Quantum Embeddings, Dynamical Mean Field Theory: an introduction. Part II

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Outline (part I & II)

- Introduction
- Mott transition
- Quantum impurity models
- DMFT: basic formalism
- The Mott transition in DMFT.
- Towards realism: Hund's metal
- Cluster extensions of DMFT.
- Quantum impurity solvers: an overview.
- Two particle quantities: susceptibilities, transport.
- Outlook

DMFT recap

- A quantum impurity model

$$S_{\text{eff}} = -\int\int_0^\beta d\tau d\tau' c_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + \int_0^\beta d\tau\ U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$G_{\sigma\text{imp}}(\tau) \equiv -\left\langle T c_\sigma(\tau) c_\sigma^\dagger(0)\right\rangle_{S_{\text{eff}}}$$

$$\Sigma_{\sigma\text{imp}}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}_\sigma^{-1}(i\omega_n) - G_{\sigma\text{imp}}^{-1}[\mathcal{G}](i\omega_n)$$

- In a self consistent bath
  - Bethe lattice/semicircular dos.

$$\mathcal{G}_\sigma^{-1}(i\omega_n) = i\omega_n + \mu - \underbrace{t^2 G_{\sigma\text{imp}}(i\omega_n)}_{\Delta_\sigma(i\omega_n)}$$

  - General lattice

$$G_{\sigma\text{imp}}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\text{imp}}[\mathcal{G}](i\omega_n)}$$

Beyond Hubbard model

- Several orbitals (indices a, b)

$$H = -\sum_{\langle ij \rangle ab} (t_{ij})_{ab} c^\dagger_{i\sigma a} c_{i\sigma b} + \sum_i H_{int}(\{c^\dagger_{i\sigma a}, c_{i\sigma a}\})$$

Orbital indices

Local interaction

- Hopping is a matrix in orbital indices $\epsilon(k)_{ab}$
- The interaction will be more complex than density-density interactions.
- A first step toward realism (still a tight-binding model, cf DFT + DMFT later to use Wannier)

Multi-orbital DMFT

- G, Σ, Δ are matrices in the orbital space

$$S_{\rm eff} = -\int_0^\beta \sum_{ab} c^\dagger_{\sigma a}(\tau)\mathcal{G}^{-1}_{\sigma,ab}(\tau-\tau')c_{\sigma b}(\tau') + \int_0^\beta d\tau\, H_{\rm int}(\tau)$$

$$G^{\rm imp}_{\sigma ab}(\tau) \equiv -\left\langle T c_{\sigma a}(\tau) c^\dagger_{\sigma b}(0)\right\rangle_{S_{\rm eff}}$$

Orbital index

$$\Sigma_{\sigma\rm imp}[\mathcal{G}](i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(i\omega_n) - G^{-1}_{\sigma\rm imp}[\mathcal{G}](i\omega_n)$$

Matrix equation

- Bethe lattice/semicircular dos.

$$\mathcal{G}^{-1}_\sigma(i\omega_n) = (i\omega_n+\mu)\mathbf{1} - \underbrace{t^2 G_{\sigma\rm imp}(i\omega_n)}_{\Delta_\sigma(i\omega_n)}$$

- General lattice

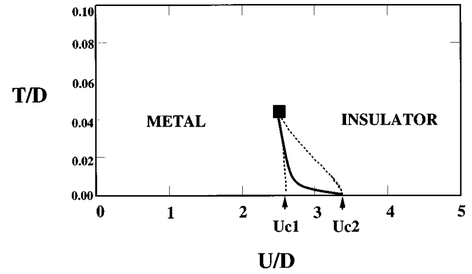
$$G^{\rm imp}_\sigma[\mathcal{G}](i\omega_n) = \sum_k \Big((i\omega_n+\mu)\mathbf{1} - \hat{\epsilon}_k - \Sigma^{\rm imp}_\sigma[\mathcal{G}](i\omega_n)\Big)^{-1}$$

Difference with 1 orbital case

- For fully symmetric model with N orbitals, density-density interaction.

$$H = -\sum_{i,j}\sum_{\sigma=1}^{N} t_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + \frac{U}{2}\sum_{i}\left[\sum_{\sigma=1}^{N}\left(d^{\dagger}_{i\sigma} d_{i\sigma} - n\right)\right]^2$$

  - Similar to N=1. $U_{c1} \sim \sqrt{N}$ $U_{c2} \sim N$ *S. Florens et al. 2002*

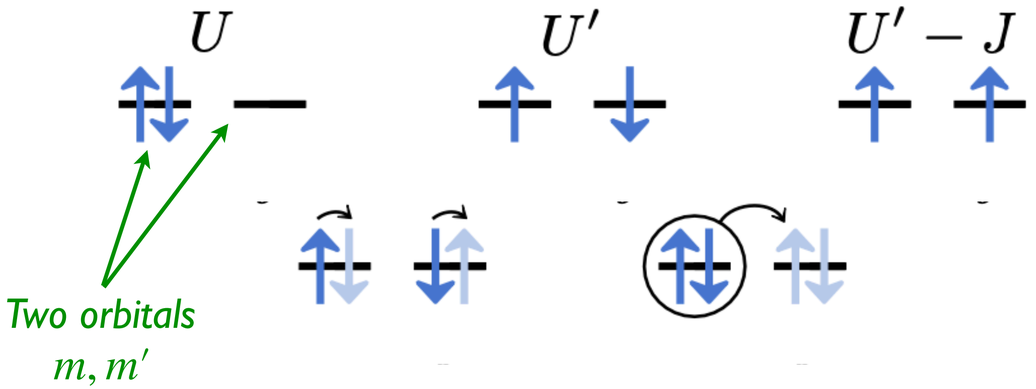


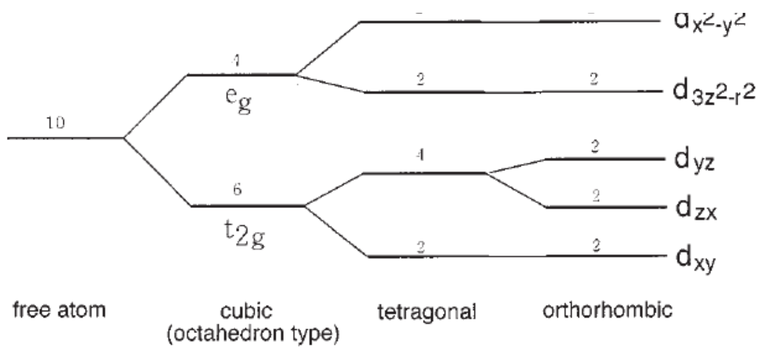
- But interactions are more complex in real materials
  - Hund's coupling, crystal field, spin-orbit,…
  - New physical phenomena !

Kanamori Hamiltonian

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J \sum_{m\neq m'} d^{+}_{m\uparrow} d_{m\downarrow}\, d^{+}_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow} d^{+}_{m\downarrow}\, d_{m'\downarrow} d_{m'\uparrow}$$

- Relevant for a class of materials, e.g. 3d, 4d transition metal oxides
- For t_{2g} (3 bands), cubic symmetry.
- Spherical symmetry : $U' = U - 2J$
- More complex H for more orbitals, less symmetry e.g. Slater …





J : Hund's coupling

- Symmetry case $U' = U - 2J,\ t_{2g}$ orbitals

$$\hat{N} = \sum_{m\sigma} \hat{n}_{m\sigma}, \quad \vec{S} = \frac{1}{2} \sum_{m} \sum_{\sigma\sigma'} d^{\dagger}_{m\sigma} \vec{\tau}_{\sigma\sigma'} d_{m\sigma'}, \quad L_m = i \sum_{m'm''} \sum_{\sigma} \epsilon_{mm'm''} d^{\dagger}_{m'\sigma} d_{m''\sigma},$$

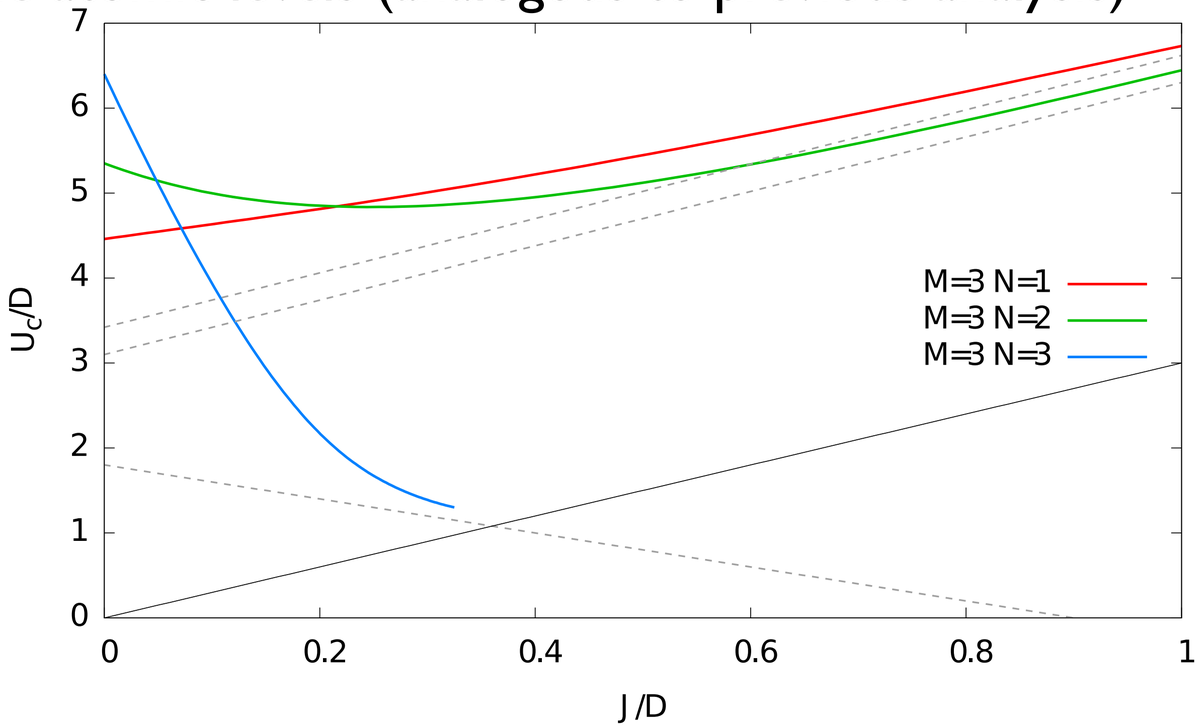
$$H_{t_{2g}} = (U - 3J) \frac{\hat{N}(\hat{N} - 1)}{2} - 2J\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2} J \hat{N}.$$

- Hund's rules ("align spins in different orbitals")
  - Maximal S
  - Maximal angular momentum L

Hund's metals

Cf ***A.Georges, G. Kotliar, Physics Today, April 2024***
review A. Georges. L. De Medici, J. Mravlje, arXiv:1207.3033

- Hund's coupling J has 2 effects
  - High energy effect: Mott gap from the atomic levels (analogous to previous analysis)
    - J enhances U_c
      away from half-filling ($N = 1,2$)
    - J reduces U_c
      at half-filling $N = 3$



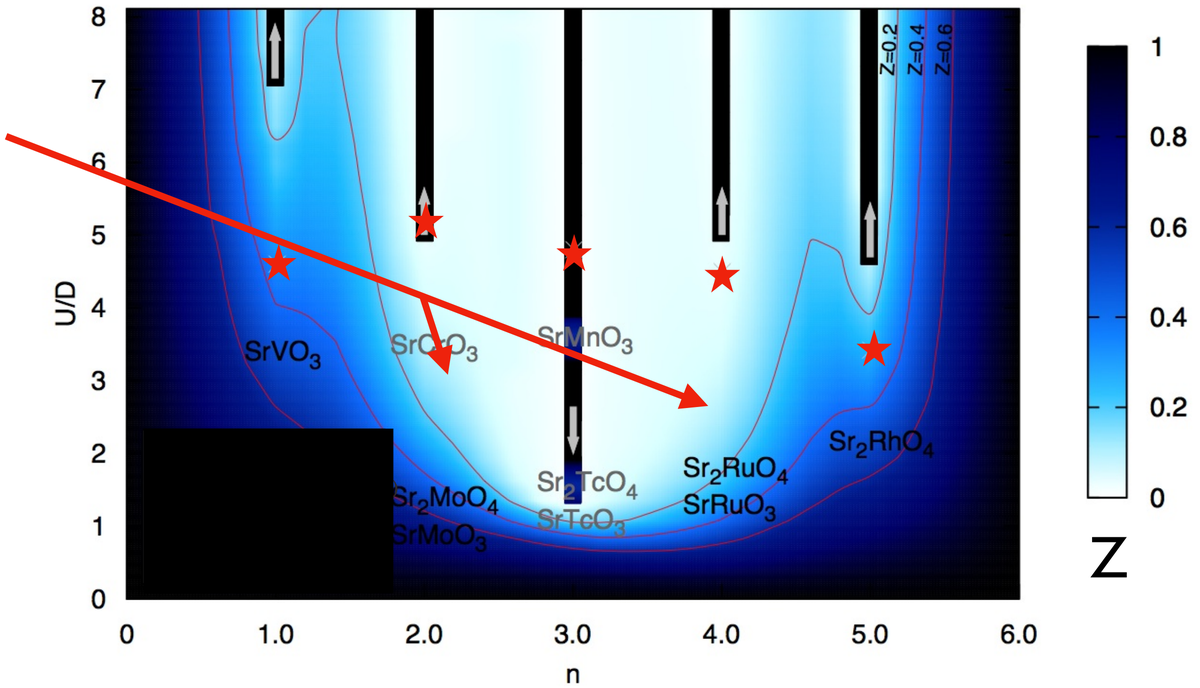
DMFT, Bethe lattice, M=3 bands, fillings N =1,2,3
from arXiv:1207.3033

Hund's metals

- Low energy effect of J (N=2):
  - Reduce the coherence temperature, Z.

Strongly correlated metal far from Mott transition

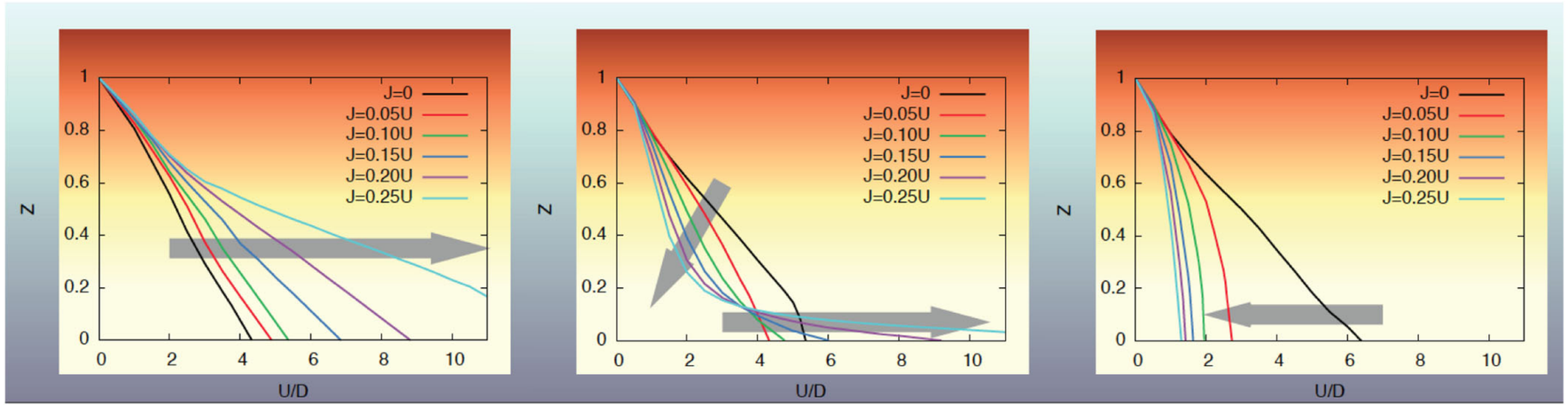
DMFT, low T, phase diagram (paramagnetic phase only)



$U' = U - 2J$

J = 0.15U

Z vs U for N=1,2,3



L. De Medici et al. PRL 107, 256401 (2011)

Coherence of spin and orbital degrees of freedom at distinct scales

- Spin/orbital fluctuates on different scales.
- Renormalization group picture.
- DMFT : an effective Kondo problem

