

# Quantum materials

Orsay

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**European Research Council**

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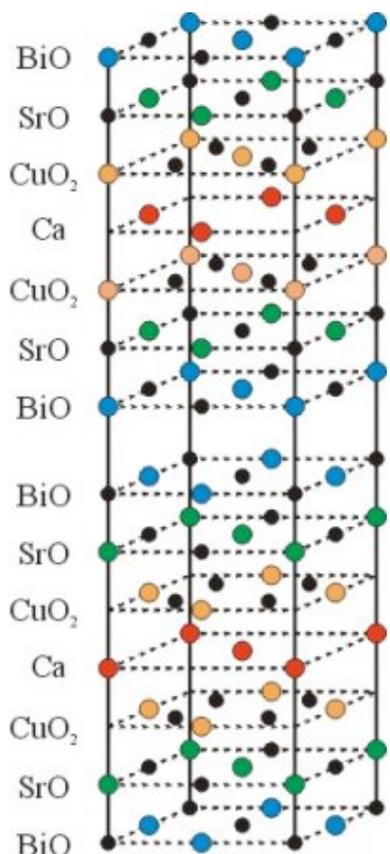
# Strongly Correlated Systems

Quantum many-body systems, fermions (or bosons),  
with interactions, at low temperature

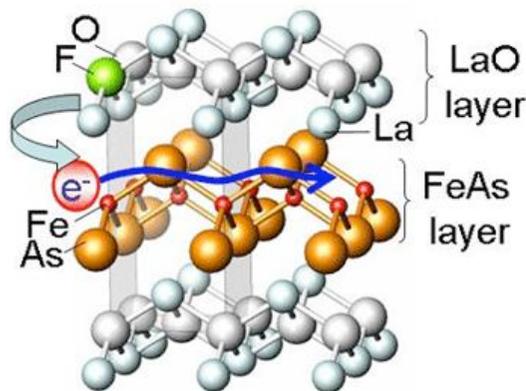
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## Materials

High Temperature superconductors  
Transition metal oxides,

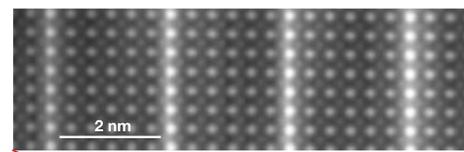


Cuprate (1986)



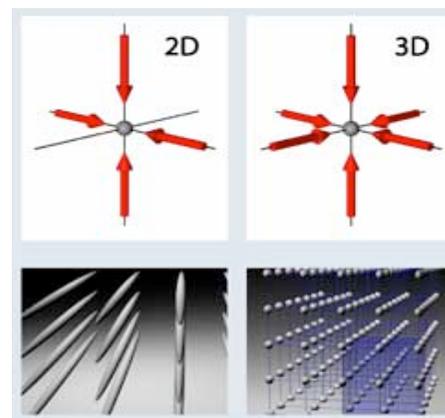
Fe-Based (2008)

Correlated metal/superconductors  
at interface of oxides



*SrTiO<sub>3</sub>/LaTiO<sub>3</sub>*  
*Ohtomo et al, Nature 2002*

Ultra-cold atoms in optical lattices



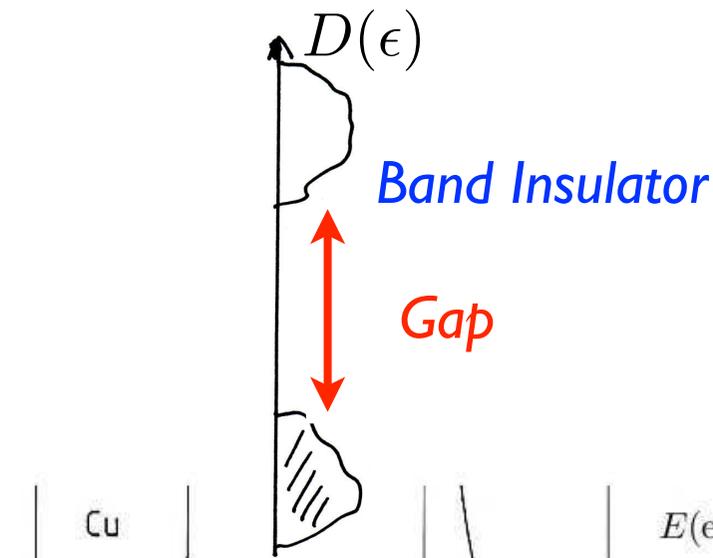
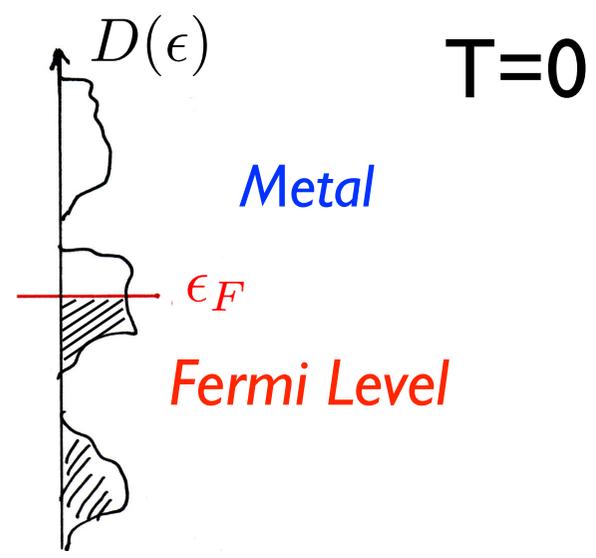
“Artificial solids”  
of atoms & light

# Standard solid state physics

- Bands. Fermi surface.

