Outline of lectures : refresher in many-body theory

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0.1 Prologue

Below, I make reference to the following free lecture notes. If you feel you are missing some prerequisites, everything is in these lecture notes.

http://www.physique.usherbrooke.ca/tremblay/cours/phy-892/N-corps.pdf

Many of these lectures are on YouTube (PHY892 Problème à N-corps / Many-Body problem Playlist)

https://studio.youtube.com/channel/amstremblay

0.2 Lecture 1 Second quantization and perturbation theory

(30 minutes) What are corelations (Reza Nourafkan)

0.2.1 Second quantization

(30 minutes) Chapter 81 : Handeling many-interacting particles : Second quantization

81.1 Fock space : Creation-annihilation operators

Number operator

81.2 Change of basis

87.2.1 Position and momentum basis

87.2.2 Wave functions

81.3 One-body operators

81.4 Two-body operators

0.2.2 The Hubbard model

(30 minutes) Chapter 82 The Hubbard model to illustrate some of the concepts

82.1 The Hubbard model

$$H = \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow} \tag{1}$$

0.2.3 Interaction representation, time-ordering product

(30 minutes) Chapter 83 Perturbation theory (interaction representation)

$$e^{-\beta \widehat{K}} = e^{-\beta \widehat{K}_0} \widehat{U}(\beta) \tag{2}$$

$$\widehat{U}(\beta) \equiv T_\tau \left[e^{-\int_0^\beta \widehat{K}_1(\tau) d\tau} \right] \tag{3}$$

$$\widehat{K}_1(\tau) \equiv e^{\widehat{K}_0 \tau} \widehat{K}_1 e^{-\widehat{K}_0 \tau}. \tag{4}$$

0.3 Lecture 2 Green's functions, Matsubara formalism, self-energy, Wick's theorem

0.3.1 Green's functions in the Matsubara formalism

(40 minutes) Chapter 29 Matsubara Green Functions

29.1.1 Photoemission and fermion correlation functions

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} \langle m| c^\dagger_{\mathbf{k}_{||}} |n\rangle \langle n| c_{\mathbf{k}_{||}} |m\rangle \delta(\omega - (K_m - K_n)) \tag{5}$$

29.1 Definition for fermions

$$\mathcal{G}_{\alpha\beta}(\tau) = -\left\langle T_\tau c_\alpha(\tau) c^\dagger_\beta(0) \right\rangle \tag{6}$$

$$= -\left\langle c_\alpha(\tau) c^\dagger_\beta(0) \right\rangle \theta(\tau) + \left\langle c^\dagger_\beta(0) c_\alpha(\tau) \right\rangle \theta(-\tau). \tag{7}$$

29.3 Antiperiodicity and Fourier representation (Matsubara frequencies)

$$\mathcal{G}_{\alpha\beta}(ik_n) = \int_0^\beta d\tau e^{ik_n \tau} \mathcal{G}_{\alpha\beta}(\tau) \tag{8}$$

29.5 Lehmann representation

$$A(\mathbf{k}; \omega') = e^{\beta\Omega} \sum_{mn} \left(e^{-\beta K_n} + e^{-\beta K_m} \right) \langle n| c(\mathbf{k}) |m\rangle \langle m| c^\dagger(\mathbf{k}') |n\rangle 2\pi\delta(\omega' - (K_m - K_n)) \tag{9}$$

Spectral weight and how it is related to $\mathcal{G}_{\mathbf{k}}(ik_n)$ and to photoemission

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto A_{\mathbf{k}}(\omega) f(\omega) \tag{10}$$

29.8 Non-interacting case

$$\mathcal{G}_{\mathbf{k}}(ik_n) = \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{11}$$

29.7 Spectral weight

Obtaining the spectral weight from $\mathcal{G}_{\mathbf{k}}(ik_n)$, the problem of analytic continuation

$$\mathcal{G}_{\mathbf{k}}(ik_n) = \int \frac{d\omega'}{2\pi} \frac{A_{\mathbf{k}}(\omega')}{ik_n - \omega'} \quad (12)$$

$$G^R_{\mathbf{k}}(\omega) = \int \frac{d\omega'}{2\pi} \frac{A_{\mathbf{k}}(\omega')}{\omega + i\eta - \omega'} \quad (13)$$

29.2 Time-ordering in practice

0.3.2 The notion of self-energy, what it means, what it hides

(20 minutes) Chapter 17 Self-energy

18.3 Importance of poles of $G^R_{\mathbf{k}}$, Dyson's equation

$$\mathcal{G}_{\mathbf{k}}(ik_n) = \mathcal{G}^0_{\mathbf{k}}(ik_n) + \mathcal{G}^0_{\mathbf{k}}(ik_n)\,\Sigma_{\mathbf{k}}(ik_n)\,\mathcal{G}_{\mathbf{k}}(ik_n) \quad (14)$$

$$G^R_{\mathbf{k}\uparrow}(\omega)^{-1} = G^{(0)R}_{\mathbf{k}\uparrow}(\omega)^{-1} - \Sigma^R_{\mathbf{k}\uparrow}(\omega) \quad (15)$$

85.3 A few properties of the self-energy

$$\mathrm{Im}\,\Sigma^R_{\mathbf{k}\uparrow}(\omega) < 0 \quad (16)$$

0.3.3 Wick's theorem, response functions, RPA

(30 minutes) 86 and C3 Wick's theorem (hybridization function)

85.4 Anderson Impurity problem, hybridization function

$$G^R_{\uparrow}(\omega)^{-1} = G^{(0)R}_{\uparrow}(\omega)^{-1} - \Delta^R_{\uparrow}(\omega) - \Sigma^R_{\uparrow}(\omega)\,. \quad (17)$$

39 Lindhard function

39.1 Definition

39.1 Non-interacting limit

41.1 Density-density correlations, RPA

56.3 Hartree-Fock and RPA

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U\chi_0(q)} \quad (18)$$

$$\chi_{ch}(q) = \frac{\chi_0(q)}{1 + \frac{1}{2}U\chi_0(q)} \quad (19)$$

56.4 RPA and violation of the Pauli exclusion principle

$$\frac{T}{N}\sum_q \left(\frac{\chi_0(q)}{1 - \frac{1}{2}U\chi_0(q)} + \frac{\chi_0(q)}{1 + \frac{1}{2}U\chi_0(q)} \right) \neq 2n - n^2 \quad (20)$$