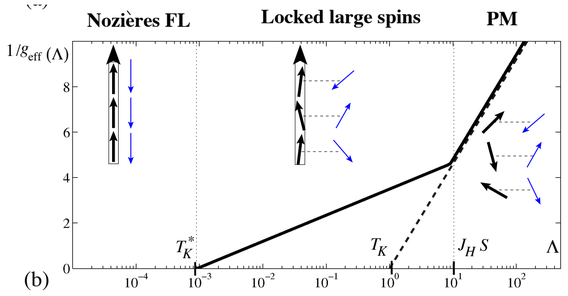
Incoherent

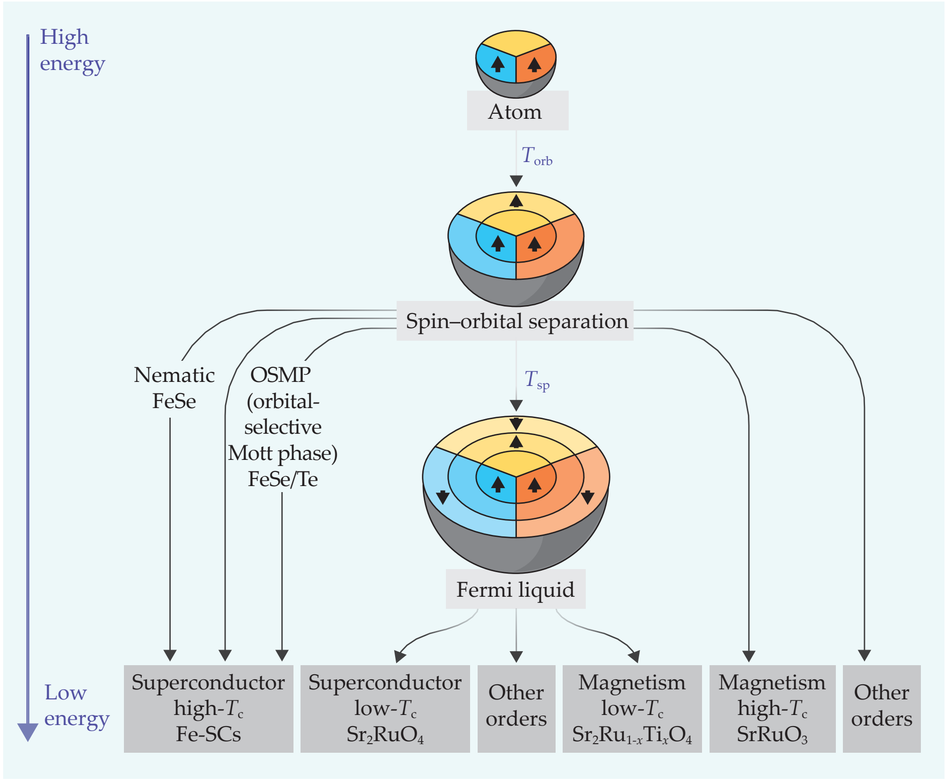
T_{orb}

Non Fermi liquid metal with fluctuating spins No orbital fluctuations

T_{spin}

Fermi liquid





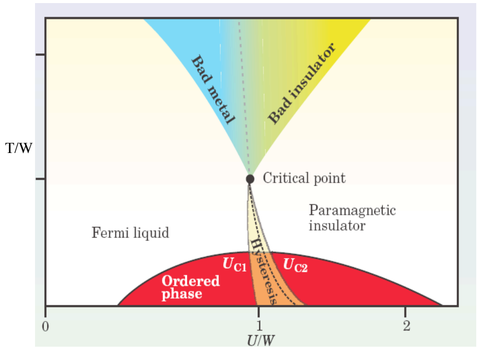
From A.Georges, G. Kotliar, Physics Today, April 2024

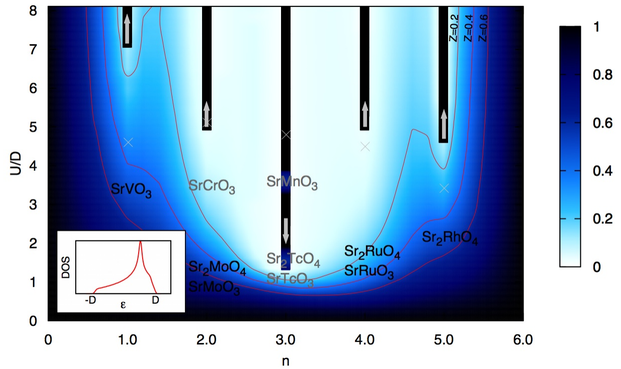
Now well understood from a Renormalization Group perspective, cf. recent work by von Delft, Lee, Weichselbaum et al., Aron, Kotliar et al., Horvat, Žitko, Mravlje, Kugler et al.,

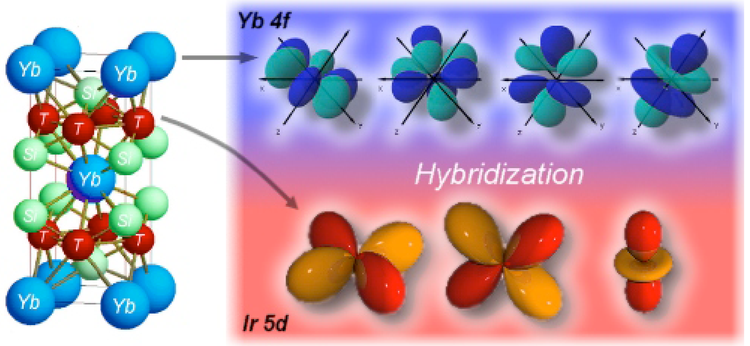
Different routes to correlations

- Mott physics; U
- Hund metals; J
- Heavy fermions. Orbitally selective Mott phase.

DMFT can be applied to all of them





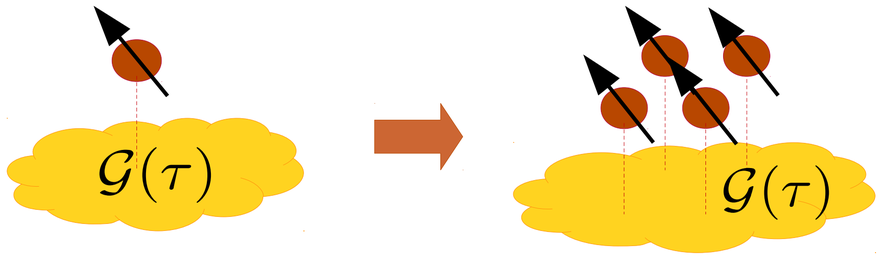


Cluster extensions of DMFT

Idea

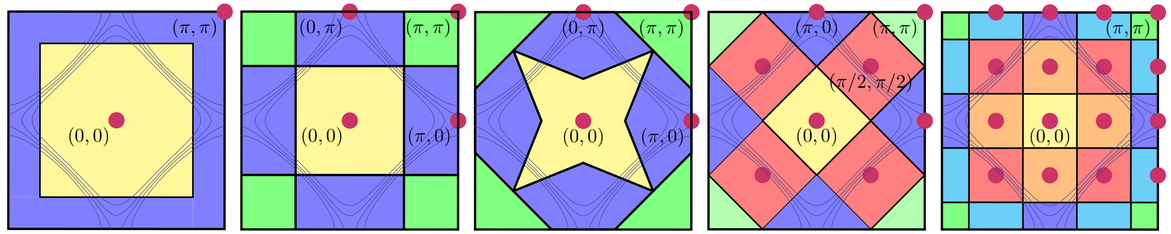
- A small cluster of atoms instead of 1 atom OR patches in the Brillouin zone for $\Sigma_{\text{lattice}}(k, \omega)$

Real space (CDMFT)



Lichtenstein, Katsnelson 2000
Kotliar et al. 2001

Reciprocal space (DCA)
Brillouin zone patching



Hettler et al. '98, ...

- For a review, cf *T. Maier al. Rev. Mod. Phys. 77, 1027 (2005)*

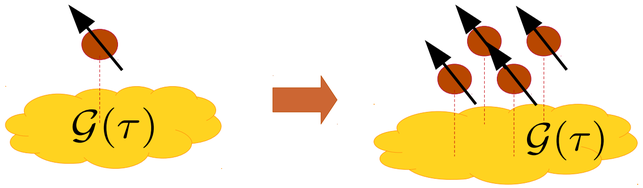
Motivations

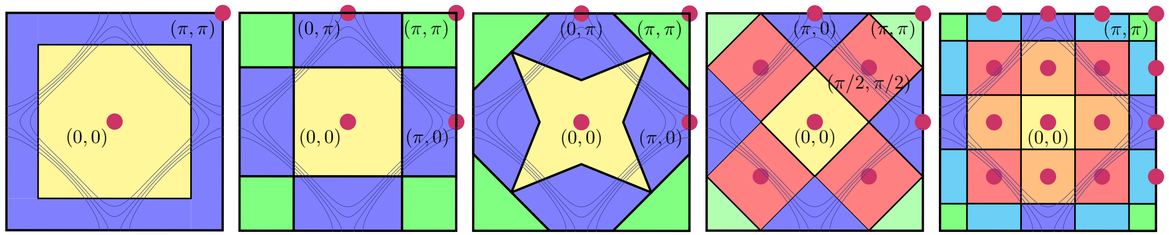
- Control :
  Interpolate between DMFT (1 site) and the full lattice (infinite number of sites).
  At large cluster size L, we have the exact solution

- k dependence of the lattice self-energy $\Sigma_{\text{lattice}}(k, \omega)$
  Different cluster methods are different parametrization of k dependence.

- Effect of *short range* spatial correlations

- Some order parameters requires more than 1 site, e.g. d-wave superconductivity.



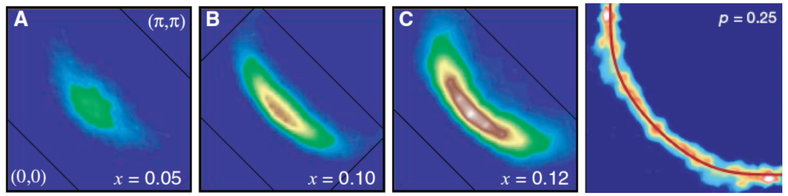


High Tc superconductors :DMFT is not enough

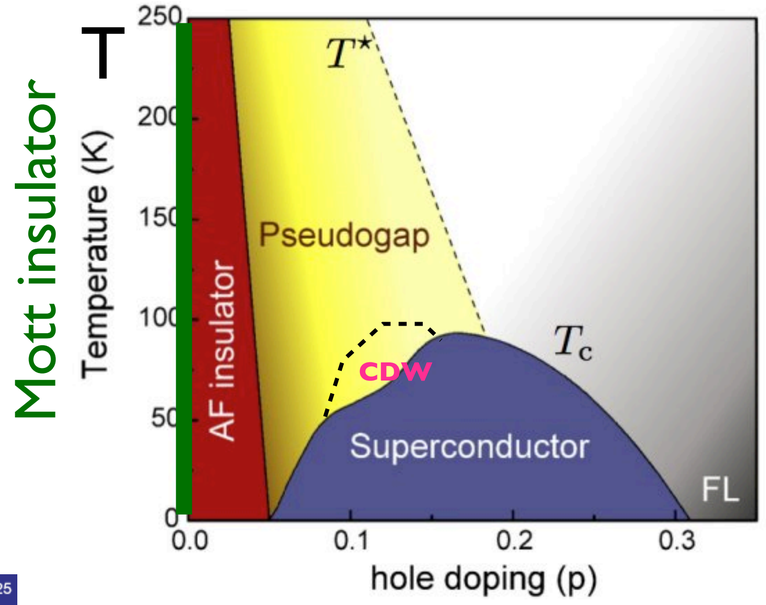
Normal Phase
Local self-energy
is not enough !

DMFT

$$\Sigma_{\sigma \mathrm{latt}}(k, i\omega_n) = \Sigma_{\sigma \mathrm{imp}}(i\omega_n)$$

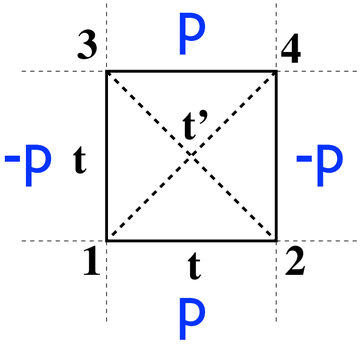


Node Antinode dichotomy in cuprates (ARPES)



SC
d-wave order
1 site is not enough !

d-SC order



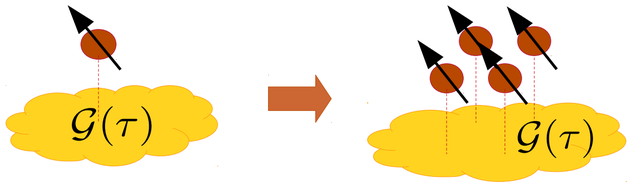
$P = \langle c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} \rangle$

- Σ, Z, m* does depend on k !
- Super-exchange J ? Spin singlets ?
  Cut divergence of m* close to Mott

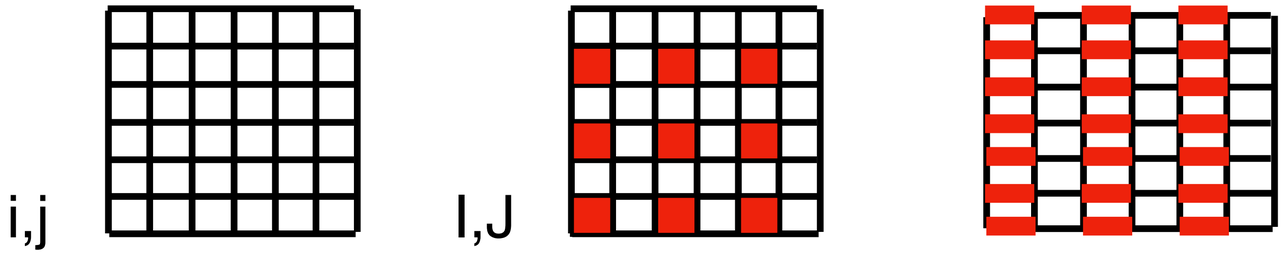
Cellular DMFT (CDMFT)

- Real space method

Lichtenstein, Katsnelson 2000
Kotliar et al. 2001



- DMFT on a superlattice of clusters



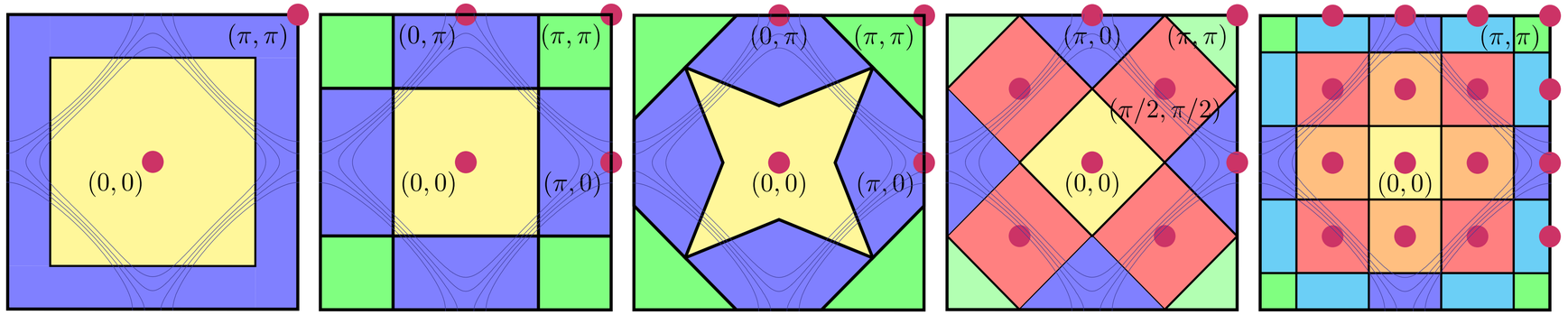
Superlattice

- Breaks translation invariance !

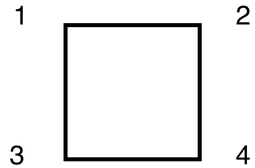
- *Cf Lecture by David Sénéchal next Monday*

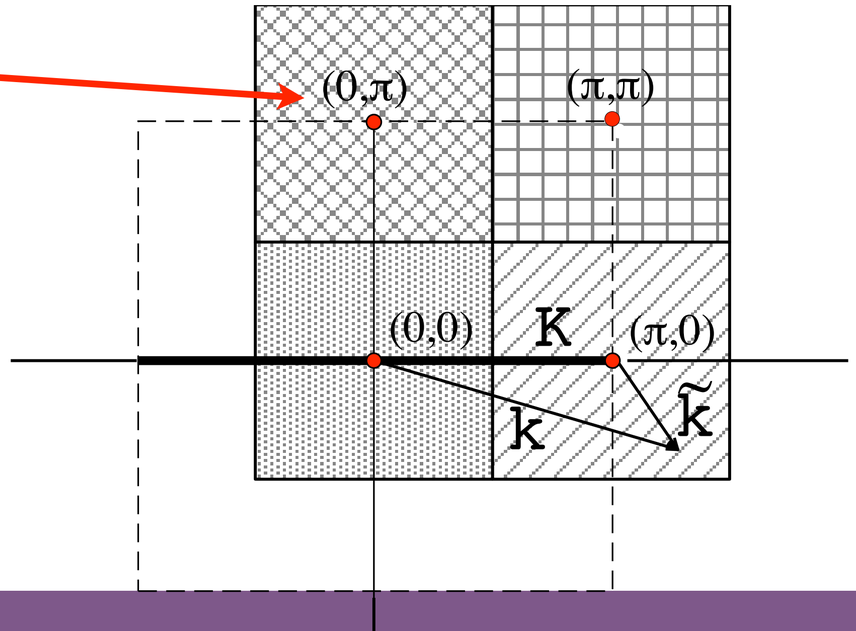
DCA

- Cut BZ in N_c patches (e.g. N_c = 2, 4, 8, 16)



- Red points : centre of the patches : K_c.
  - Momenta of a finite, cyclic cluster, e.g. 2x2





