



# Quantum cluster theories: Nonlocal dynamical fluctuations beyond DMFT and the dynamical cluster approximation.



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# Outline

- Models for strongly correlated electron systems
- A brief review of DMFT and its applications
- DMFT: Pitfalls
- Beyond DMFT: Cluster approaches
- Applications of Quantum cluster theories



# Minimal Models

## Hubbard model

$$\hat{H} = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + \epsilon_d \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

## Periodic Anderson Model

$$\begin{aligned} \hat{H} = & \epsilon_c \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{(i,j),\sigma} c_{i\sigma}^\dagger c_{j\sigma} + V \sum_{i,\sigma} (f_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.}) \\ & + \sum_{i,\sigma} \left( \epsilon_f + \frac{U}{2} f_{i-\sigma}^\dagger f_{i-\sigma} \right) f_{i\sigma}^\dagger f_{i\sigma}. \end{aligned}$$



# Solving the models

## Quantum many body theory approach

### Single-particle Green's function or propagator

$$G_{ij;\sigma}(t) = -i \langle 0 | T\{c_{i\sigma}(t)c_{j\sigma}^\dagger(0)\} | 0 \rangle$$

Density of states  
(Photoemission)Scattering rates and  
self-energy

### Many-particle Green's function or propagator

$$G(t_1, t_2, \dots) = \langle \phi | T \mathcal{A}(t_1) \mathcal{B}(t_2) \cdots \mathcal{R}(t_r) | \phi \rangle$$

Charge, spin and orbital  
susceptibilitiesElectrical and thermal  
conductivitiesVertex functionsBinder  
Cumulant, bond-order



# Solving the models

# Hubbard model

$$\hat{H} = \boxed{- \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + \epsilon_d \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}} \boxed{\text{limit} + U \sum_i n_{i\uparrow} n_{i\downarrow}}$$

Usual method of solution:  $H=H_0 + H_I$

## Known limit

## Perturbation

Not useful when  $H_0 \sim H_I$

Other small parameters:  $1/N$     $SU(N)$ : Symmetry of the spin-sector

**Question:** Is there a limit where simplification occurs but the band and atomic limits are treated on an equal footing?

**Answer:** Limit of infinite dimensions.



# Dynamical mean field theory- Philosophy

Ising model  $H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i = -h_o S_o - \sum_i J_{io} \hat{S}_o \hat{S}_i + H^{(o)}$

Trace out all  $S_i$  except  $S_o$   $\sum_{S_i, i \neq o} e^{-\beta H} \equiv e^{-\beta H_{\text{eff}}[S_o]}$ .

$$H_{\text{eff}} = \text{const} + \sum_{n=1}^{\infty} \sum_{i_1 \cdots i_n} \frac{1}{n!} \eta_{i_1} \cdots \eta_{i_n} \langle S_{i_1} \cdots S_{i_n} \rangle_c^{(o)} \quad J_{io} S_o \equiv \eta_i$$

$J_{ij} = J = J_o / d^{||i-j||}$   Mean field approximation  $H_{\text{eff}} = -h_{\text{eff}} S_o$

$$h_{\text{eff}} = h + \sum_i J_{oi} \langle S_i \rangle^{(o)}.$$

Effective field – self consistently determined  $h_{\text{eff}} = h + z J m$

Magnetization  $m = \tanh \beta h_{\text{eff}}$  (from the single-spin partition function)

**Philosophy** - Reduce a lattice problem to a single-site embedded in a self-consistently determined host.



# Dynamical mean field theory

Hubbard model

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

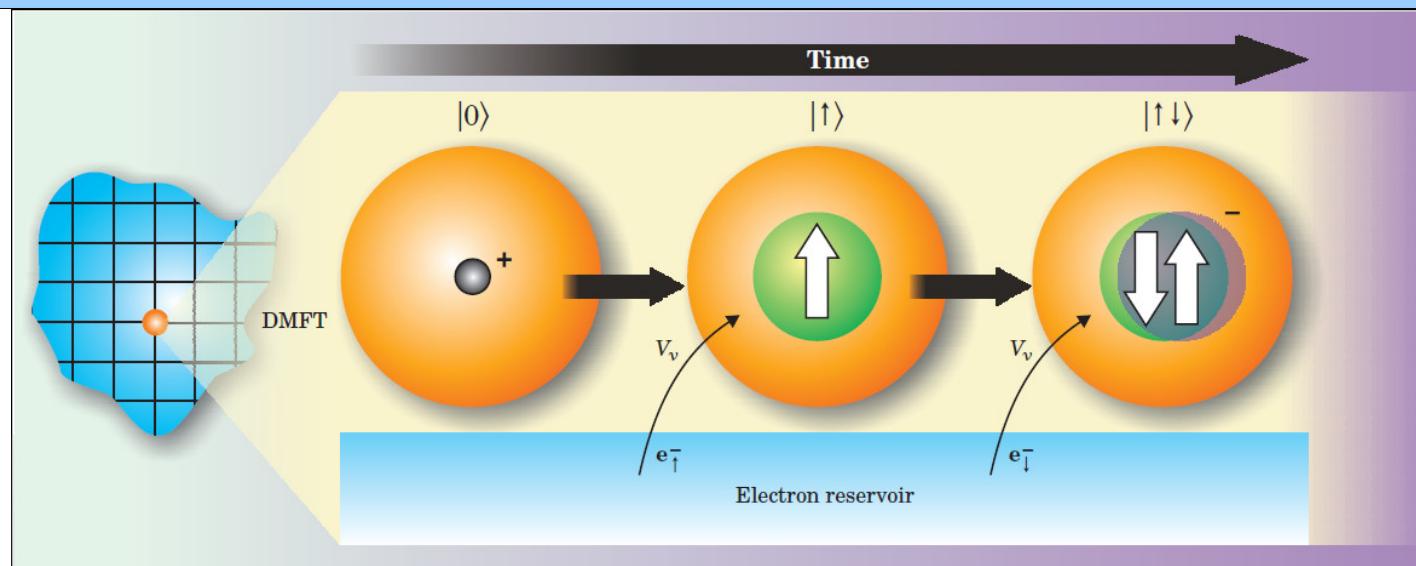
With  $t = \frac{t_*}{\sqrt{2d}}$   $S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{o\sigma}^+(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta d\tau n_{o\uparrow}(\tau) n_{o\downarrow}(\tau).$

Dynamical mean field  $\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{oi} t_{oj} G_{ij}^{(o)}(i\omega_n).$



# Dynamical mean field theory

- Mean field theory for quantum many body systems on a lattice.
- Maps lattice models to self-consistent impurity models
- Self energy and Vertex function become purely local and momentum independent.
- Ignores spatial fluctuations but accounts for quantum local temporal fluctuations.
- Exact in the limit of infinite dimensions.