Non-interacting electrons

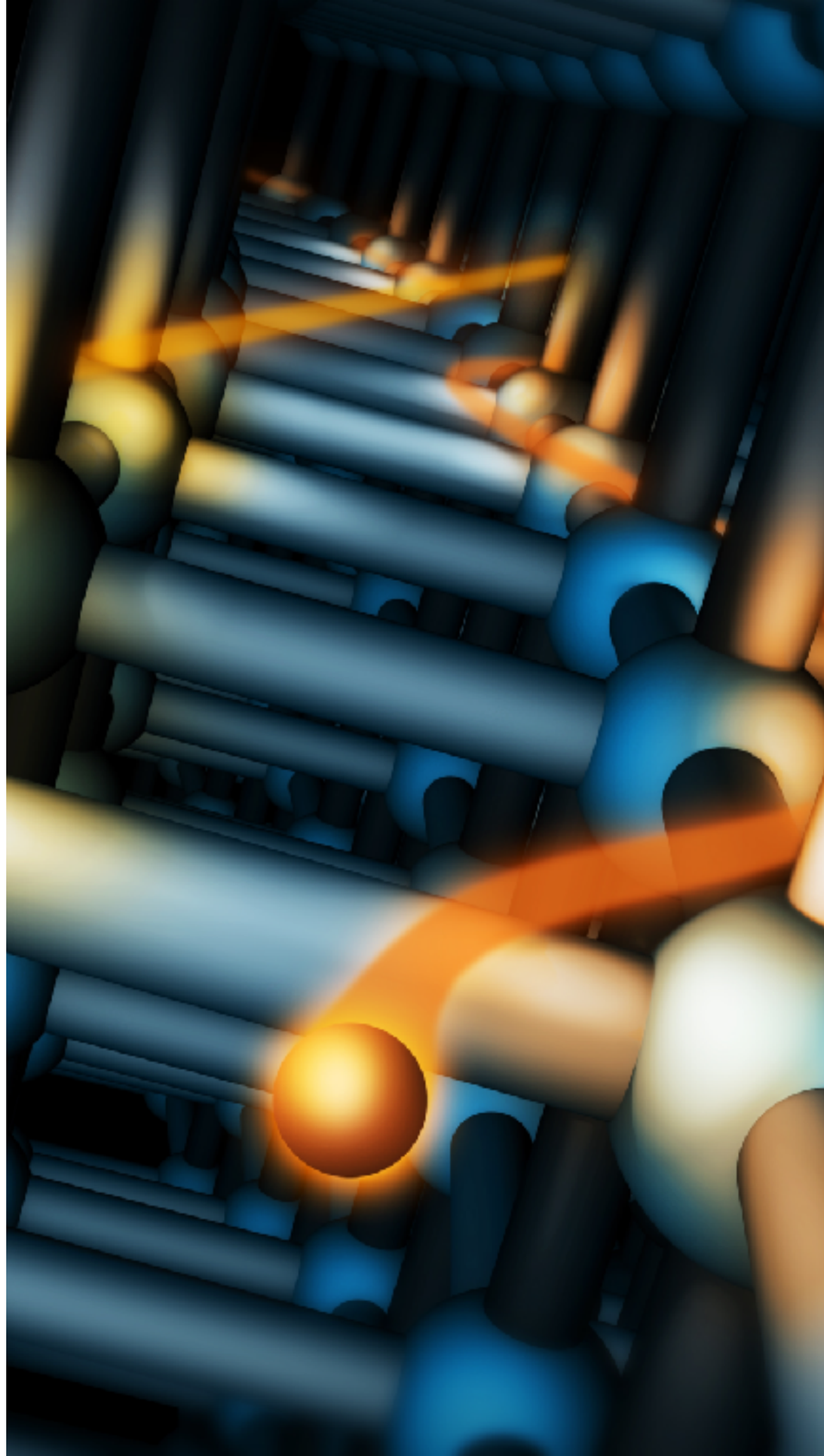
- A wave function composed of a *single* Slater determinant

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1\sigma_1) & \phi_2(\mathbf{r}_1\sigma_1) & \dots & \phi_N(\mathbf{r}_1\sigma_1) \\ \phi_1(\mathbf{r}_2\sigma_2) & \phi_2(\mathbf{r}_2\sigma_2) & \dots & \phi_N(\mathbf{r}_2\sigma_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N\sigma_N) & \phi_2(\mathbf{r}_N\sigma_N) & \dots & \phi_N(\mathbf{r}_N\sigma_N) \end{vmatrix}$$

Slides taken with permission from a course by
Reza Nourafkan

ELECTRON CORRELATION PECULIARITY

QUANTUM MECHANICS, INDISTINGUISHABLE PARTICLES



CORRELATION IN EVERYDAY LIFE

IN A MANY BODY SYSTEM, THE BEHAVIOUR OF A GIVEN ENTITY IS NOT INDEPENDENT OF THE OTHERS!

CORRELATION IN MATHEMATICS & NATURAL SCIENCES

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

$$C_{AB} = \langle AB \rangle - \langle A \rangle \langle B \rangle$$

- Spatial

$$\langle n(\mathbf{r}, t) n(\mathbf{r}', t) \rangle \neq \langle n(\mathbf{r}, t) \rangle \langle n(\mathbf{r}', t) \rangle$$

- Temporal

$$\langle n(\mathbf{r}, t) n(\mathbf{r}, t') \rangle \neq \langle n(\mathbf{r}, t) \rangle \langle n(\mathbf{r}, t') \rangle$$

MANY-BODY PROBLEM IN SOLIDS

- Many-body Hamiltonian of an electronic system

$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i \hat{\nabla}_i^2 + \frac{1}{2}\sum_{i\neq i'}\frac{e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_{i'}|} - \sum_{i\hat{\alpha}}\frac{Z_\alpha e^2}{|\hat{\mathbf{r}}_i - \hat{\mathbf{R}}_\alpha|}$$
$$-\sum_\alpha \frac{\hbar^2}{2M_\alpha}\hat{\nabla}_\alpha^2 + \frac{1}{2}\sum_{\alpha\neq\alpha'}\frac{Z_\alpha Z'_\alpha e^2}{|\hat{\mathbf{R}}_\alpha - \hat{\mathbf{R}}_{\alpha'}|}$$

- Many-body wave-function for N electrons

$$\Psi(\mathbf{r}_1\sigma_1, \ldots, \mathbf{r}_N\sigma_N)$$

MANY-BODY PROBLEM IN SOLIDS

- Trial many-body wave function for an N electrons system

$$\Psi(\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N) = \sum_i c_i\psi_i(\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N)$$

$$\langle\Psi|\hat{H}|\Psi\rangle = \sum_{ij} c_i^* c_j \langle\psi_i|\hat{H}|\psi_j\rangle$$

- Many-body basis set?
  - Product of one-particle wave-functions
    - Choose M (M>N) single particle basis function (spin-orbital)

$$\{\phi_{1\sigma_1}(\mathbf{r}),\phi_{2\sigma_2}(\mathbf{r}),\ldots,\phi_{M\sigma_M}(\mathbf{r})\}$$

    - Electrons are indistinguishable fermions

$$(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2) = -\Psi(\mathbf{r}_2\sigma_2,\mathbf{r}_1\sigma_1)$$

WHY IS THE PROBLEM OF ELECTRONIC STRUCTURE HARD?

- N electrons system and M (M>N) single particle basis function

$$\Psi(\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N)=\sum_i c_i\psi_i(\mathbf{r}_1\sigma_1,\ldots,\mathbf{r}_N\sigma_N)$$

- Number of Slater determinants

$$\binom{M}{N}=\frac{M!}{N!(M-N)!}$$

- Two carbon atoms (N=12). Suppose M=36

more that 10^9 determinants

Dimensionality

IT IS HOPELESS TO LOOK FOR AN EXACT SOLUTION OF A MANY-BODY SYSTEM

How we are going to proceed?

HARTREE-FOCK METHOD

- A wave function composed of a *single* Slater determinant

$$= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1\sigma_1) & \phi_2(\mathbf{r}_1\sigma_1) & \dots & \phi_N(\mathbf{r}_1\sigma_1) \\ \phi_1(\mathbf{r}_2\sigma_2) & \phi_2(\mathbf{r}_2\sigma_2) & \dots & \phi_N(\mathbf{r}_2\sigma_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{r}_N\sigma_N) & \phi_2(\mathbf{r}_N\sigma_N) & \dots & \phi_N(\mathbf{r}_N\sigma_N) \end{vmatrix}$$

- The single-electron functions are chosen *cleverly* to produce the best approximation possible $\delta\langle\psi|H|\psi\rangle/\delta\phi_i^* = 0$

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 + \sum_\alpha \frac{Z_\alpha e^2}{|\mathbf{r}-\mathbf{R}_\alpha|} \right)\phi_i(\mathbf{r}) + \left(\sum_j^{occ} \int d\mathbf{r}'\phi_j^*(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\phi_j(\mathbf{r}') \right)\phi_i(\mathbf{r})$$

Hatree-potential

$$- \left(\sum_j^{occ} \int d\mathbf{r}'\phi_j^*(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\phi_i(\mathbf{r}') \right)\phi_j(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

Exchange-potential

SLATER DETERMINANTS ARE UNCORRELATED

- The repulsion energy between two electrons is calculated between an electron and the average electron density for the other electrons

It doesn't take into account the fact that the electron will push away the other electrons as it moves around

- Probability density of finding two electrons

$$\rho(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \sum_{\sigma_3 \ldots \sigma_N} \int d\mathbf{r}_3 \ldots d\mathbf{r}_N |\psi(\mathbf{r}_1\sigma_1, \ldots, \mathbf{r}_N\sigma_N)|^2$$

$$= \frac{1}{N(N-1)} \sum_{kl} \left[|\phi_k(\mathbf{r}_1\sigma_1)|^2 |\phi_l(\mathbf{r}_2\sigma_2)|^2 - \phi_k^*(\mathbf{r}_1\sigma_1)\phi_k(\mathbf{r}_2\sigma_2)\phi_l^*(\mathbf{r}_2\sigma_2)\phi_l(\mathbf{r}_1\sigma_1) \right]$$

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\sigma_1\sigma_2} \rho(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$$

Opposite spin orbitals are uncorrelated!

