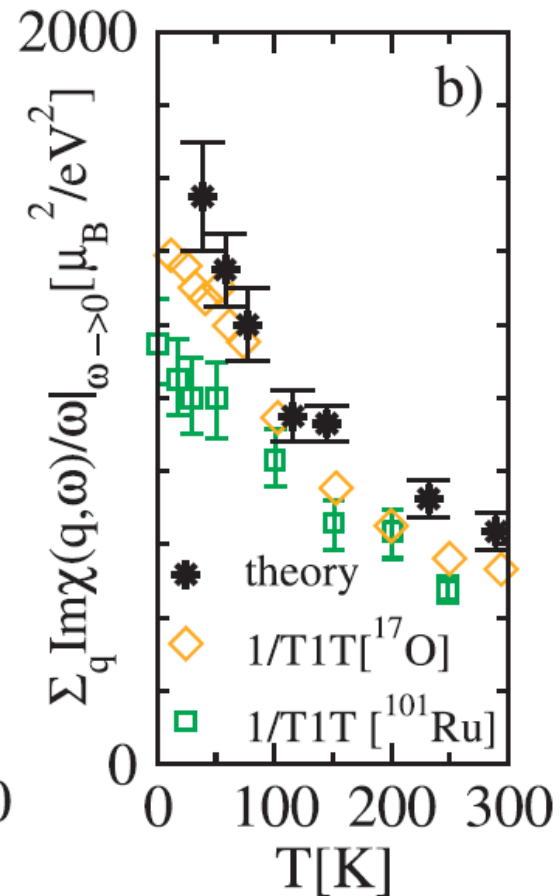
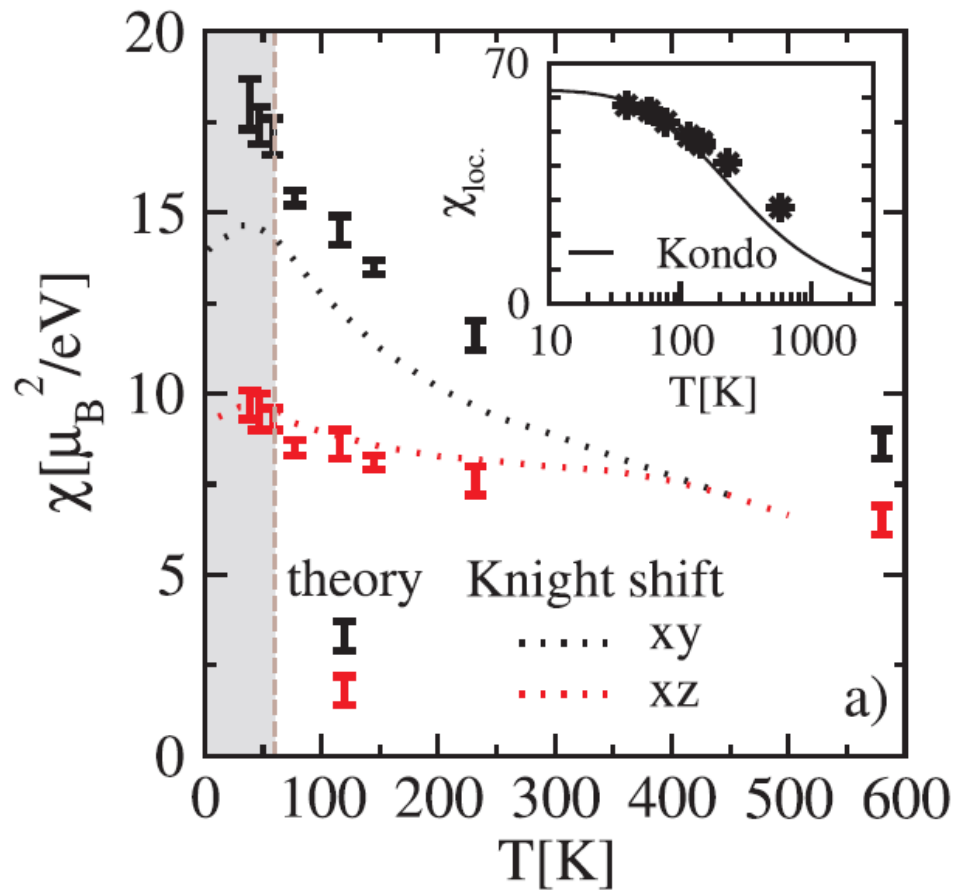