Density of states

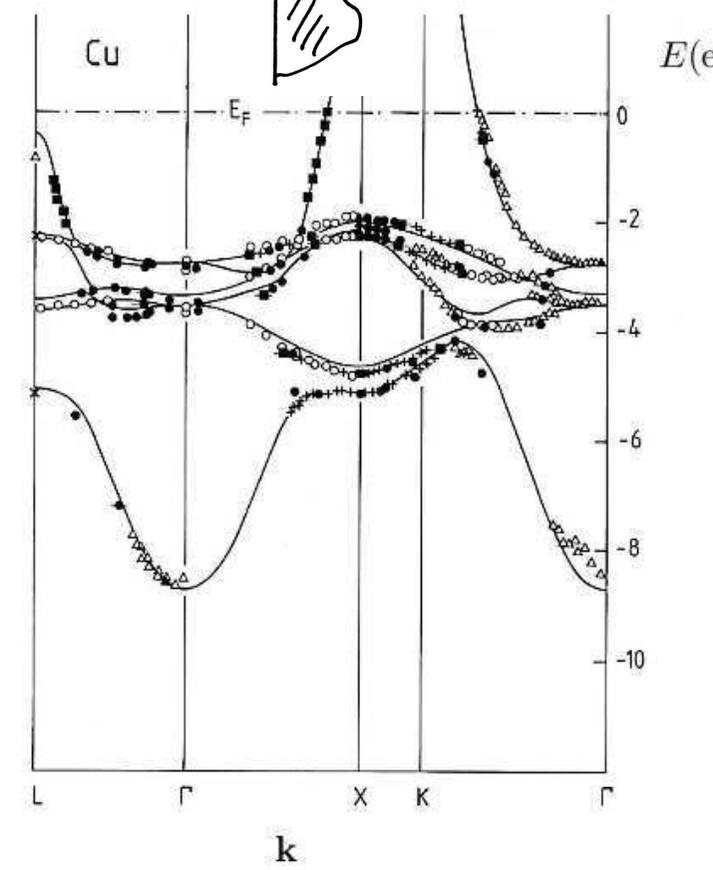
$$D(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k)$$



- Interaction  $\approx$  kinetic energy  $\approx$  1-50 eV

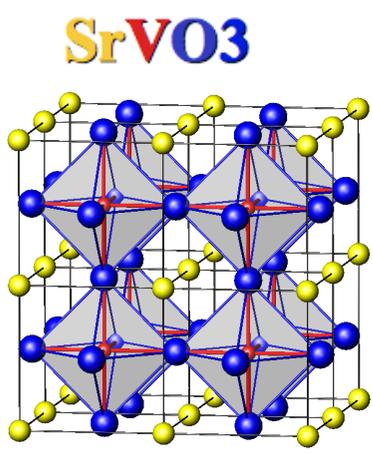
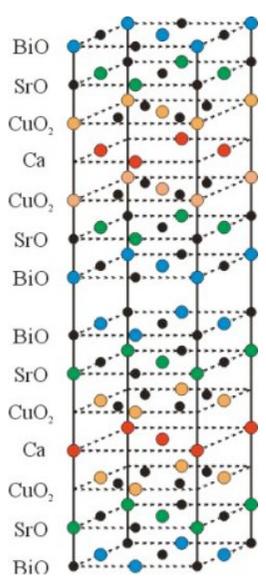
But

- Fermi liquid theory (Landau)  
Low energy renormalization group fixed point  
Quasi-particles: effective mass  $m^*$ , lifetime, ...
- Density functional theory (Kohn).  
Independent electrons + effective potential.



# Strongly Correlated Systems

- New phases, new phenomena.
- True many-body problem. No effective one electron picture.
- Exponential complexity with the number of fermions !



Periodic Table of the Elements

Transition Metals

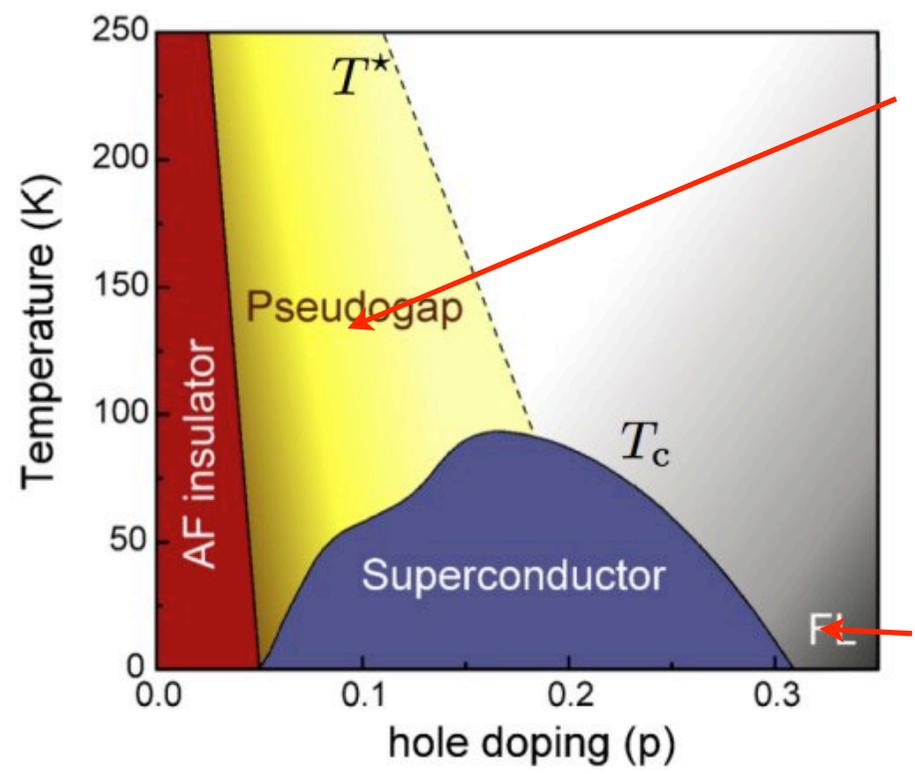
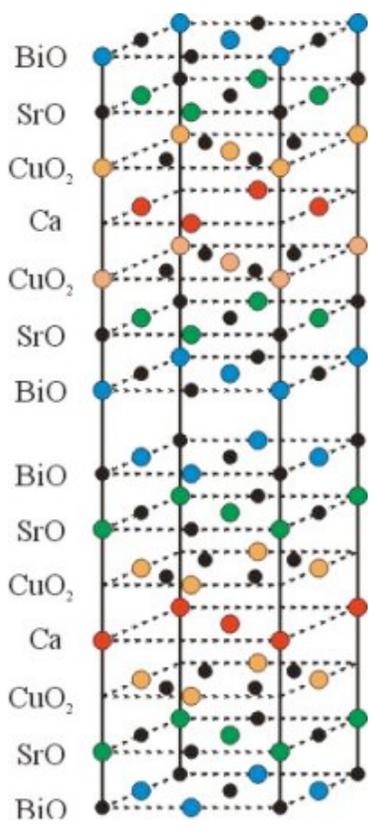
1A 1 H hydrogen 1.008	2A 4 Be beryllium 9.012	3A 5 B boron 10.81	4A 6 C carbon 12.01	5A 7 N nitrogen 14.01	6A 8 O oxygen 16.00	7A 9 F fluorine 19.00	8A 10 Ne neon 20.18										
11 Na sodium 22.99	12 Mg magnesium 24.31	13 Al aluminum 26.98	14 Si silicon 28.09	15 P phosphorus 30.97	16 S sulfur 32.07	17 Cl chlorine 35.45	18 Ar argon 39.95										
19 K potassium 39.10	20 Ca calcium 40.08	21 Sc scandium 44.96	22 Ti titanium 47.88	23 V vanadium 50.94	24 Cr chromium 52.00	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.39	31 Ga gallium 69.72	32 Ge germanium 72.58	33 As arsenic 74.92	34 Se selenium 78.96	35 Br bromine 79.90	36 Kr krypton 83.80
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.94	43 Tc technetium (98)	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3
55 Cs cesium 132.9	56 Ba barium 137.3	57 La* lanthanum 138.9	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.9	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.5	81 Tl thallium 204.4	82 Pb lead 207.2	83 Bi bismuth 208.9	84 Po polonium (209)	85 At astatine (210)	86 Rn radon (222)
87 Fr francium (223)	88 Ra radium (226)	89 Ac~ actinium (227)	104 Rf rutherfordium (261)	105 Db dubnium (262)	106 Sg seaborgium (263)	107 Bh bohrium (264)	108 Hs hassium (265)	109 Mt meitnerium (266)	110 Ds darmstadtium (271)	111 Uuu (272)	112 Uub (277)	114 Uuq (290)	116 Uuh (298)	118 Uuo (?)			
Lanthanide Series*		58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium 147	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.0	71 Lu lutetium 175.0		
Actinide Series~		90 Th thorium 232.0	91 Pa protactinium (231)	92 U uranium (238)	93 Np neptunium (237)	94 Pu plutonium (242)	95 Am americium (243)	96 Cm curium (247)	97 Bk berkelium (247)	98 Cf californium (249)	99 Es einsteinium (254)	100 Fm fermium (253)	101 Md mendelevium (256)	102 No nobelium (254)	103 Lr lawrencium (260)		