KOHN–SHAM APPROACH

- It is not essential to tabulate the complete many-body wave function
- The Kohn-Sham approach to DFT defines *an auxiliary system of independent fermions* that is chosen to reproduce the ground state *electron density* but not all properties
- DFT guarantees us that such an auxiliary system exist end even more provides us a generator for its external potential

$$(-\frac{\hbar^2}{2m_e}\nabla^2 + v_{eff}(\mathbf{r}))\phi_i(\mathbf{r}) = \epsilon_i\phi_i(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_i f_i|\phi_i(\mathbf{r})|^2$$

$$v_{eff}(\mathbf{r}) = v_{ext}(\mathbf{r}) + v_H([n],\mathbf{r}) + v_{xc}([n],\mathbf{r})$$

Universal exchange-correlation functional

WHAT IS MEANT BY ELECTRON CORRELATION?

- Chemist: what is not captured in Hartree-Fock method
  - Correlation energy

$$E_{\text{corr}} = \langle \Psi | H | \Psi \rangle - E_{\text{HF}}$$

$$|\Sigma(\omega) - \Sigma_{HF}|$$

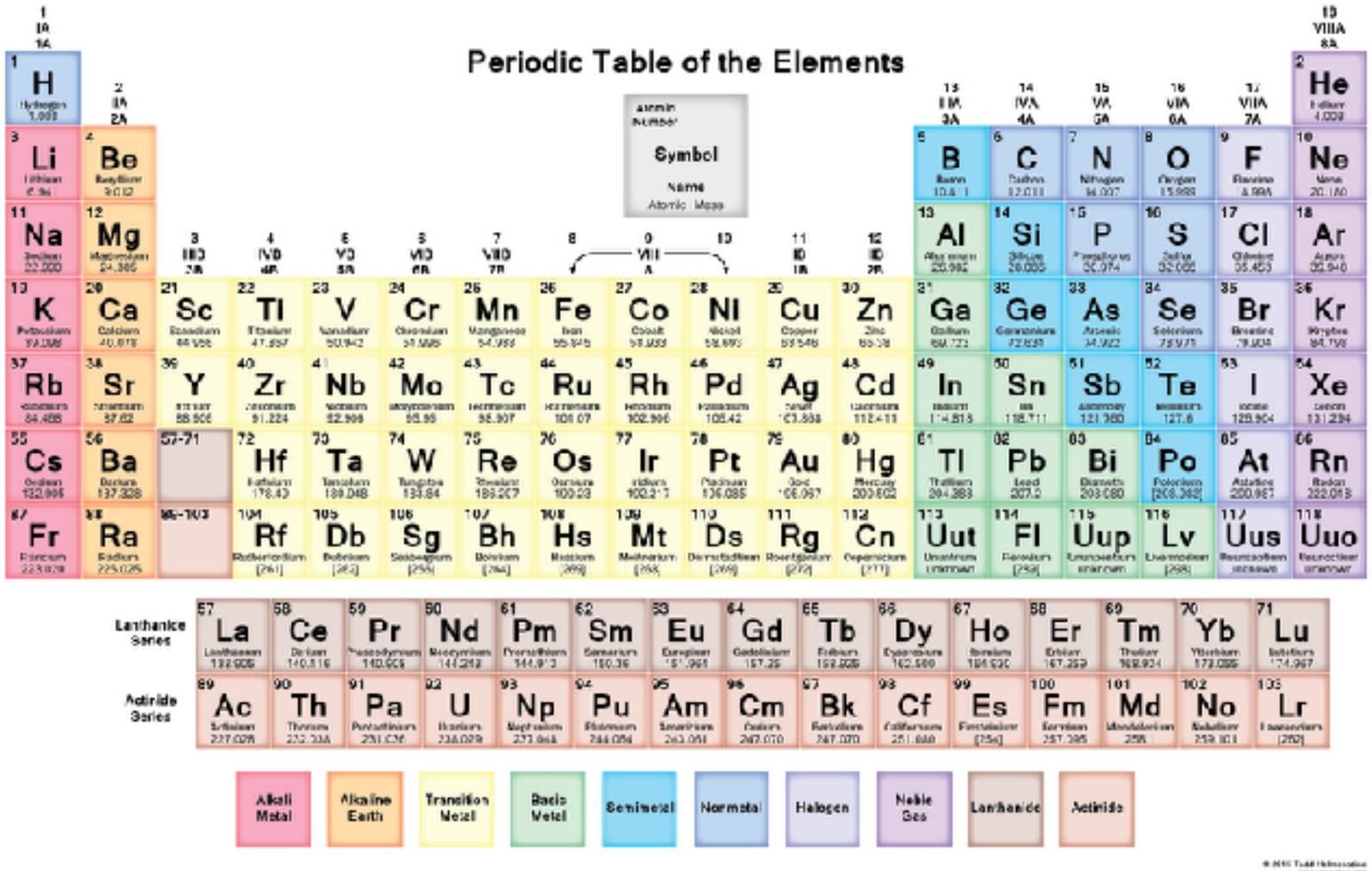
- Physicist: what is not captured in Khon-Sham approach in LDA/GGA approximation
  - Correlation energy