- Self energy Σ constant by pieces on the patches

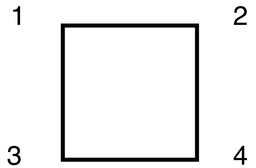
DCA

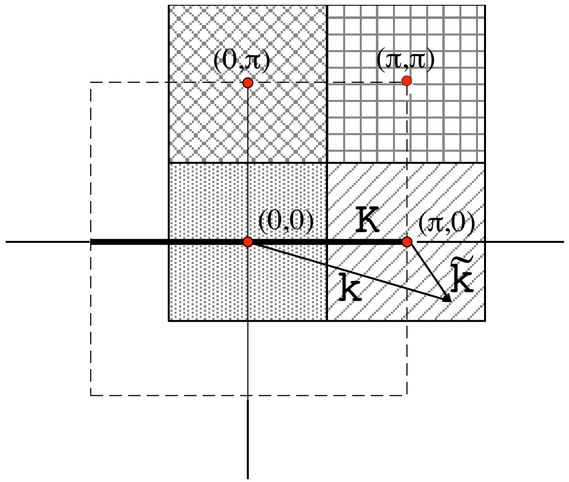
- Impurity model is a cyclic finite cluster sites a, b with K_c momenta.

$$S_{\text{eff}} = -\int_0^\beta \sum_{ab} c^\dagger_{\sigma a}(\tau)\mathcal{G}^{-1}_{\sigma,ab}(\tau-\tau')c_{\sigma b}(\tau') + \sum_a \int_0^\beta d\tau\ U n_{\uparrow a}(\tau) n_{\downarrow a}(\tau)$$

$$G^{\text{imp}}_{\sigma ab}(\tau) \equiv -\left\langle T c_{\sigma a}(\tau) c^\dagger_{\sigma b}(0)\right\rangle_{S_{\text{eff}}}$$

- Action is written in real space (U is local)
- Self consistency condition in reciprocal space.
  Due to cyclicity, the matrix is diagonal in K_c





$$\Sigma_{\sigma\text{imp}}[\mathcal{G}](K_c, i\omega_n) \equiv \mathcal{G}^{-1}_\sigma(K_c, i\omega_n) - G^{-1}_{\sigma\text{imp}}[\mathcal{G}](K_c, i\omega_n)$$

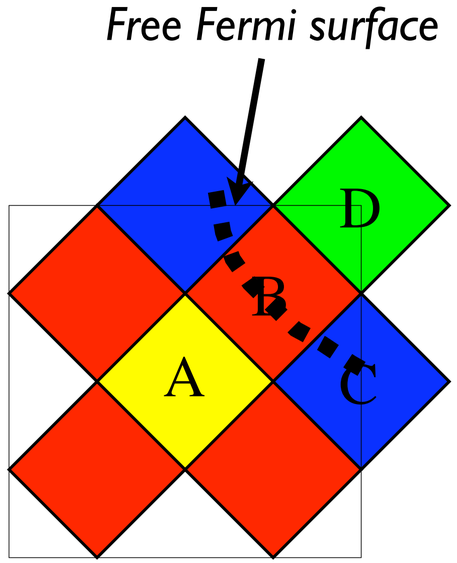
$$G^{\text{imp}}_\sigma[\mathcal{G}](K_c, i\omega_n) = \int d\epsilon D_C(\epsilon) \frac{1}{i\omega_n + \mu - \epsilon - \Sigma^{\text{imp}}_\sigma[\mathcal{G}](K_c, i\omega_n)}$$

Density of state of patch C

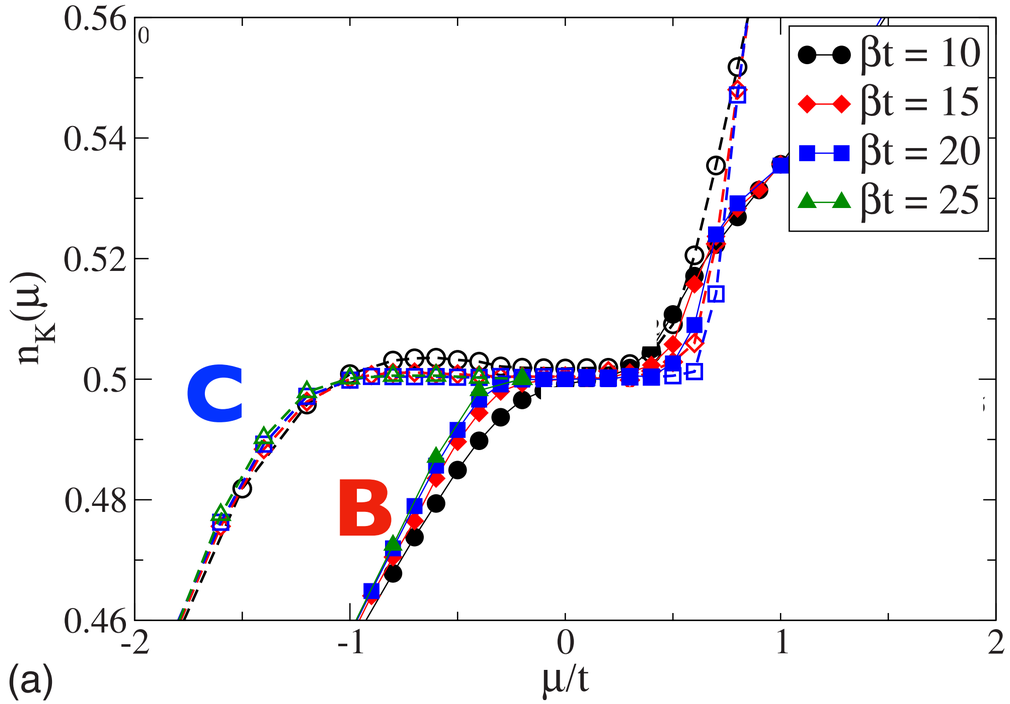
$$D_c(\epsilon) \equiv \sum_{\tilde{k}} \delta(\epsilon - \epsilon_{K_c+\tilde{k}})$$

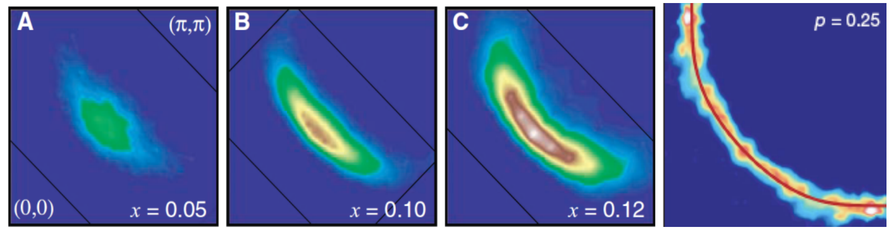
Example: 8 sites DCA clusters

E. Gull, P. Werner and A.J. Millis, OP, PRB 2009



Patches for 8 sites clusters

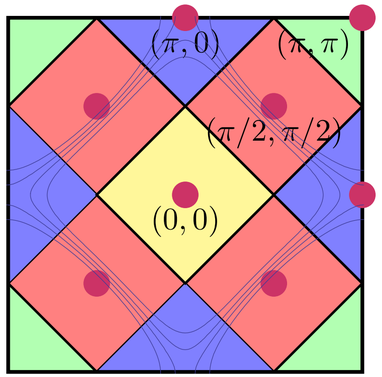


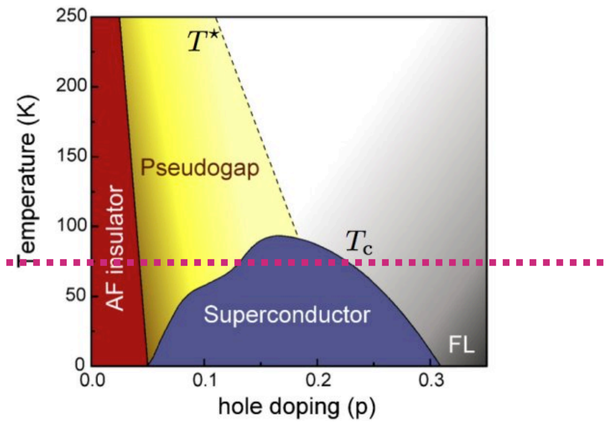


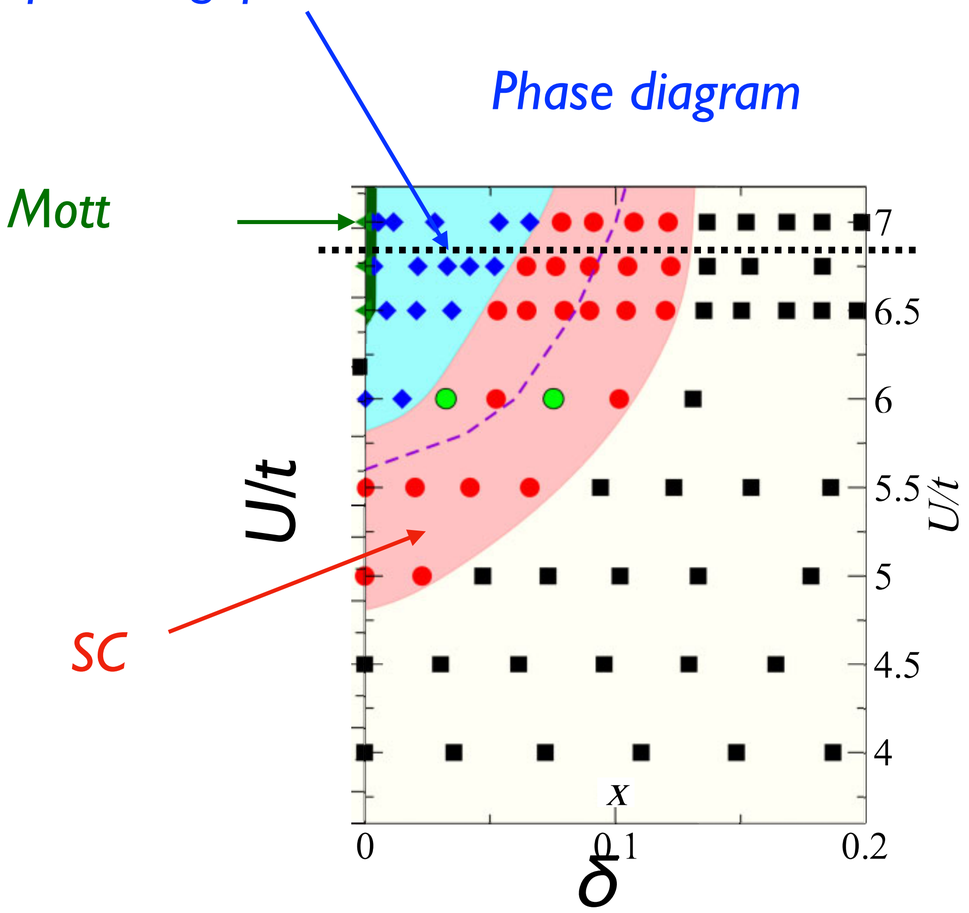
- $n_K(\mu)$: occupation of each patch
- 2 steps transition: at intermediate doping, C insulating, B is metallic.

8 patches DCA : Superconducting phase vs pseudo-gap

E. Gull, O.P., A. Millis PRL 110, 216405 (2013)







Nambu spinors

$$\psi_i = \begin{pmatrix} c_{i\uparrow} \\ c^\dagger_{i\downarrow} \end{pmatrix}$$

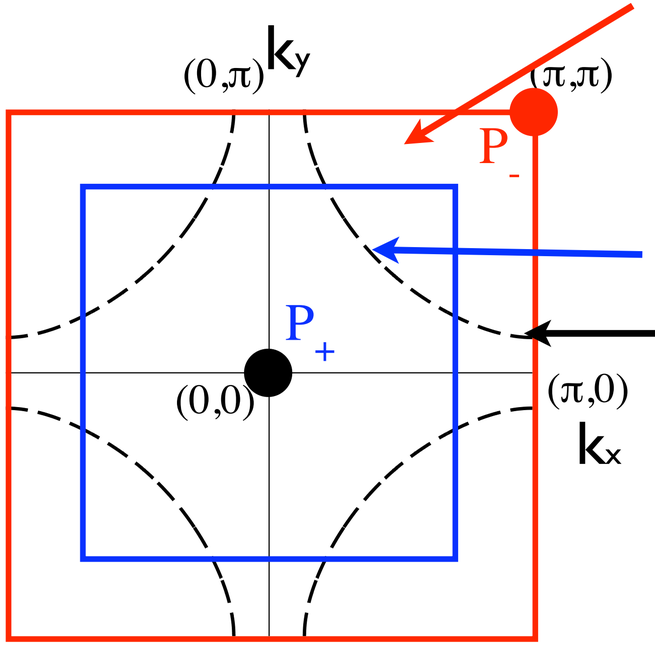
$$\hat{G}(\mathbf{k},\tau) \equiv -\langle T\Psi_{\mathbf{k}}(\tau)\Psi^+_{\mathbf{k}}(0)\rangle = \begin{pmatrix} G(\mathbf{k},\tau) & F(\mathbf{k},\tau) \\ F(\mathbf{k},\tau)^* & -G(-\mathbf{k},-\tau) \end{pmatrix}.$$

Anomalous Green function

$$F(\mathbf{k},\tau) \equiv -\langle T c_{\mathbf{k}\uparrow}(\tau) c_{-\mathbf{k}\downarrow}(0)\rangle.$$

Tutorial : Minimal two-patches DCA for Fermi Arcs

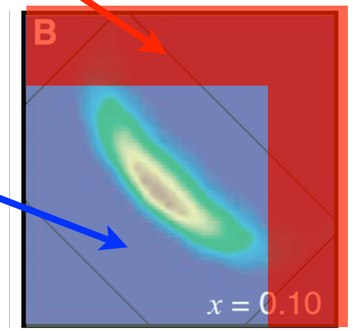
M. Ferrero, P. S. Cornaglia, L. De Leo, O. Parcollet, G. Kotliar, A. Georges, EPL and PRB 2009



Outer patch P- : Antinodes

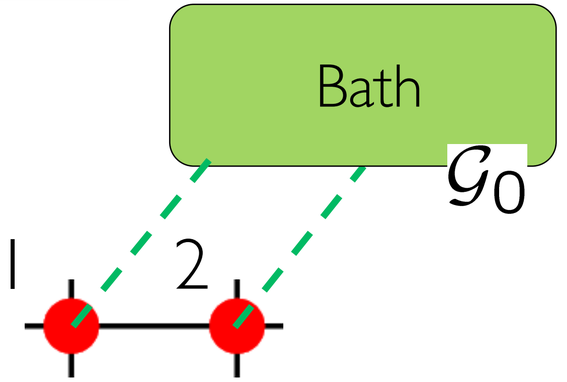
Inner patch P+ : Nodes

Free Fermi surface



$$\mu = 1, 2$$

$$c_{\pm} = (c_1 \pm c_2)/\sqrt{2}$$



- At $\delta = 0.16$, outer patch P- becomes insulating
  [how ? Cf Tutorial !]

Two-site Anderson impurity model

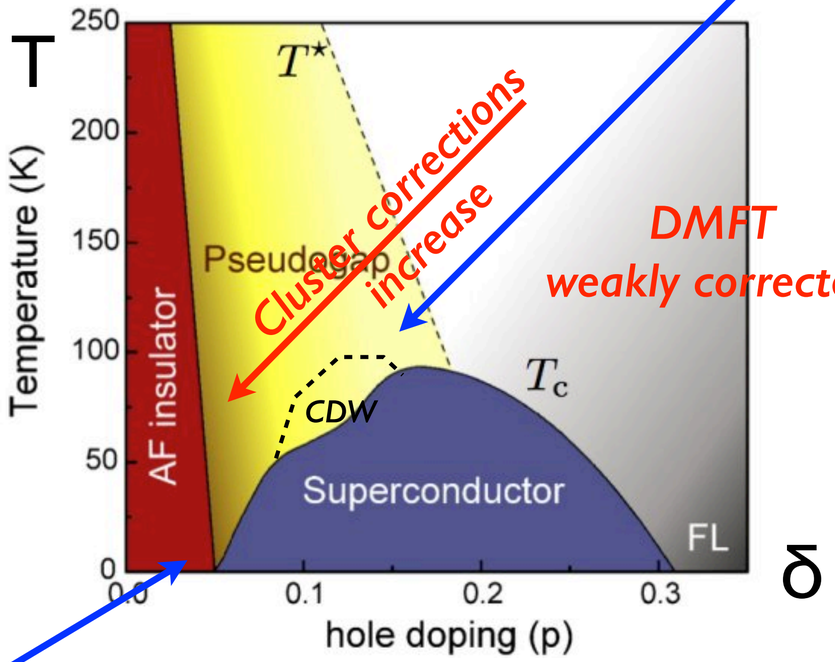
DMFT is high temperature method

"Top to Bottom"

Start from high T/doping

R.G.