Rare earth and actinides

A famous example

# High temperature superconductors

(Bednorz, Muller 1986)



*Unconventional normal metal*

*Fermi liquid*



- A family of copper oxides with high critical temperature (90, 100K).
- Physics **qualitatively different** from conventional superconductors.
- Physical mechanism ? “Glue” for Cooper pairs ?

# A simple model for theoretical physicists

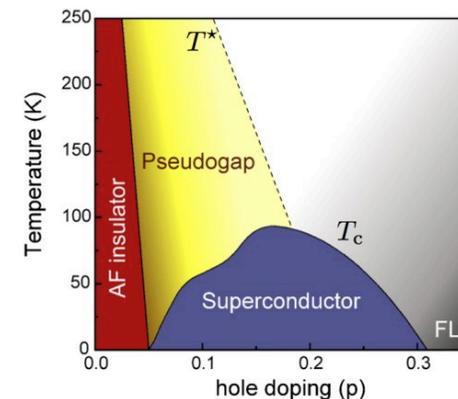
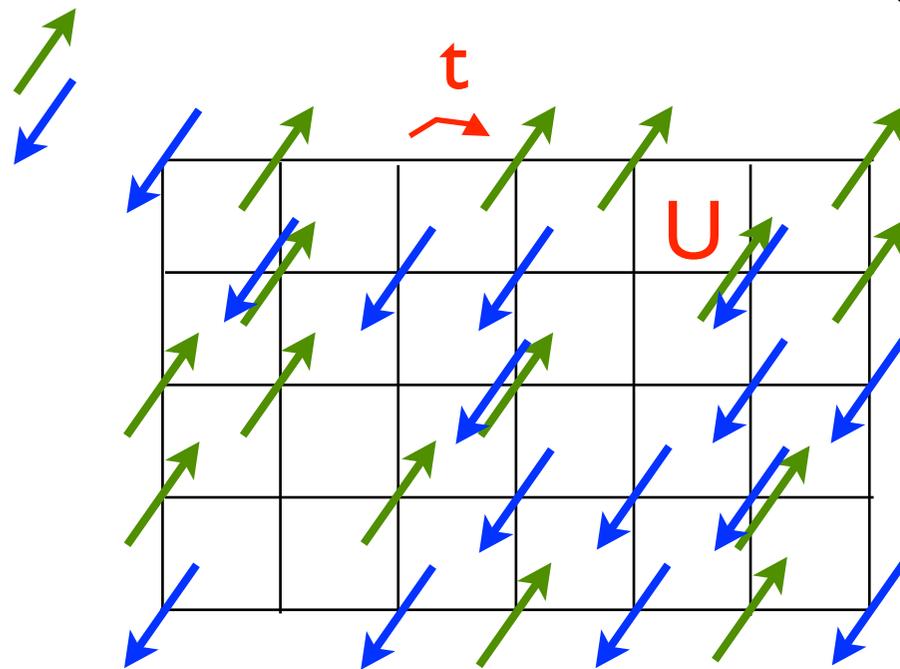
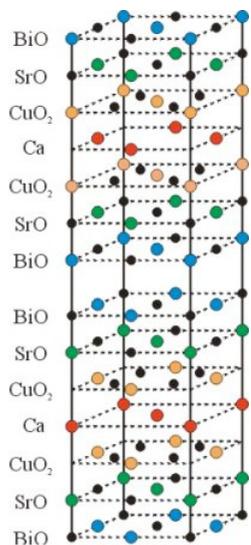
## Hubbard model Hamiltonian

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

$$n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$$

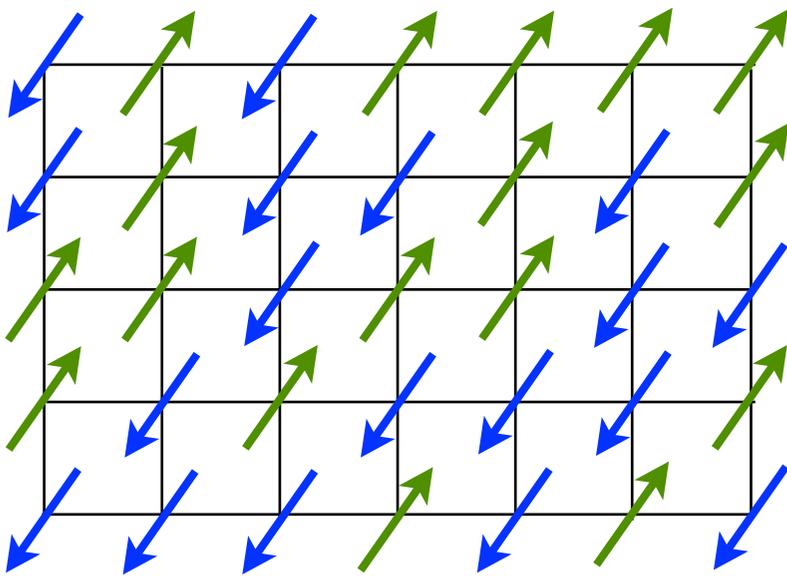
$$\delta = 1 - \langle n_\uparrow + n_\downarrow \rangle$$