$$E_{\text{corr}} = \langle \Psi | H | \Psi \rangle - E_{\text{LDA/GGA}}$$

$$|\Sigma(\omega) - v_{xc}^{LDA/GGA}|$$

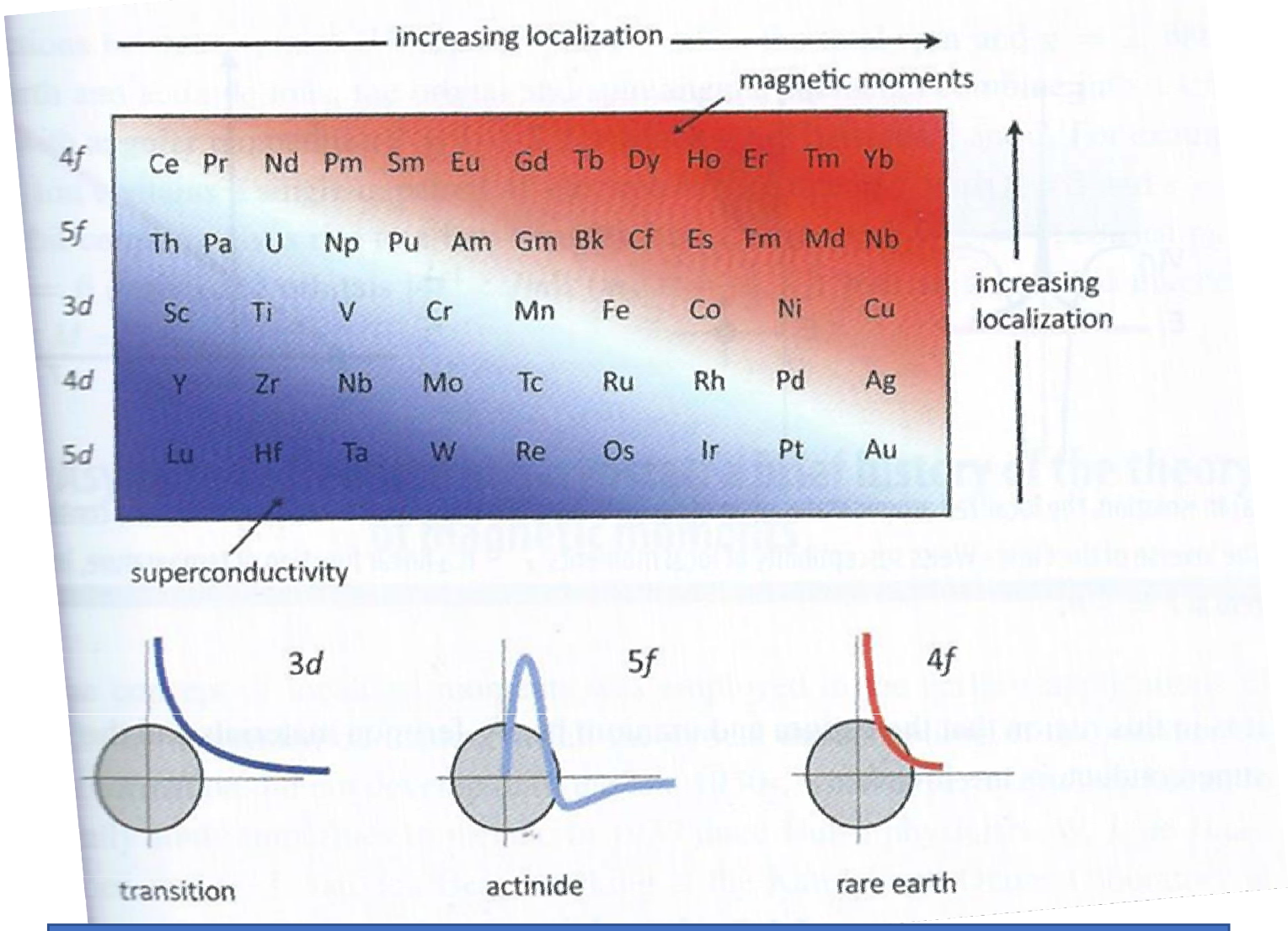
WEAK VS STRONG CORRELATIONS

- A weakly-correlated system is one for which a mean-field approximation or a low-order perturbation expansion around it suffices



J.L. Smith, E.A. Kmetko *

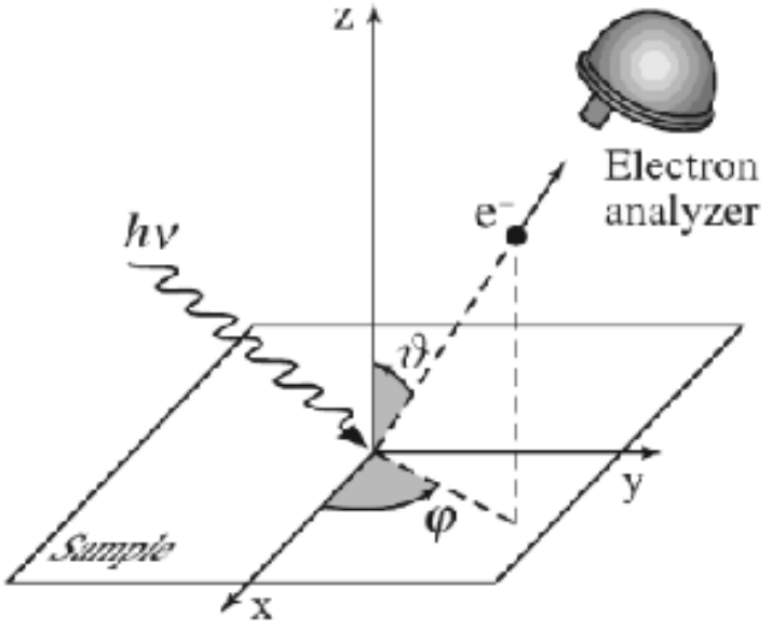
Journal of the Less Common Metals
Volume 90, Issue 1, March 1983, Pages 83-88



ELECTRON CORRELATION SIGNATURES

Thermodynamic and transport properties which are fundamentally different from mean-field theory or Landau Fermi-liquid theory predictions

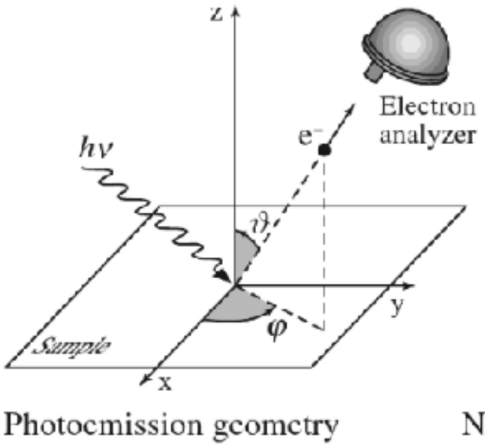
Photoemission: measuring single-electron E(**k**)



Photocmission gcomctry N

Fermi liquid

T. Valla, A. V. Fedorov, P. D. Johnson, and S. L. Hulbert
P.R.L. **83**, 2085 (1999).



Photocmission geometry

N

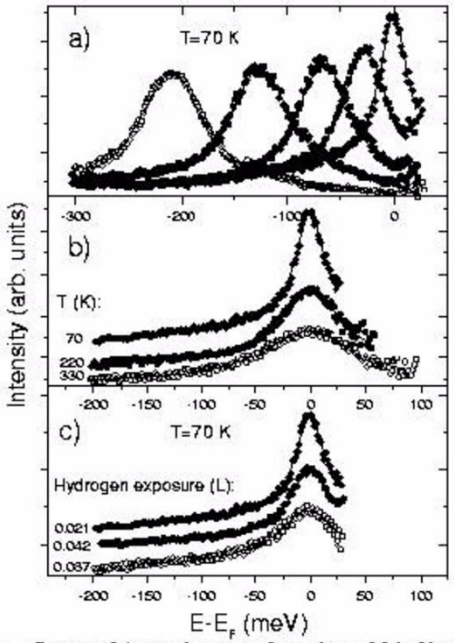


FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen exposure (c) is shown.

taintics from the fits to peaks such as those shown in Fig. 2(a). The peak width shows a minimum at $\omega = 0$, a

