Quantum materials

Orsay

May 14th 2017

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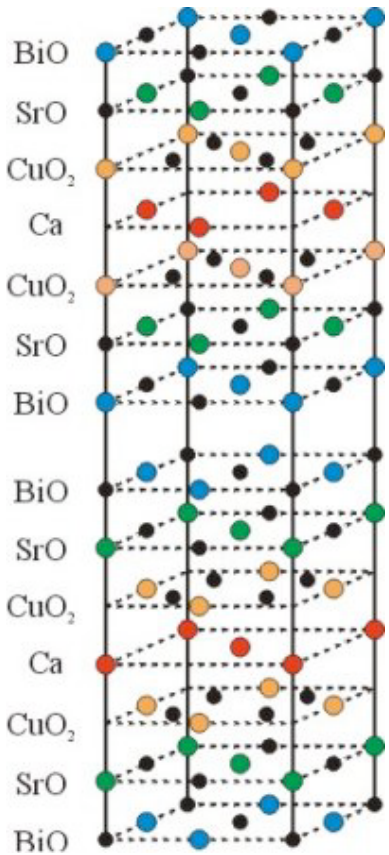
European Research Council

Established by the European Commission

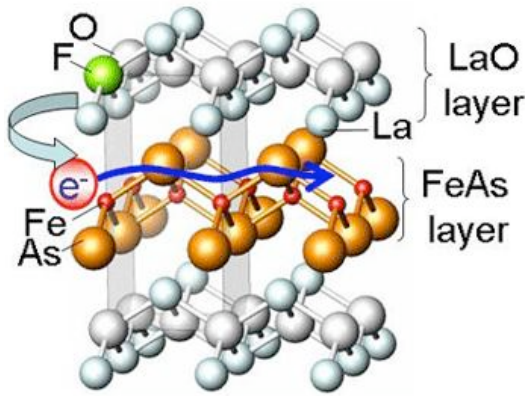
Strongly Correlated Systems

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

Materials
High Temperature superconductors
Transition metal oxides,

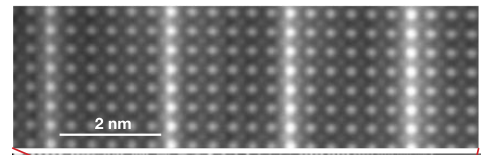


Cuprate (1986)



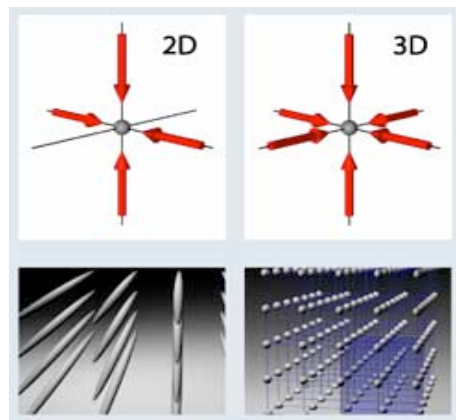
Fe-Based (2008)

Correlated metal/superconductors
at interface of oxides



SrTiO3/LaTiO3
Ohtomo et al, Nature 2002

Ultra-cold atoms in optical lattices



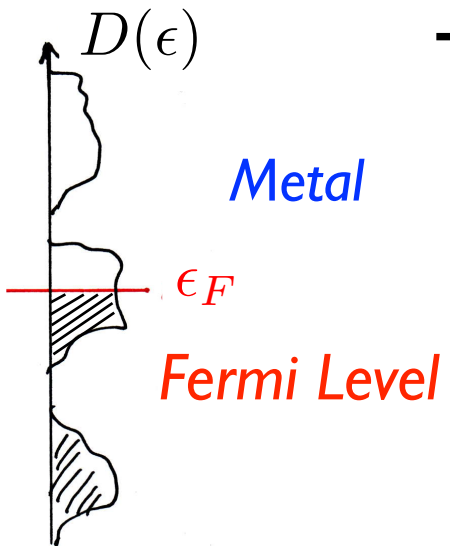
"Artificial solids"
of atoms & light

Standard solid state physics

- Bands. Fermi surface.

Density of states

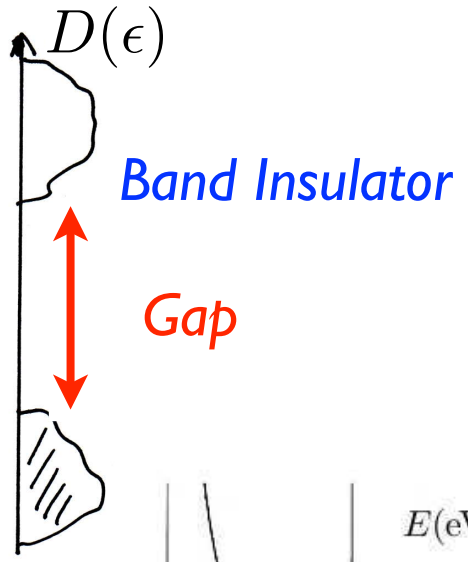
$$D(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k)$$