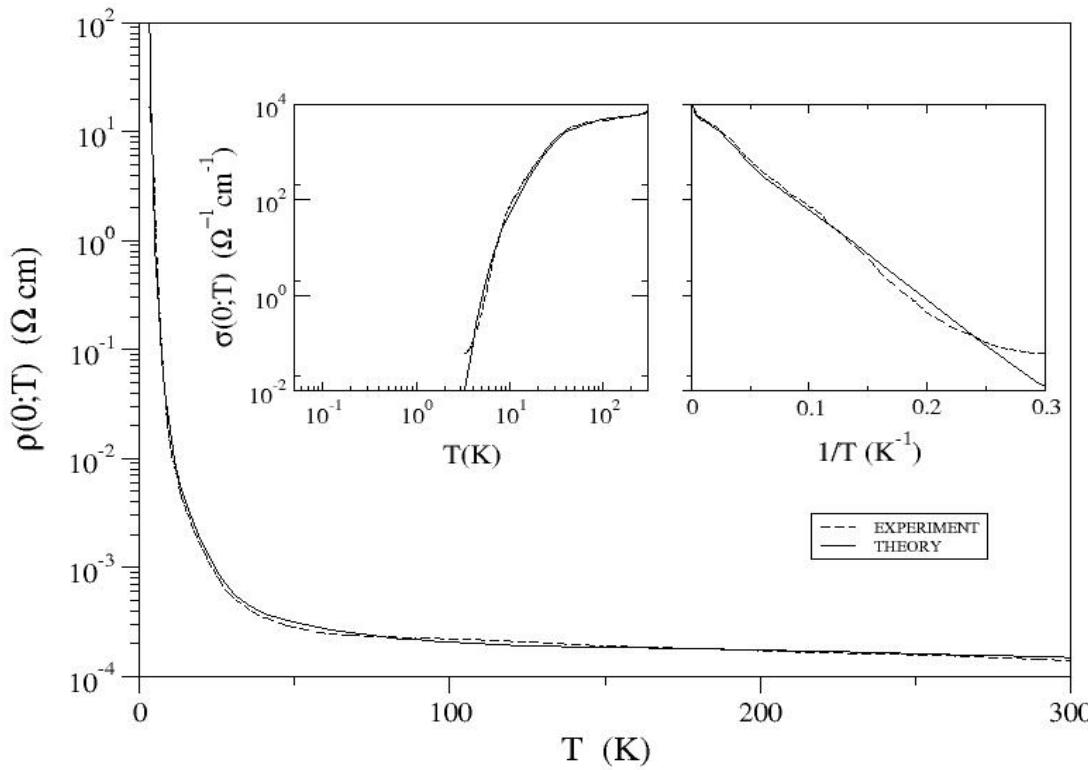
# Applications



# Heavy fermions

Periodic Anderson

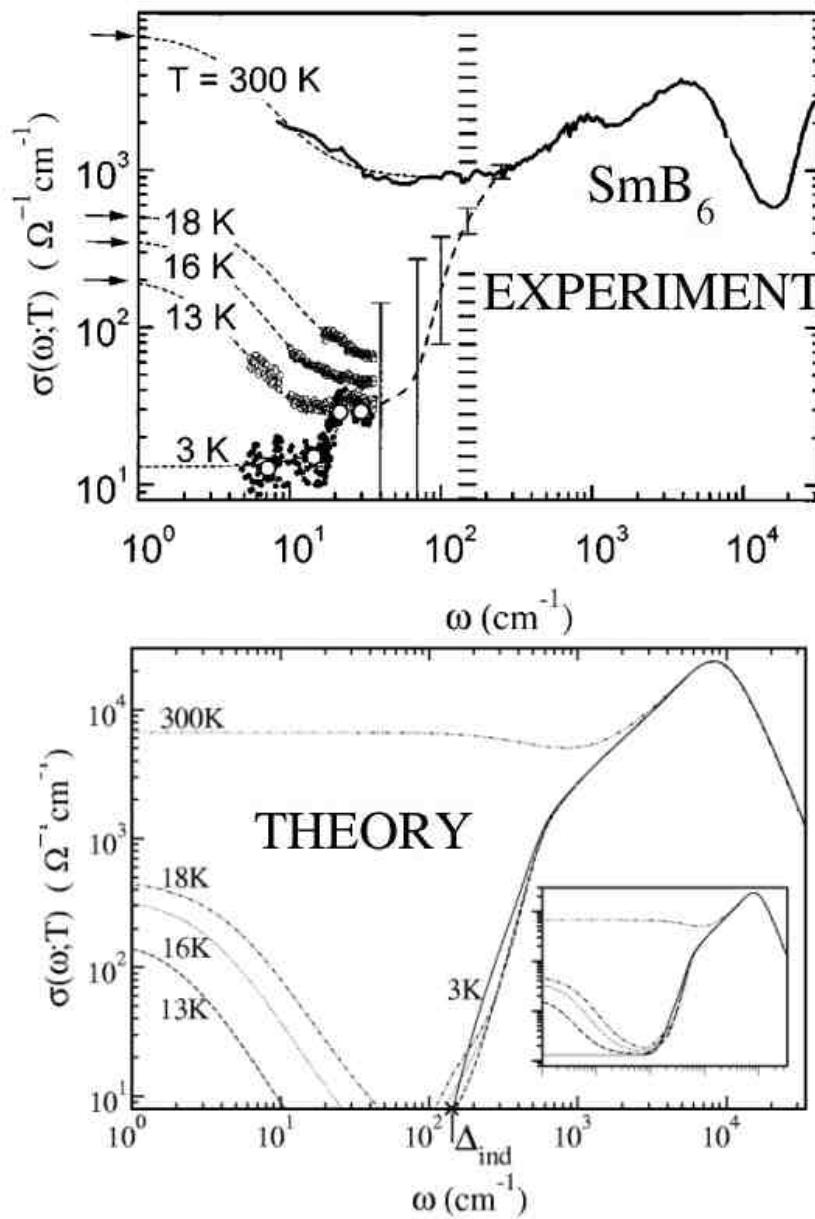
$$\hat{H} = \epsilon_c \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{(i,j),\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + V \sum_{i\sigma} (f_{i\sigma}^\dagger c_{i\sigma} + \text{h.c.}) + \sum_{i\sigma} \left( \epsilon_f + \frac{U}{2} f_{i,-\sigma}^\dagger f_{i,-\sigma} \right) f_{i,\sigma}^\dagger f_{i,\sigma}$$



**$\text{SmB}_6$**   
DC Resistivity

$$\Delta_g = 8.75 \text{ meV} = 101 \text{ K}$$

N. S. Vidhyadhiraja et al J. Phys. Condens. Matter Vol.15 pp.4045-4087 (2003).  
Gorshunov et al Phys. Rev. B, Vol.59, pp.1808-1814 (1999).



***SmB<sub>6</sub>***

Optical conductivity

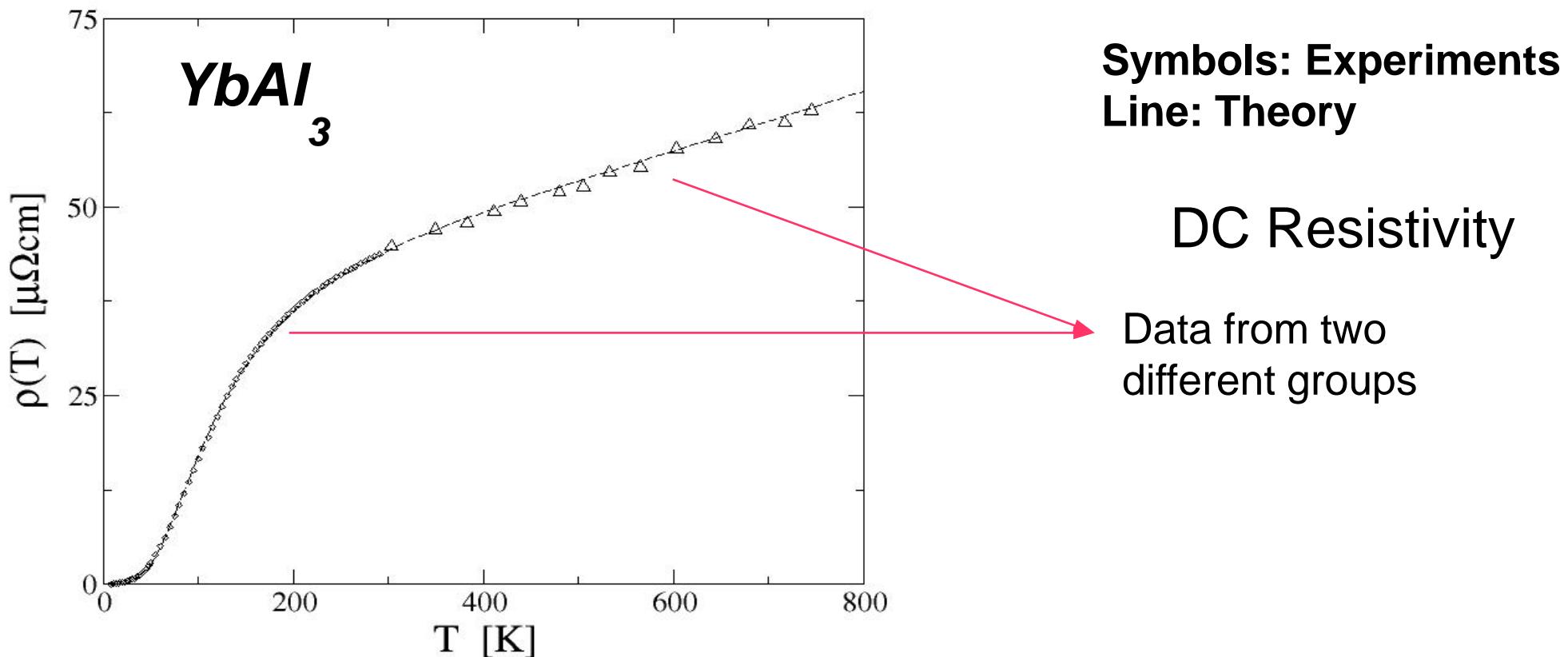
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## Heavy Fermions – Dynamical Mean Field Theory



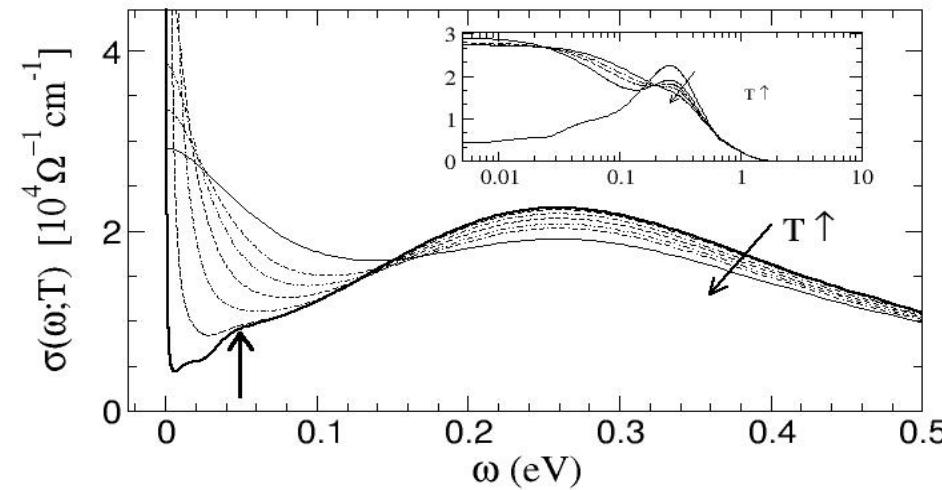
Rowe et al J. Phys. D: Appl. Phys **35** 2183-2186 (2002).