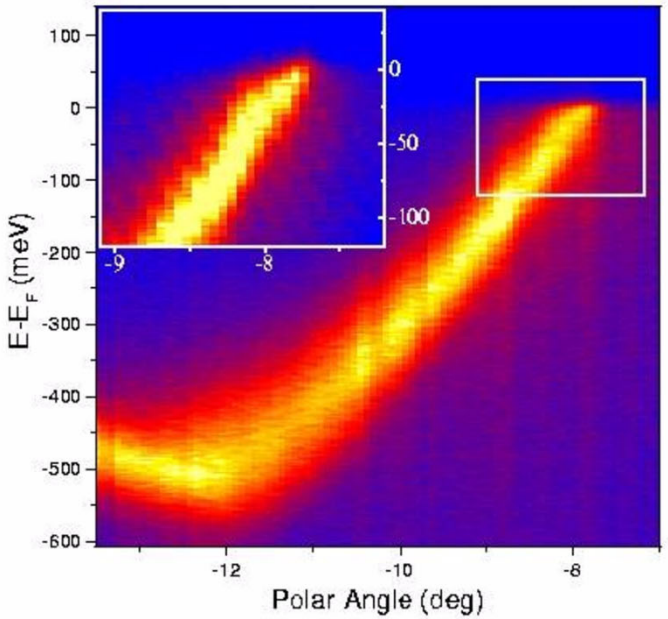
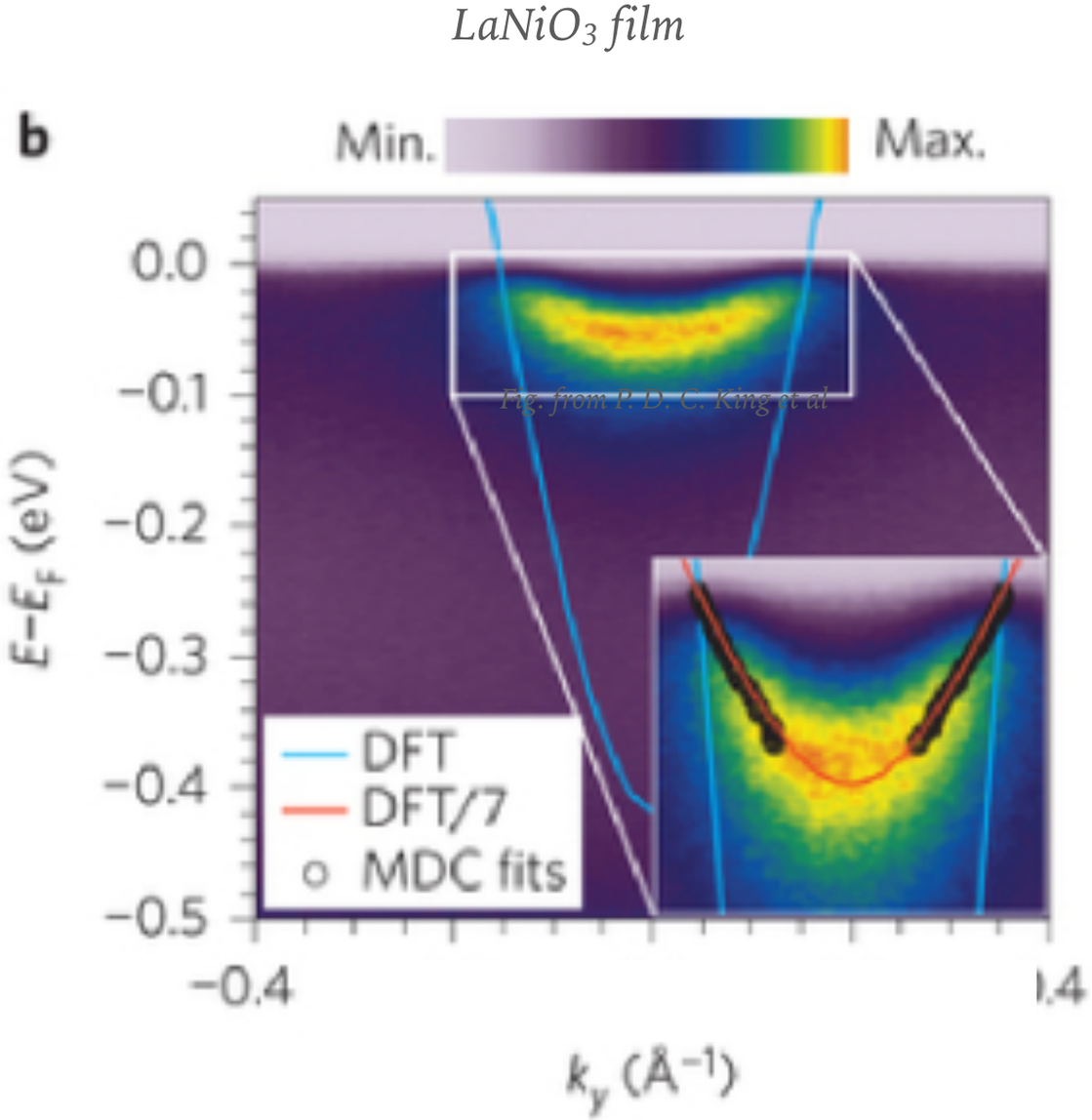


FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\overline{\Gamma} - \overline{\mathrm{N}}$ line of the SBZ at 70 K Shown in the inset is the spectrum of the region around k_F taken with special attention to the surface cleanliness.

SIGNATURES OF ELECTRON CORRELATION

- Correlation-induced phase transition
- Differences between LDA band masses and measured masses
- Satellites in photoemission
- Non-linear T dependance of the electronic contribution in specific heat
- Small Drude weights
- .....



A. Georges http://arxiv.org/abs/cond-mat/0403123

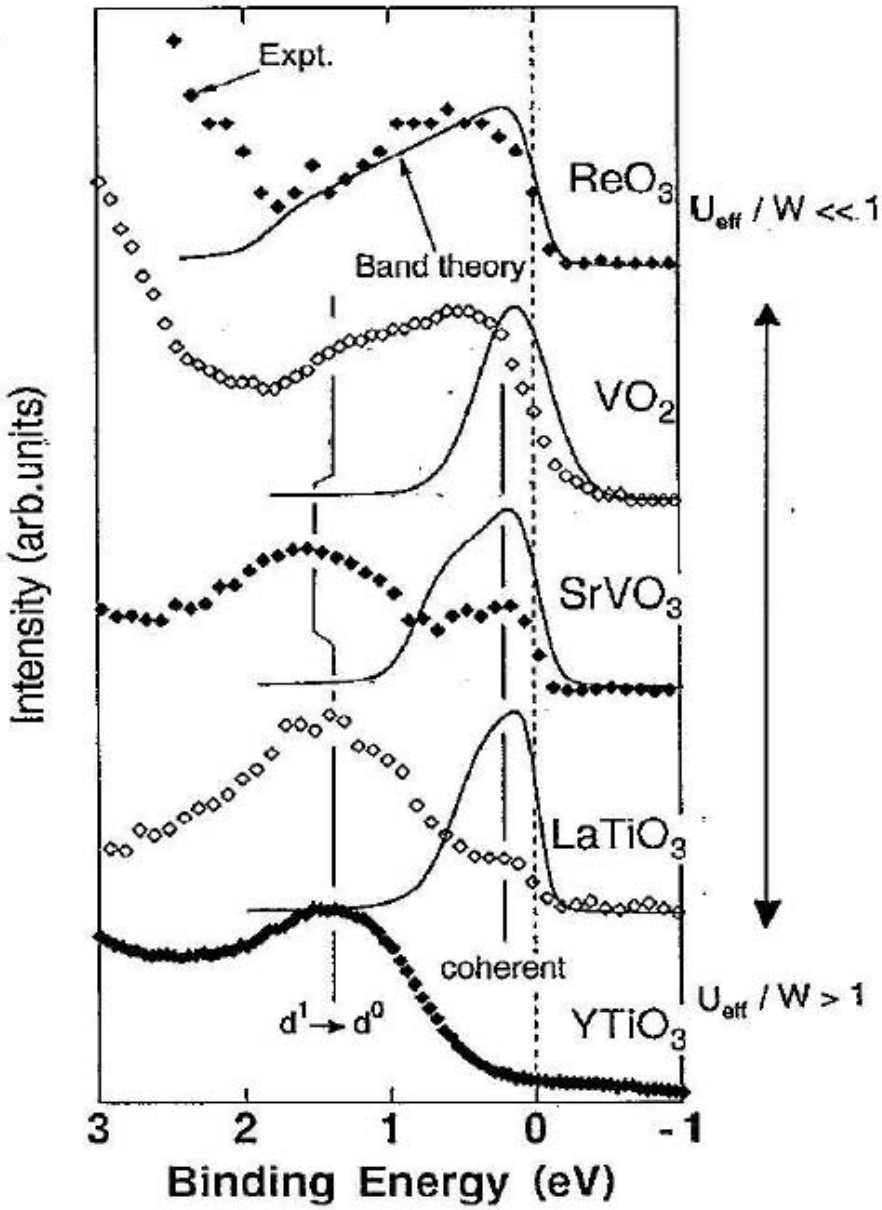
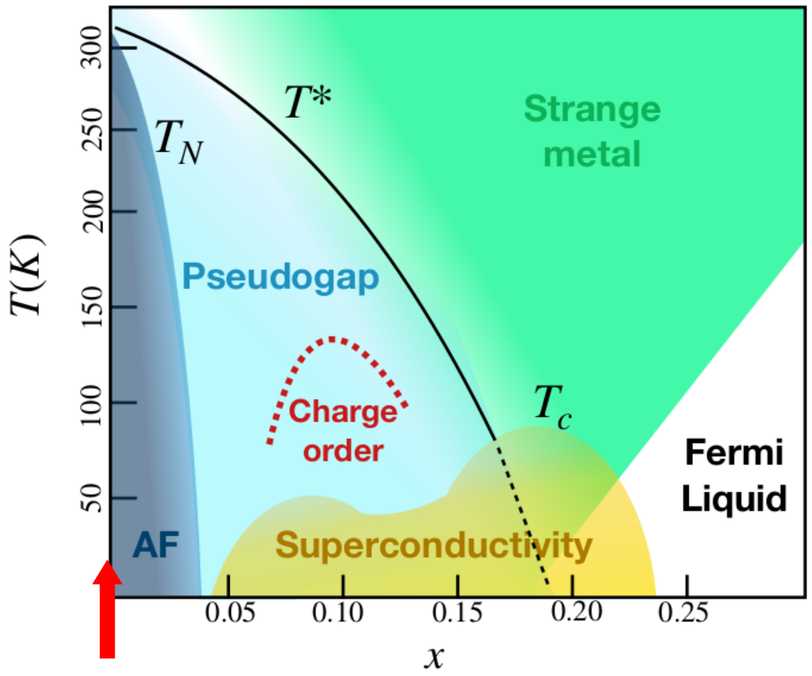