Ingle et al., PRB'05

Magnetic response

Pauli susceptibility

$$1/T_1 \sim T$$

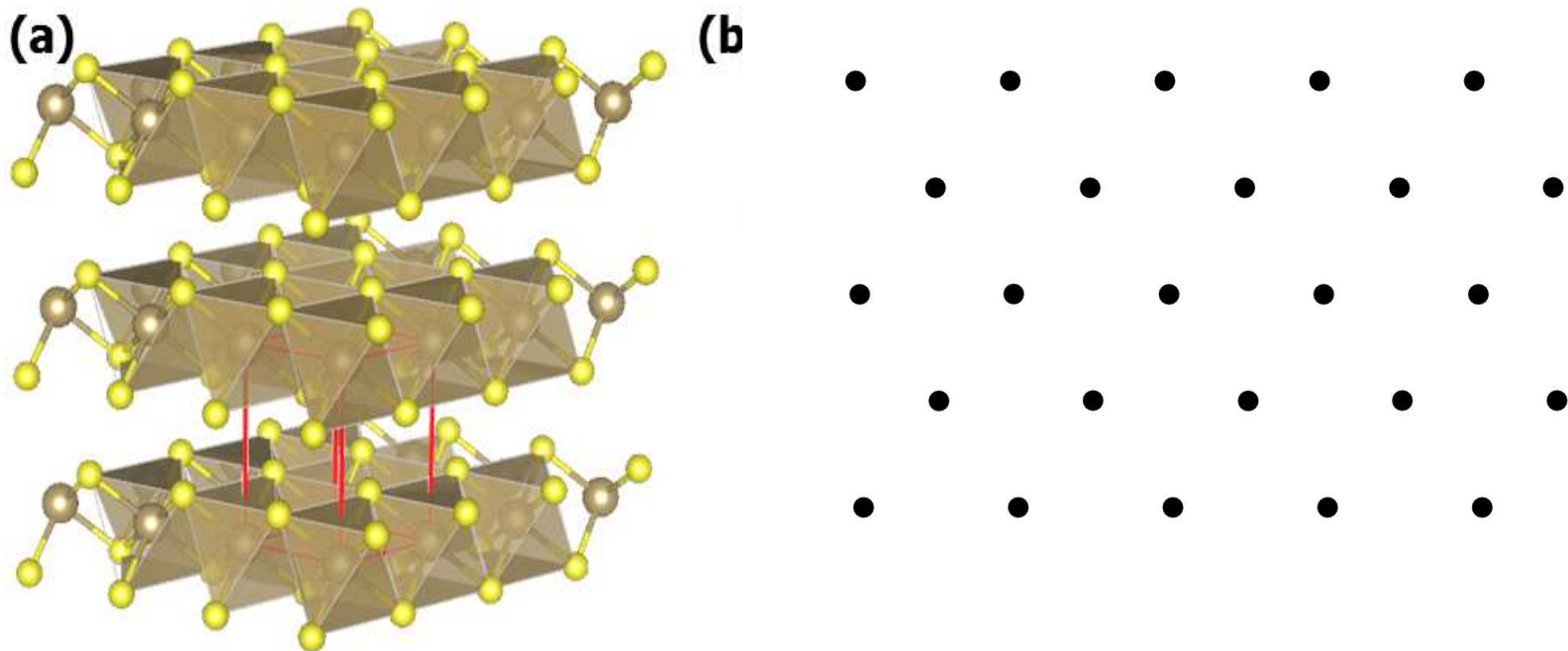


Fact 8: Many correlated electron systems are well described by
LDA+DMFT