N.S.Vidhyadhiraja , Logan J. Phys. Condens. Matter Vol.17 pp.2959-2976 (2005);

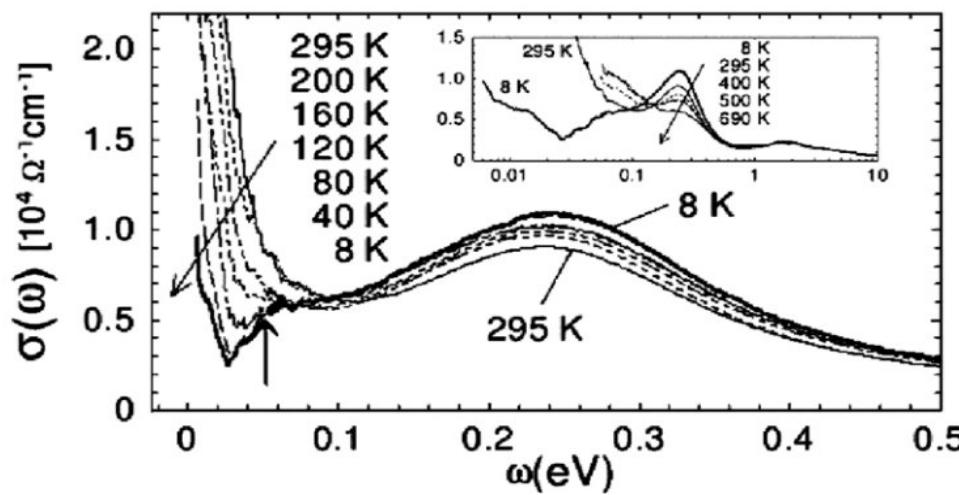


## $\text{YbAl}_3$

### Optical conductivity



Theory



Experiment

Okamura et al J. Phys. Soc. Japan Vol.73 pp.2045 (2004).

NSV , Logan J. Phys. Condens. Matter Vol.17 pp.2959-2976 (2005);



# Heavy Fermions – Dynamical Mean Field Theory

**$SmB_6$ ,  $YbB_{12}$ ,  $Ce_2Bi_4Pt_3$ ,  $CeB_6$ ,  $CeAl_3$ ,  $CeCoIn_5$ ,  
 $YbAl_3$ ,  $CeOs_4Sb_{12}$ ,  $CeFeGe_3$ ,  $CeRhSi_2$ ,**  
 **$Ce_2Ni_3Si_5$**

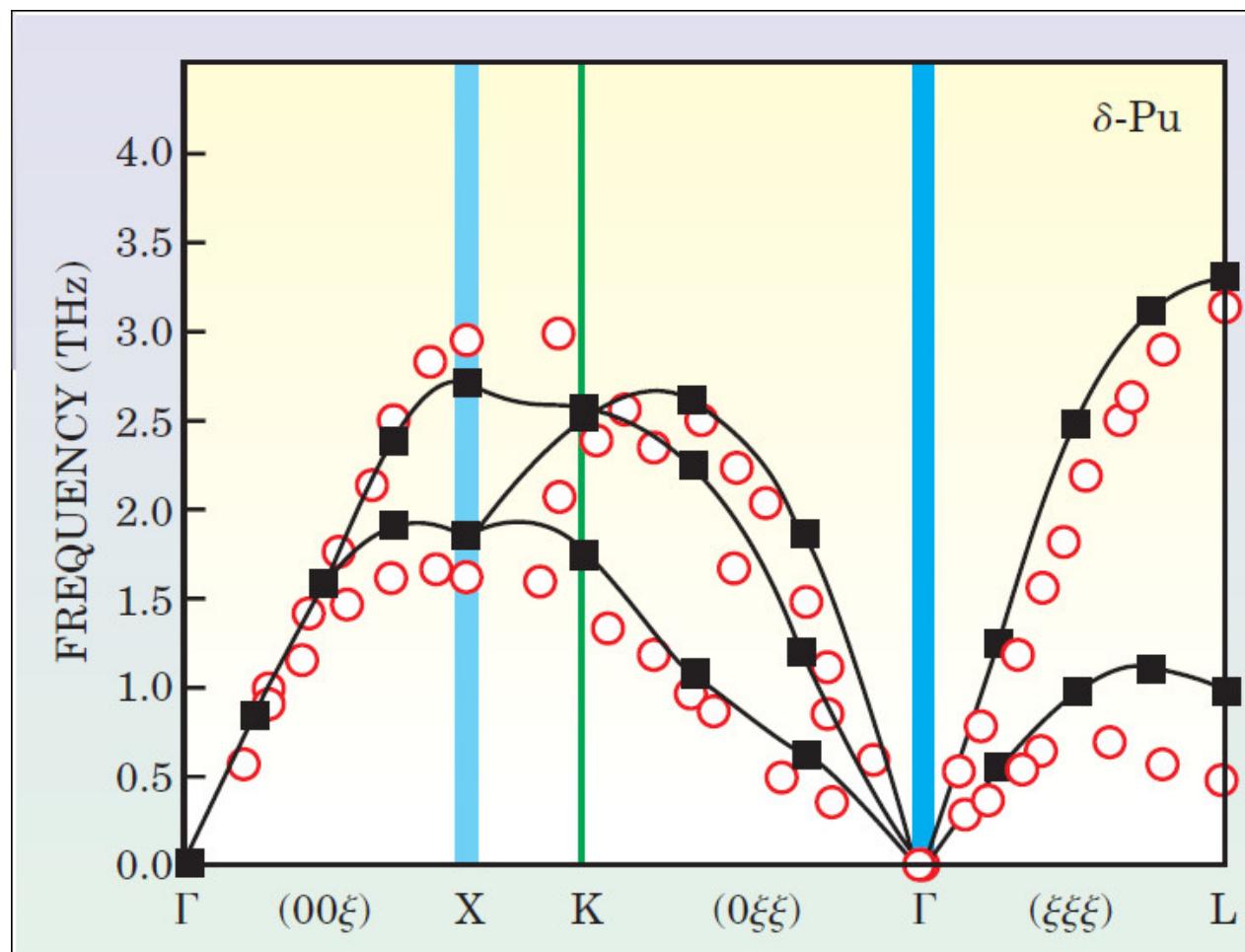
**$Ce_{1-x}La_xB_6$ ,  $Ce_{1-x}La_xAl_3$**