FIGURE 10. Photoemission spectra of several d^1 transition metal oxides, reproduced from Ref. [88]. The effects of correlations increases from ReO_3 (a weakly correlated metal) to $YTiO_3$ (a Mott insulator). The plain lines are the d.o.s obtained from band structure calculations. A lower Hubbard band around -1.5 eV is clearly visible in the most correlated materials, both in the metallic and insulating case.

Identifying the correlated subspace

Which degrees of freedom are correlated? Can be identified from DFT

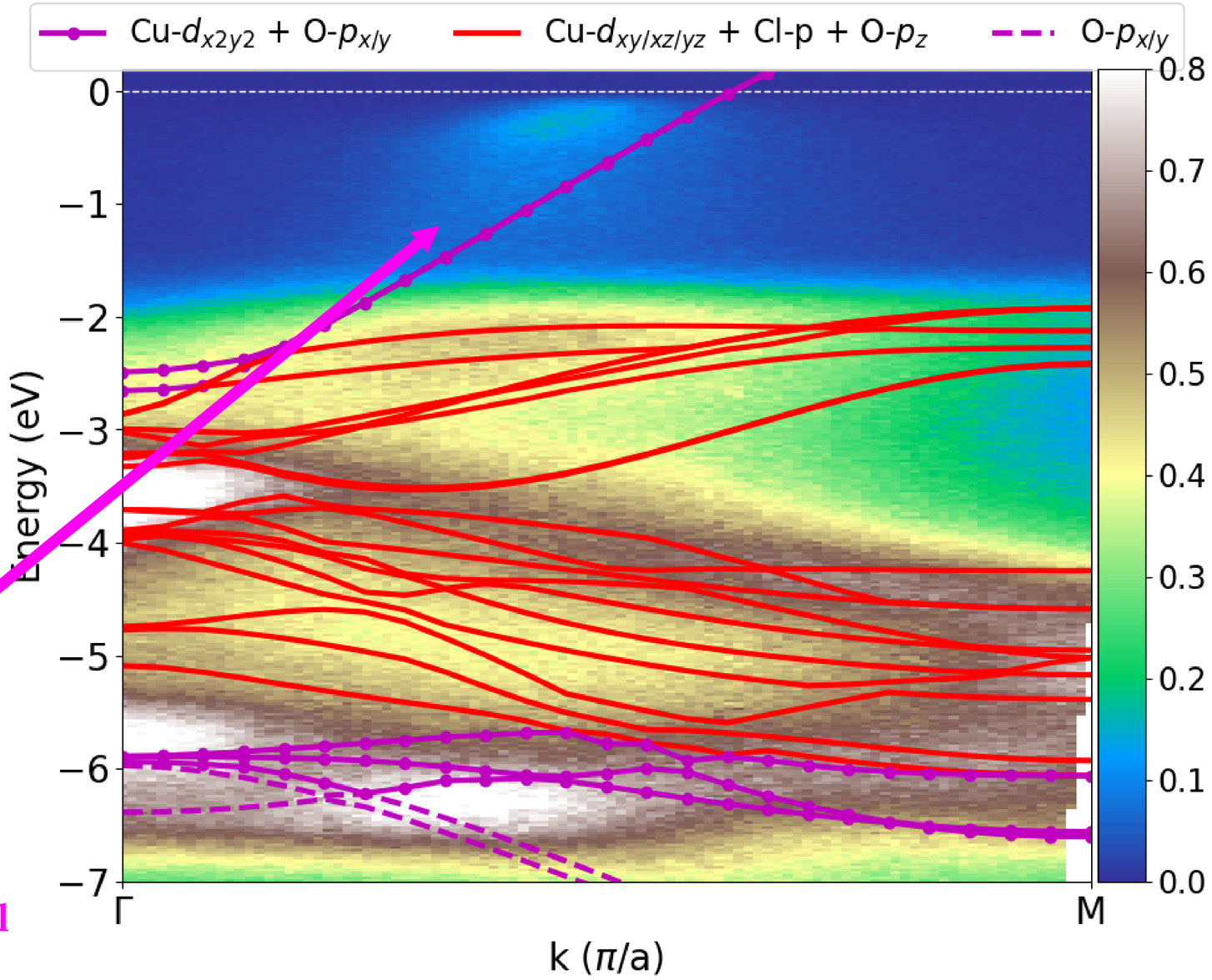
At x=0, should be an **insulator**:



Isolated band seems to be the culprit

Confirmed by **photoemission** data (@SOLEIL)