Electron, spin +1/2  
 Electron, spin -1/2

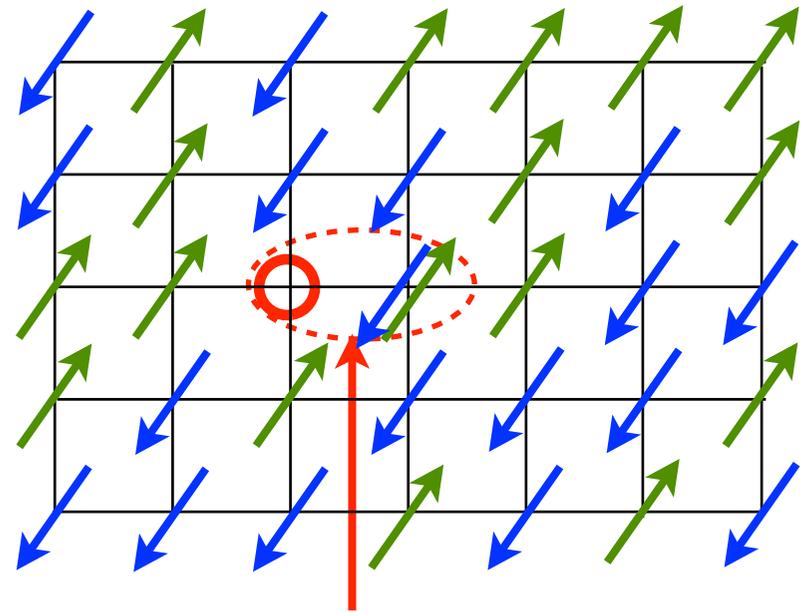


- Simplest possible model, almost a caricature.

- One electron per site on average (half-filled band).
- Should be a textbook metal.
- If  $U$  is large enough, it is an insulator : **charge motion frozen.**

