Lecture 3
Impurity solvers for DMFT

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Outline

- Lecture 1 : Introduction to DMFT
- Lecture 2 : Beyond DMFT. Clusters.
- Lecture 3 : Impurity solvers :
  - Why specific algorithm for DMFT effective impurities ?
  - Continuous time Quantum Monte Carlo: CT-INT and CT-HYB
  - Discussion

Solving DMFT : iterative method

Impurity solver

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

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

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

$\mathcal{G}$

$G_{\rm imp}$, $\Sigma_{\rm imp}$

Self consistency condition

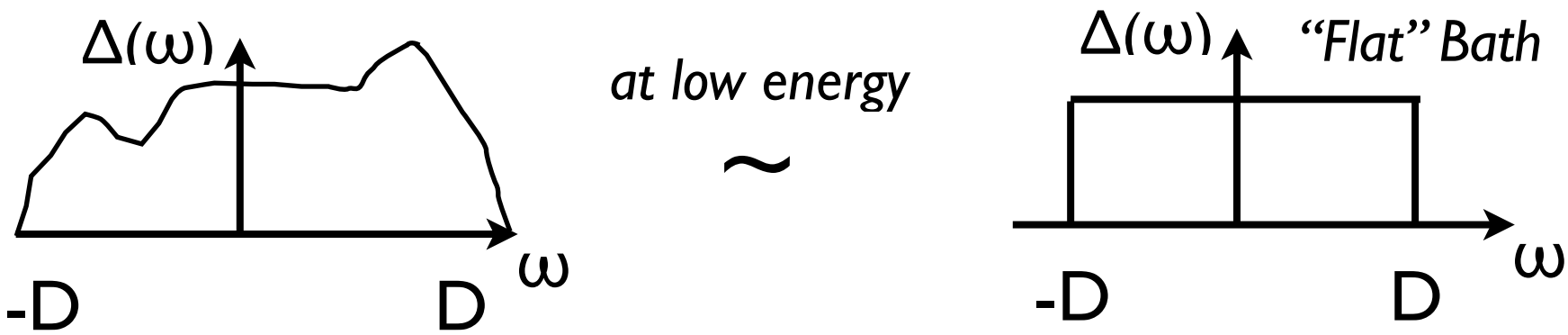
$$G_{\sigma\rm imp}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\rm imp}[\mathcal{G}](i\omega_n)}$$

Why do we need specific algorithms ?

Impurity model : non-DMFT case

- Anderson impurity in a metallic host (structureless bath)
- Typical energy scale of the bath Δ = D ~ eV
  very high energy scale (U.V. cut-off).
- Low energy, universal regime: separation of scales, scaling laws