(C) Benjamin Bacq-Labreuil



A. Georges http://arxiv.org/abs/cond-mat/0403123

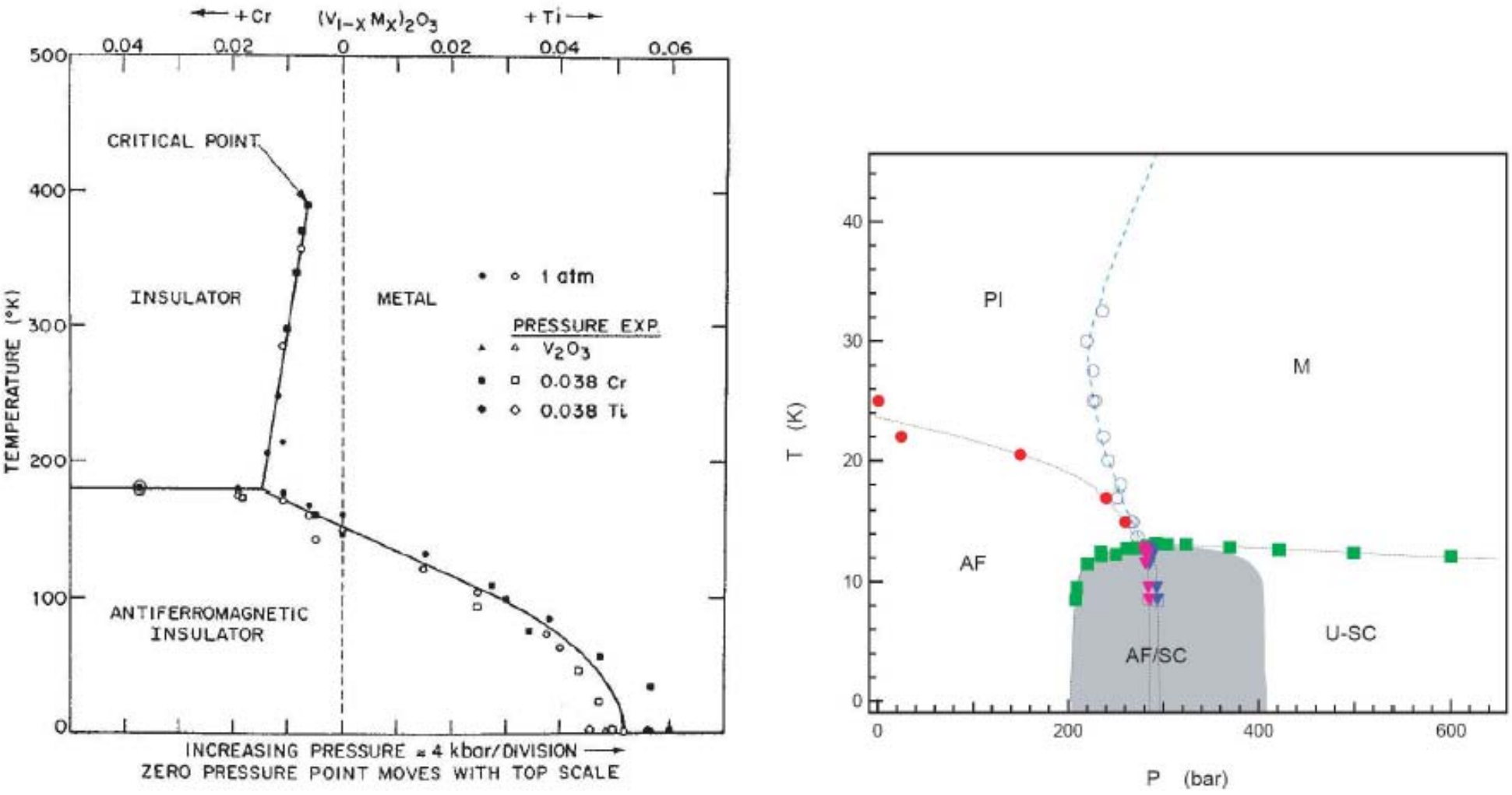
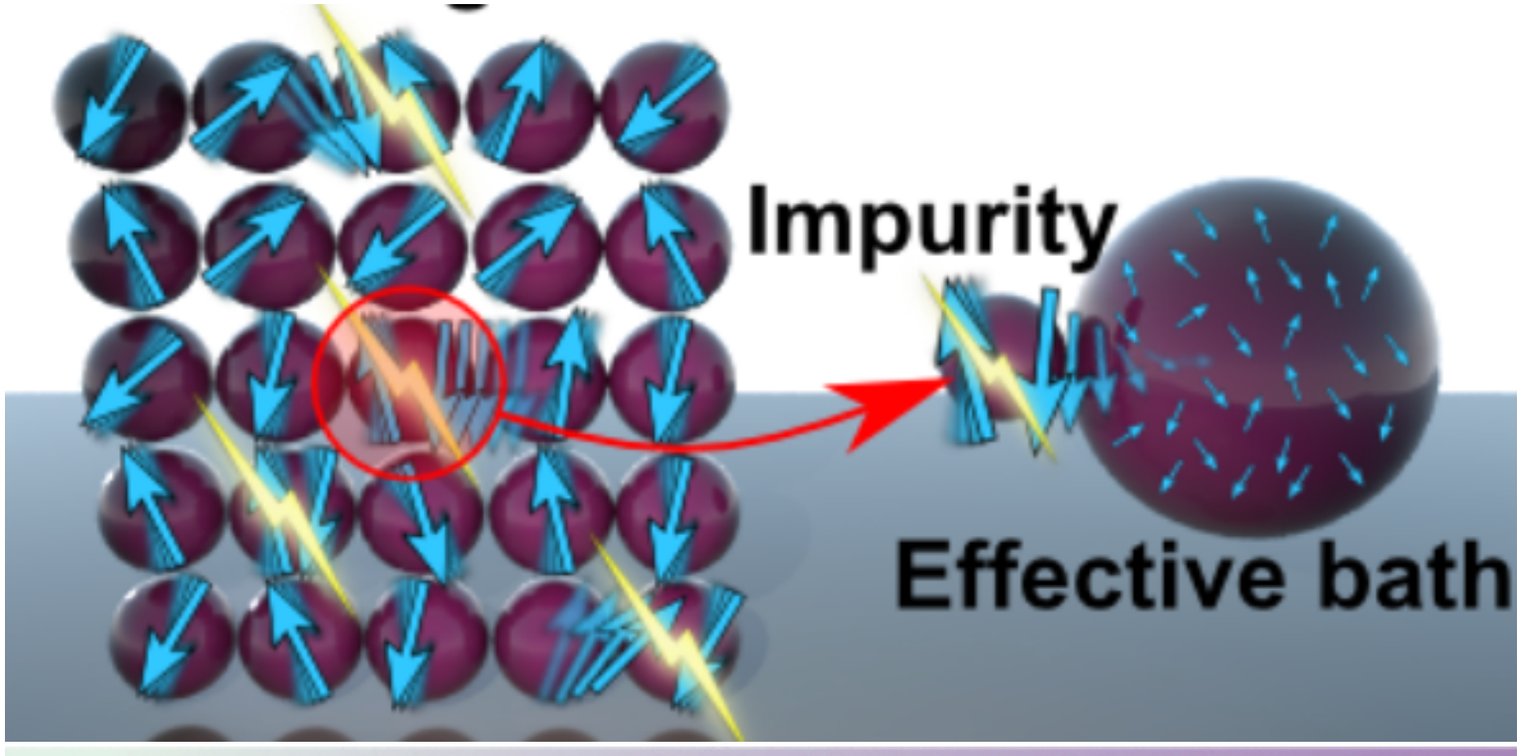
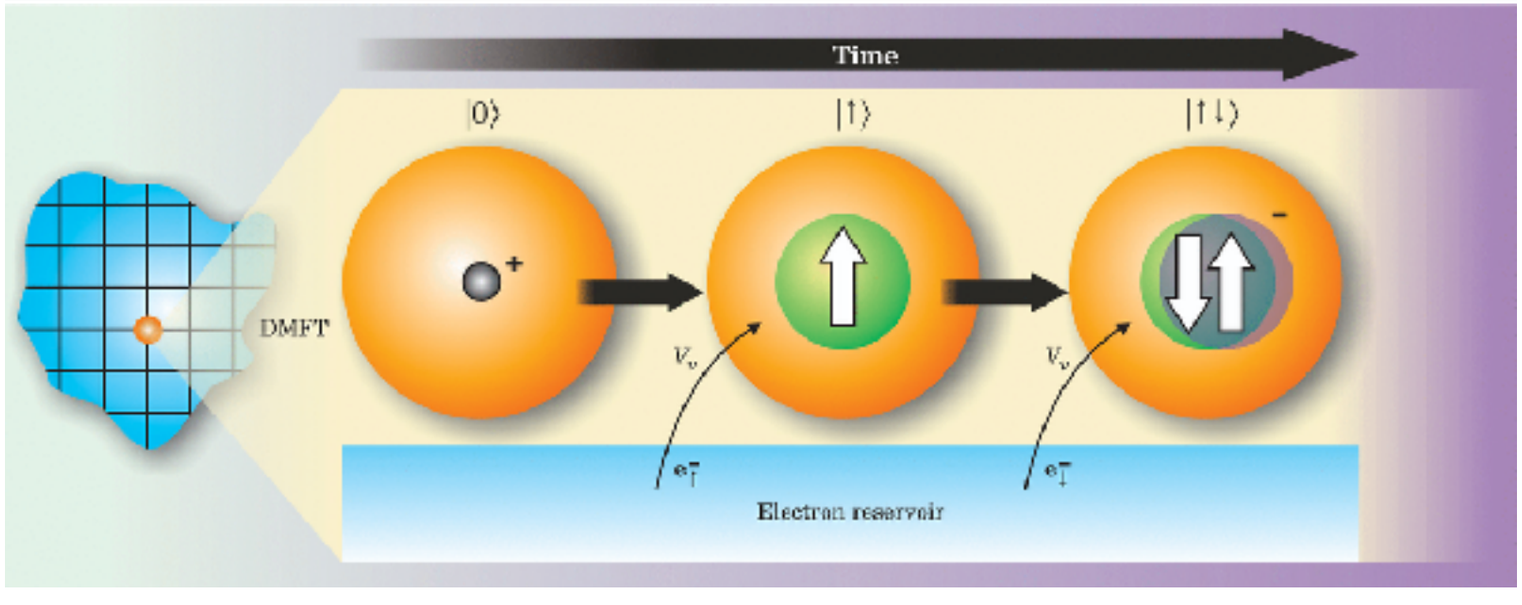


FIGURE 7. Left: Phase diagram of $(V_{1-x}\,Cr_x)_2O_3$ as a function of either Cr-concentration x or pressure (after[75]). Increasing x by 1% produces similar effects than *decreasing* pressure by $\sim$ 4kbar, for this material. Right: Phase diagram of κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl as a function of pressure (after [76]).