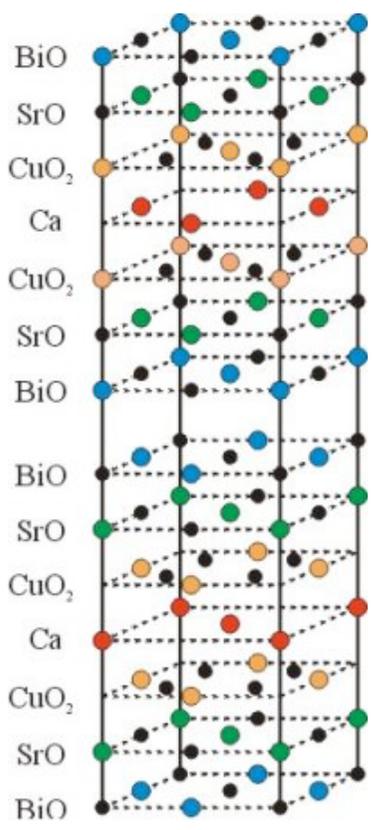


Mott insulator

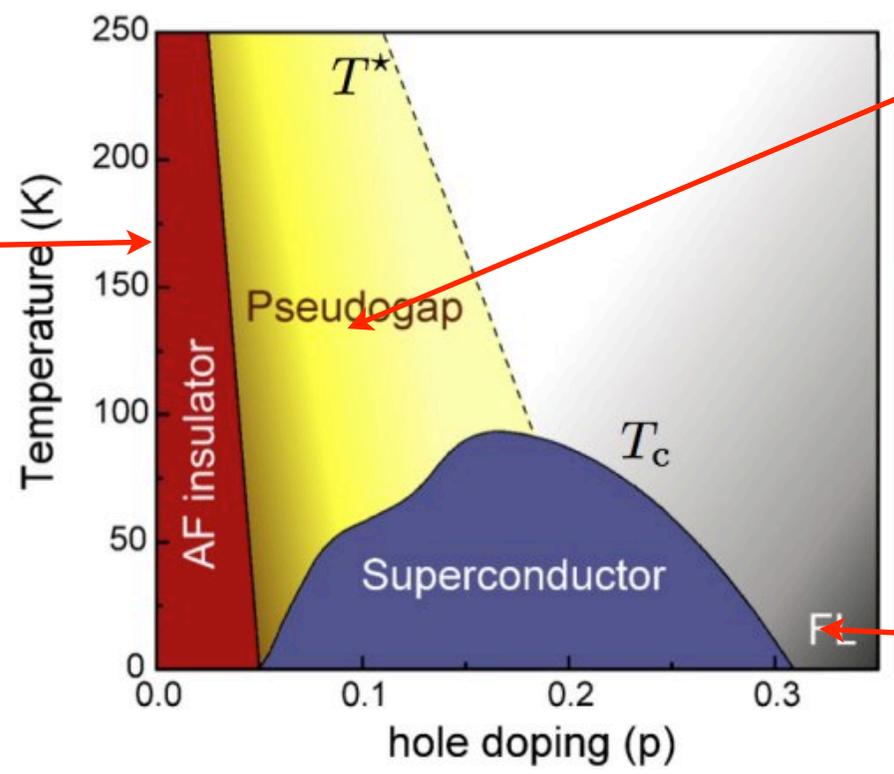


Large Coulomb repulsion  $U \sim eV \sim 10^4 K$

# Doped Mott insulators



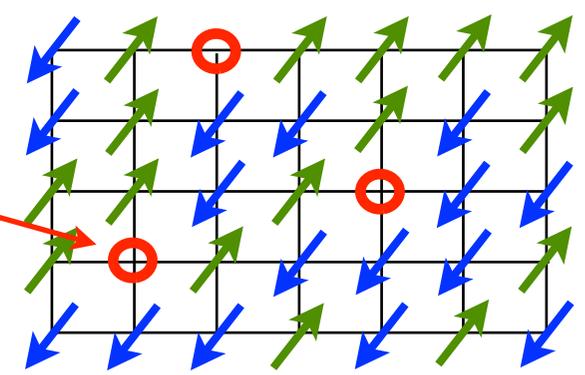
*Mott insulator*



*Unconventional normal metal*

*Fermi liquid*

*Holes = charge carriers*



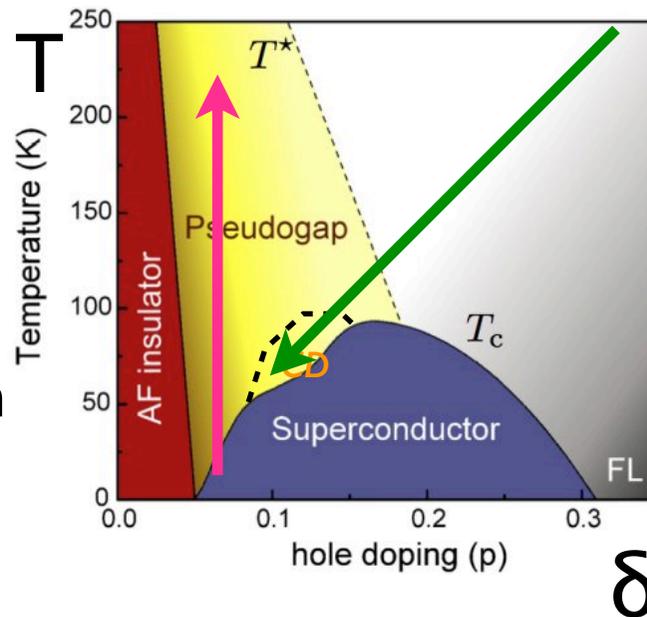
- Can we solve the Hubbard model ?
- Does it describe the high-Tc superconductors ? (*Anderson's conjecture 1987*).

How to solve Hubbard model ?

# A new era

- Quantitative, reliable methods & algorithms in non-perturbative regimes for  $d > 1$
- with a control parameter.
- beyond simple models, towards a real ab-initio computation.

“Bottom to Top”  
 Understand the quantum entanglement of the many-body ground state  
*DMRG, PEPS, ...*



“Top to Bottom”  
 From high T/doping

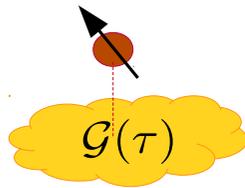
*Cluster DMFT,  
 diagrammatic QMC,  
 Trilex, Quadrilex ...*

- Compute partition function  $Z$
- Markov chain with local ergodic moves
- Direct approach of the Hubbard model
  - Infamous fermionic sign problem !
  - Exponentially difficult (with size,  $1/T$ ).
- Indirect routes
  - *Diagrammatic QMC*  
Expansion coef. in  $U$ , up to order 8, with QMC.  
Sum the series ?
  - *DMFT ...*

# Dynamical Mean Field Theory (DMFT)

A. Georges, G. Kotliar 92.

- An atom coupled to an effective self-consistent bath
- “Impurity model” : still a quantum many-body problem (interaction on the atom).



$$\Sigma(k, \omega) \approx \Sigma_{\text{impurity}}(\omega)$$

$$S_{\text{eff}} = - \int_0^\beta c_a^\dagger(\tau) G_{0ab}^{-1}(\tau - \tau') c_b(\tau') + \int_0^\beta d\tau H_{\text{local}}(\{c_a^\dagger, c_a\})(\tau)$$

$$G_{0ab}^{-1}(i\omega_n) = (i\omega_n + \mu)\delta_{ab} - \Delta_{ab}(i\omega_n)$$

← Interaction  
← Bath

- DMFT is a good starting point when **atomic physics is important**, e.g. U, Mott transition, Hund coupling, atomic multiplet.

# Control

- DMFT is not exact.

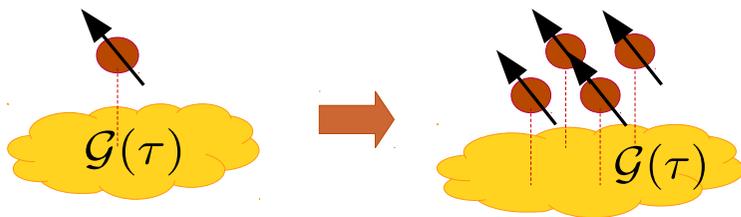
$$\Sigma(k, \omega) \approx \Sigma_{\text{impurity}}(\omega)$$

- Cluster method

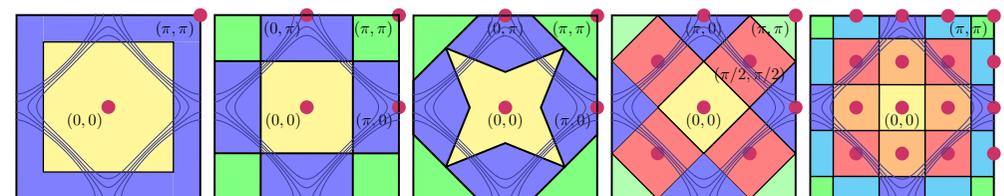
- Systematic expansion starting from DMFT.

- Control parameter = size of cluster / momentum resolution.

*Real space clusters*



*Reciprocal space clusters  
Brillouin zone patching*



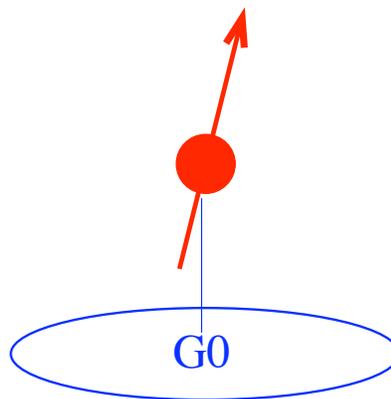
- Beyond : Trilex, ...