T=0

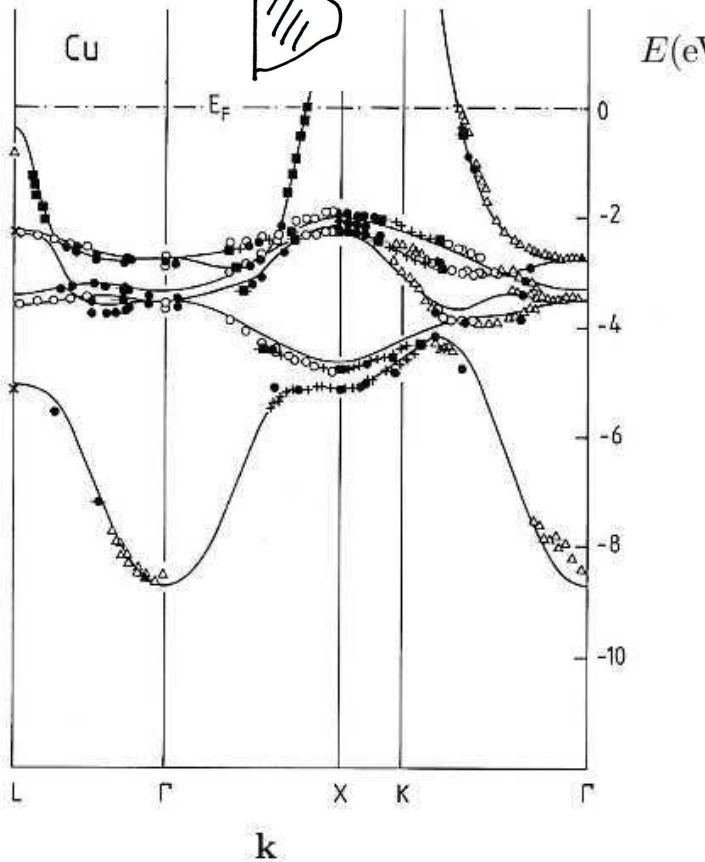
Metal

Fermi Level



Band Insulator

Gap



- Interaction ≈ kinetic energy ≈ 1-50 eV

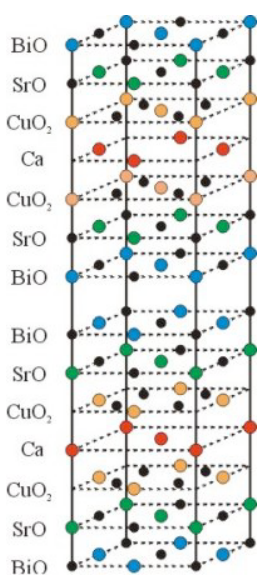
But

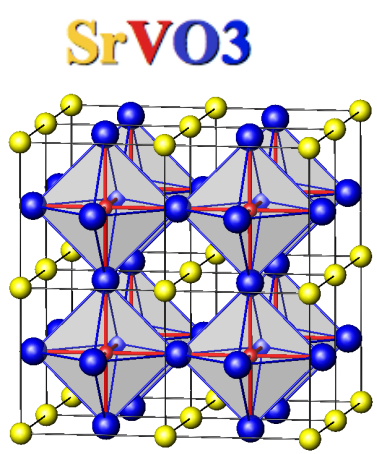
- Fermi liquid theory (Landau)
  Low energy renormalization group fixed point
  Quasi-particles: effective mass m*, lifetime, ...

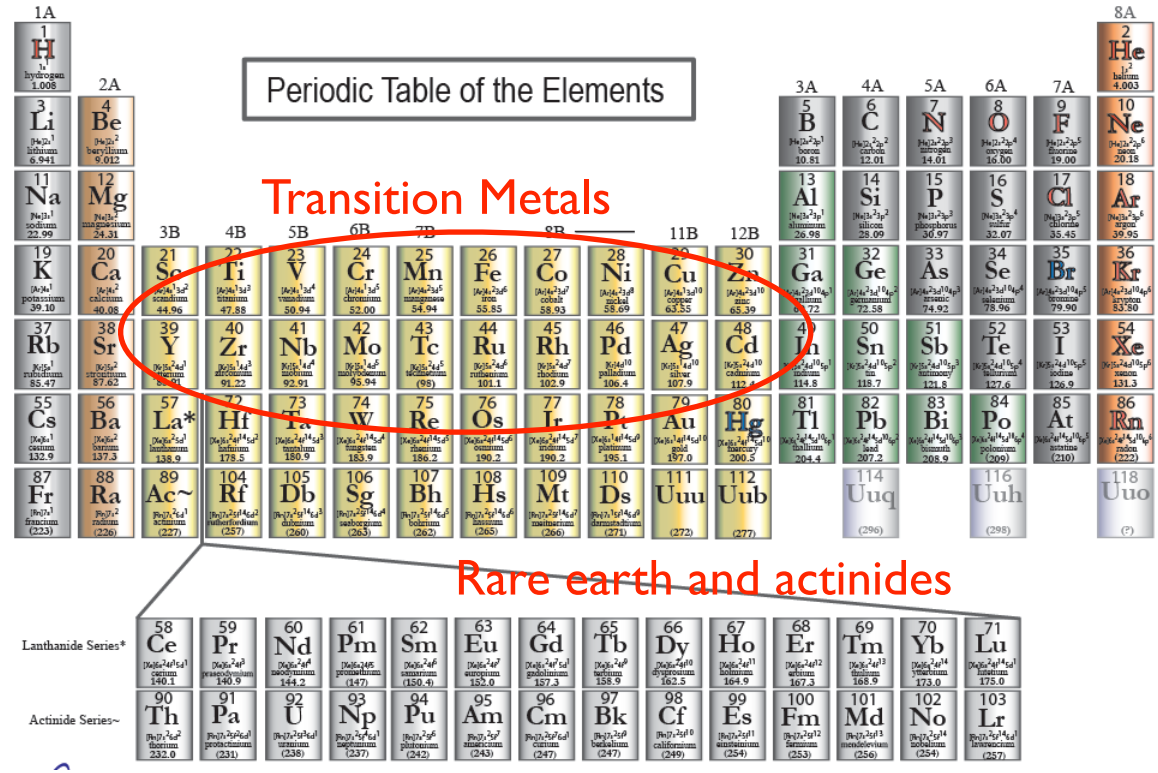
- Density functional theory (Kohn).
  Independent electrons + effective potential.