Diagrammatic methods

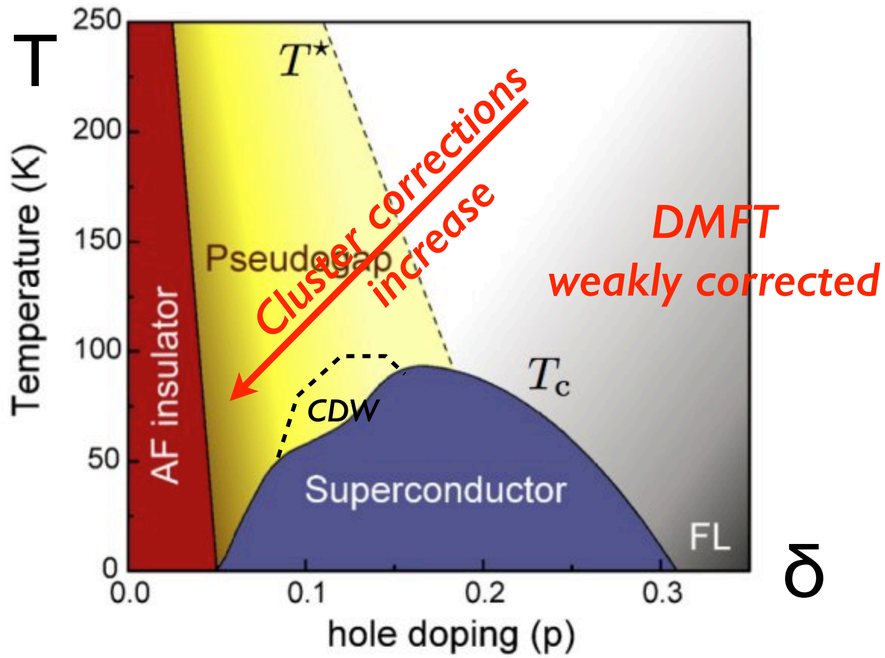


"Bottom to Top"

Study the many-body ground state

DMRG, PEPS, MERA

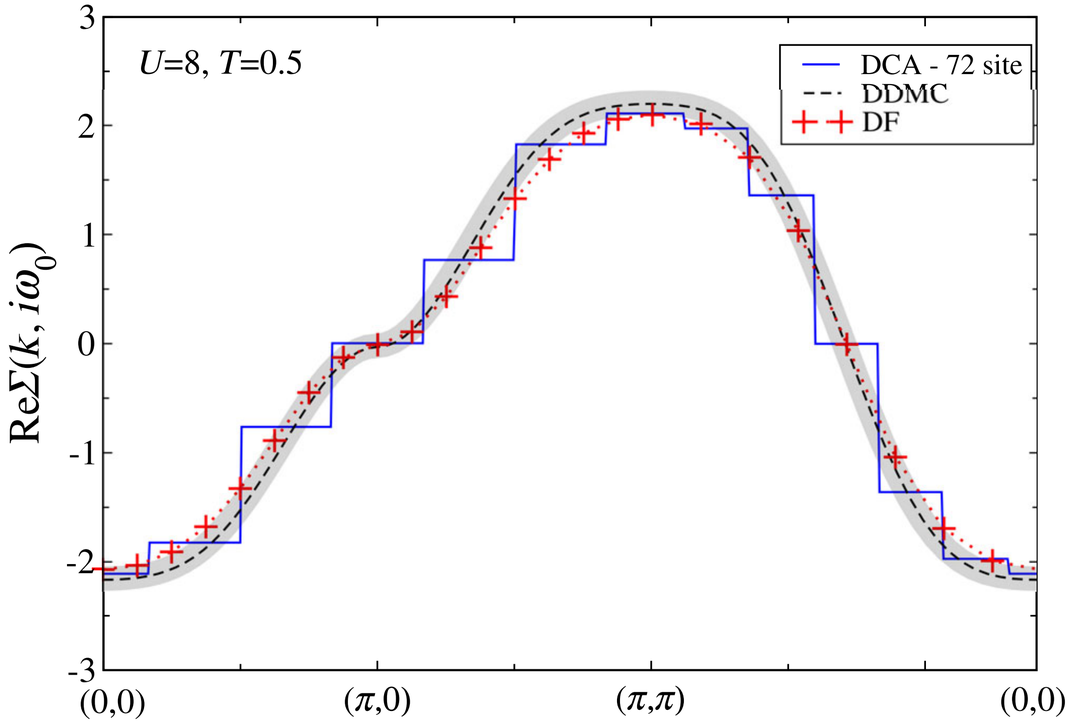
Large vs minimal clusters



- At high T or δ, intermediate U:
  - Solvers are limited (sign problem !) for large clusters in some regimes
- At lower T, δ
  - Small clusters capture some important effects (pseudogap, d-SC).
    Minimal cluster ? Physical picture ?

Converging large clusters at high T

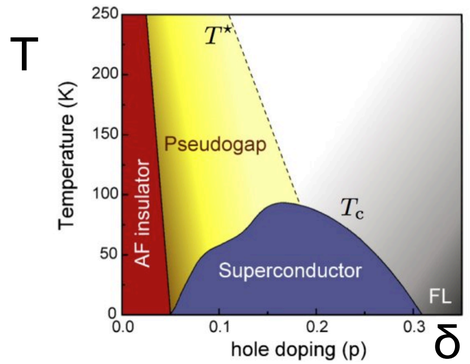
- Compare to e.g. diagrammatic QMC, DQMC
- Systematic benchmarks for new methods on these points



DCA 72 sites, *J. LeBlanc et al. Phys. Rev. X 5, 041041 (2015)*

Cluster DMFT & Hubbard model

- Emergence of some consensus on robust features of the Hubbard model



A lot of authors & works since 2000, e.g. Capone, Civelli, Ferrero, Georges, Gull, Haule, Imada, Jarrell, Kotliar, Lichtenstein, Katsnelson, Maier, Millis, Sordi ,Tremblay, Werner, OP, ...

Pseudo-gap

- Emerging from Mott insulator
- Nodes/antinodes. Fermi Arcs

d-wave SC

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

- *Cf Lecture by David Sénéchal next Monday : ED, cluster DMFT and application.*

Quantum impurity solvers

Quantum impurity solvers : the bottleneck !

$$S_{\text{eff}} = -\int\int_0^\beta d\tau d\tau' c_a^\dagger(\tau)\mathcal{G}_{ab}^{-1}(\tau-\tau')c_b(\tau') + \int_0^\beta d\tau H_{\text{loc}}(\{c_a^\dagger, c_a\})(\tau)$$

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

Bath

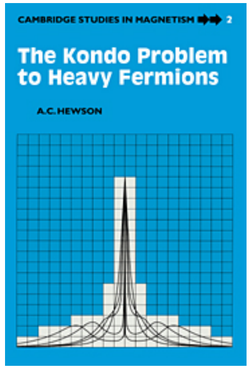
Interaction

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

- Compute G, $G^{(2)}$
- For multi orbital model (e.g. Kanamori), clusters
- Real time/imaginary time.
- …

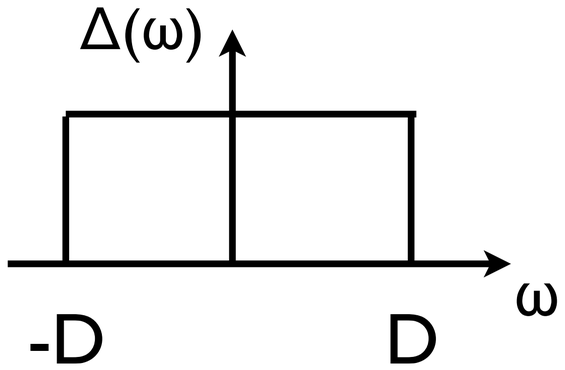
Why do we need specific algorithms
to solve DMFT
quantum impurity models ?

The pre-DMFT toolbox



- Many sophisticated approaches to quantum impurity models.
  - Integrability (Bethe Ansatz) in the universal regime
    A. Tsvelik, P. Wiegmann/ N. Andrei, 1980
  - Boundary Conformal Field Theory *Cardy; Affleck, Ludwig, 1991* Bosonization.

- Not sufficient for DMFT
  - Low-energy solution only.
  - DMFT baths have structure !

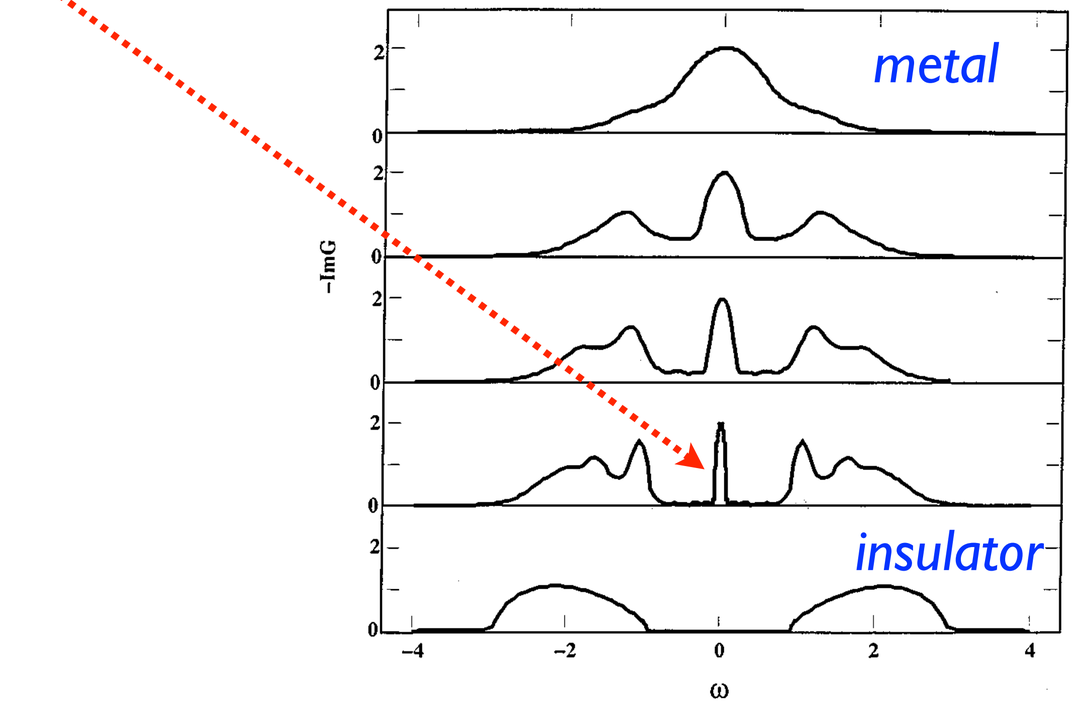


$$T, \omega, T_K << D$$

DMFT baths have structure in ω !

- We want to compute the full ω dependency

DMFT bath evolution close to Mott transition (IPT solution)



A. Georges et al., Rev. Mod. Phys. 68, 13, (1996)

The DMFT solver toolbox

- Exact/Controlled algorithms
  - Continuous Time Quantum Monte Carlo (CTQMC). *Cf Lecture by M. Ferrero today*
  - Exact diagonalization (ED). *Cf lecture by D. Sénéchal on Monday*
  - Numerical Renormalization group (NRG). *Cf Lecture by F. Kugler on Monday*
  - Tensor network (DMRG).

- Approximate solvers
  - Iterated Perturbation Theory (IPT). *Cf TRIQS tutorial*
  - NCA family (NCA, OCA, …)
  - Slave bosons / Hartree-Fock / "Hubbard I" (= atomic self-energy)

Continuous Quantum Monte Carlo (CTQMC)

CTQMC algorithms

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

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

Bath

Interaction

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

- Expansion in interaction : CT-INT
  A.N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005)
- Expansion in Δ(ω), around the atomic limit : CT-HYB
  P. Werner, A. Comanac, L. de' Medici, M. Troyer, A. J. Millis, PRL 97, 076405 (2006);
  P .Werner, A.J. Millis, Phys. Rev. B 74, 155107 (2006)
- Continuous time determinantal : CT-AUX
  *E.Gull, P.Werner, **O.P.**, M.Troyer EPL (2008)*

CT-HYB : principle

- Explicit expansion in power of Δ.

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

n-body correlators of the bath (Wick)

n-body correlators of the impurity

- Compute the sums & integrals with Monte Carlo.
- $\langle n \rangle \sim \beta \,|\, \Delta \,|$. In practice, often $n \sim 100 - 1000$

- *Cf Lecture by Michel Ferrero on QMC, and CT-INT.*

CT-HYB : what can we compute ?

- Imaginary time Green function $G_{ab}(\tau)$, self-energy $\Sigma_{ab}(i\omega_n)$
- Two-body functions $G^{(2)}_{abcd}(\tau_1, \tau_2, \tau_3, \tau_4) \equiv - \langle T_\tau c^\dagger_a(\tau_1) c_b(\tau_2) c^\dagger_c(\tau_3) c_d(\tau_4) \rangle$
- Impurity (many-body) density matrix.
- Impurity dominant states
  - Which states of the impurity contribute the most to the path integral ?

    - *Cf TRIQS tutorial*

CTHYB: Pros

- Treat the full multiplets, with any impurity interaction e.g. Kanamori, Slater, spin orbit
- Can also handle some retarded interaction $U(\tau)$ (for DMFT extension, e.g. GW + DMFT).
- CTHYB is a standard algorithm for material computations.

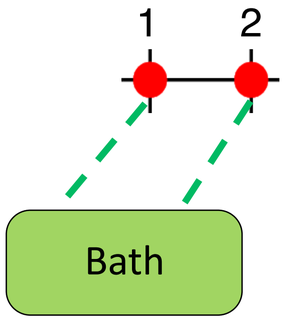
CTHYB: Cons

- Fermionic sign problem.
- Limited to imaginary time. The analytical continuation issue.
- Slow. Convergence $\sim 1/\sqrt{N_{\text{samples}}}$
- Scales poorly
  - at low T (asymptotically $\sim \beta^3$)
  - with number of orbitals (a priori exponential, as the impurity itself is solved exactly).

Fermionic sign problem

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

- Massive cancellation in the sum. *Cf Lecture by M. Ferrero.*
- A major limitation of the algorithm.
  - Exponentially hard at low T (error bars grows).
  - Not present for DMFT 1 band, but in clusters, off-diagonal $\Delta_{ab}(\omega)$, spin-orbit, …
  - Not physical. Depends on the basis.
    e.g. dimer cluster (2 site) : no sign in $c_{even/odd} = (c_1 \pm c_2)/\sqrt{2}$
  - Not predictable a priori.



The analytical continuation problem

- Spectral representation

$$G(\tau) = \int d\epsilon A(\epsilon) K(\tau, \epsilon) \qquad K(\tau, \epsilon) \equiv -\frac{e^{-\epsilon\tau}}{1 + e^{-\beta\epsilon}} \qquad A(\omega) = -\frac{1}{\pi} \mathrm{Im} G^R(\omega + i0^+)$$

- Matrix $K(\tau, \epsilon)$ is of low-rank (badly conditioned i.e. hard to invert).
  - $A(\omega) \to G(\tau)$: easy
  - $G(\tau) \to A(\omega)$ is impossible / very hard, specially at large ω. Inverse Laplace transform.

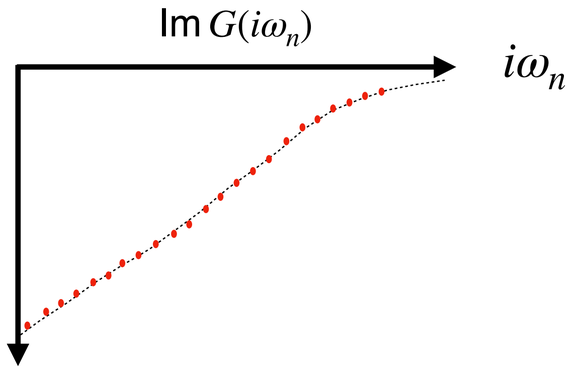
How to address this issue ?

1. Extract the physics from imaginary time data.
2. Use a real time solver (cf later), if possible.
3. Use analytic continuation techniques.

Interpret imaginary time/frequency results

- Thermodynamic quantities are directly computed, e.g.
  - e.g. density $n(\mu)$
  - energy $\langle H \rangle$
- How does the Green function $G(i\omega_n)$ look like ?

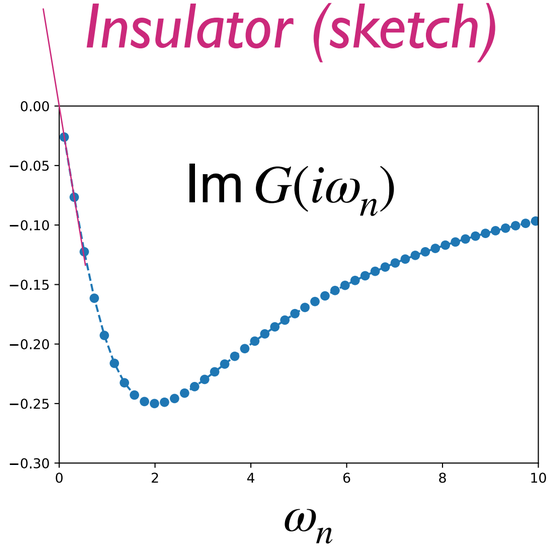
Metal (sketch)



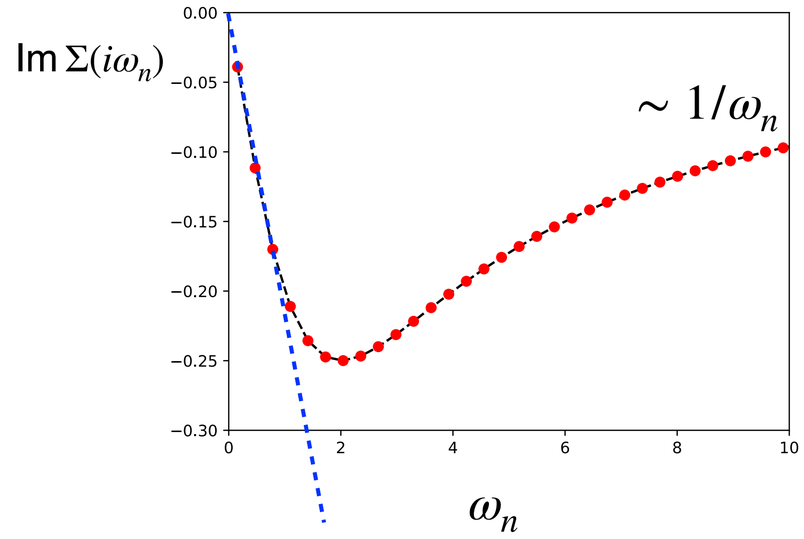
$$\omega_n = \frac{(2n+1)\pi}{\beta}$$

$$G(i\omega_n) = \int d\omega \frac{A(\omega)}{i\omega_n - \omega}$$

Insulator (sketch)



Matsubara self-energy in a metal



- Fermi liquid properties (low energy)
  - Quasi-particle residue Z
  - Coherent scale E_{FL}
  - $Re\Sigma^R(0) = \Sigma(i\omega_n \to 0)$

$$\Sigma^R(\omega) = \Sigma^R(0) + \left(1 - \frac{1}{Z}\right)\omega - i\frac{\omega^2 + (\pi T)^2}{E_{FL}} + O(\omega^3, T^3)$$

$$\text{Im}\,\Sigma(i\omega_n) = \left(1 - \frac{1}{Z}\right)\omega_n + \frac{\omega_n^2 - (\pi T)^2}{E_{FL}} + O(\omega^3, T^3)$$

- Testing FL form with first Matsubara frequency : $\text{Im}\,\Sigma(i\omega_0 = i\pi T) \sim T + O(T^3)$

Transport

- Transport requires the spectral function, or $\Sigma(\omega)$ in real frequencies.
- Example : optical c-axis conductivity

Fermi function

$$\sigma_c(\Omega) = \frac{2e^2 c}{\hbar ab} \int d\omega \frac{f(\omega) - f(\omega + \Omega)}{\Omega} \frac{1}{N} \sum_{\mathbf{k}} t_\perp^2(\mathbf{k}) A(\mathbf{k}, \omega) A(\mathbf{k}, \Omega + \omega)$$

- Fermi functions "zoom" at low frequencies.
- What to do ?
  - Real time/frequency solver [recommended]
  - Analytic continuation [at your own peril …]

Analytic continuation techniques

- Padé approximants
  - Approximate $G(z)$ by a rational function.