*Algorithms to solve the impurity model ?*

# A local many-body problem

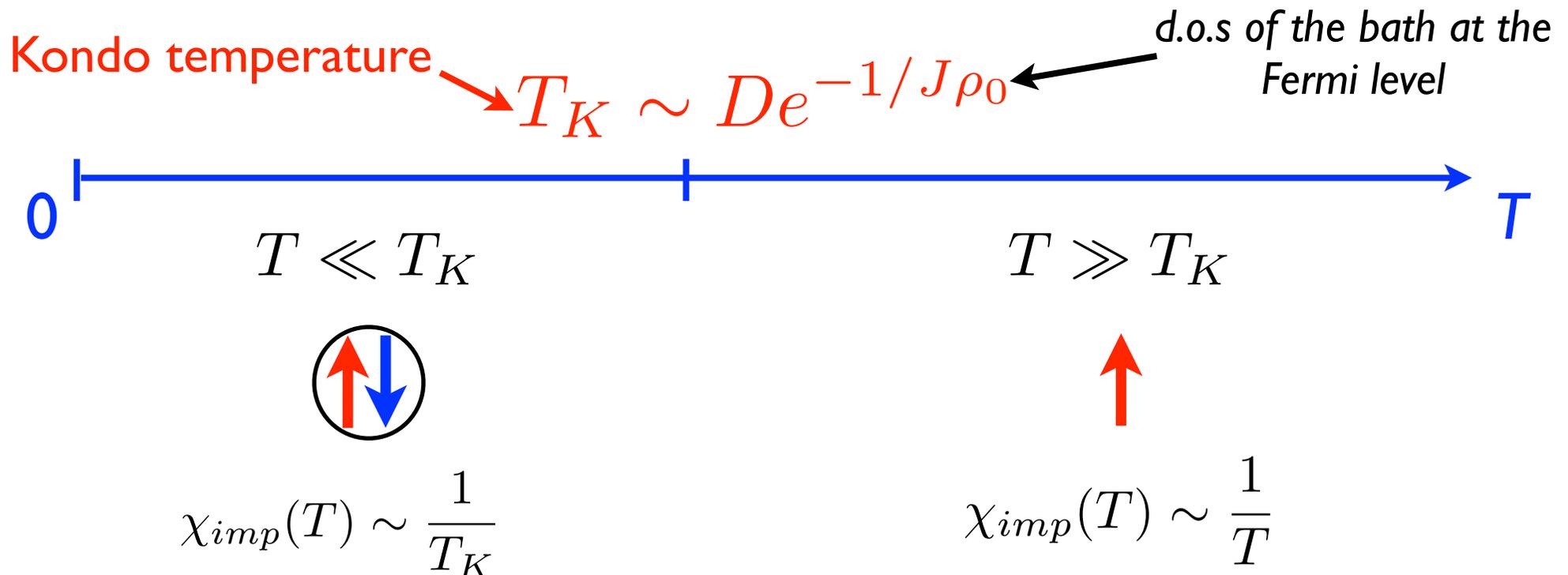
- The simplest version : Kondo model.
- 1 spin + 1 Fermi sea of non-interacting electrons, with a local magnetic (exchange) interaction

$$H = \sum_{k\sigma\alpha} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J_K \vec{S} \cdot \sum_{\substack{kk' \\ \sigma\sigma'}} c_{k\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}$$



# Kondo effect

- Not so easy !
- A confinement problem. Screening of the spin by the bath.
- I+I Field Theory with asymptotic freedom (similar to QCD)



Algorithms are key

- In simplest case, single site problem :
  - No sign problem.
  - Solvable in polynomial time !

$$S_{\text{eff}} = - \int_0^\beta c_a^\dagger(\tau) G_{0ab}^{-1}(\tau - \tau') c_b(\tau') + \int_0^\beta d\tau H_{\text{local}}(\{c_a^\dagger, c_a\})(\tau)$$

$$G_{0ab}^{-1}(i\omega_n) = (i\omega_n + \mu)\delta_{ab} - \Delta_{ab}(i\omega_n)$$

Interaction

$a, b = I, N$  : degree of freedom (e.g. spin, orbital index, ...) Bath

- Expansion in power of the **interactions**
- Expansion in power of **hybridization to bath** (around atomic limit)

# Expansion in interaction

- Standard perturbative technique at finite temperature.

$$S_{\text{eff}} = - \sum_{\sigma=\uparrow,\downarrow} \iint_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau) G_{0\sigma}^{-1}(\tau - \tau') c_\sigma(\tau) + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$\frac{Z}{Z_0} = 1 - U \int_0^\beta d\tau_1 \langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \rangle_0 + \frac{U^2}{2} \iint_0^\beta d\tau_1 d\tau_2 \langle T_\tau n_\uparrow(\tau_1) n_\downarrow(\tau_1) n_\uparrow(\tau_2) n_\downarrow(\tau_2) \rangle_0 \dots$$

- Using Wick Theorem :

$$\frac{Z}{Z_0} = \sum_{n \geq 0} \frac{1}{n!} \int_0^\beta d\tau_1 \dots d\tau_n (-U)^n \underbrace{\prod_{\sigma=\uparrow,\downarrow} \det_{1 \leq i, j \leq n} [G_\sigma^0(\tau_i - \tau_j)]}_{w(n, \{\tau_i\})}$$

# Expansion in hybridization

$$S_{\text{eff}} = - \int_0^\beta c_a^\dagger(\tau) G_{0ab}^{-1}(\tau - \tau') c_b(\tau') + \int_0^\beta d\tau H_{\text{local}}(\{c_a^\dagger, c_a\})(\tau)$$