Strongly Correlated Systems

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



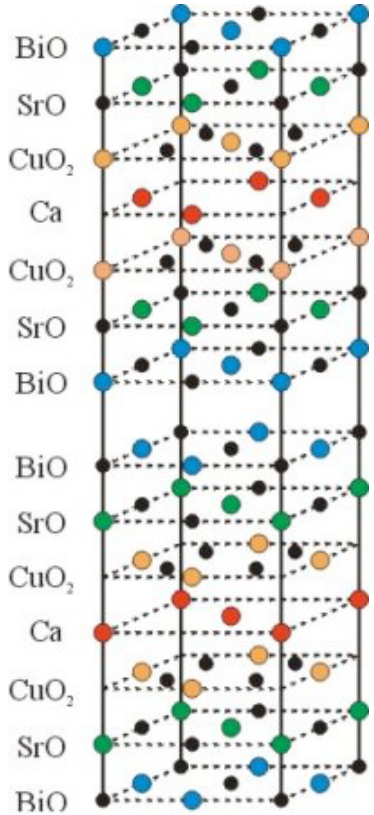


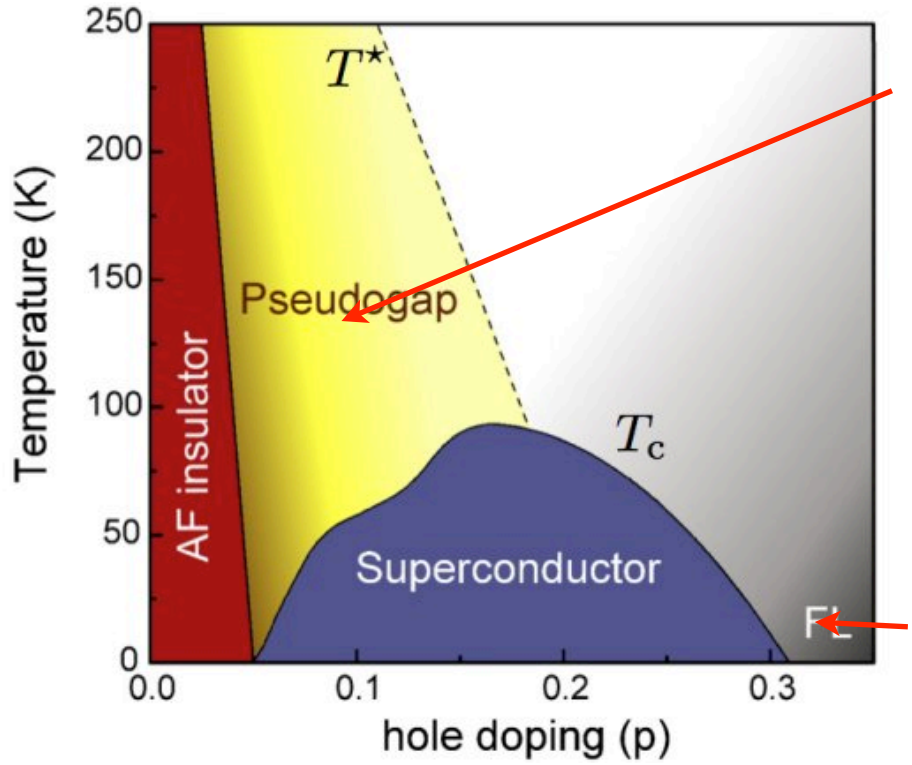


A famous example

High temperature superconductors

(Bednorz, Muller 1986)





Unconventional normal metal

Fermi liquid

$La_{2-x}Sr_xCuO_4$, $Bi_2Sr_2CaCu_2O_{8+\delta}$

- 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

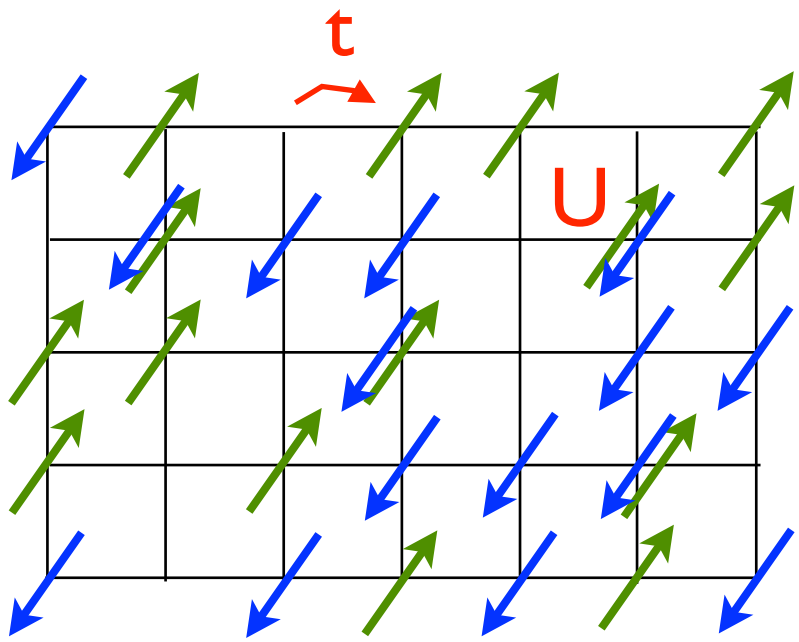
$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow},$$

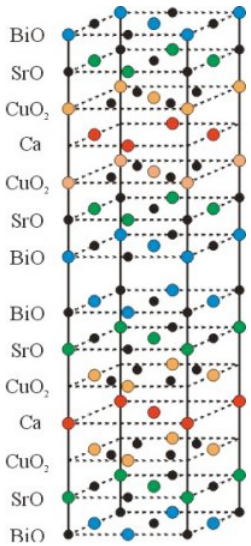
$$n_{i\sigma} \equiv c^{\dagger}_{i\sigma} c_{i\sigma}$$

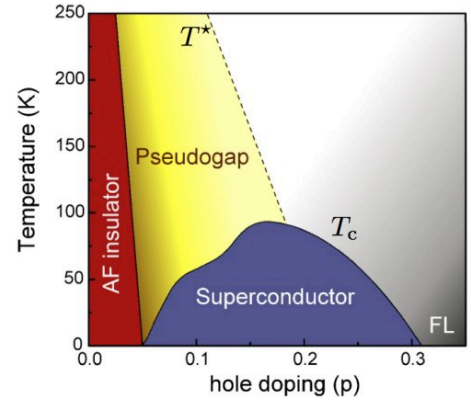
$$\delta = 1 - \langle n_{\uparrow} + n_{\downarrow} \rangle$$