***Spectral Dynamics, DC and Optical transport,  
Thermodynamics, Magnetotransport***



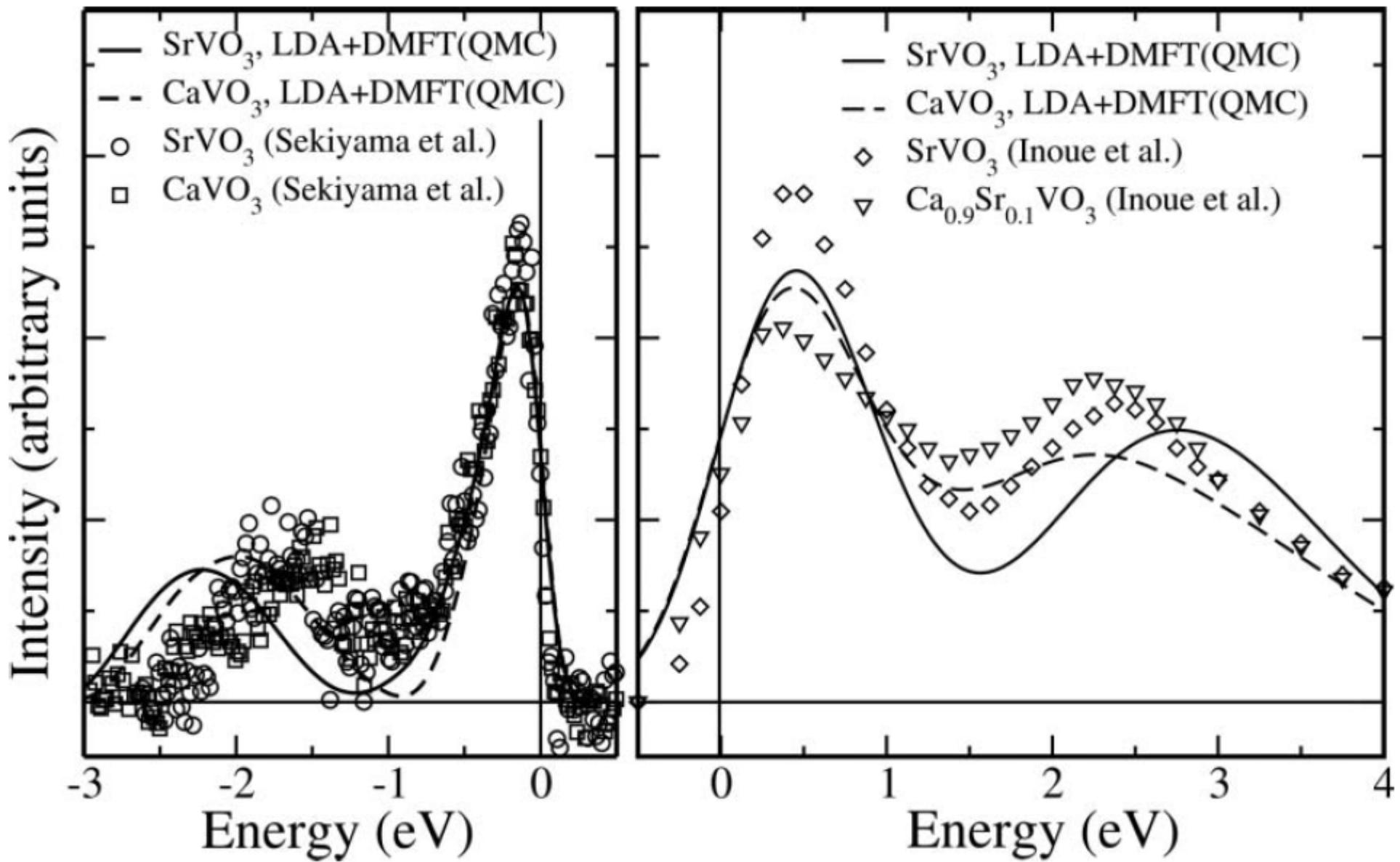
# Elemental Plutonium

Phonon spectrum computed with DMFT and compared to experiment



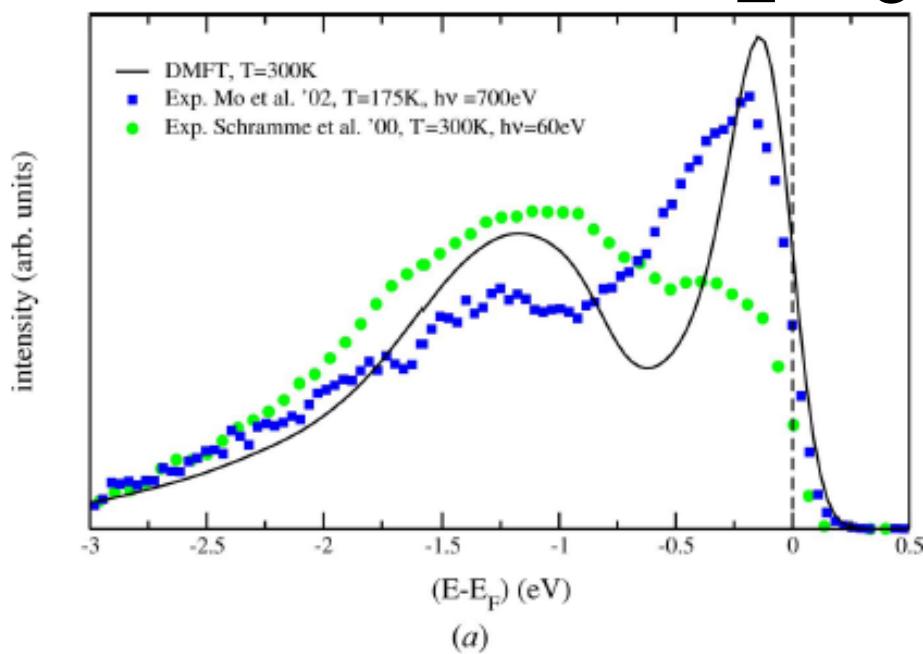


# SrVO<sub>3</sub>



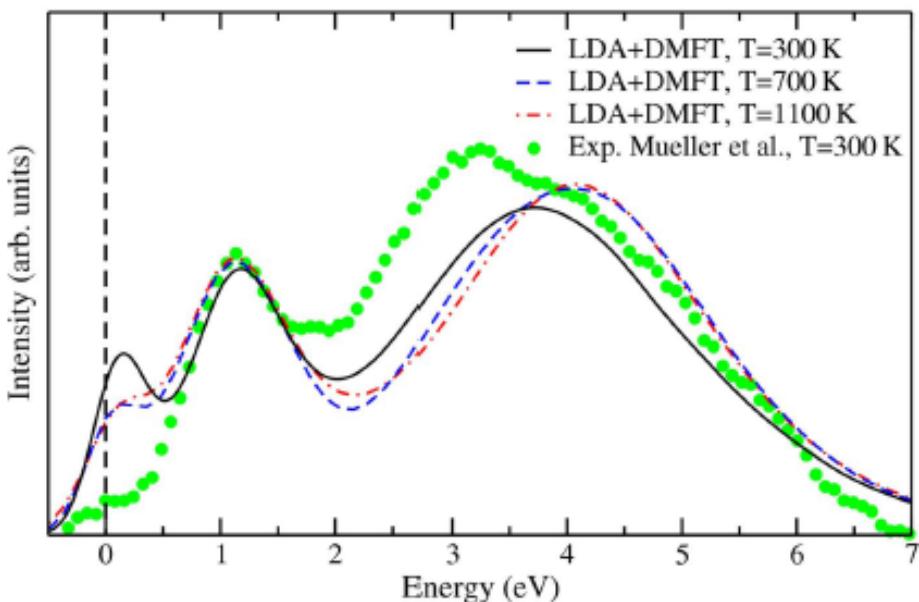


# $V_2O_3$



(a)

Photoemission  
spectra



X-ray absorption  
spectra

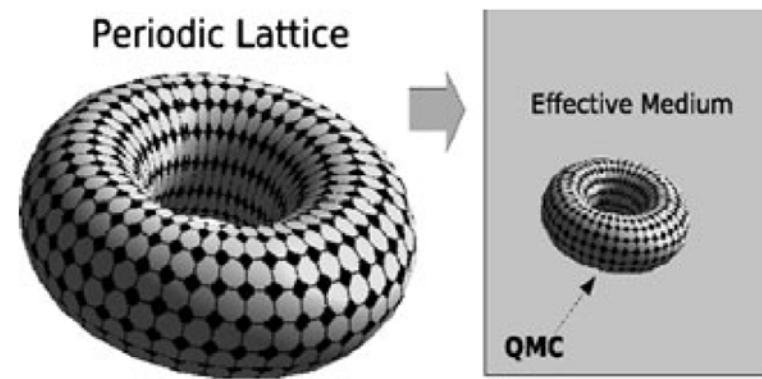


# Problems with DMFT

- Ignores non-local dynamical spatial fluctuations (implying that  $S_{ij}=0$  for  $i \neq j$ ).
- Physics specific to finite dimensions (especially 1D, 2D) is not captured.
- Ordered phases with  $\mathbf{k}$ -dependent order parameter cannot be studied.
- Might yield spurious transitions (e.g. Curie-Weiss theory for 1D Ising model)
- Other non-local phenomena such as Anderson localization also cannot be described.