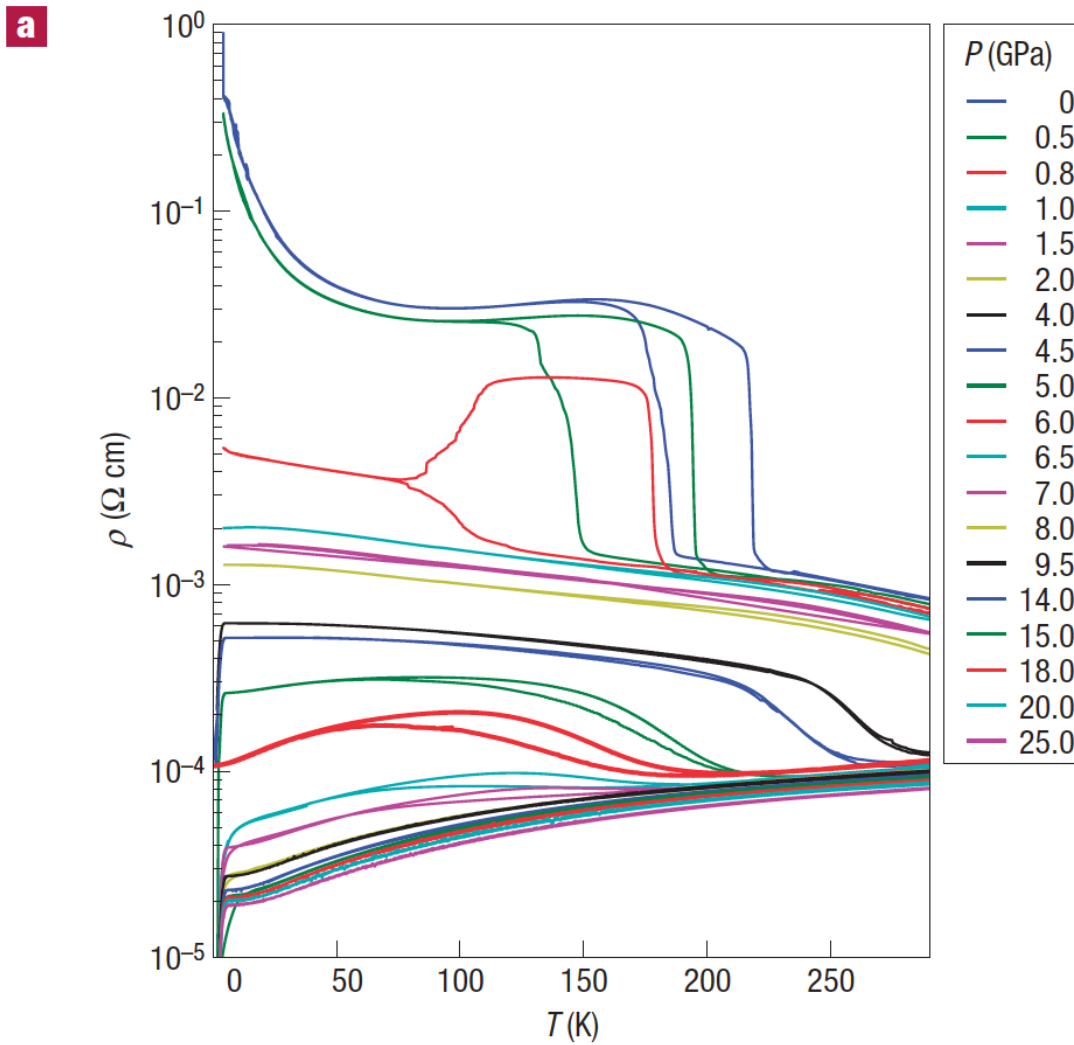


TaS₂

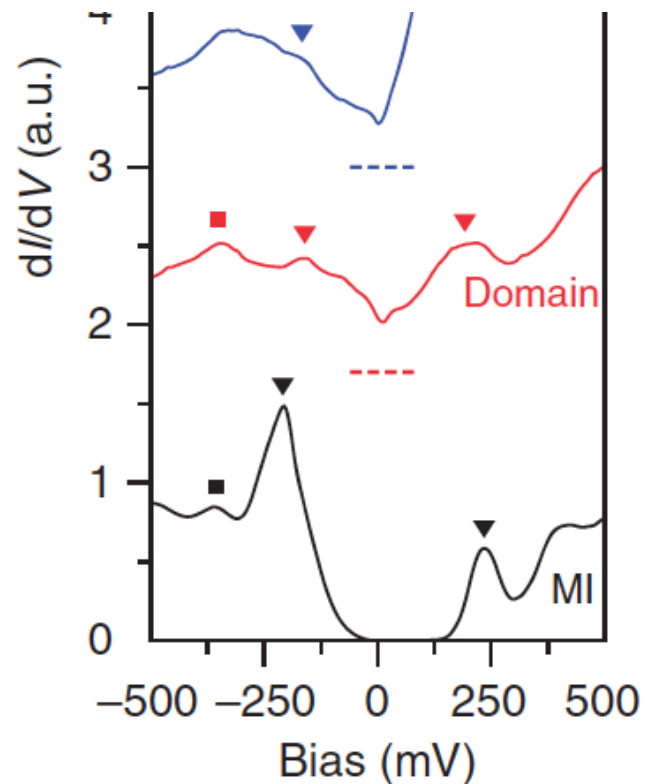
- TaS₂ one electron in Ta d-bands (local t_{2g} env.)
- Layers of triangular lattices
- 5-d electrons (small U)