Electron, spin +1/2

Electron, spin -1/2





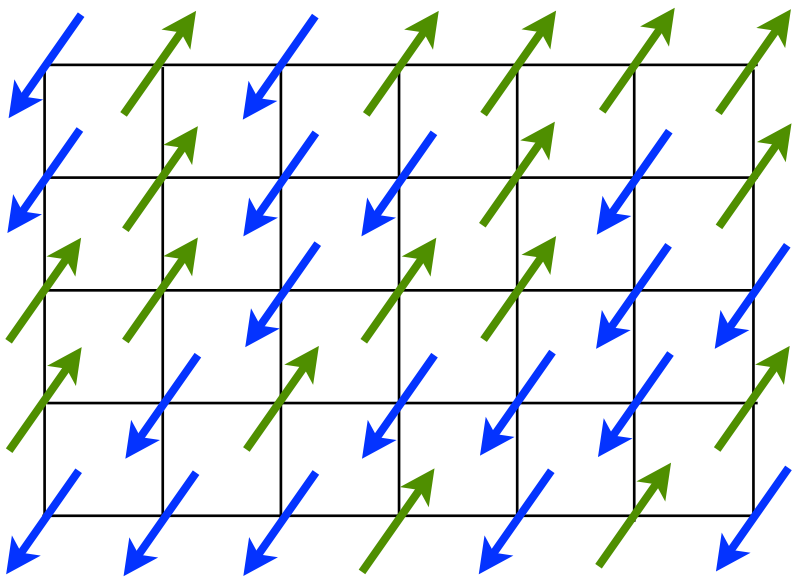


- Simplest possible model, almost a caricature.

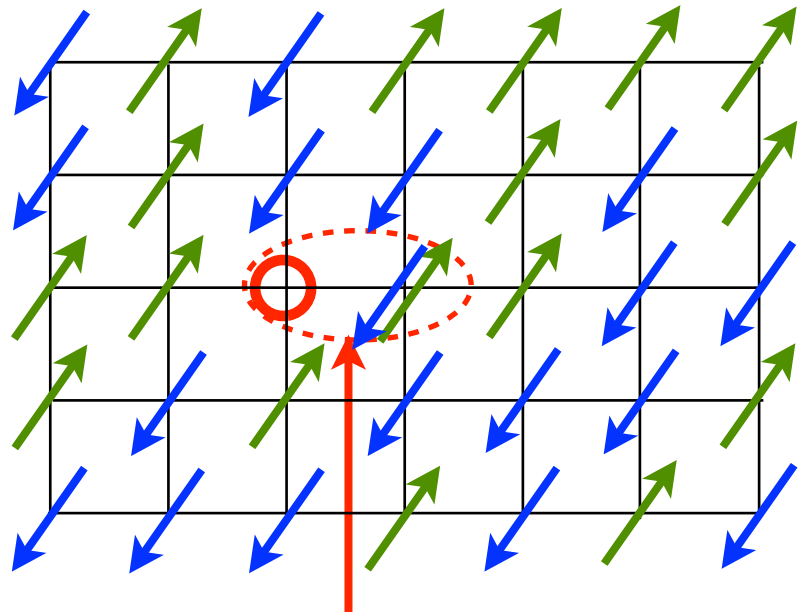
Mott insulator

N. Mott, 50's

- 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.