# Beyond DMFT: Cluster approaches



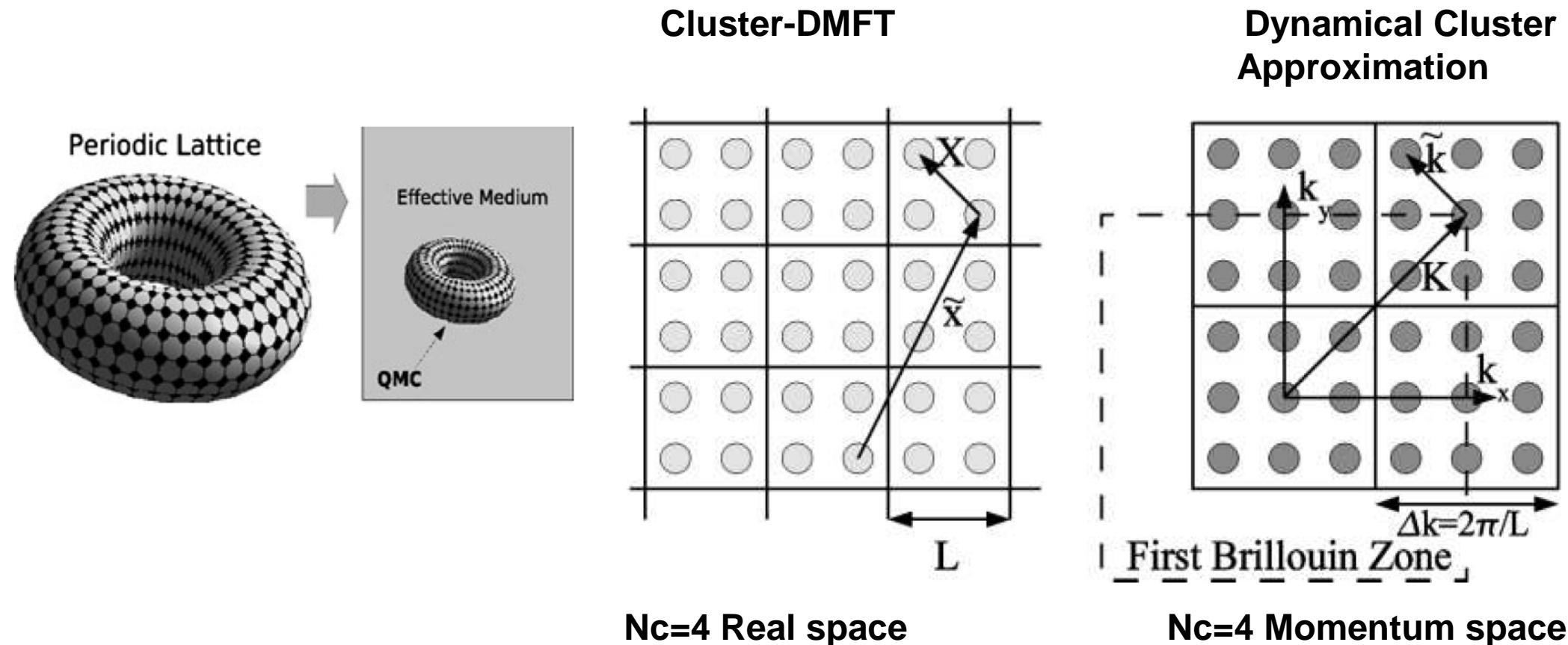
H.Fotso et al, Chapter in *Strongly Correlated Systems*, Springer (2012).

T. Maier et al, Rev. Mod. Phys 77 1027 (2005).

APS-IUSSTF lectures at Purdue - 2015



# Beyond DMFT: Cluster approaches



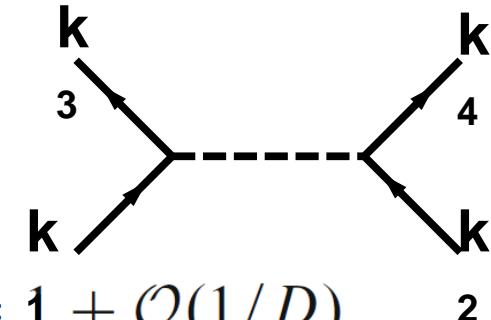


# Momentum space clusters

## - Dynamical Cluster approximation

- In an exact theory, the Laue function expressing momentum conservation would be

$$\Delta(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = \sum_{\mathbf{r}} \exp [i\mathbf{r} \cdot (\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)] \\ = N \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4},$$



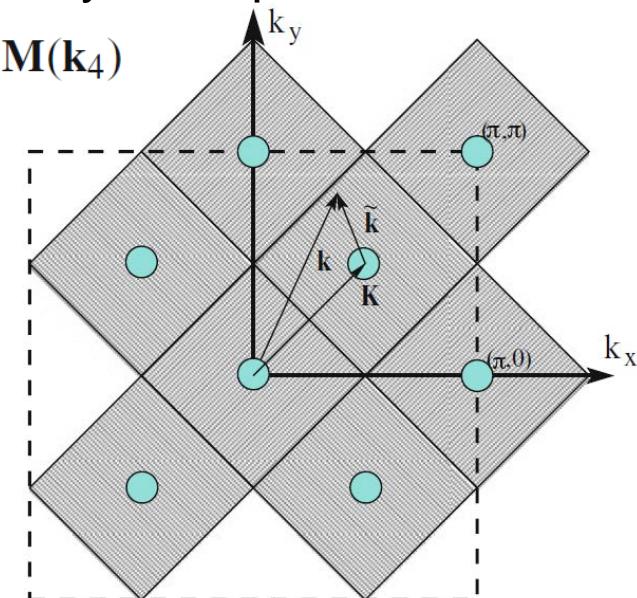
- In the limit of infinite dimensions,  $\Delta_{D \rightarrow \infty}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = 1 + \mathcal{O}(1/D)$ . hence momentum conservation can be ignored.

- In the dynamical cluster approximation, the Laue function may be expressed as  $\Delta_{\text{DCA}}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = N_c \delta_{\mathbf{M}(\mathbf{k}_1) + \mathbf{M}(\mathbf{k}_2), \mathbf{M}(\mathbf{k}_3) + \mathbf{M}(\mathbf{k}_4)}$

- $\mathbf{M}(\mathbf{k})$ : mapping of  $\mathbf{k}$  to the cluster momentum  $\mathbf{K}$

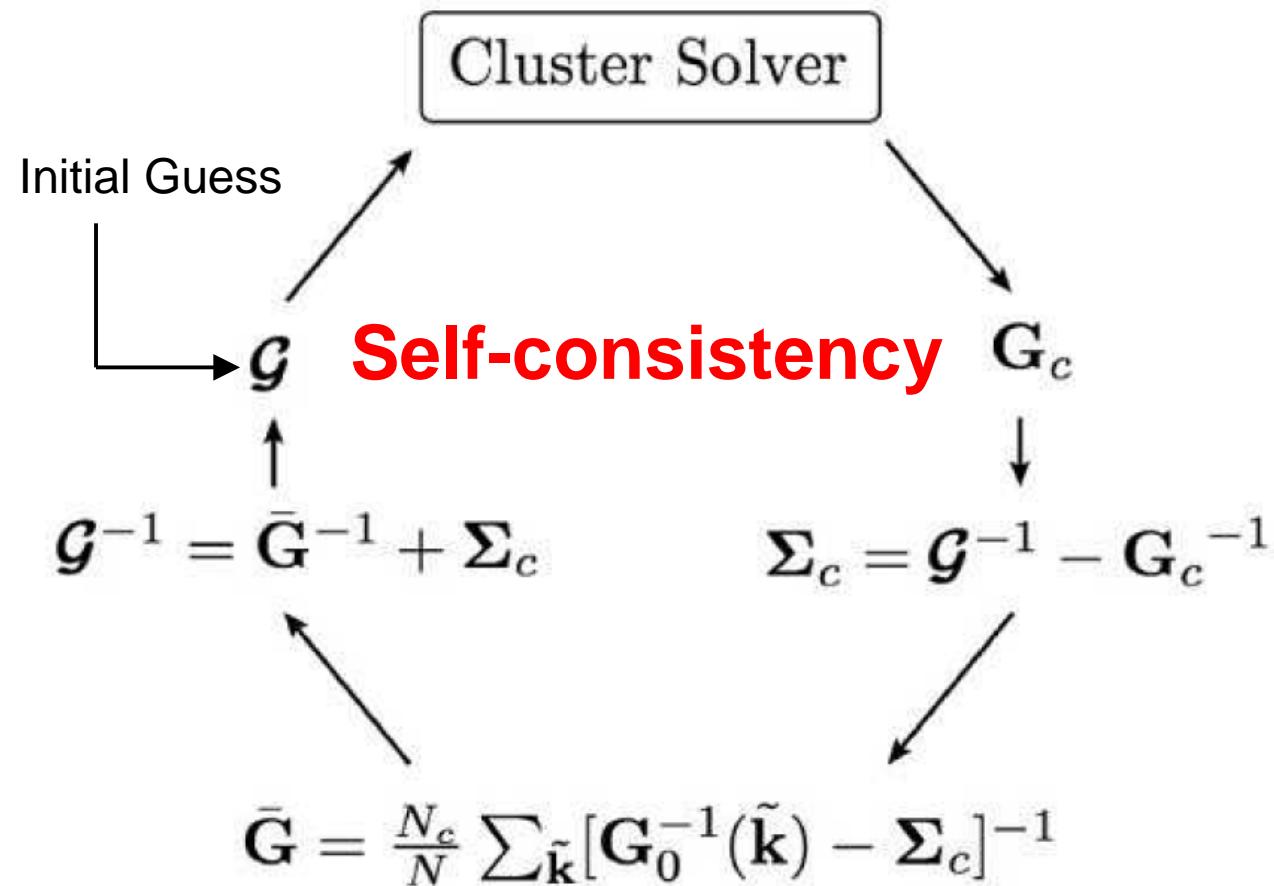
- The Green's function is given by

$$G(\mathbf{k}, z) = \frac{1}{z - (\epsilon_{\mathbf{k}} - \mu) - \bar{\Sigma}(\mathbf{M}(\mathbf{k}), z)}$$