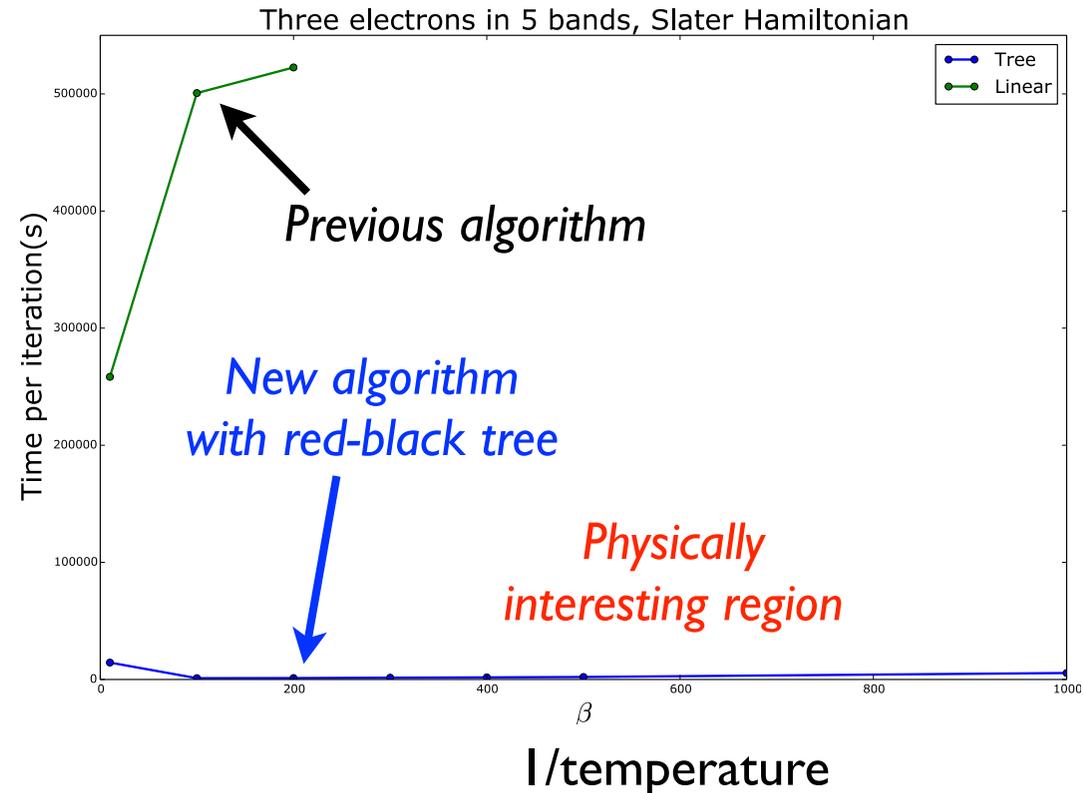
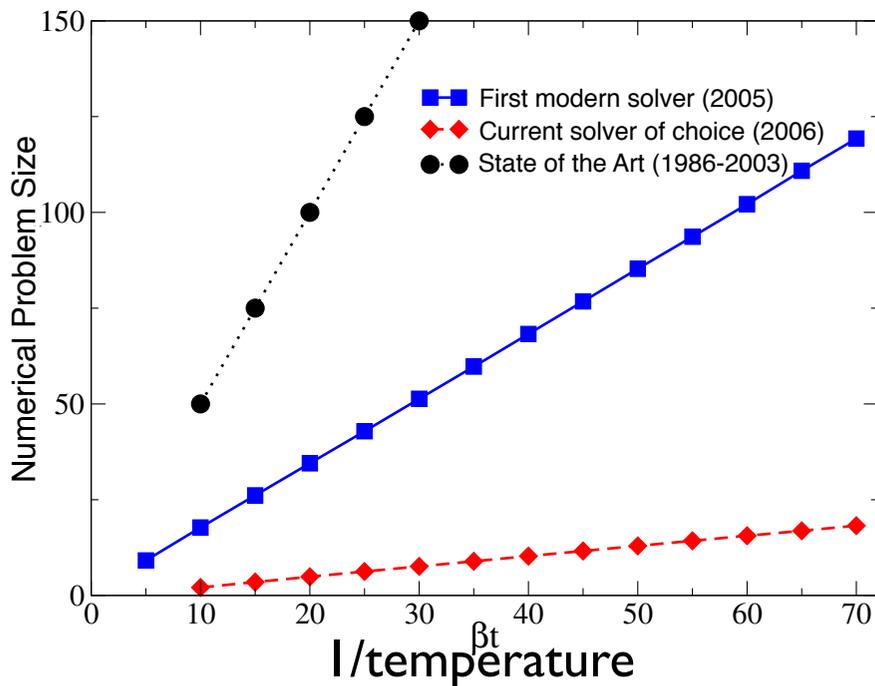
$$G_{0ab}^{-1}(i\omega_n) = (i\omega_n + \mu)\delta_{ab} - \Delta_{ab}(i\omega_n) \quad a, b = I, N$$

- Expansion in hybridization :

$$Z = \sum_{n \geq 0} \int \prod_{i=1}^n d\tau_i d\tau'_i \sum_{a_i, b_i=1, N} \underbrace{\det_{1 \leq i, j \leq n} [\Delta_{a_i, b_j}(\tau_i - \tau'_j)] \text{Tr} \left( \mathcal{T} e^{-\beta H_{\text{local}}} \prod_{i=1}^n c_{a_i}^\dagger(\tau_i) c_{b_i}(\tau'_i) \right)}_{w(n, \{a_i, b_i\}, \{\tau_i\})}$$

- $H_{\text{local}}$  = Hamiltonian of the isolated atom.

- Huge recent progress.



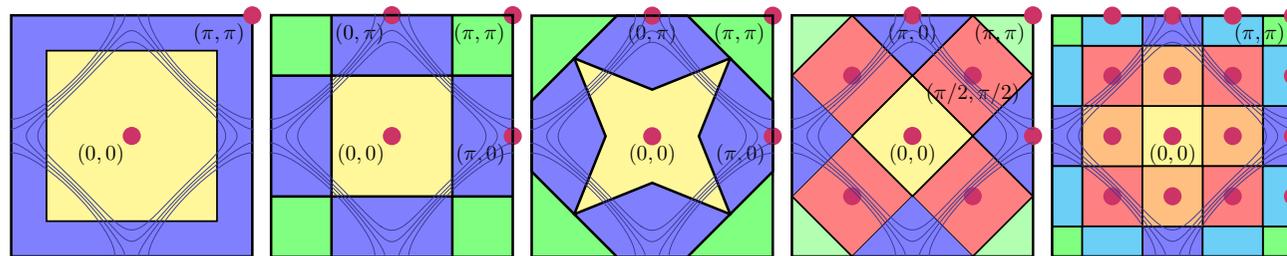
- Modern QMC.  
Typical matrix size reduced by  $\sim 30$ .  
Time speedup of factor  $30^3$   
or  $\sim 25$  years of Moore's law

- Recent progress with Red-Black trees for 5 bands systems (e.g. Fe).

**What can we do today ?**

# State of the art

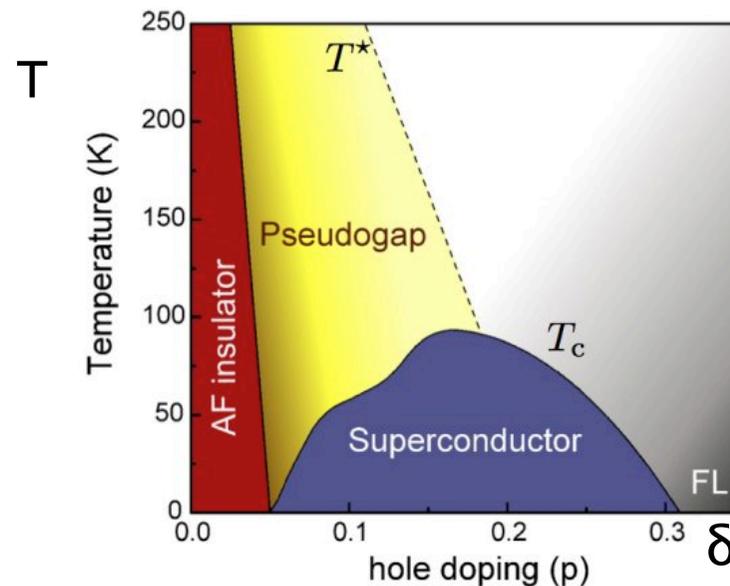
- Thanks to modern algorithms, solve up to 16 sites,  $T \approx 200\text{K}$



- Reproduce qualitatively various aspects of cuprate phase diagram.