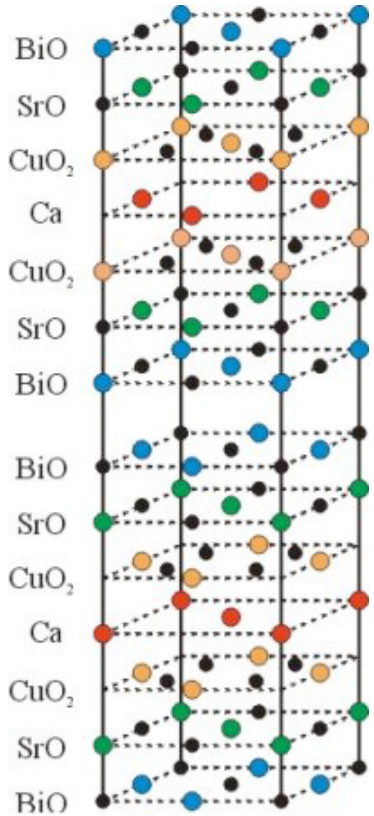


Mott insulator

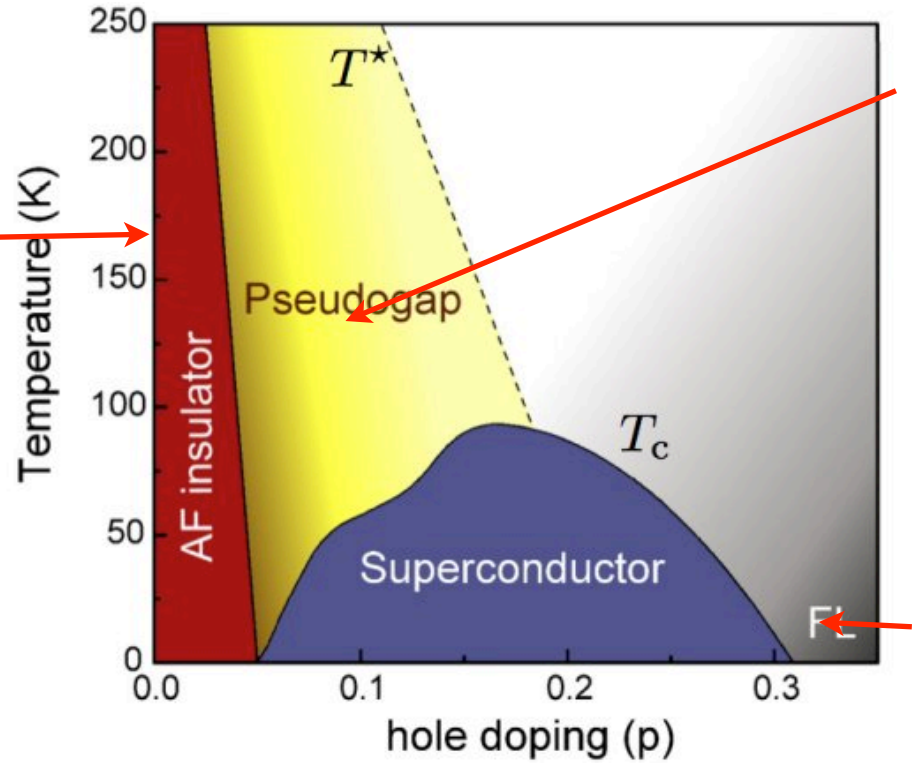


Large Coulomb repulsion U ~ eV ~ 10^4 K

Doped Mott insulators



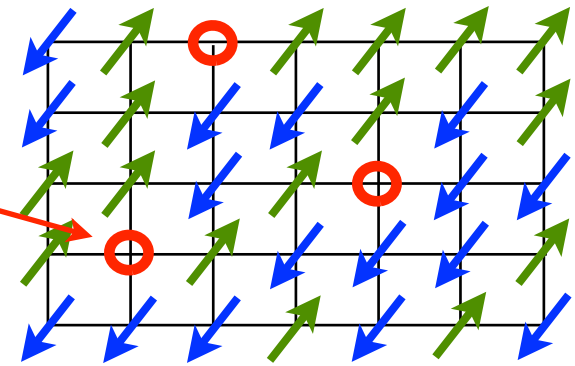
Mott insulator



Unconventional normal metal

Fermi liquid

Holes = charge carriers



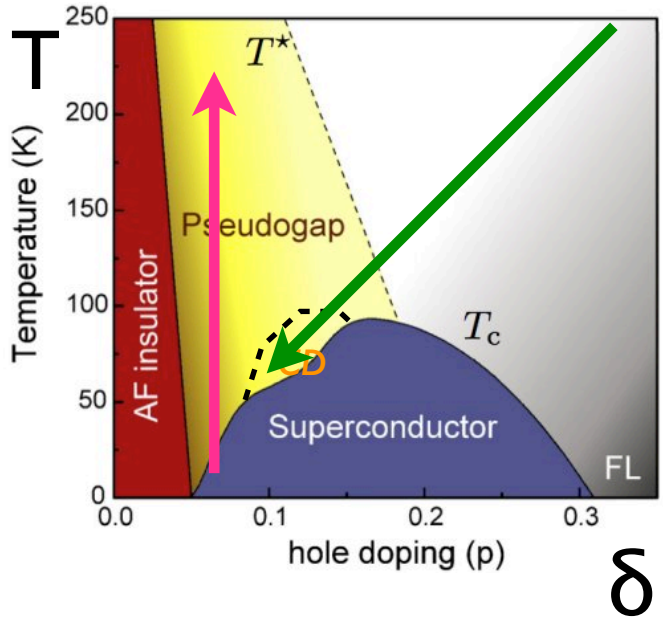
- Can we solve the Hubbard model ?
- Does it describe the high-Tc superconductors ? *(Anderson's conjecture 1987).*

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 ...

Quantum Monte Carlo

- Compute partition function Z
- Markov chain with local ergodic moves

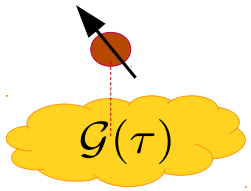
- Direct approach of the Hubbard model
  - Infamous fermionic sign problem !
  - Exponentially difficult (with size, 1/T).

- 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).



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

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

Interaction

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

Bath

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

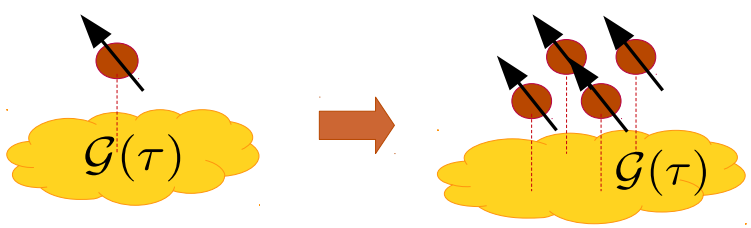
Control

- DMFT is not exact.

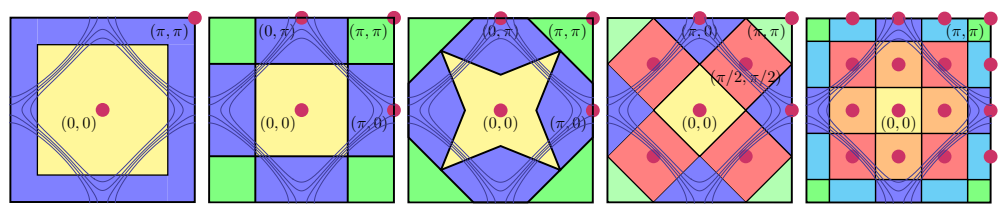
$$\Sigma(k,\omega) \approx \Sigma_{\text{impurity}}(\omega)$$

- Cluster method
  - Systematic expansion starting from DMFT.
  - Control parameter = size of cluster / momentum resolution.

Real space clusters



Reciprocal space clusters
Brillouin zone patching



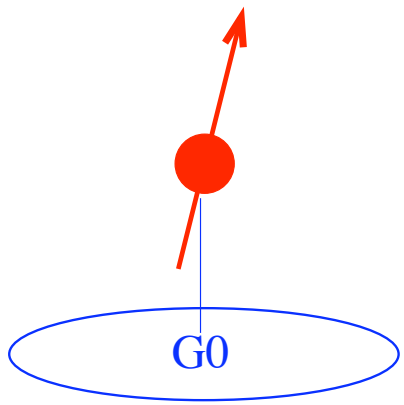
- Beyond : Trilex, ...

Algorithms to solve the impurity model ?