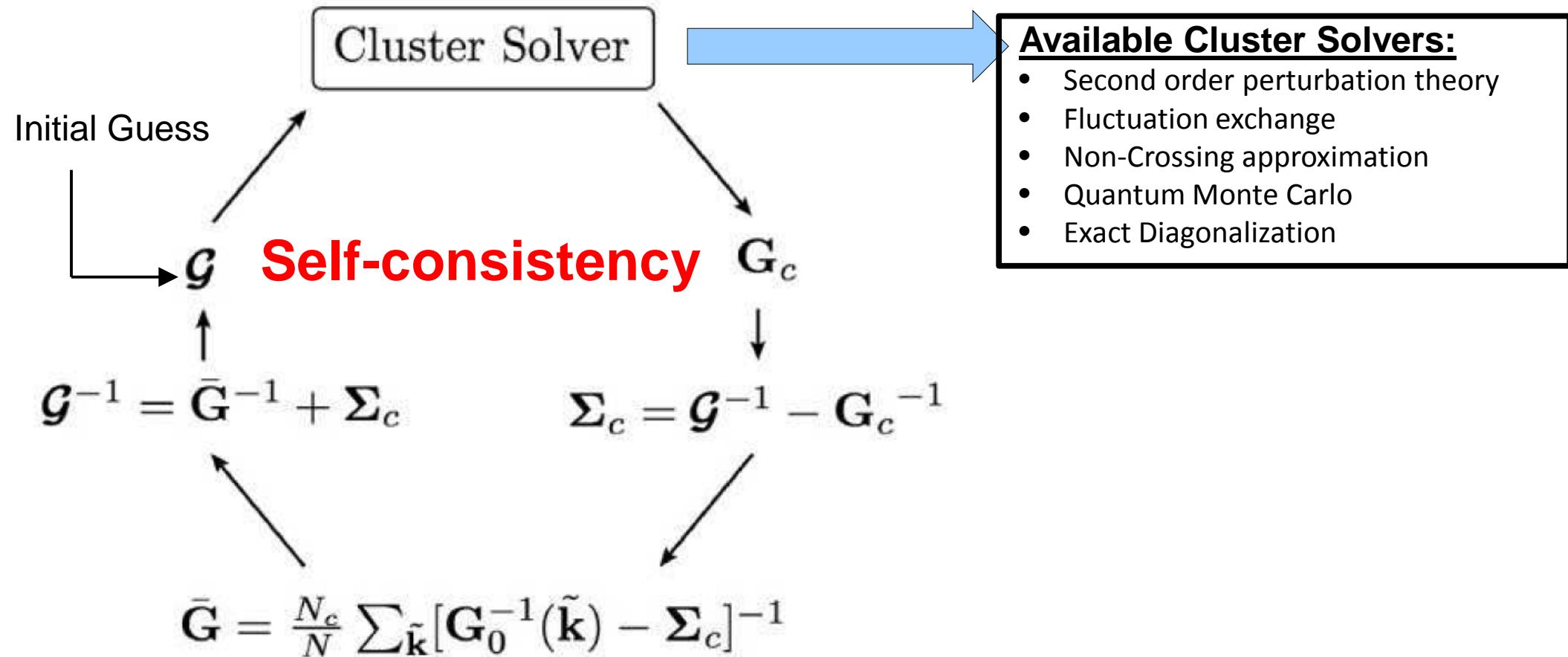


# Beyond DMFT: Cluster approaches(in practice)



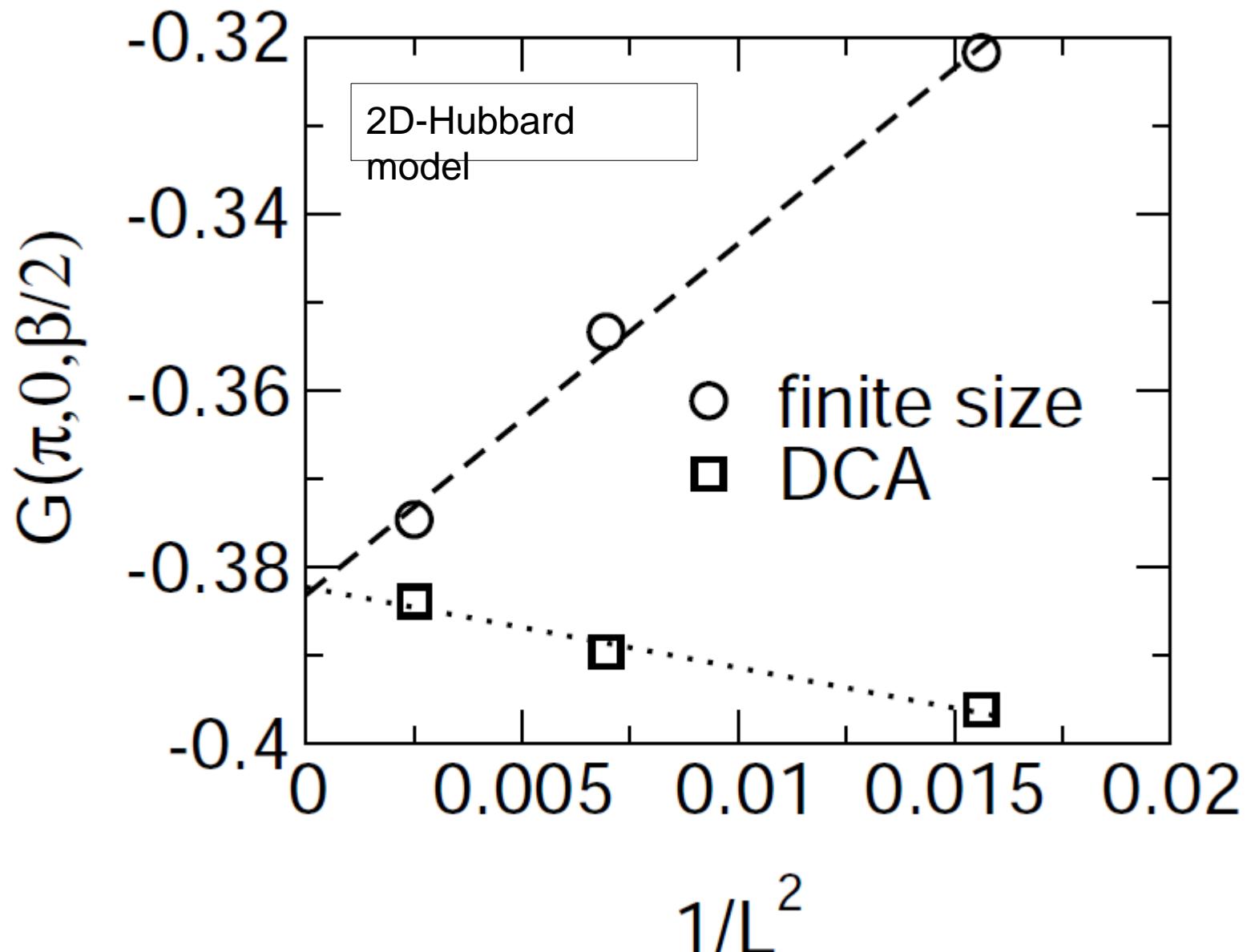


# Beyond DMFT: Cluster approaches





# Dynamical Cluster approximation (Convergence)





# Applications



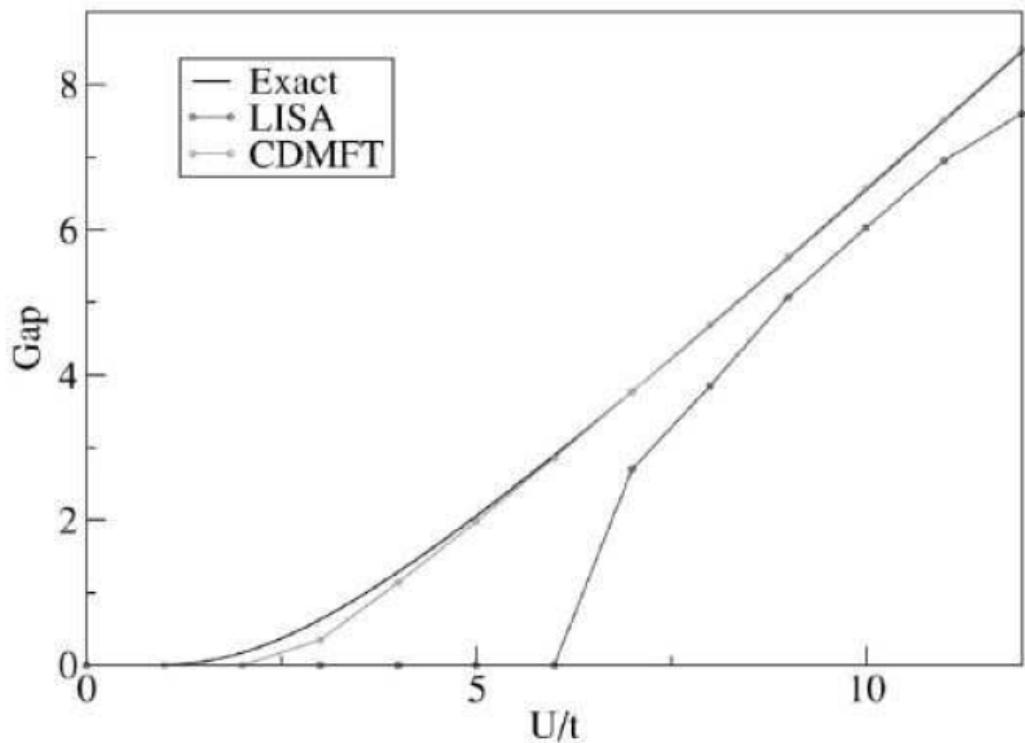
# 1D-Hubbard model

The Hamiltonian is given by:

$$\mathcal{H} = -t \sum_{i,\sigma} (c_{i+1\sigma}^\dagger c_{i\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