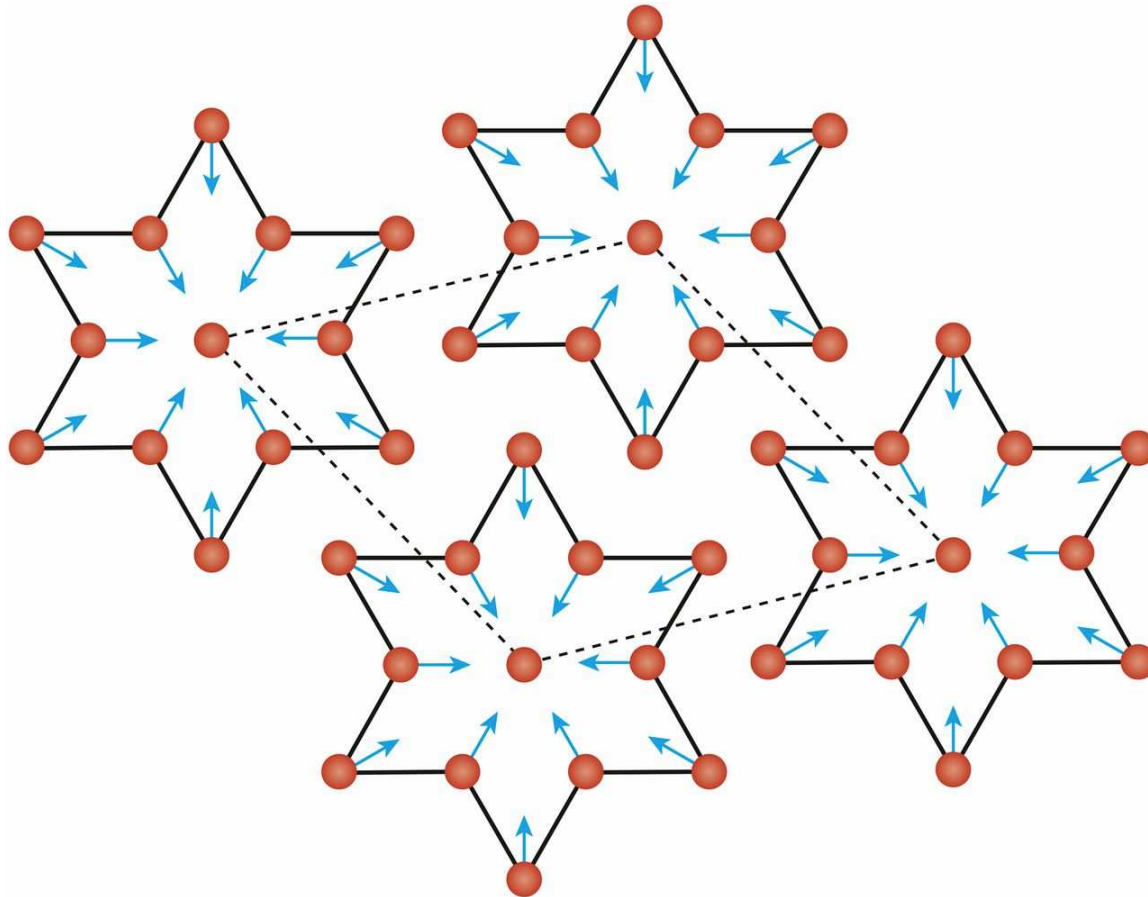
Mott transition



- STS shows insulating behavior (also optics)