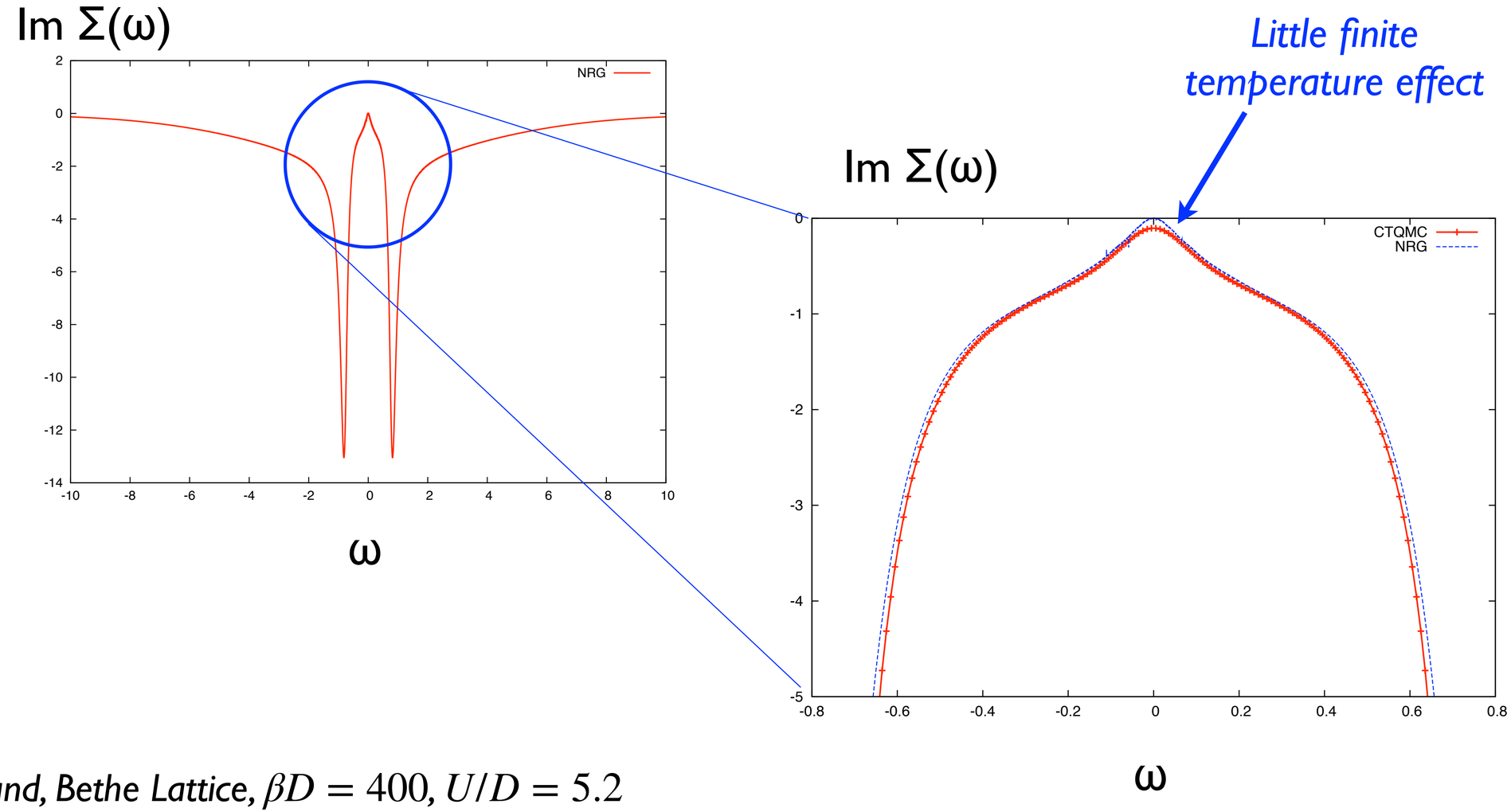
Cf TRIQS tutorial

- Maximum entropy (MaxEnt)
  Jarrell and Gubernatis, Physics Reports Vol. 269, 133, (1996).
  - The most probable $A(\omega)$ given $G(\tau)$, error bar and correlations.

- Exploit structure of the Green function, e.g. Nevalinna method [not for noisy data]
  Fei et al. Phys. Rev. Lett. 126, 056402 (2021)

CTQMC + Padé vs NRG

from M. Ferrero & P. Cornaglia

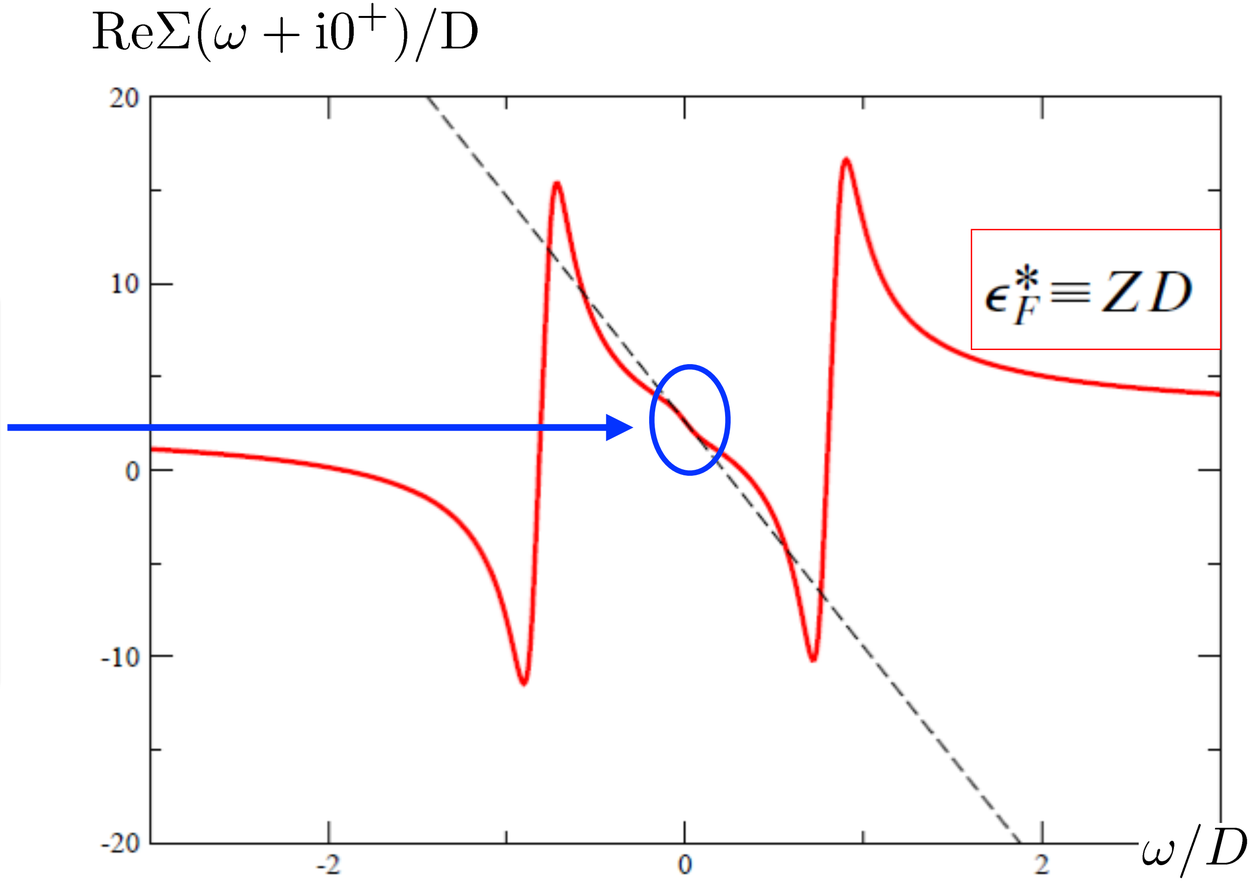


DMFT, 1 band, Bethe Lattice, $\beta D = 400, U/D = 5.2$

A lot of structure beyond the Fermi liquid

- Real part of self-energy

- Fermi liquid theory only valid here
- Kink = loss of quasi-particle coherence



courtesy M.Ferrero (Padé & compares perfectly to NRG)

Quantum impurity solvers

2. Hamiltonian solvers

- Exact diagonalization (ED). *Cf lecture by D. Sénéchal on Monday*
- Numerical Renormalization group (NRG). *Cf Lecture by F. Kugler on Monday*
- Tensor network (DMRG).

Hamiltonian form

- Write the hybridization Δ as an explicit free fermion bath

$$S = -\int\int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')d_\sigma(\tau') + \int_0^\beta d\tau\ U n_{d\uparrow}(\tau)n_{d\downarrow}(\tau)$$

$$\mathcal{G}_\sigma^{-1}(i\omega_n) \equiv i\omega_n + \epsilon_d - \underbrace{\sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}}_{\Delta_\sigma(i\omega_n)}$$

$$\downarrow$$

$$H = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_{k\sigma}\xi_{k\sigma}^\dagger\xi_{k\sigma} + \sum_{\sigma=\uparrow,\downarrow} \varepsilon_d d_\sigma^\dagger d_\sigma + U n_{d\uparrow}n_{d\downarrow} + \sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma}(\xi_{k\sigma}^\dagger d_\sigma + h.c.)$$

Exact Diagonalization solver : principle

- Fit Δ with a small bath (on Matsubara frequency, at a small fictitious temperature T_{eff})

$$Min_{V,\xi} \sum_n \left| \Delta(i\omega_n) - \sum_k \frac{|V_k|^2}{i\omega_n - \xi_k} \right|^2$$

- Diagonalize or use Lanczos algorithm to find the many-body ground state $|\psi_{GS}\rangle$
- Compute the $T = 0$ Green function $G(t) \sim \langle \psi_{GS} | c \; e^{-it(H-E_{GS})} \, c^\dagger | \psi_{GS} \rangle \quad + (\dots)$

- *Cf Lecture by David Sénéchal next Monday : ED, cluster DMFT and some application.*

Exact Diagonalization solver

- Pros :
  - 1 band DMFT: a small bath of a few sites is sufficient to capture the Mott transition
  - $T = 0$ solver (but with T_{eff}, there is a finite resolution)
- Cons:
  - Scales exponentially with number of orbital/cluster size.
    In practice, 4 sites is a maximum.
  - Poor ω resolution.
  - Convergence with bath size is hard to achieve.

Numerical Renormalization Group (NRG)

Cf Lecture by F. Kugler

- Pros :
  - Gold standard for real time solvers in equilibrium
  - Very precise a low energy
  - Now can compute vertex function, even in real time !
- Cons:
  - Scales exponentially with number of orbital/cluster size.
    In practice, 4 sites is a maximum.
  - Poor resolution at large ω

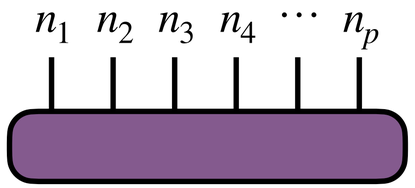
Tensor network.
DMRG

N-body wavefunctions

- Many body wave functions often have a low rank structure.
- Consider an impurity model, and N-body wave function written in the Fock states.

$$|\Psi\rangle = \sum_{n_1 n_2 n_3 \ldots n_p} \Psi_{n_1 n_2 n_3 \ldots n_p} |n_1 n_2 n_3 \ldots n_p\rangle$$

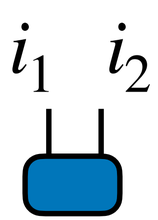
$$\Psi_{n_1 n_2 n_3 \ldots n_p} =$$



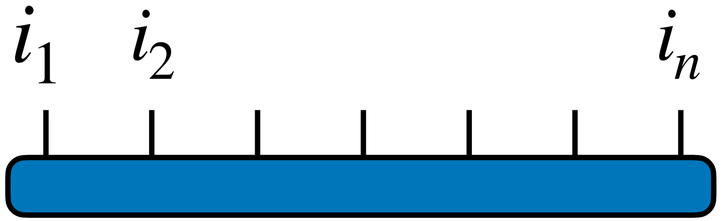
- For many systems (e.g. 1d, quantum impurities), the tensor Ψ is low rank

Tensors

- A n-dimensional array $T_{i_1 i_2 \ldots i_n}$ with the indices $i_k \in \{1, \ldots, d\}$
- Pictorial representation.
  Legs = indices.
  Contraction = connecting lines.



$A_{i_1 i_2}$



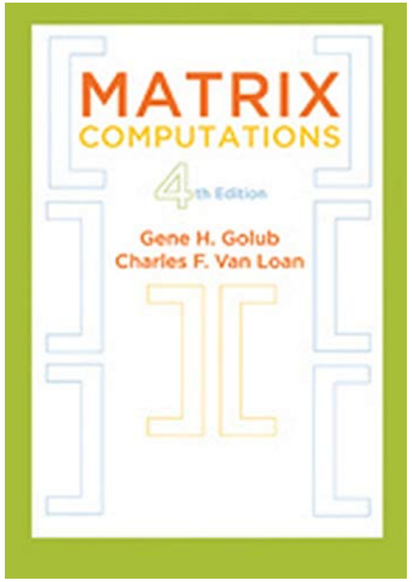
$T_{i_1 i_2 \ldots i_n}$

Low rank decomposition of tensors ?

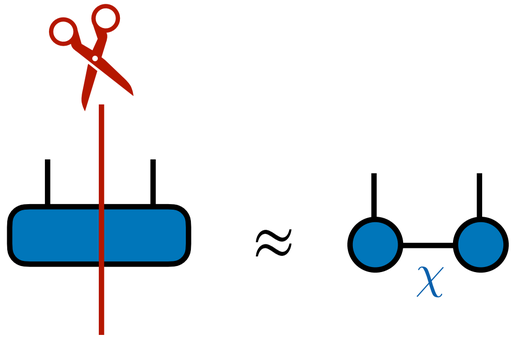
Low rank matrix

- Singular Value Decomposition (SVD) (or RRQR, RRLU …)

$$A = UDV \qquad D = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & \lambda_n \end{pmatrix}$$



- Precision ϵ: keep χ largest singular values λ_i
- $\chi = \epsilon$-rank.



$$A_{ij} = L_{ir} R_{rj} \qquad 1 \le r \le \chi$$

Low rank: save memory and computing time

Low rank tensors

- Matrix product states (MPS) = Tensor Trains.

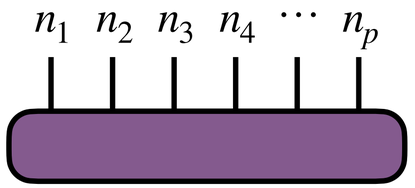
$$T_{i_1 i_2 \ldots i_n} \approx M^{i_1}_{1 r_1} M^{i_2}_{r_1 r_2} \ldots M^{i_n}_{r_{n-1} 1}$$

- *Tensor networks*
  - How to manipulate tensors in this compressed form.
  - A new (big) chapter in linear algebra…

N-body wavefunctions

$$|\Psi\rangle = \sum_{n_1 n_2 n_3 \ldots n_p} \Psi_{n_1 n_2 n_3 \ldots n_p} |n_1 n_2 n_3 \ldots n_p\rangle$$

$$\Psi_{n_1 n_2 n_3 \ldots n_p} =$$



- Variational Ansatz for ground state Ψ_{GS} in term of a low rank tensor network.
- DMRG (Density Matrix Renormalization Group). *S.White, 1992*
- Controlled by quantum entanglement / bond dimension (rank) χ

Solving quantum impurities with tensor networks

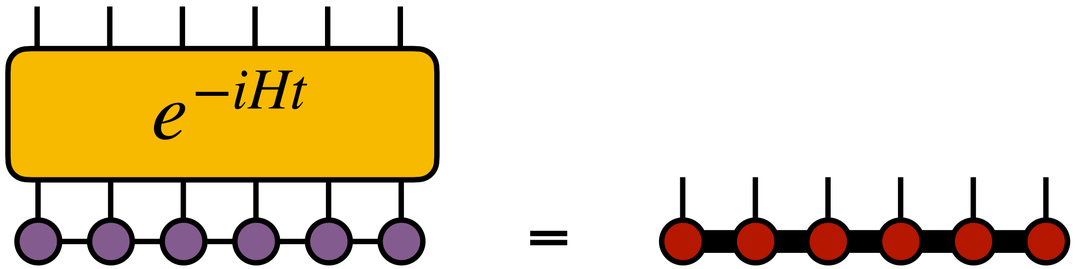
1. Fit the bath Δ with a discrete bath, as in ED (but with much larger systems).