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



- Linearise the energy close to the Fermi level

$$\epsilon(k) \propto (k - k_F)$$

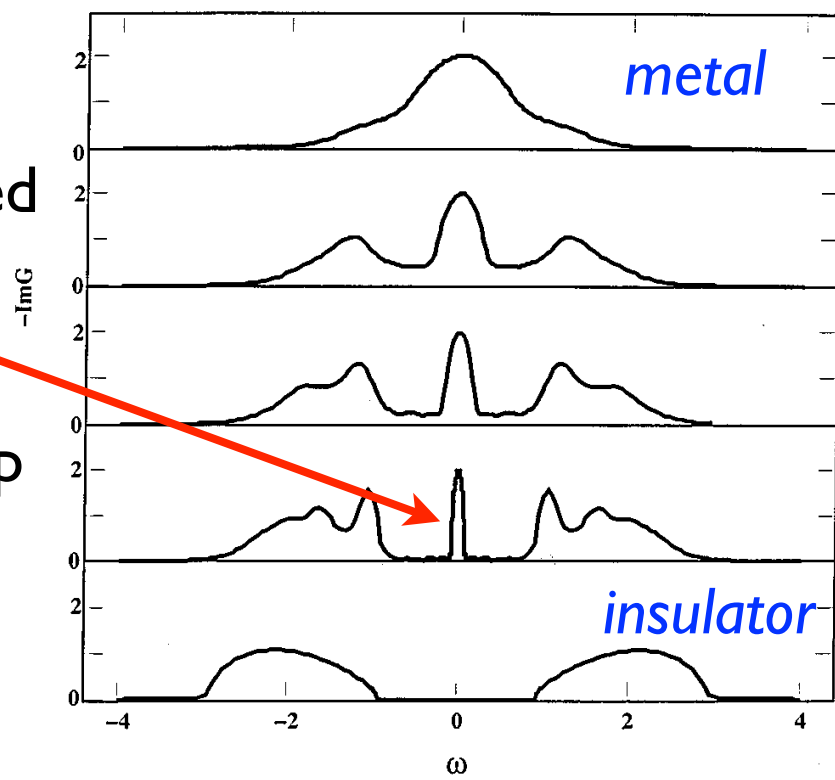
DMFT baths have a low-energy structure

- Gapped bath (insulator, superconductor) : no Kondo effect

- DMFT bath is self-consistently determined and has a structure at low energy

- Cluster DMFT : bath can have pseudo-gap

DMFT bath evolution close to Mott transition

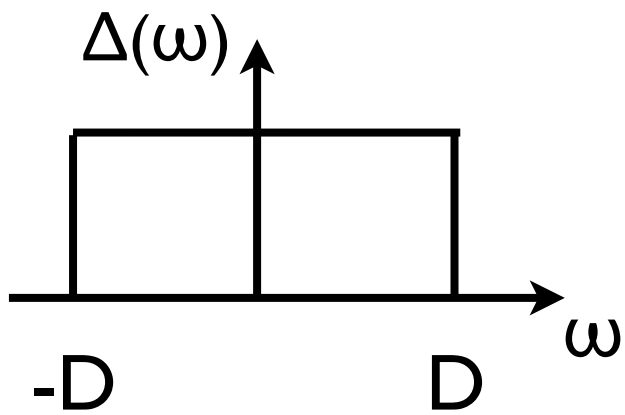


A. Georges et al., Rev. Mod. Phys. 68, 13, (1996)

Field theory methods

- Integrability (Bethe Ansatz) in the universal regime
  A. Tsvelik, P. Wiegmann/ N. Andrei, 1980;
  Thermodynamics but Green function very hard to compute.
- Boundary Conformal Field Theory *Cardy; Affleck, Ludwig, 1991*
  At low-energy fixed point.
- BUT both methods starts from a flat band.

Not sufficient to solve DMFT



Impurity solvers : a rich toolbox

- Continuous Time Quantum Monte Carlo family (CT-QMC)
- Algorithms based in Hamiltonian form
  - Exact diagonalization (ED)
  - Numerical Renormalization group (NRG)
  - Density Matrix Renormalization group (DMRG).
- Approximate solvers :
  - Iterated Perturbation Theory (IPT)
  - NCA family (NCA, OCA, …)
  - Slave boson technique.

Quantum Monte Carlo

Monte Carlo sampling

Cf Lode's talk

- Partition function and operator averaging : (assume p(x) >0)

$$Z = \int_{\mathcal{C}} dx\, p(x), \qquad \langle A \rangle = \frac{1}{Z} \int_{\mathcal{C}} dx\, A(x) p(x)$$

Configuration space

Probability of configuration x
e.g. in classical model : $p(x) \propto e^{-\beta E(x)}$

- Principle : use a Markov chain in configuration space.
  - Average replaced by average over the Markov chain.
  - Transition rate $W_{x \to y}$: probability to go from x to y
  - Detailed balance : $\dfrac{W_{x\to y}}{W_{y\to x}} = \dfrac{p(y)}{p(x)}$
  - Ergodicity property :
    It is possible to reach y from x, ∀x,y in a finite number of steps.

Metropolis algorithm

N. Metropolis et al. J. Chem. Phys. 1953

- To build the Markov chain:
  - Propose moves in the configuration space
  - Accept them with some probability, such that :

Proposition probability (chosen)

Acceptance probability (computed)

$$W_{x\to y} = W^{\text{prop}}_{x\to y} \times W^{\text{acc}}_{x\to y}$$

$$W^{\text{acc}}_{x\to y} \equiv \min\left(1, \underbrace{\frac{p(y)W^{\text{prop}}_{y\to x}}{p(x)W^{\text{prop}}_{x\to y}}}_{R_{x\to y}}\right)$$

The sign problem

- What if p(x) is not always positive ? Use |p(x)| as the probability !

$$\langle A \rangle = \frac{1}{Z} \int_{\mathcal{C}} dx\, A(x) p(x) = \frac{\int_{\mathcal{C}} dx \left(A(x)\, \mathrm{sign}(p(x)) \right) |p(x)|}{\int_{\mathcal{C}} dx \left(\mathrm{sign}(p(x)) \right) |p(x)|}$$

- The denominator (average of sign (p(x)) can decay exponentially as temperature is lowered or in large volume limit.
- The QMC is correct if <sign>≠1, but becomes untractable when <sign>≈0 (large error bars).
- A major limitation of Quantum Monte Carlo (specially for fermions)
- The sign problem depends on the basis/rewriting of Z !

Monte Carlo

- A QMC algorithm :
  - Rewrite Z, ideally as a sum of positive terms.
  - Find local ergodic moves
- Advantages :
  - QMC is a very flexible technique
  - QMC is massively parallel by construction.
- Drawbacks :
  - Convergence is slow, like $1/\sqrt{\text{time}}$
  - Sign problem may be severe !

Monte Carlo is just a technique to compute sums.
How to rewrite Z, which move to use, etc... is your choice !