- Small gap (0.1eV)

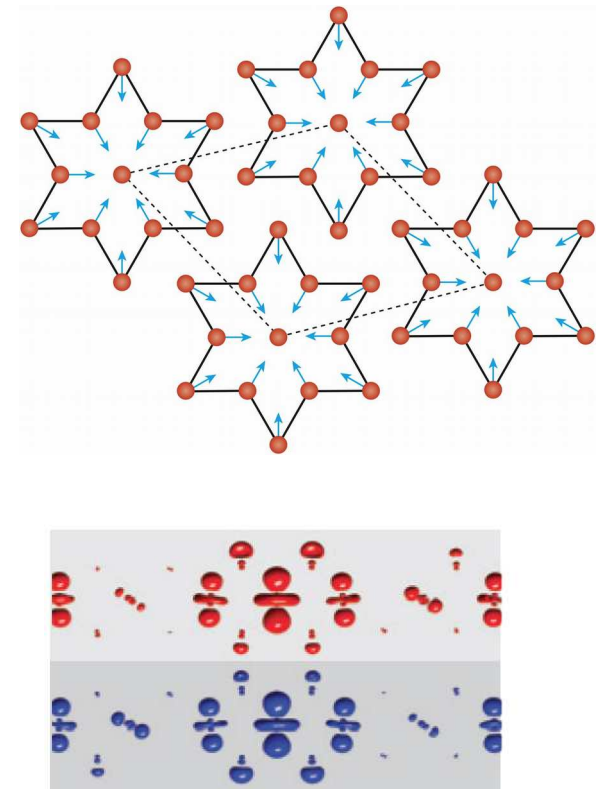
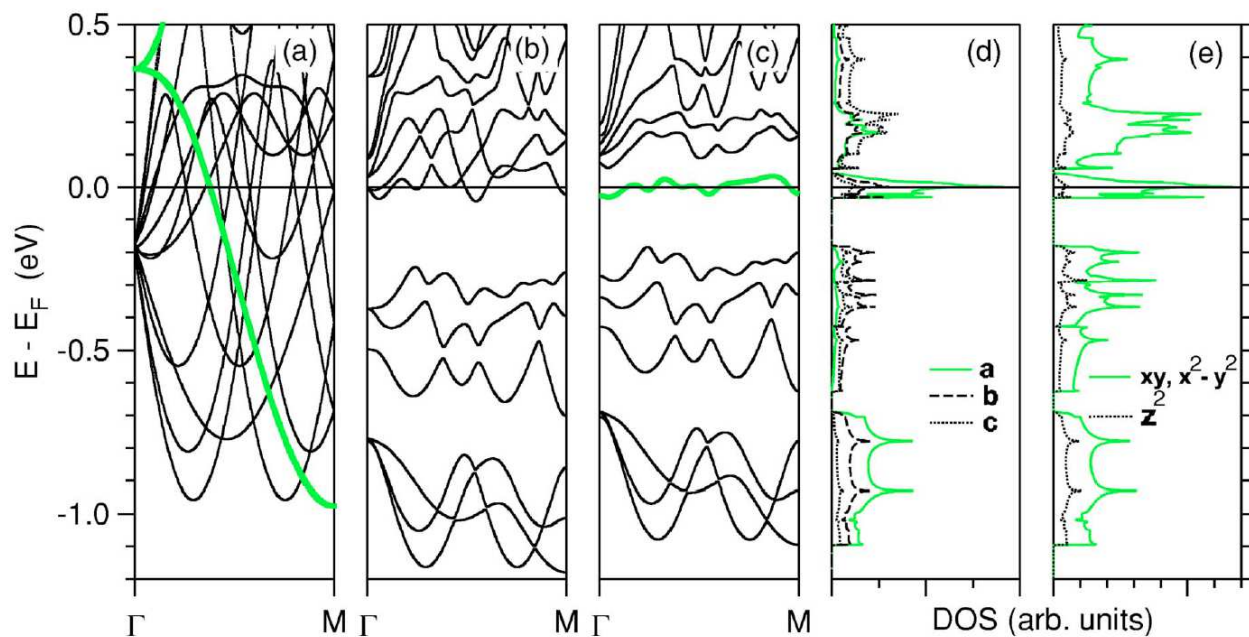