## Pseudo-gap

- Emerging from Mott insulator



## *d*-wave SC

- In various clusters sizes (4, 8, 16, ...).
  - Behavior of  $T_c$ , gap vs  $\delta$
- Still many issues : mechanism ? converge ?

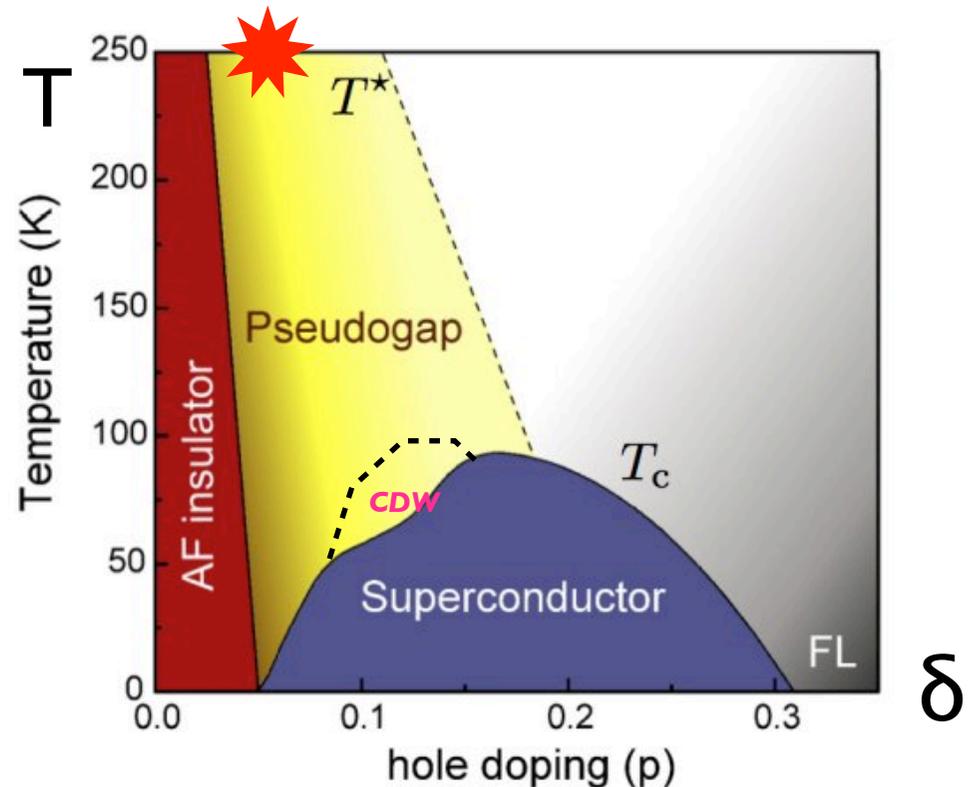
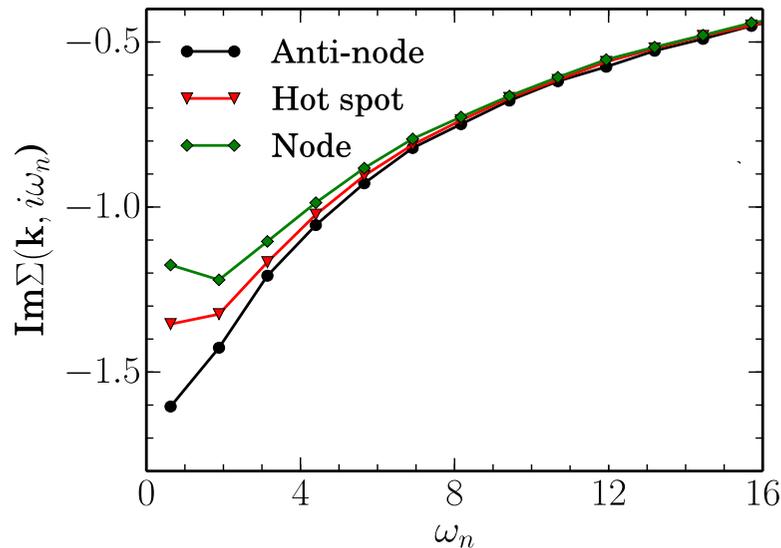
# Pseudogap : exact solution at high temperature

- Converge cluster methods and diagrammatic QMC at one point.
- Exact solution of Hubbard model at a non trivial point with the pseudo-gap !

W.Wu, M. Ferrero et al. Arxiv:1608.08402

$$U=5.6t \quad t'=-0.3t$$

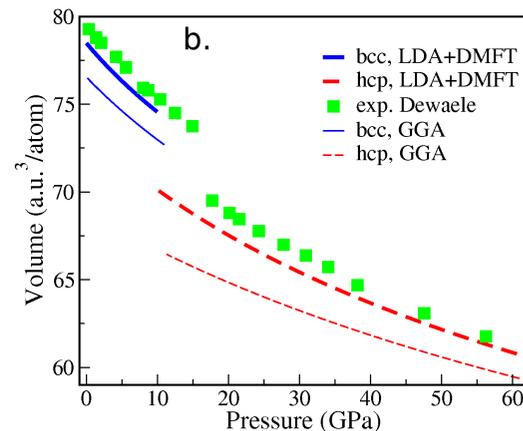
$$\delta = 4\% \quad T = 0.2t$$



# Ab-initio electronic structure for strongly correlated materials

- Combine electronic structure methods based on Density Functional Theory (DFT) and DMFT methods.
- **Predictive** ab-initio method for strongly correlated materials.

*Equation of state and transport in  $\epsilon$ -Fe,  
e.g. volume vs pressure (Pourovskii et al PRB 2014)*



# The TRIQS project

## Toolbox for Research in Interacting Quantum Systems

Computer Physics Communication, 2015-2016

- Open source, since 2012.
- Contributors in my group, Polytechnique, Collège de France, Orsay, Hambourg, Graz, ETH Zurich, Michigan University, Columbia University NYC, ....

## Contributors

People

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# Summary

- Strongly correlated quantum systems
- A new era with controlled methods and algorithms.
- Cluster DMFT methods reproduce many aspects of the high temperature superconductors.
- Still a lot of work on algorithms, benchmarks, applications.

Thank you for your attention