BEYOND MEAN-FIELD APPROACHES

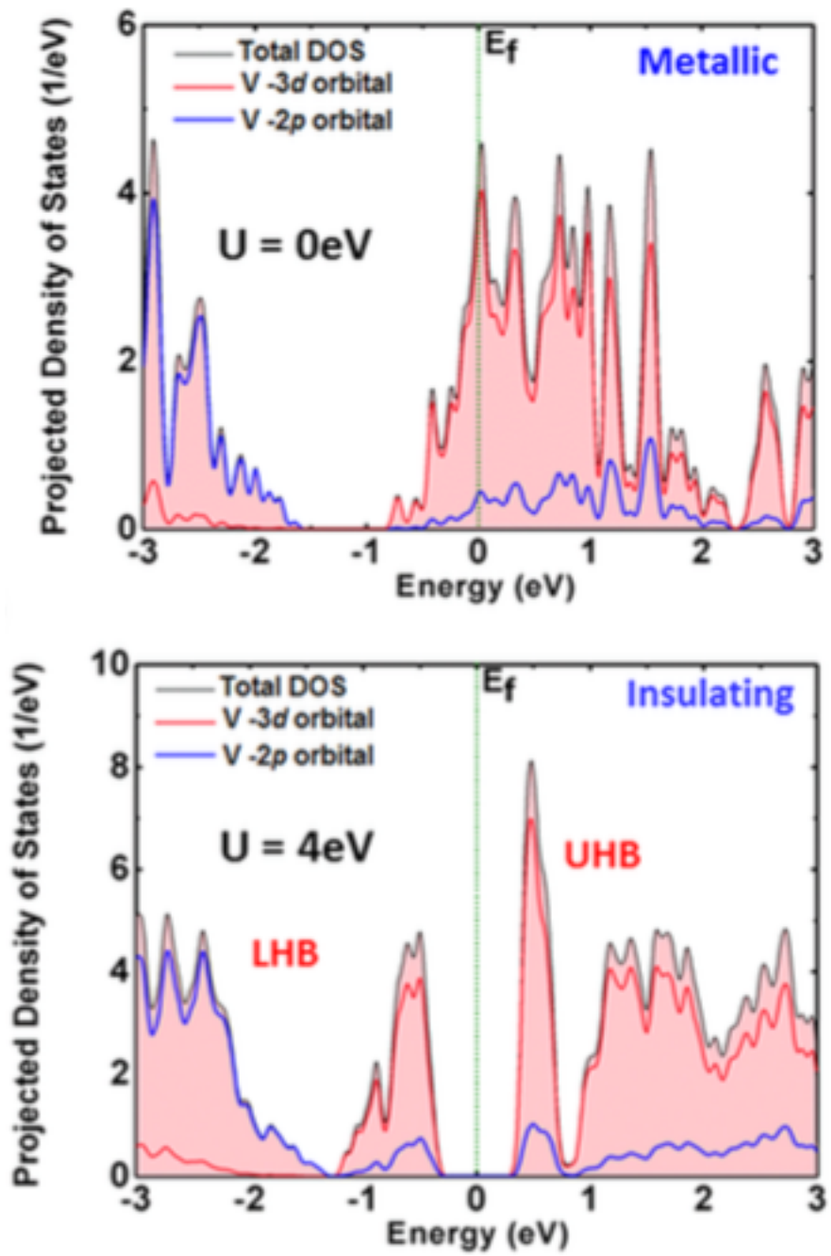
- Dynamical mean-field theory

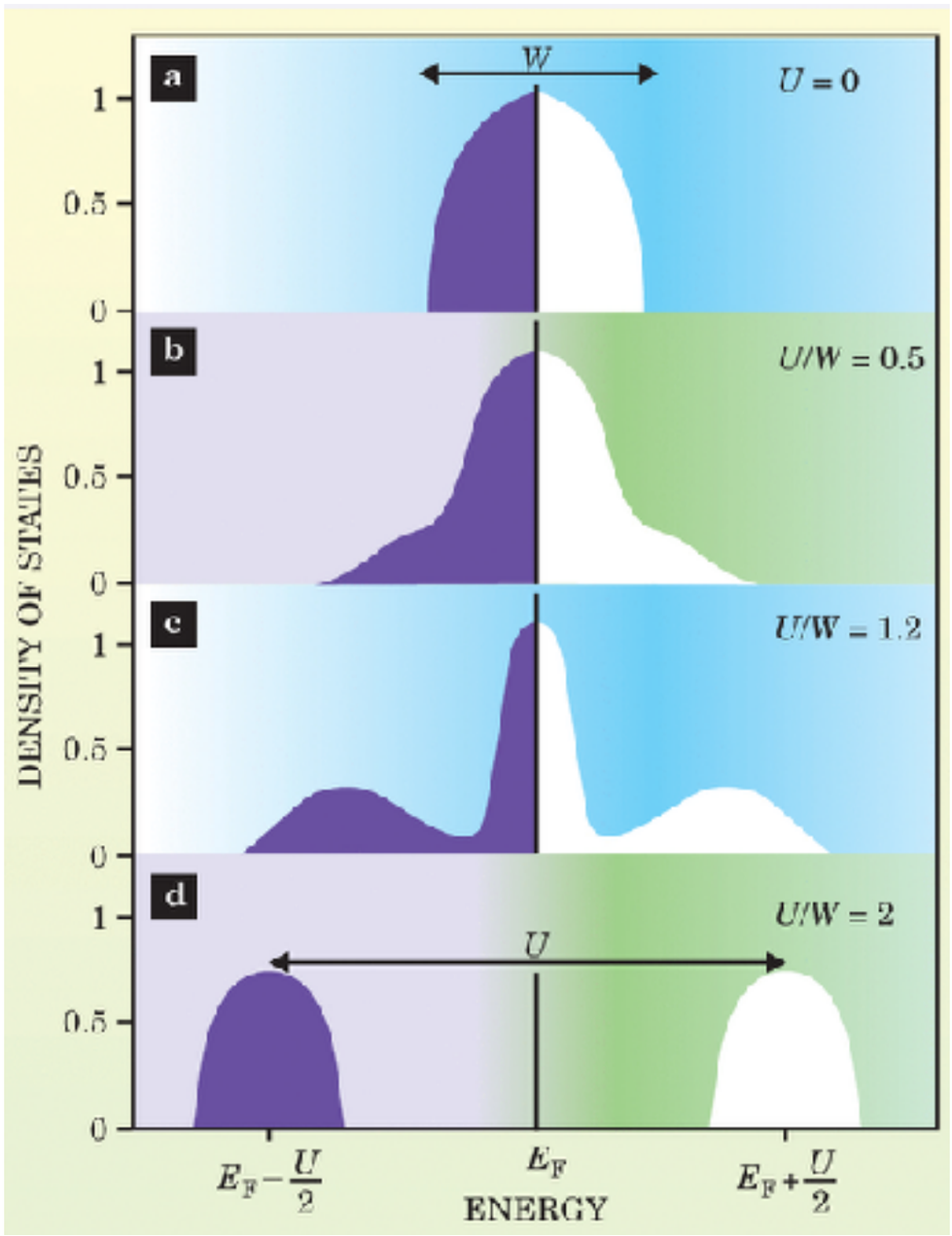




CORRELATION DRIVEN METAL-INSULATOR TRANSITION

- VO_2





SUMMARY

- Most materials with interesting properties such as heavy fermion, high T_c superconductor, giant magnetoresistance, multiferroic etc. are strongly correlated
- Ordered states are usually weakly correlated
- Methods such as QMC (model Hamiltonian) or LDA+DMFT take into account some correlation effects