- Actually, a set of structural transitions. Mott state is realized in CDW at low-T.



Narrow band close to FL following structural transition

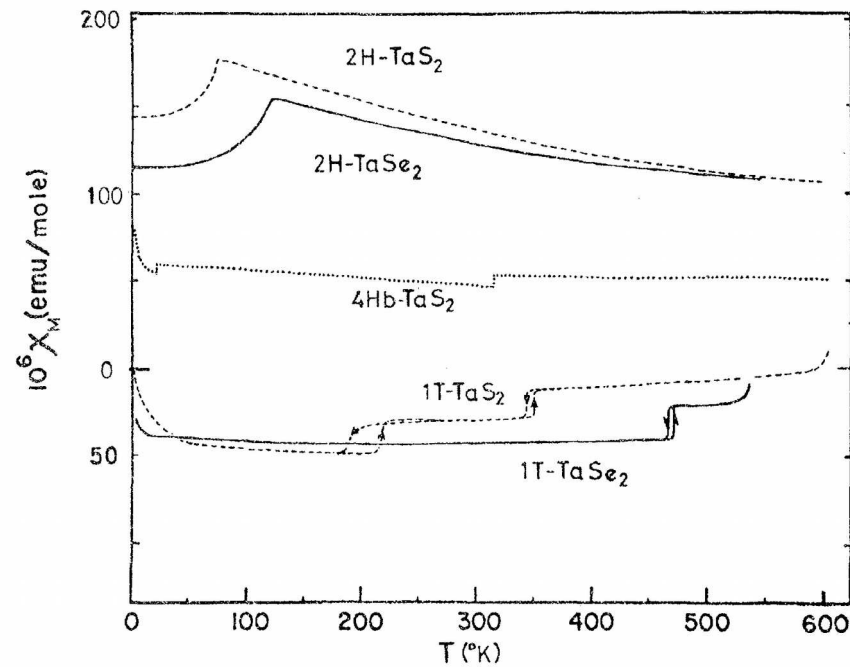
- 1 band per cluster of 13 Ta atoms relevant at low energies