A local many-body problem

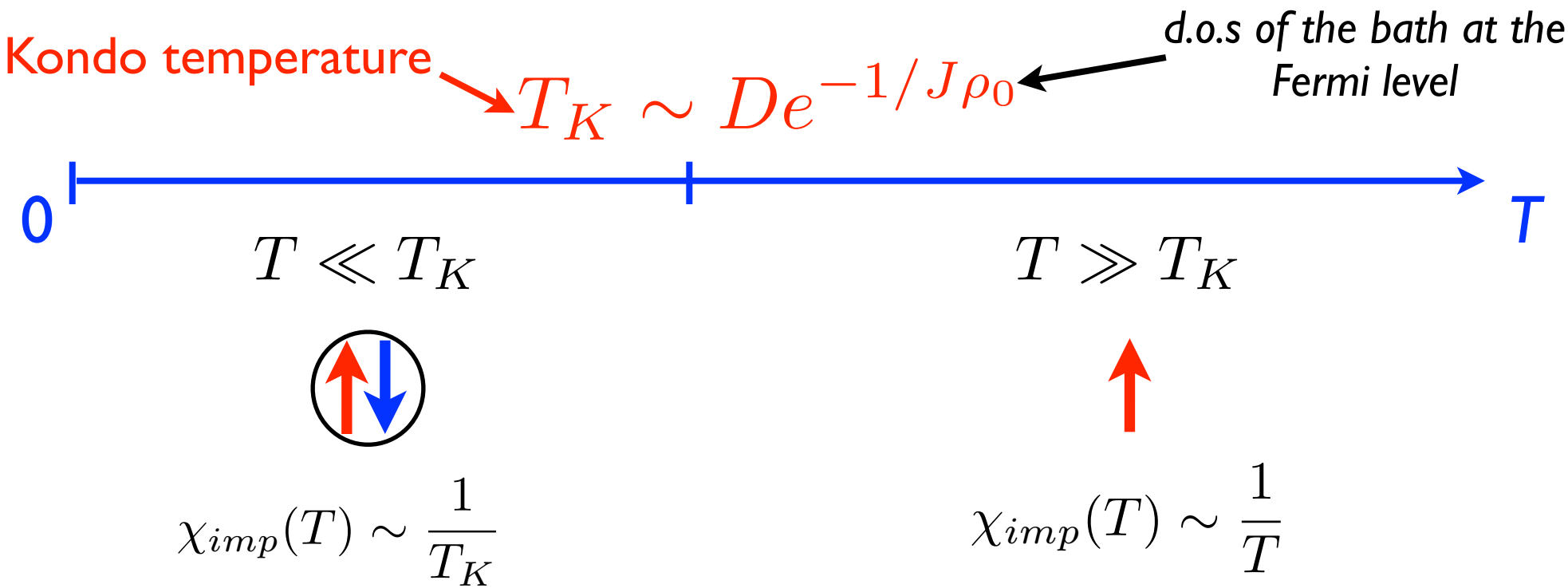
- The simplest version : Kondo model.
- 1 spin + 1 Fermi see of non-interacting electrons, with a local magnetic (exchange) interaction

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



Kondo effect

- Not so easy !
- A confinement problem. Screening of the spin by the bath.
- 1+1 Field Theory with asymptotic freedom (similar to QCD)



Algorithms are key

QMC for impurity models

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

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

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

Interaction

Bath

a,b = 1,N : degree of freedom (e.g. spin, orbital index, ...)

- 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.

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

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

- Using Wick Theorem :

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

Expansion in hybridization

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

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

a,b = 1,N

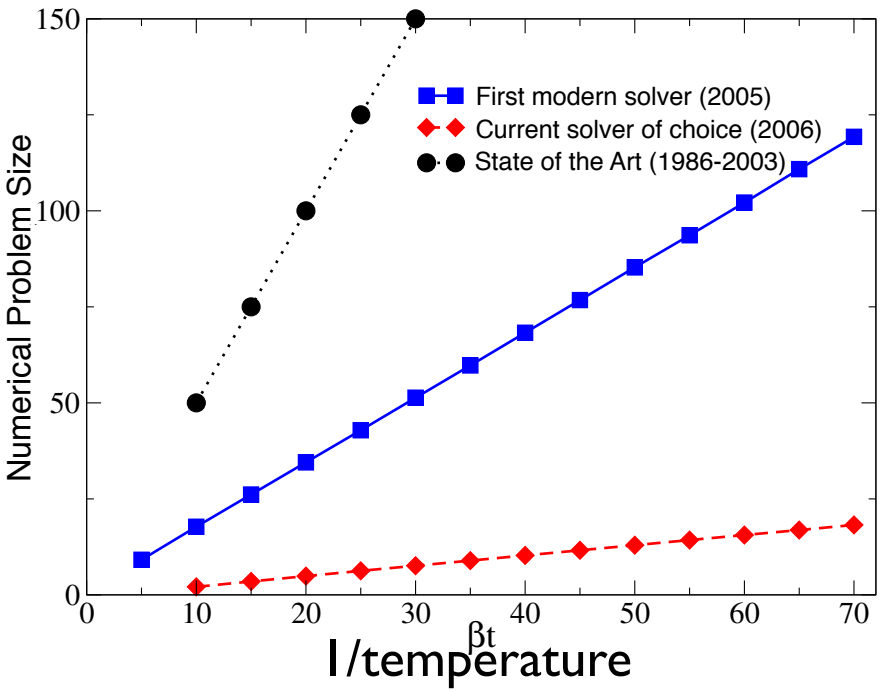
- Expansion in hybridization :