**Kinetic energy      Coulomb repulsion**

**Exact result:** Non-zero gap in the density of states for all  $U>0$ .

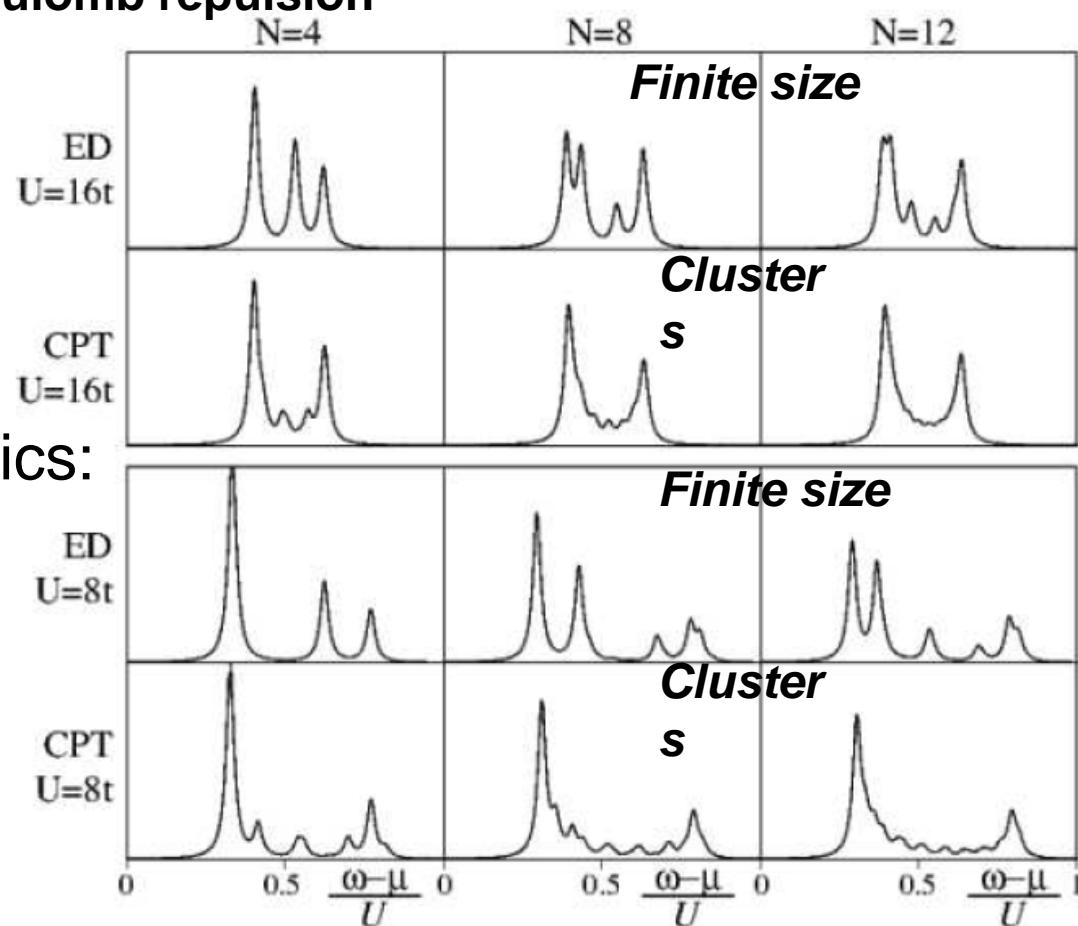




# 1D-Hubbard model

The Hamiltonian is given by:

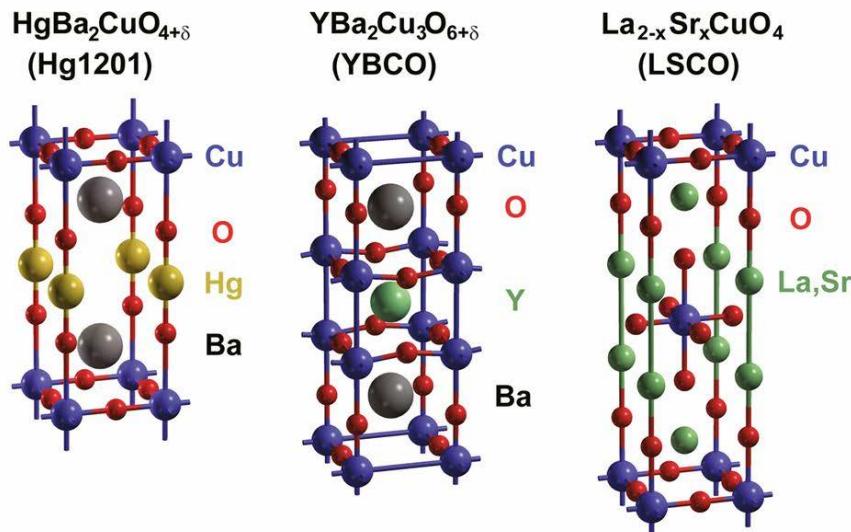
# **Exact result: Luttinger liquid physics: Spin-charge separation**



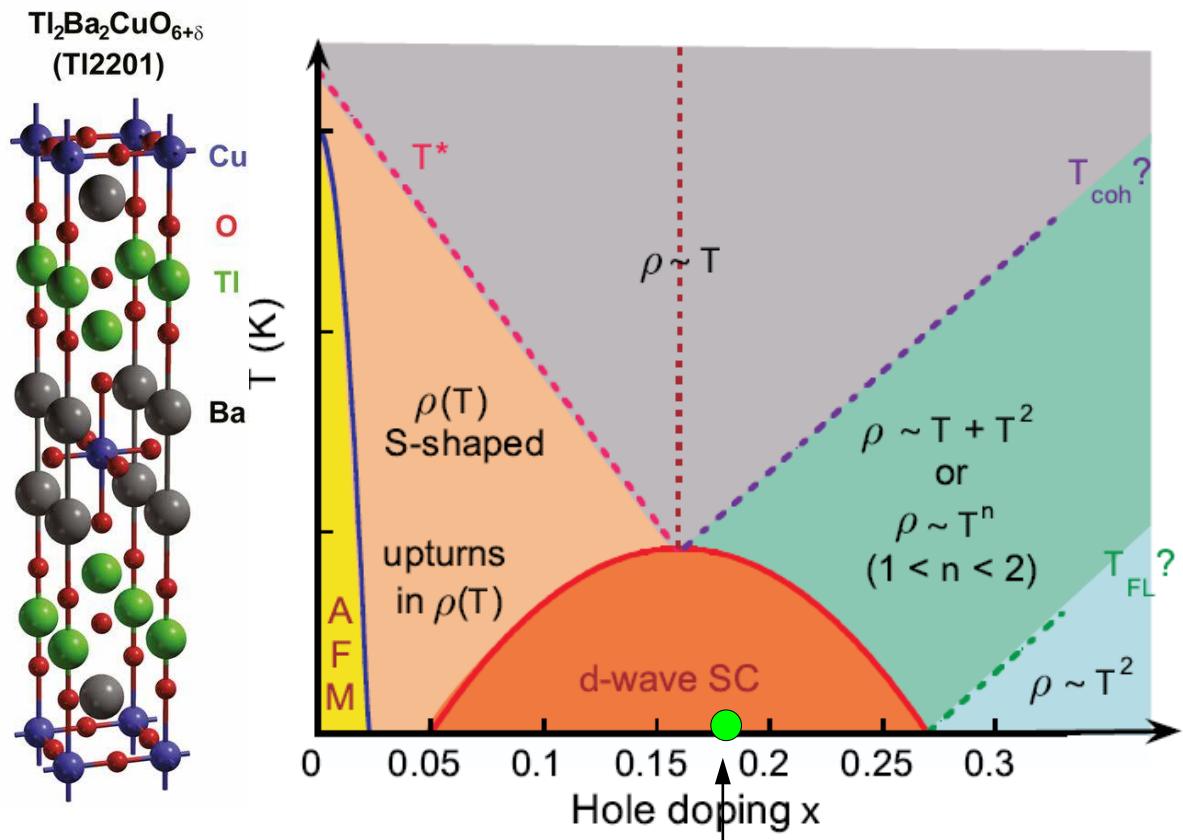
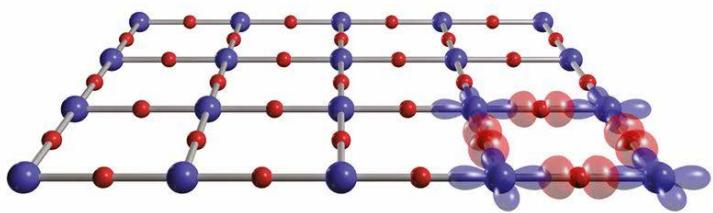