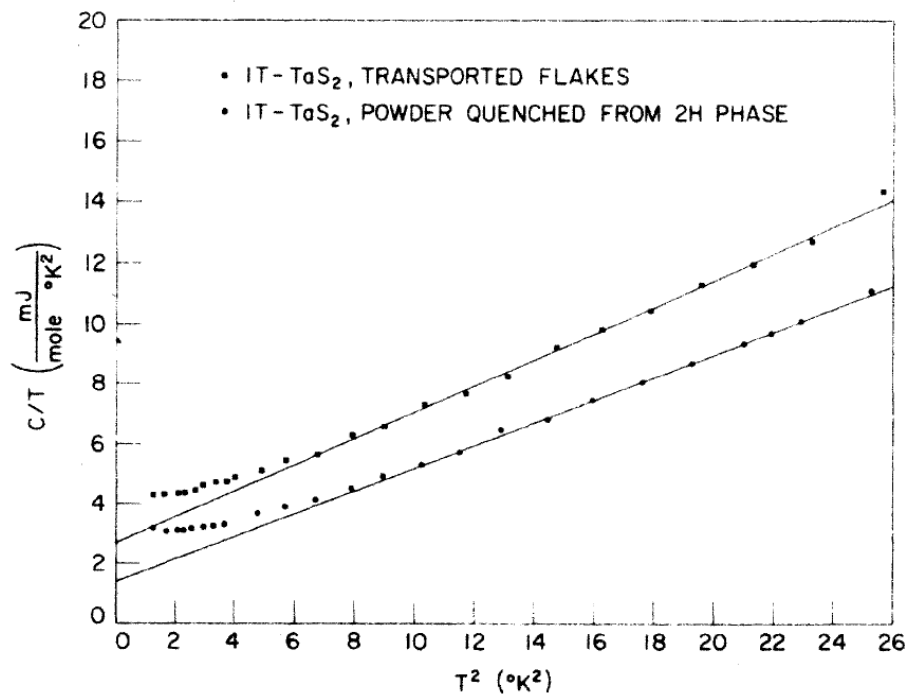
- If it is a Mott insulator, what do spins do ?

Mott insulator, but Pauli susceptibility?

- Pauli magnetic susceptibility

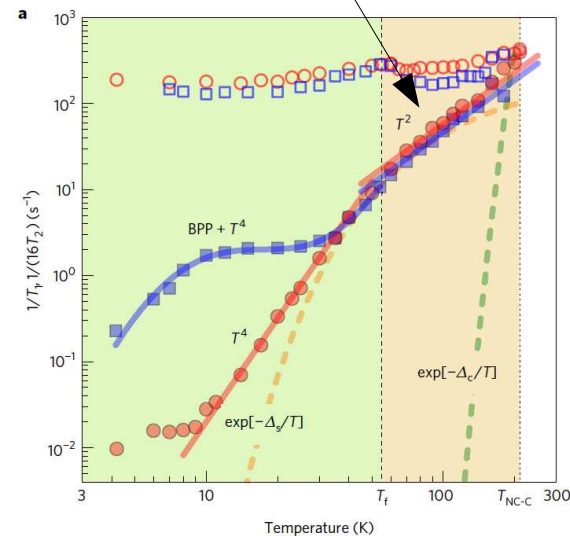


- Finite linear in T specific heat. Like in metals.



Collaboration with F5/F7

- Klanjsek et al, Nphys'17
- No magnetic order (muon spectroscopy)
- $1/T_1$ shows unusual T^2 dependence
- Spin liquid!



Summary

- Atomistic/ band-structure point of view on correlated electron systems
- LDA describes band-structure of many compounds well, but breaks down when U is strong
- Mott transition ; DMFT
- Sr_2RuO_4 : low coherence scale & Hund's coupling
- TaS_2 Mott insulator at small U ; spin-liquid behavior

Fact 1: there is a thing called DFT and it describes the bandstructure of many compounds well

Fact 2: Several experimental techniques exist that allow quantitative comparison with theory

Fact 3: strong Coulomb repulsion leads to a breakdown of band theory and occurrence of Mott insulator

Fact 4: orbitals matter!

Fact 5: Mott insulators are magnets

Fact 6: DOS of correlated metals consists of quasiparticle peak and Hubbard bands

Fact 7: in Fermi liquids $\rho \sim T^2$

Fact 8: Many correlated electron systems are well described by DMFT (LDA+DMFT)

Thank you!