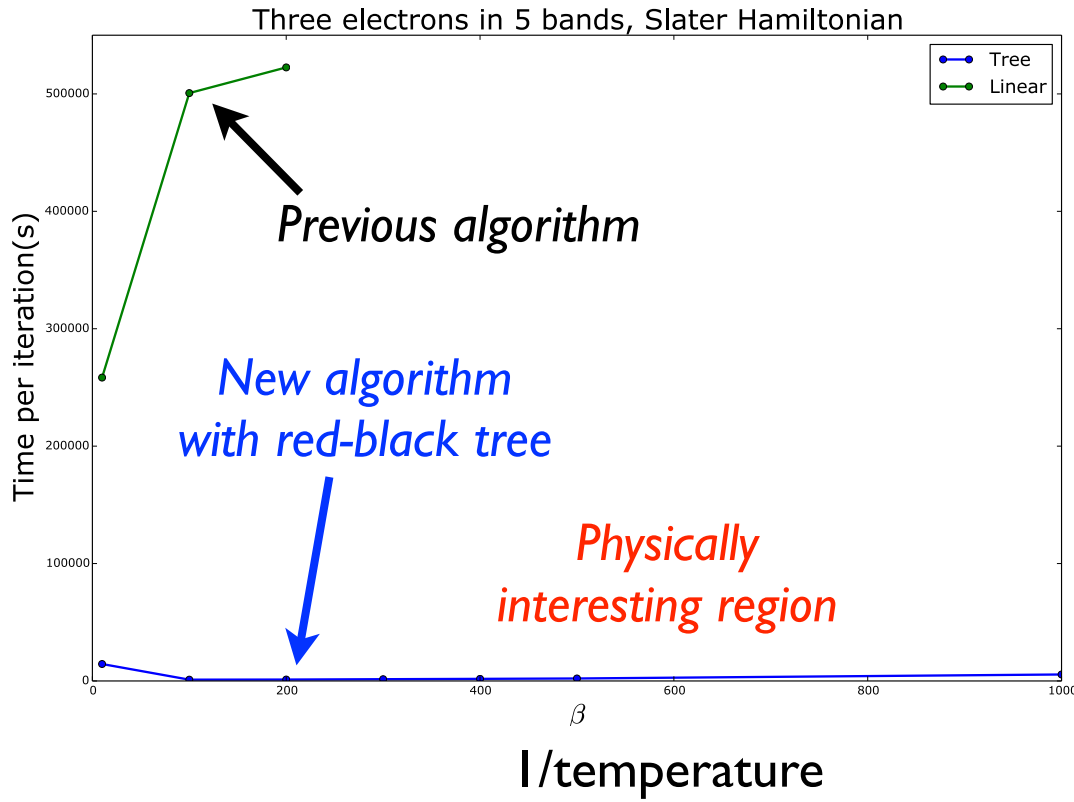
$$Z = \sum_{n\geq 0} \int_< \prod_{i=1}^n d\tau_i d\tau_i' \sum_{a_i,b_i=1,N} \underbrace{\det_{1\leq i,j\leq n} \left[\Delta_{a_i,b_j}(\tau_i - \tau_j')\right] \mathrm{Tr}\left(\mathcal{T} e^{-\beta H_{\rm local}} \prod_{i=1}^n c_{a_i}^\dagger(\tau_i) c_{b_i}(\tau_i')\right)}_{w(n,\{a_i,b_i\},\{\tau_i\})}$$

- Hlocal = Hamiltonian of the isolated atom.

Algorithms

- Huge recent progress.





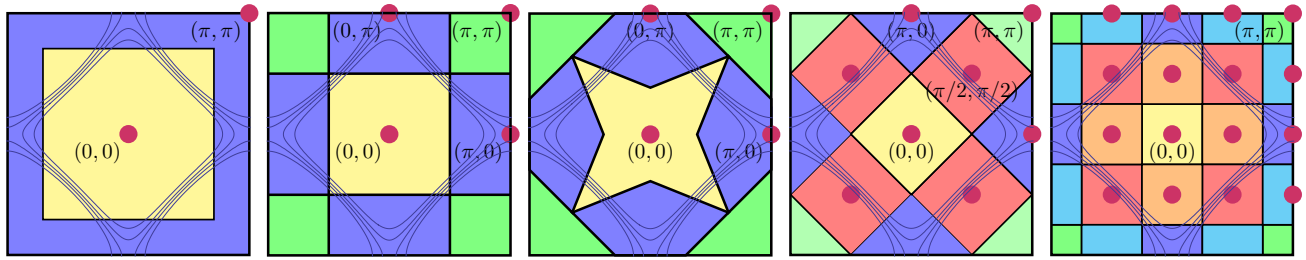
- Modern QMC.
  Typical matrix size reduced by ~30.
  Time speedup of factor 30^3
  or ~25 years of Moore's law

- 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 ≈200K

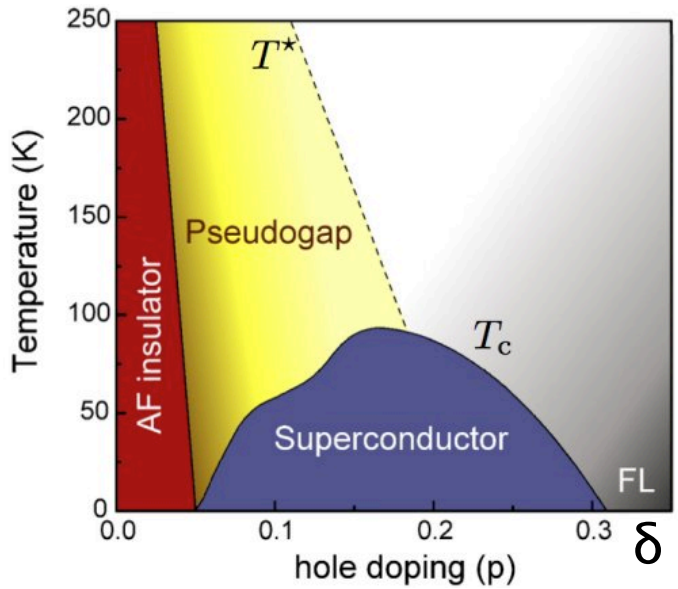


- Reproduce qualitatively various aspects of cuprate phase diagram.

Pseudo-gap

- Emerging from Mott insulator

T



d-wave SC

- In various clusters sizes (4, 8, 16, ...).
- Behavior of Tc, gap vs δ

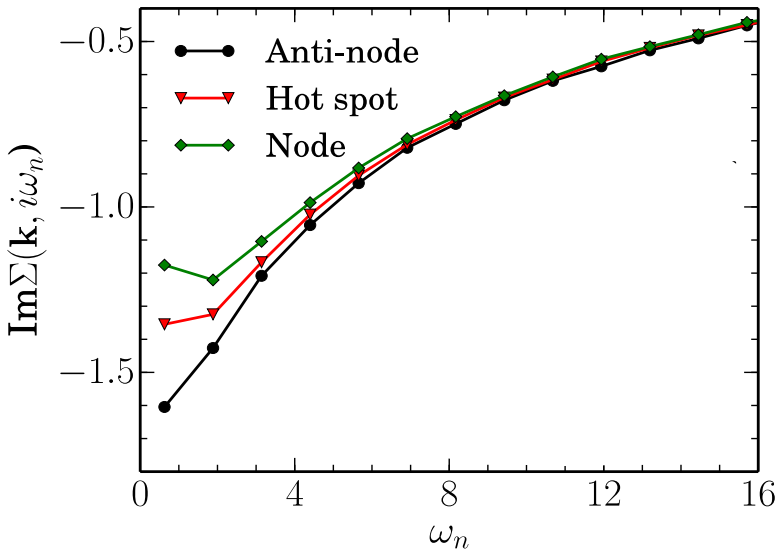
- Still many issues : mechanism ? converge ?