2. Use DMRG algorithm to find the many-body ground state $|\psi_{GS}\rangle$

- Use low rank tensor Ansatz for $|\psi_{GS}\rangle$ and minimize the energy $\langle\psi_{GS}|H|\psi_{GS}\rangle$.

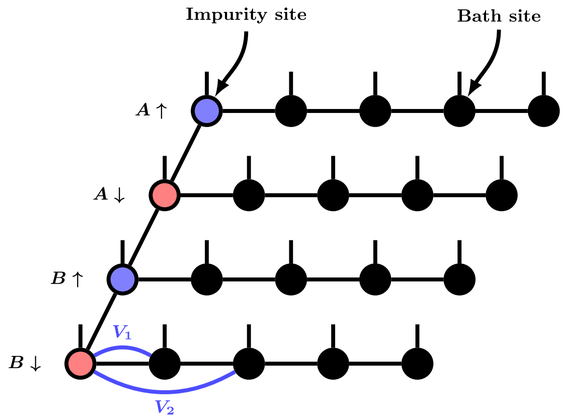
3. Use time evolution algorithm in tensor networks to compute the $T = 0$ Green function

$$G(t) \sim \langle\psi_{GS}|\, c\; e^{-it(H-E_{GS})}\, c^\dagger\, |\psi_{GS}\rangle \quad + (\dots)$$



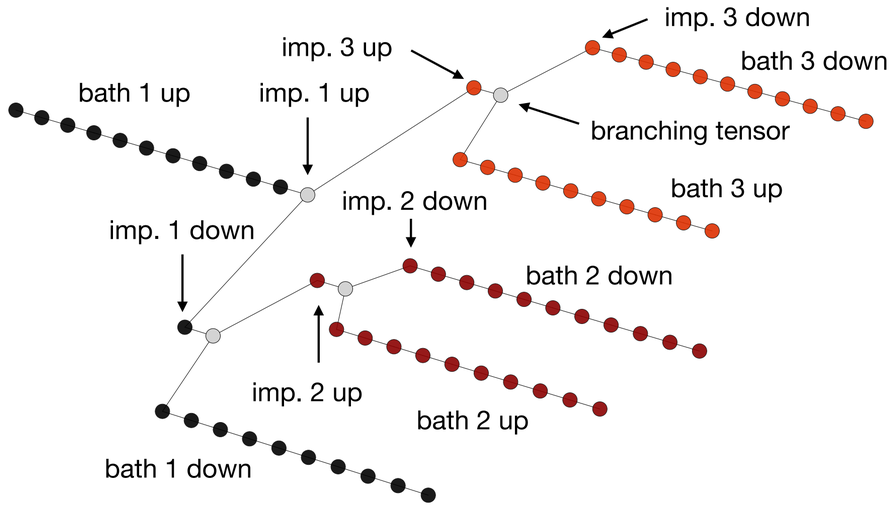
Many details left from this introduction

- Bath fitting
- Need to go beyond MPS (fork tensor)



Fork Tensor Product State (ForkTPS)

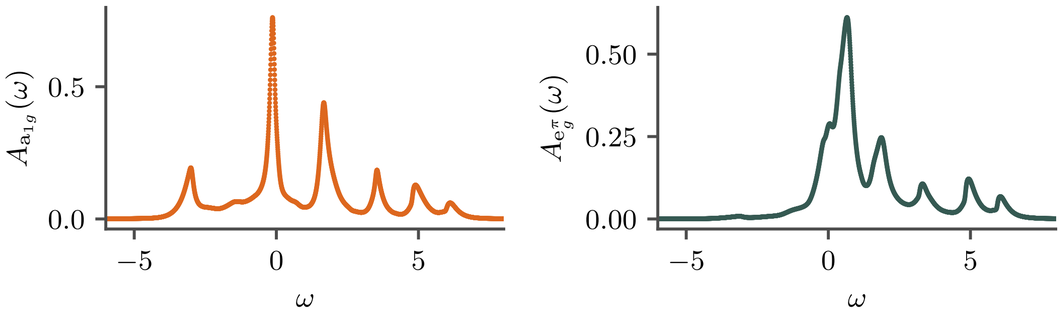
D. Bauernfeind et al. Phys. Rev. X 7, 031013 (2017)



M. Grundner, P. Westhoff, F. B. Kugler, O.P., U. Schollwöck arXiv:2312.11705

Tensor network solver

- Pros :
  - Real time (or imaginary time)
  - Large baths size L (up to several hundreds).
  - Larger impurities than NRG (5 bands or more).
  - Good resolution at high frequencies (see multiplets in $A(\omega)$)
  - $T = 0$ or finite T (purification or METTS = Maximally Entangled Typical Thermal State)

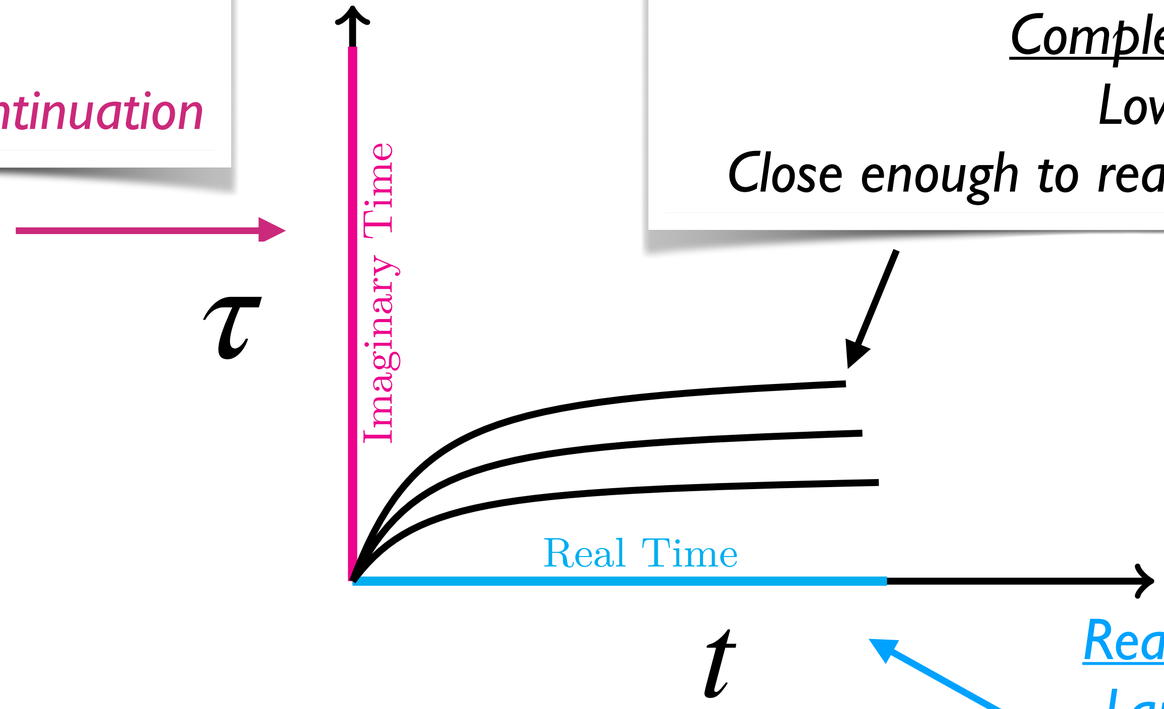


- Cons:
  - Convergence vs L still very slow $\Delta\omega \sim 1/L$
  - Growth of entanglement/rank at long time t
    Poor ω resolution at low frequencies
  - Not open source code to use [but we are working on it at the Flatiron Institute]

A recent development : complex time

X. Cao, Y. Lu, M. Stoudenmire, O. P.
arXiv:2311.10909
M. Grundner, P. Westhoff, F. B. Kugler, O.P. , U. Schollwöck
arXiv:2312.11705

Imaginary time
Low χ
Requires analytic continuation



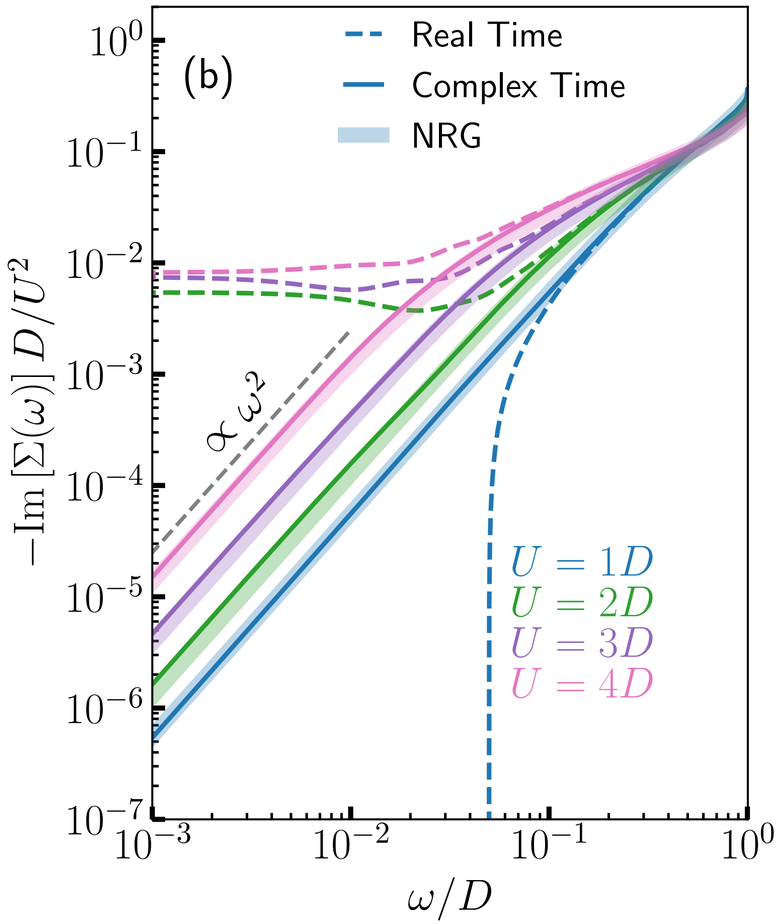
Complex time
Low χ
Close enough to real axis to reconstruct

Real time
Large χ
Long time limitation

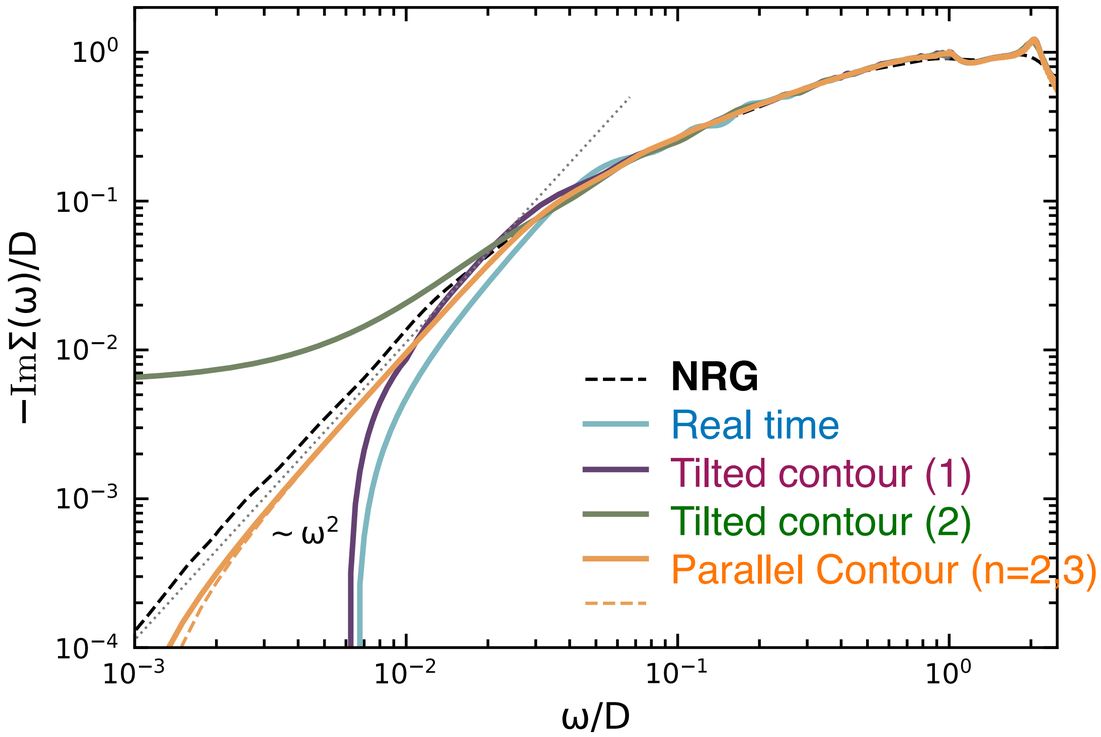
Excellent low energy results !

- Fermi liquid Im $\Sigma(\omega) \sim \omega^2$

Similar to NRG, but potentially much larger systems !



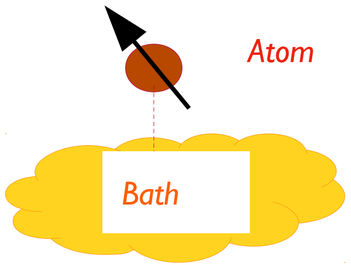
Anderson impurity model
1 orbital, flat bath of bandwidth D



Hubbard-Kanamori 3 bands

Quantum impurity solvers: challenges

- **Larger,** more complex systems (spin orbit, low symmetry, many orbitals, large clusters)
- *Faster* (explore parameter space, e.g. compute structure).
- High precision (e.g. for transport at low T)
  - Low frequency, temperature.
  - Transport computations (require high precision self-energy at low ω)
- Real time, out of equilibrium.



Algorithm development is crucial here !

Two body quantities

Susceptibilities

- Static susceptibility at simple q : solve DMFT in ordered phase

$$\chi \propto \frac{\partial m}{\partial h}\Big|_{h=0}$$

- Need a more general method for
  - Frequency dependency
  - Momentum dependency (incommensurate order)
  - General χ tensor (multiple possible instabilities)

Kubo formula

- Quantum linear response theory
  Response of operator A to a field coupled to B

$$\chi_{AB}(t-t') = -i\theta(t-t')\langle [A(t), B(t')] \rangle$$

- A, B : quadratic in the fundamental operators

$$A = A_{ab} c_a^\dagger c_b \qquad B = B_{cd} c_c^\dagger c_d$$

E.g. : susceptibilities $A = B = \sum_{i\sigma} (-1)^\sigma c_{\sigma i}^\dagger c_{\sigma i}$, conductivity (A = B = J)

- Requires the computation of two-particle Green functions

$$\sim \langle c_a^\dagger(t) c_b(t) c_c^\dagger(0) c_d(0) \rangle$$

Two particle Green functions

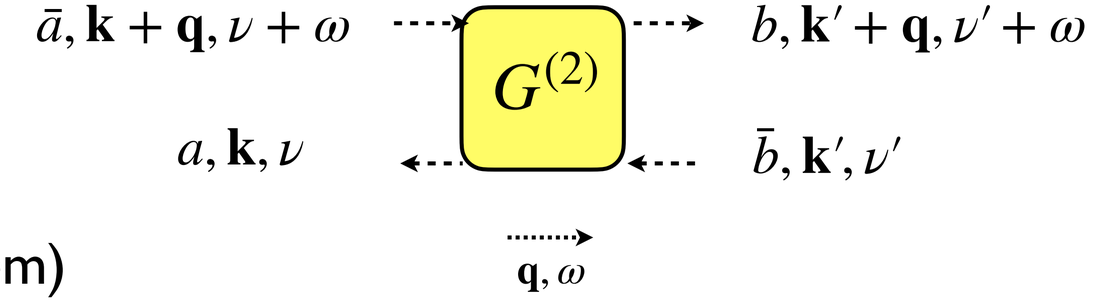
- Definition

$$G^{(2)}_{\bar{a}a\bar{b}b}(x_1, x_2, x_3, x_4, \tau_1, \tau_2, \tau_3, \tau_4) \equiv -i\langle T_\tau c^\dagger_{\bar{a}}(x_1, \tau_1) c_a(x_2, \tau_2) c^\dagger_{\bar{b}}(x_3, \tau_3) c_b(x_4, \tau_4)\rangle$$

a,b : multi-index orbital, spin

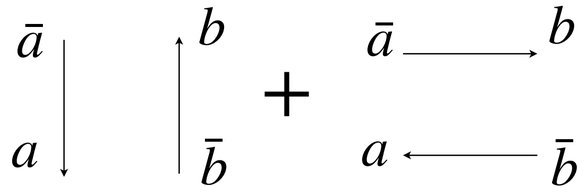
- Rank 4 tensor, with 3 frequencies/momenta

$$G^{(2)}_{\bar{a}a\bar{b}b}(k, k', q, \nu, \nu', \omega) =$$



- Non interacting case (Wick theorem)

$$G^{(2)}_{\bar{a}a\bar{b}b} =$$



$G_{0a\bar{a}}G_{0b\bar{b}}$ $\quad -G_{0a\bar{b}}G_{0b\bar{a}}$

Two particle Green functions

- Definition

$$G^{(2)}_{\bar{a}a\bar{b}b}(x_1, x_2, x_3, x_4, \tau_1, \tau_2, \tau_3, \tau_4) \equiv -i\langle T_\tau c^\dagger_{\bar{a}}(x_1, \tau_1) c_a(x_2, \tau_2) c^\dagger_{\bar{b}}(x_3, \tau_3) c_b(x_4, \tau_4)\rangle$$