# 2D-Hubbard model and high $T_c$ cuprate superconductors

A



B



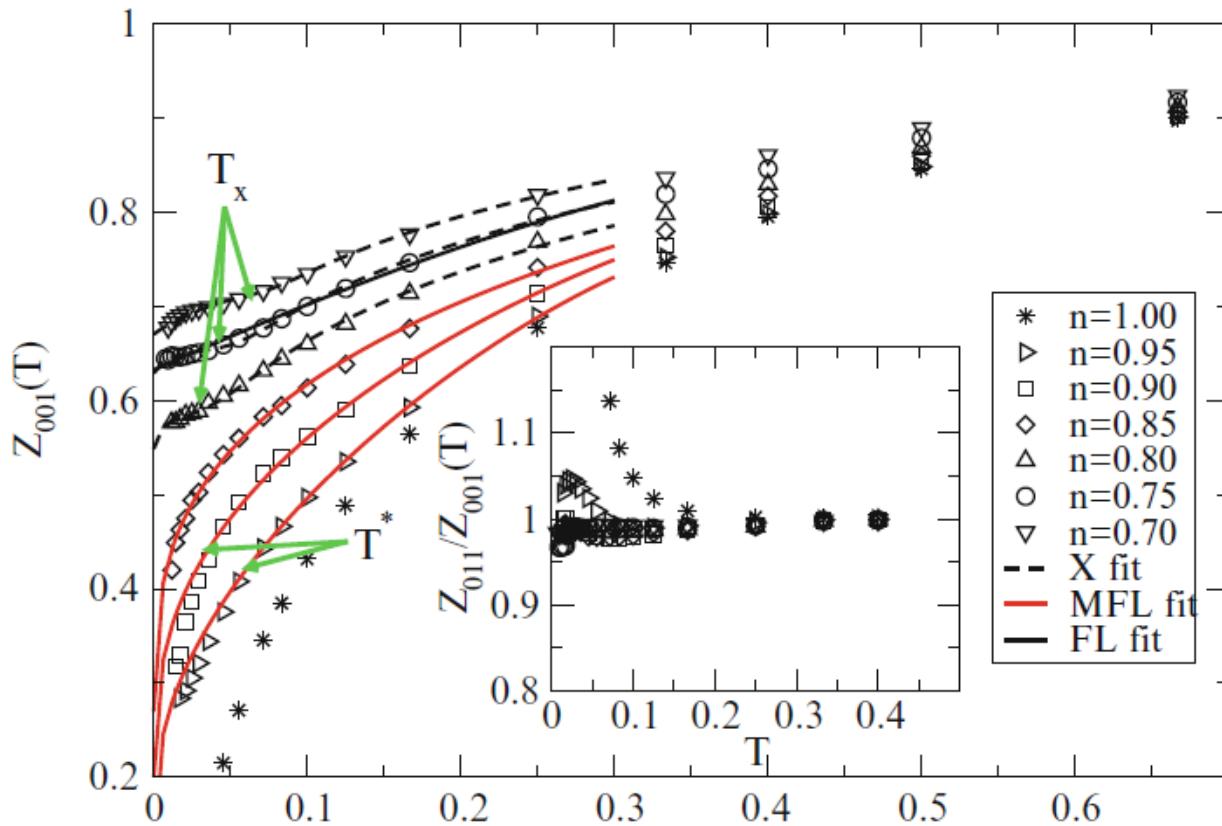


# 2D-Hubbard model

The Hamiltonian is given by:

$$\mathcal{H} = -t \sum_{i,\sigma} (c_{i+1\sigma}^\dagger c_{i\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

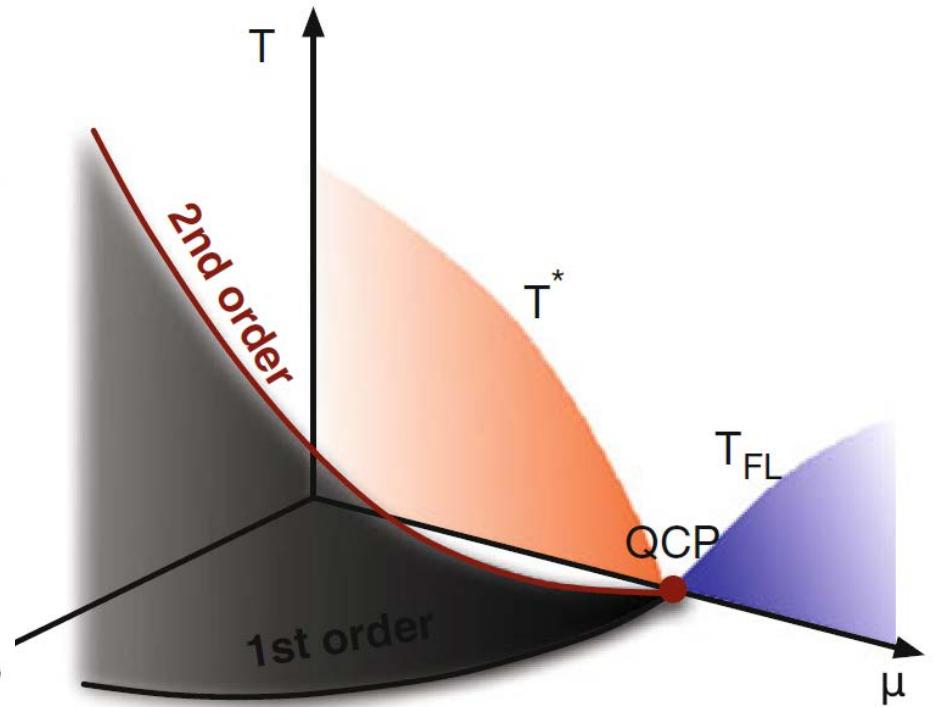
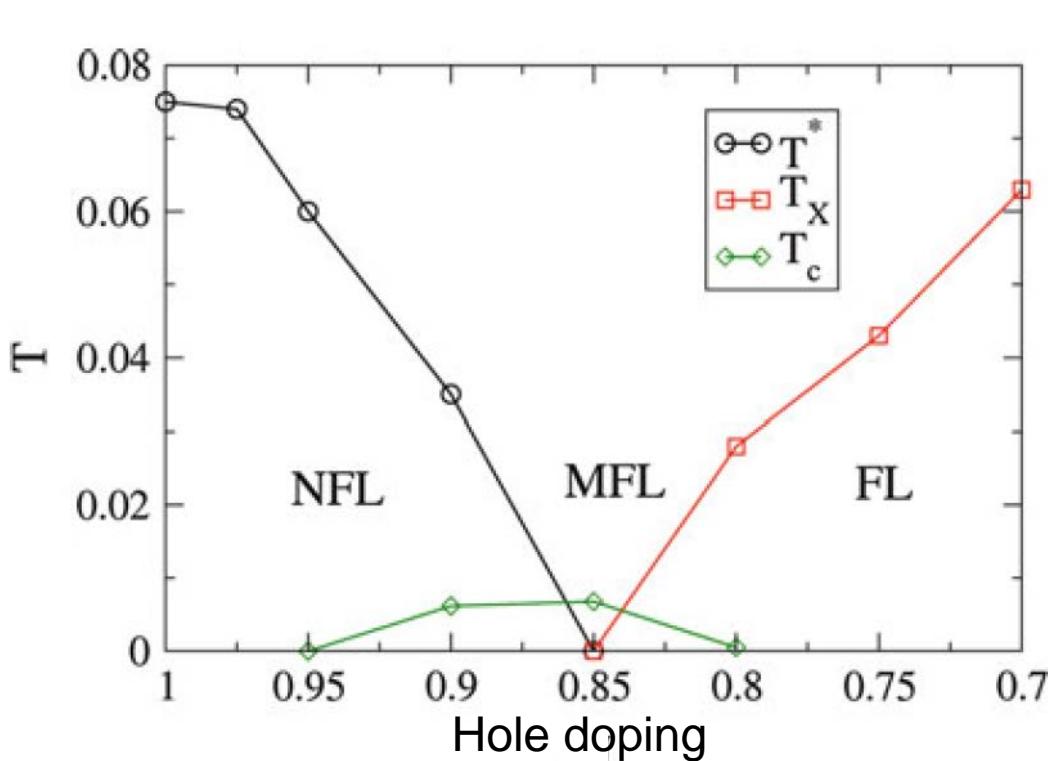
**Kinetic**                                   **Coulomb repulsion**





# 2D-Hubbard model

## (Nature of the quantum critical point)



**Inference:** QCP enhances pairing susceptibility, but not the pairing interaction.