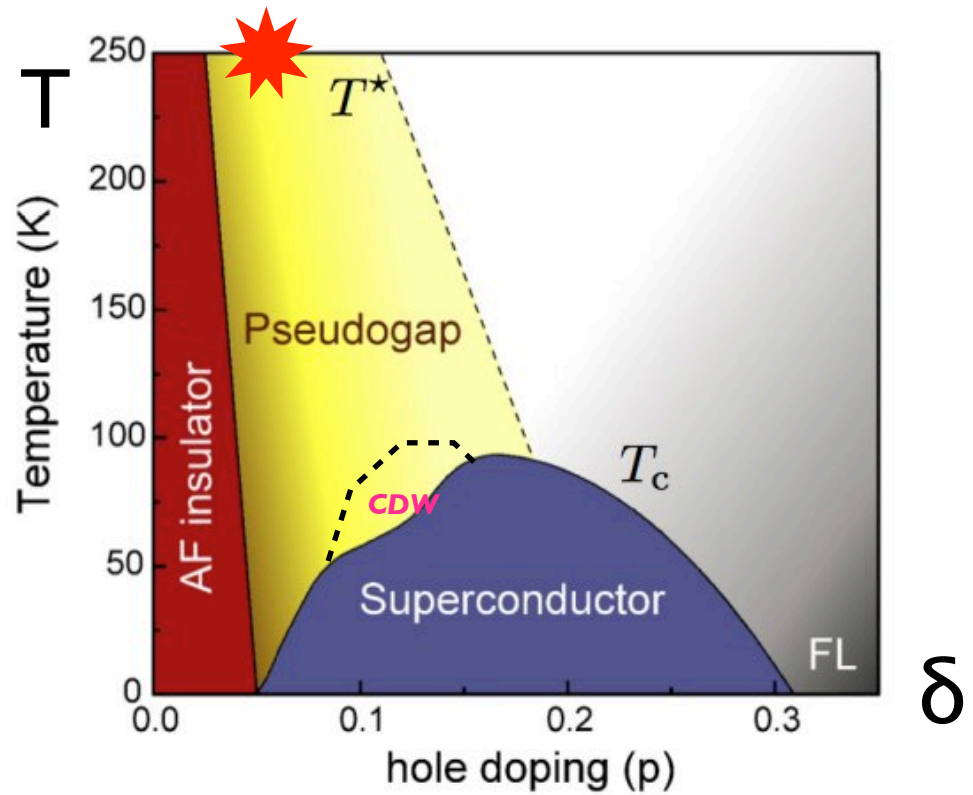
Pseudogap : exact solution at high temperature

- 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 t'= -0.3t
δ = 4% T = 0.2t

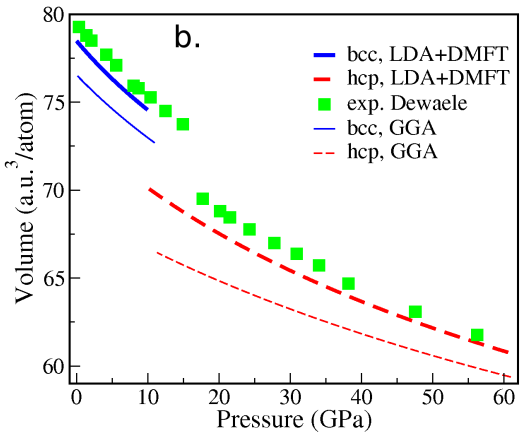




Ab-initio electronic structure for strongly correlated materials

- 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 ε-Fe,
e.g. volume vs pressure *(Pourovskii et al PRB 2014)*



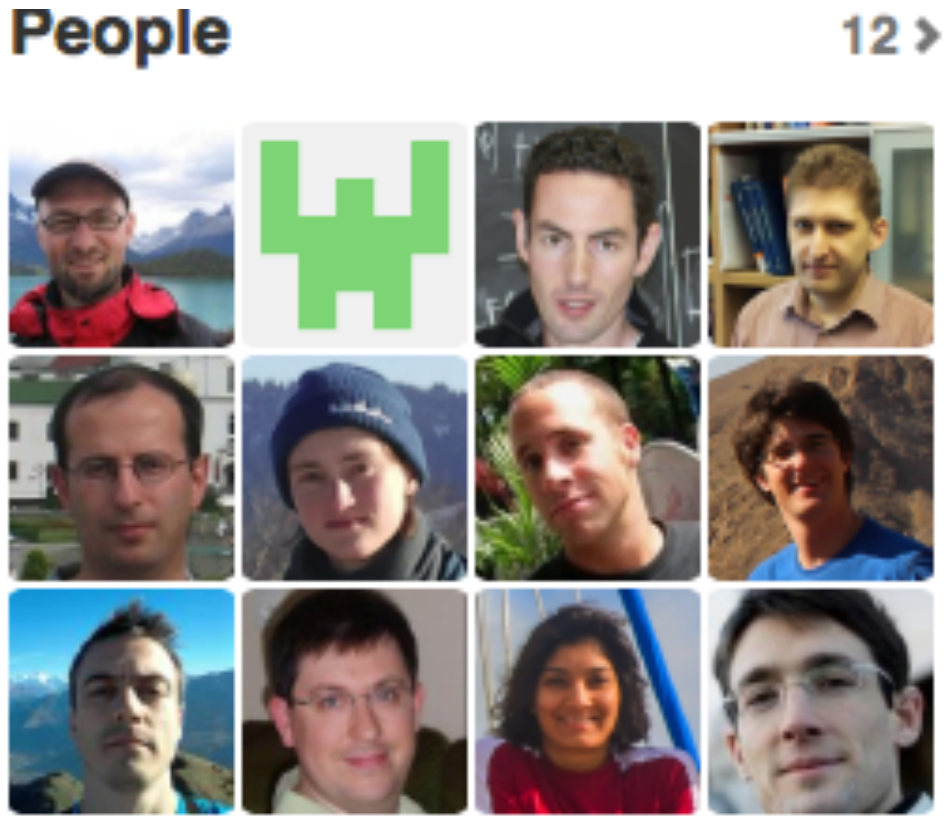
The TRIQS project

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



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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