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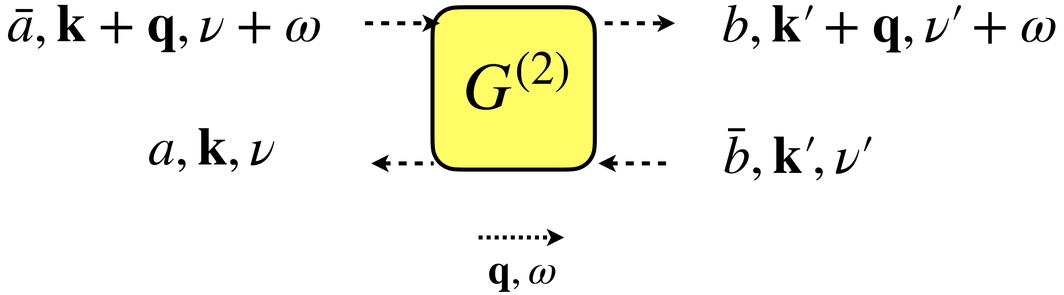
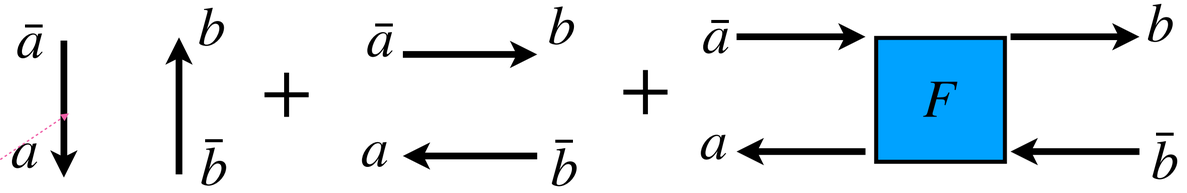


- Perturbative expansion

$$G^{(2)}_{\bar{a}a\bar{b}b} =$$



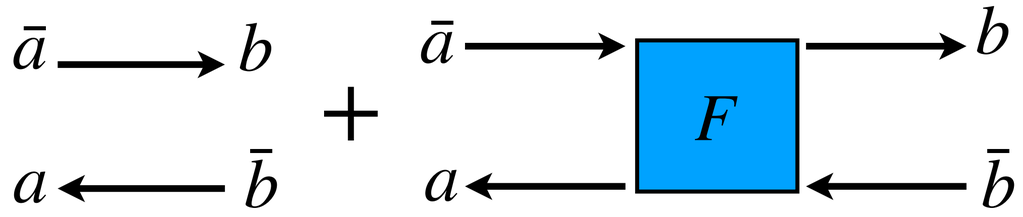
Full propagator $G_{a\bar{a}}G_{b\bar{b}}$ $-G_{a\bar{b}}G_{b\bar{a}}$ *reducible vertex F*

- In Fermi liquid, interactions between quasi-particles.

Generalized susceptibilities

- Generalized susceptibility (remove disconnected part, <A>)

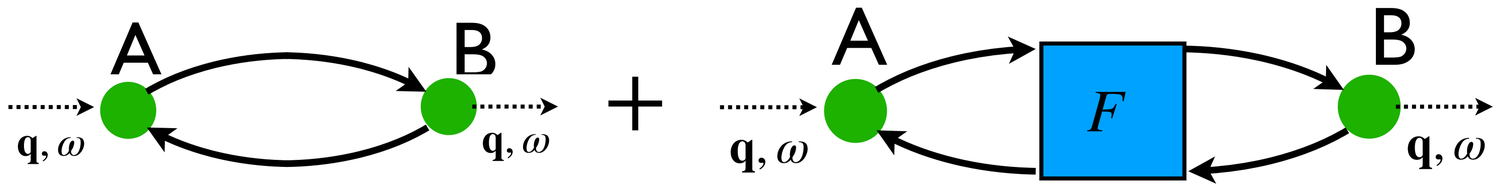
$$\tilde{\chi}_{\bar{a}a\bar{b}b} = \tilde{\chi}_{0\ \bar{a}a\bar{b}b} + \tilde{\chi}_{0\ \bar{a}a\bar{b}b} F \tilde{\chi}_{0\ \bar{a}a\bar{b}b}$$



- Susceptibility : contract with A and B, sum over frequencies/momenta

$$\chi(q,\omega) = \sum_{\nu\nu' kk'} \tilde{\chi}_{\bar{a}a\bar{b}b}(q,k,k',\omega,\nu,\nu') A_{\bar{a}a}(k) B_{\bar{b}b}(k')$$

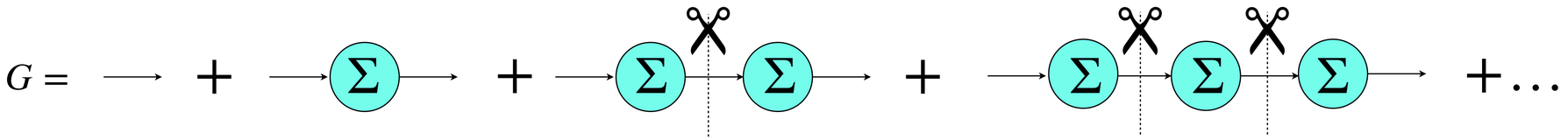
$$\chi_{AB}(q,\omega) =$$



Lindhard function *Vertex corrections*

Reminder : Dyson Equation

- Dyson equation for the one particle Green function

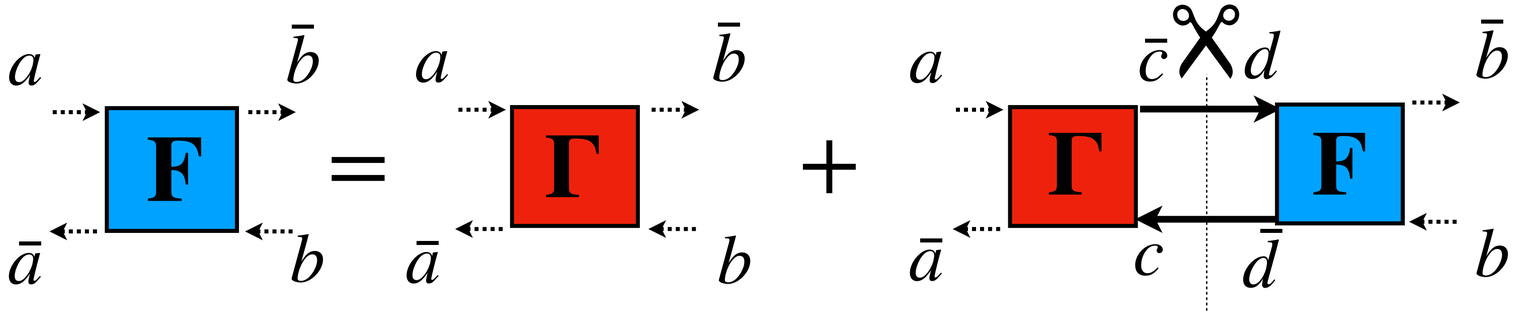


- Self-energy : 1PI (particle irreducible) diagrams

$$G = G_0 + G_0 \Sigma G \qquad \Sigma = G_0^{-1} - G^{-1}$$

Bethe-Salpeter equation

- Reducibility in particle-hole channel



$$F^{\nu\nu'\omega}_{a\bar{a}b\bar{b};kk'q} = \Gamma^{\nu\nu'\omega}_{a\bar{a}b\bar{b};kk'q} + \sum_{c\bar{c}d\bar{d},k_1,\nu_1} \Gamma^{\nu\nu_1\omega}_{ab\bar{a}\bar{b};kk_1q}\tilde{\chi}^{\nu_1\omega}_{0c\bar{c}d\bar{d},k_1k_1q}F^{\nu_1\nu'\omega}_{d\bar{d}b\bar{b};k_1k'q}$$

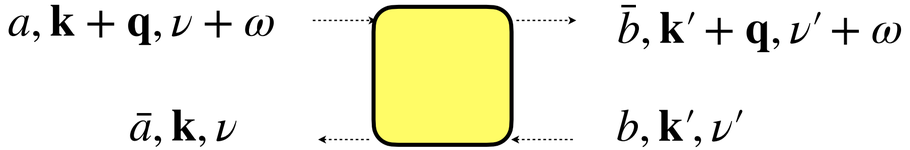
- Matrix equation

$$F = \Gamma + \Gamma\tilde{\chi}F$$

grouping indices

$I = (a, \bar{a}, k, \nu) \qquad J = (b, \bar{b}, k', \nu')$

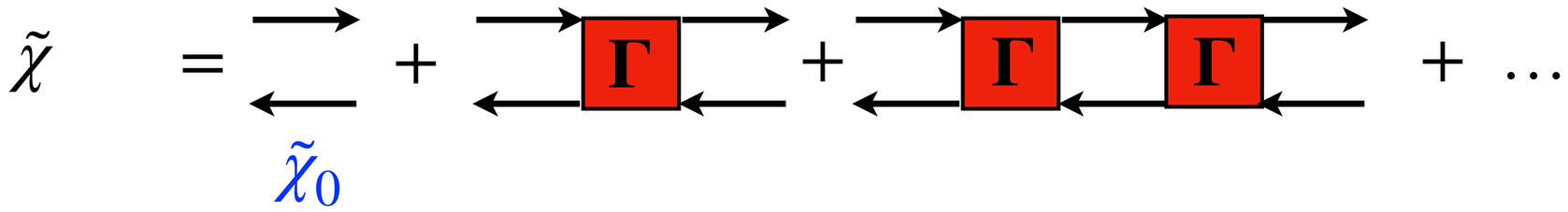
diagonal in (q,ω)



- $\Gamma_{a\bar{a}b\bar{b}}(k, k', q, \nu, \nu', \omega)$: Irreducible vertex in the particle-hole channel

Bethe-Salpeter equation

- Relation (exact) between the irreducible vertex Γ and χ



$$\tilde{\chi} = \tilde{\chi}_0 + \tilde{\chi}_0 \Gamma \tilde{\chi} \Longleftrightarrow \Gamma = \tilde{\chi}^{-1} - \tilde{\chi}_0^{-1}$$

- Approximations for Γ
  - RPA : $\Gamma \propto U$
  - DMFT ?

DMFT

Cf. A. Georges et al. Rev. Mod. Phys. 1996

$$\Gamma_{lattice}(k, k', q, \nu, \nu', \omega) \approx \Gamma_{imp}(\nu, \nu', \omega)$$

- Since

$$\Gamma^{lattice}_{ijkl} = \frac{\delta^2 \Phi}{\delta G_{ji} \delta G_{lk}}$$

- and DMFT approximation is

$$\Phi[G] \approx \sum_i \phi_{atomic}[G_{ii}]$$

$$\Gamma^{lattice}_{ijkl} \approx \delta_{i=j=k=l} \Gamma_{imp}$$

$$\Sigma^{latt}_{ij} = \frac{\delta \Phi}{\delta G_{ji}} = \delta_{ij} \Sigma^{imp}$$

Susceptibilities in DMFT

Cf. A. Georges et al. Rev. Mod. Phys. 1996

M. Jarrell et al., '90

- Solve DMFT
- Compute impurity two-particle functions
- Use BSE for impurity and lattice

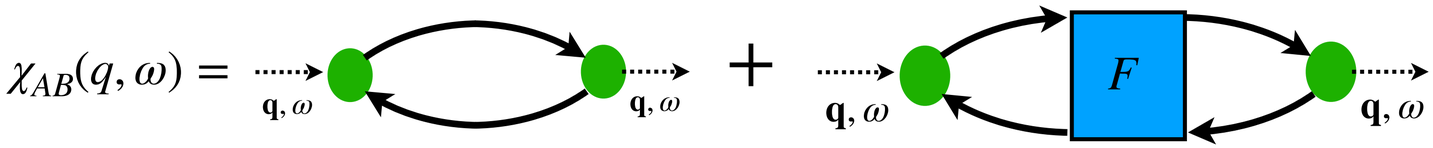
$$G_{imp} \longrightarrow \tilde{\chi}_{imp,0} \longrightarrow \Gamma_{imp} \longrightarrow \Gamma_{lattice} \longrightarrow \tilde{\chi}_{lattice} \longrightarrow \chi_{lattice}(q,\omega)$$

$$G^{(2)}_{imp} \longrightarrow \tilde{\chi}_{imp} \nearrow$$

$$\Gamma_{imp} = \tilde{\chi}^{-1}_{imp} - \tilde{\chi}^{-1}_{imp,0} \qquad \tilde{\chi}^{-1}_{lattice} = \Gamma_{lattice} + \tilde{\chi}^{-1}_{lattice,0}$$

Does not feedback in DMFT self-consistency loop

Are vertex corrections important ?

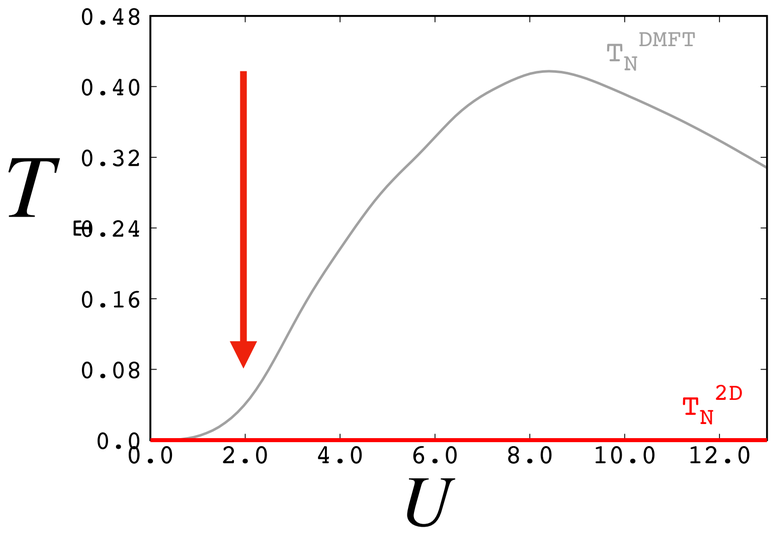


- Magnetic susceptibility
  - Non interacting case. Lindhard function $\chi_{\text{charge}} = \chi_{\text{spin}} \propto G_0 G_0$
  - Mott insulator: charge gap vs low energy spin excitations
- Conductivity
  - Cancellation of vertex corrections by symmetry in DMFT, but not in cluster.

Simple example

M. Jarrell 92
Curves from T. Schaefer

- 1 band Hubbard model, 2d square lattice, DMFT.



Ornstein-Zernike form

$$\chi(q, i\Omega_0) = \frac{A}{(q - Q_{AF})^2 + \xi^{-2}}$$

$$Q_{AF} = (\pi, \pi)$$

$$\chi(q = (\pi, q_y), \omega = 0)$$

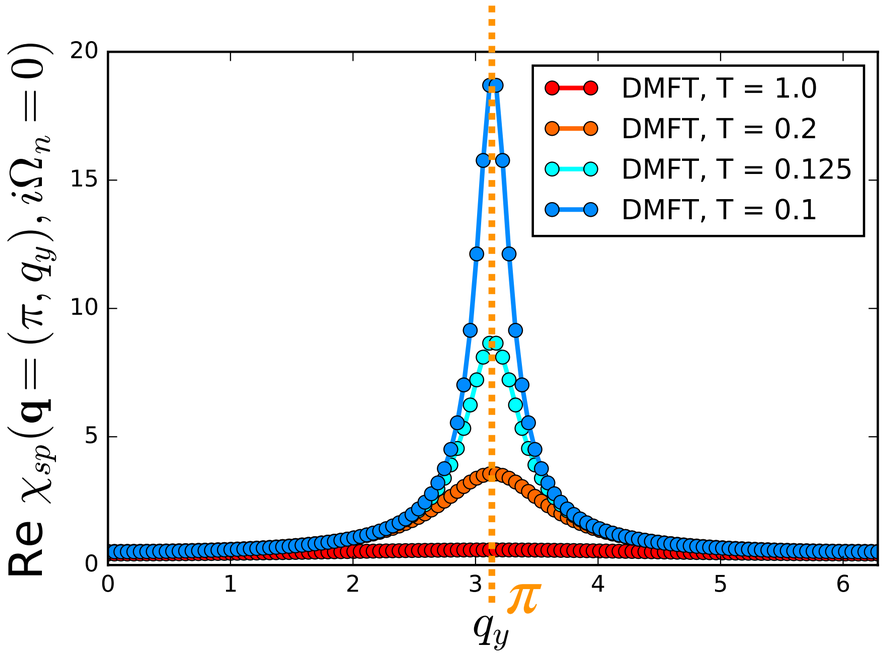
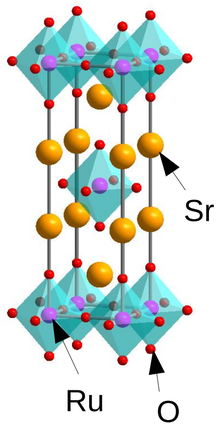
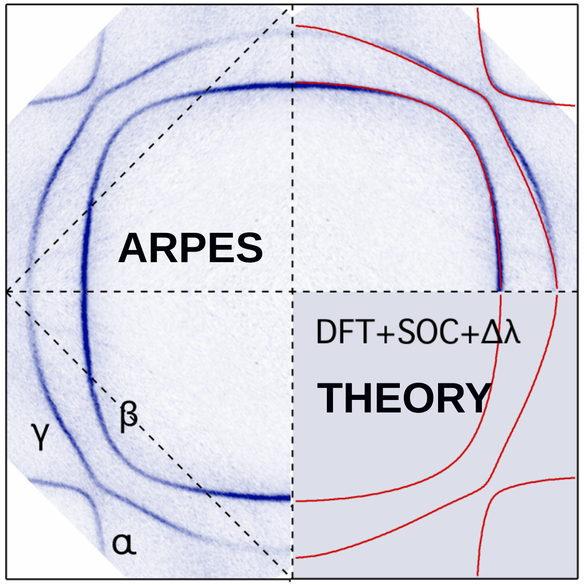


Illustration with a Hund metal

Sr_2RuO_4

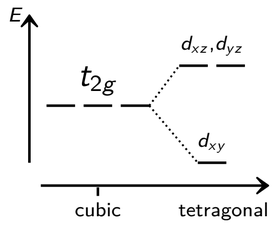
- A correlated Hund's metal ($U = 2.3$ eV, $J = 0.4$ eV)
- Spin orbit coupling ($\lambda = 0.1 - 0.2$ eV)
- Fermi liquid for $T < T_{FL} \approx 25K$
- Superconductivity $T_c \approx 1.5K$
- 3 sheet Fermi surface
- Clean samples/experiments.

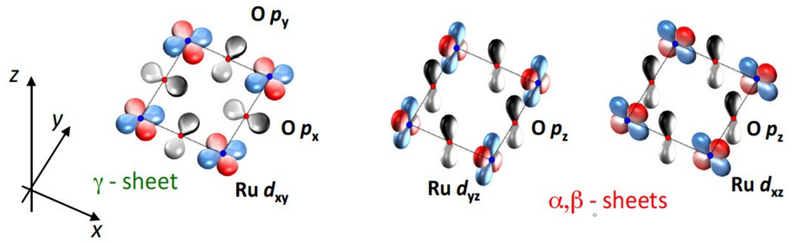




Fermi surface. Theory vs ARPES

A. Tamai, M. Zingl et al. Phys. Rev. X 9, 021048 (2019)



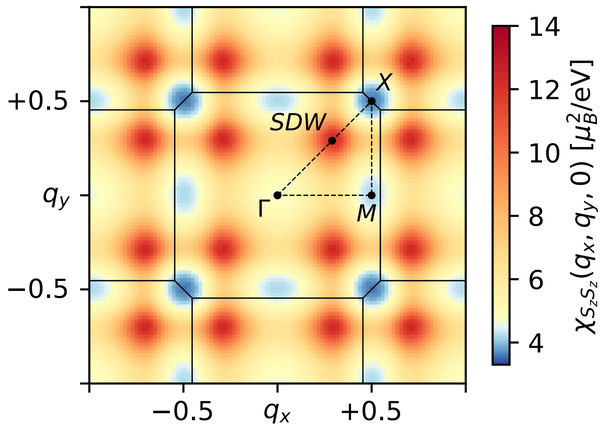


Sr_2RuO_4 : spin response

Magnetic response

nature of magnetic fluctuations ?

$$\chi_{\text{spin}}(q, \omega = 0)$$



H. Strand, et al
Phys. Rev. B 100, 125120 (2019)

- Bethe Salpeter + DMFT vertex computation
- Quasi-local spin fluctuations due to Hund's coupling

.

Sr_2RuO_4 : Spin-orbital separation

- Inelastic x-ray spectra

RIXS spectral vs DMFT

nature communications

Article

https://doi.org/10.1038/s41467-023-42804-3

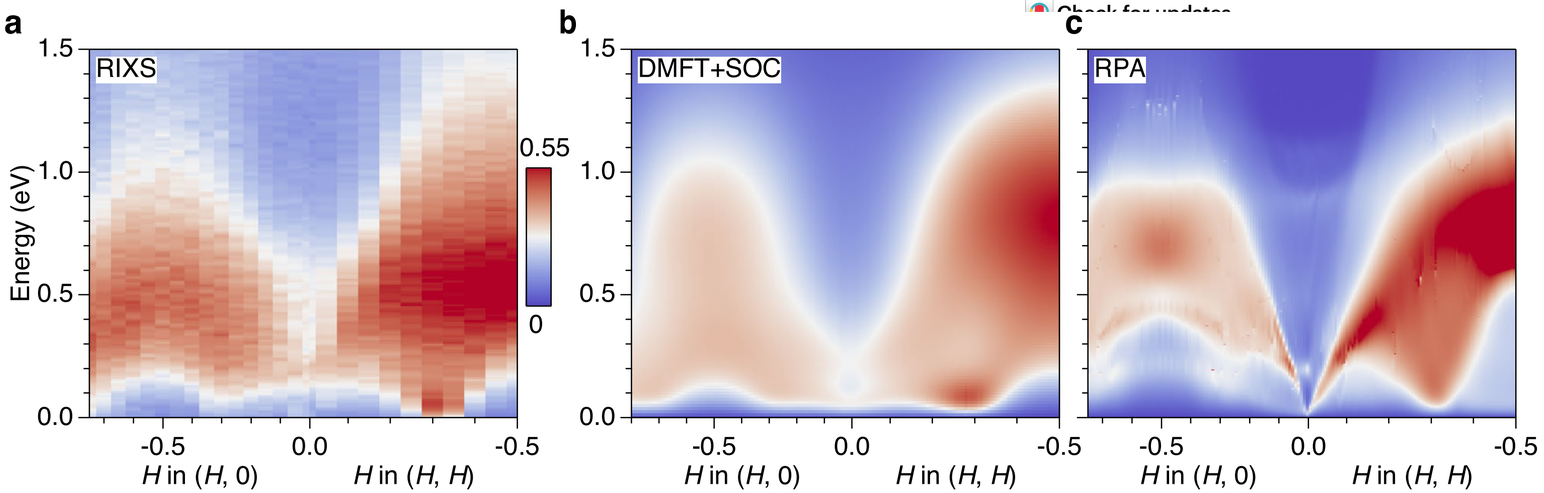
Distinct spin and orbital dynamics in Sr_2RuO_4

Received: 24 March 2023

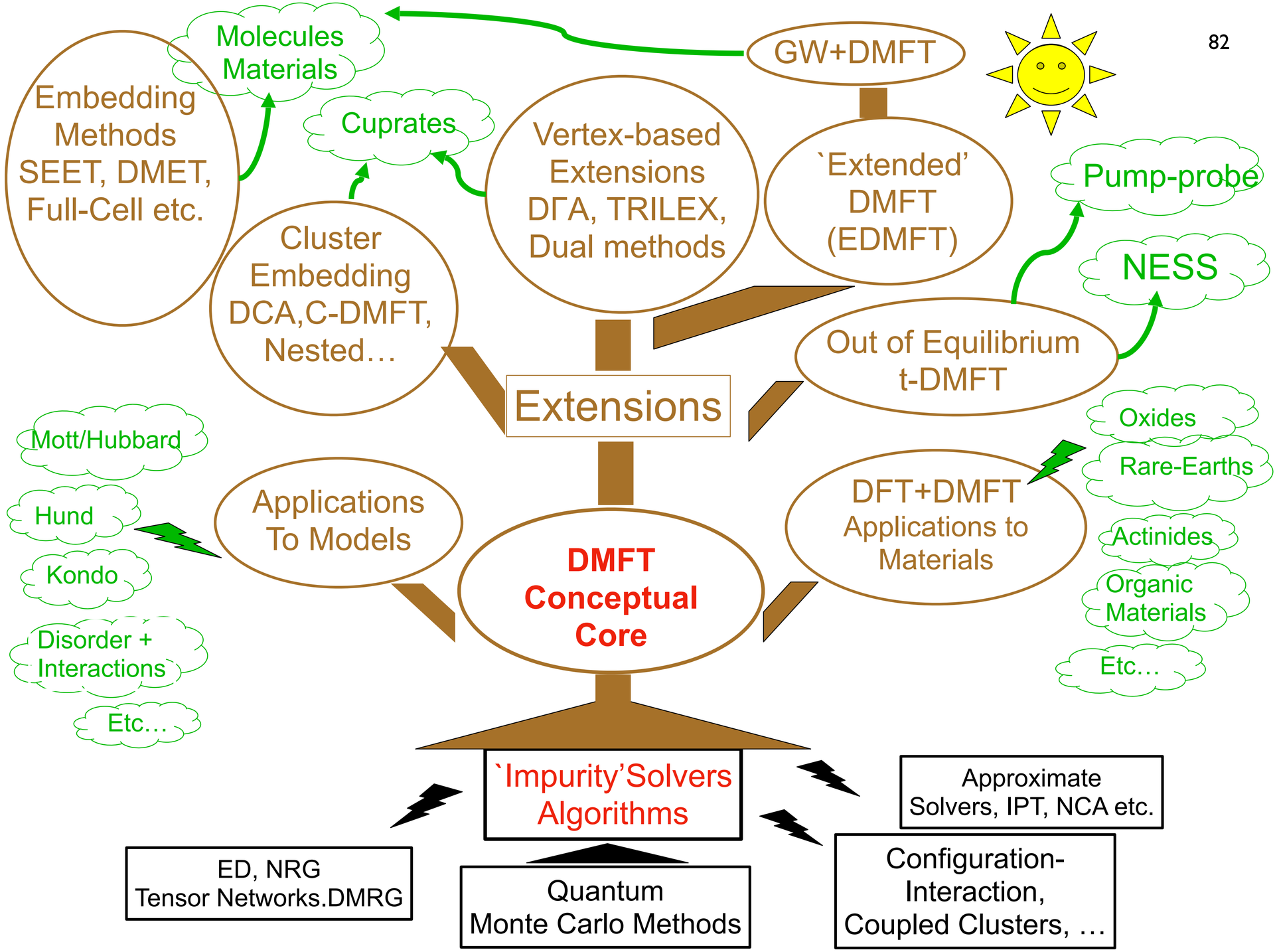
Accepted: 20 October 2023

Published online: 03 November 2023

H. Suzuki[1,2,3,15] ✉, L. Wang[1,15], J. Bertinshaw[1], H. U. R. Strand[4,5], S. Käser[1,6], M. Krautloher[1], Z. Yang[1], N. Wentzell[7], O. Parcollet[7,8], F. Jerzembeck[9], N. Kikugawa[10], A. P. Mackenzie[9], A. Georges[7,11,12,13], P. Hansmann[1,6,9], H. Gretarsson[1,14] ✉ & B. Keimer[1] ✉



Conclusion


Molecules
Materials
GW+DMFT
Embedding
Methods
SEET, DMET,
Full-Cell etc.
Cuprates
Vertex-based
Extensions
DΓA, TRILEX,
Dual methods
`Extended'
DMFT
(EDMFT)
Pump-probe
NESS
Cluster
Embedding
DCA,C-DMFT,
Nested…
Out of Equilibrium
t-DMFT
Extensions
Mott/Hubbard
Hund
Kondo
Disorder +
Interactions
Etc…
Applications
To Models
DMFT
Conceptual
Core
DFT+DMFT
Applications to
Materials
Oxides
Rare-Earths
Actinides
Organic
Materials
Etc…
`Impurity'Solvers
Algorithms
ED, NRG
Tensor Networks.DMRG
Quantum
Monte Carlo Methods
Approximate
Solvers, IPT, NCA etc.
Configuration-
Interaction,
Coupled Clusters, …

Related lectures

- Tutorials : TRIQS, abinit +DMFT.
- Lectures:
  - M. Ferrero today: CTQMC
  - D. Sénéchal on Monday: ED, cluster and application
  - S. Beck and A. Hampel on Monday: applications to materials.
  - F. Kugler on Tuesday: NRG
  - A. Toschi on Wednesday: Extensions of DMFT based on vertex (DΓA)
  - P. Werner, M. Eckstein on Wednesday: Non equilibrium DMFT.

DMFT : some references

- The classic.
  A. Georges, G. Kotliar, W. Krauth and M. Rozenberg,
  Rev. Mod. Phys. 68, 13, (1996)

- On realistic computations (DFT + DMFT)
  G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C. Marianetti,
  Rev. Mod. Phys. 78, 865 (2006)

- On Quantum Monte Carlo (DMFT) Impurity solvers
  E. Gull et al.
  Rev. Mod. Phys. 83, 349 (2011)

- On Cluster DMFT methods
  T. Maier et al.
  Rev. Mod. Phys. 77, 1027 (2005)

- On Vertex and DMFT extensions
  G. Rohringer et al. Rev. Mod. Phys. 90, 025003 (2018)

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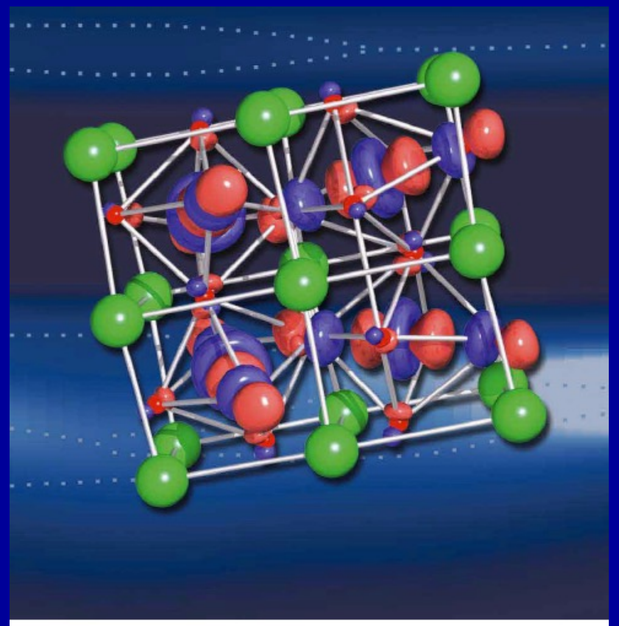

The LDA+DMFT approach to strongly correlated materials

Eva Pavarini, Erik Koch, Dieter Vollhardt, and Alexander Lichtenstein (Eds.)

German Research School for Simulation Sciences

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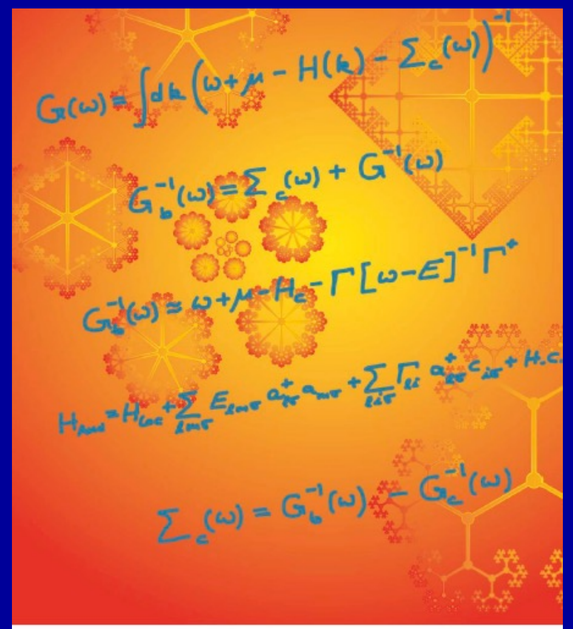

DMFT at 25: Infinite Dimensions

Eva Pavarini, Erik Koch, Dieter Vollhardt and Alexander Lichtenstein (Eds.)

German Research School for Simulation Sciences

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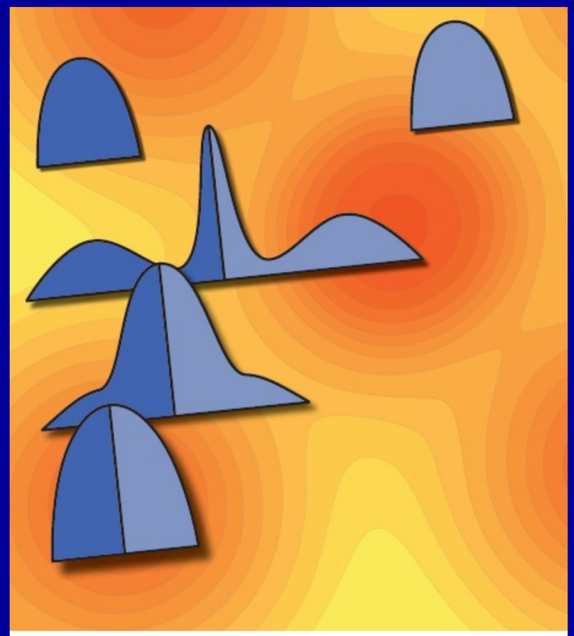

DMFT: From Infinite Dimensions to Real Materials

Eva Pavarini, Erik Koch, Alexander Lichtenstein, and Dieter Vollhardt (Eds.)

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https://www.cond-mat.de/events/correl.html

Also: recent book by V.Turkowski (Springer)

Thank you for your attention