Continuous Time QMC

- Perform an expansion in a coupling constant and sum it with MC
- Original idea by N. Prokofiev : continuous time QMC (1996)
- For impurity problems :
  - Expansion in U : CT-INT
    A.N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005)
  - Expansion in $\Delta(\omega)$, 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)

Continuous time QMC : principle

- Write a perturbative expansion of the partition function :

$$H = H_a + H_b$$

$$Z = \mathrm{Tr}\, T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right]$$

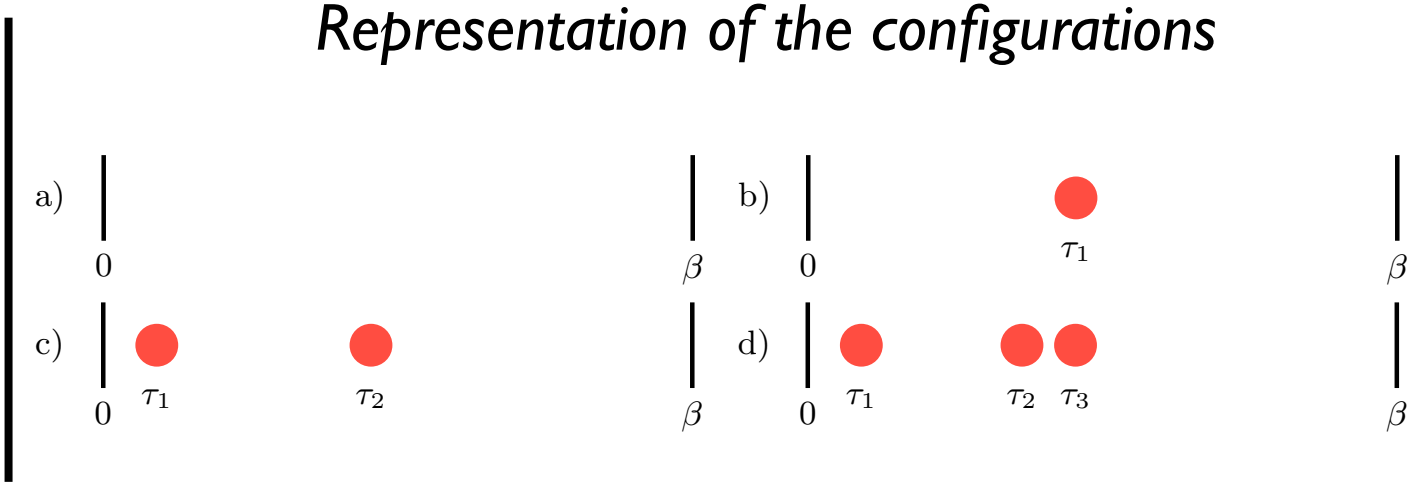
$$= \sum_{n\geq 0}(-1)^n \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n \,\mathrm{Tr}\left[e^{-\beta H_a} H_b(\tau_n) H_b(\tau_{n-1}) \ldots H_b(\tau_1)\right]$$

$$= \sum_{n\geq 0} \sum_{\tau_1<\tau_2<\ldots\tau_n} \sum_{\gamma\in\Gamma_n} \underbrace{(\Delta_\tau)^n w(n,\gamma,\tau_1,\ldots,\tau_n)}_{p(x)} = \sum_{x\in\mathcal{C}} p(x)$$

Configurations

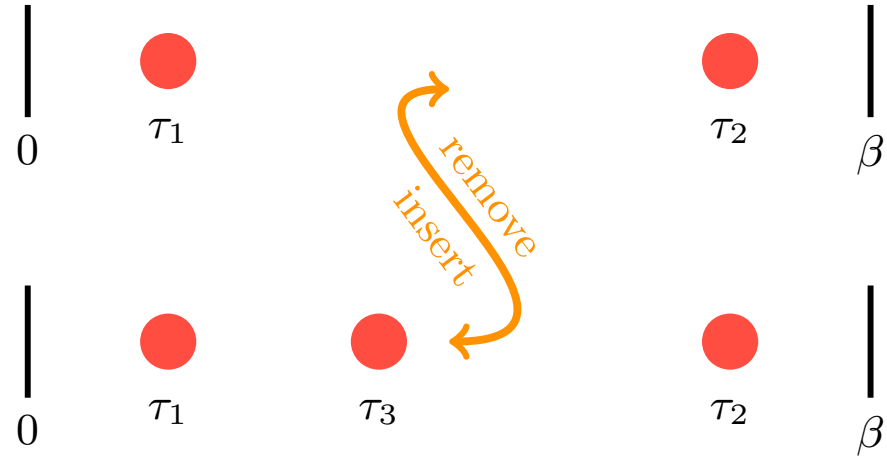
$$x = (n, \gamma, \tau_1, \tau_2, \ldots \tau_n)$$

Representation of the configurations



Continuous time QMC : principle (II)

A CT-QMC move



- Move : add/remove one interaction term (= change n by 1), e.g.
  x = (n, ...) configuration with n vertices
  y = (n+1, ...) configuration with n+1 vertices

$$W^{prop}_{x\to y} = \frac{\Delta_\tau}{\beta} \qquad W^{prop}_{y\to x} = \frac{1}{n+1}$$

- The Metropolis rate has a finite limit. *Prokofiev (1996)*

$$R_{x\to y} = \frac{p(y)W^{\rm prop}_{y\to x}}{p(x)W^{\rm prop}_{x\to y}} = \frac{w(y)(\Delta_\tau)^{n+1}}{w(x)(\Delta_\tau)^{n}}\frac{\beta}{\Delta_\tau(n+1)}$$

The algorithm can be formulated directly in continuous time

Which perturbative expansion ?

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

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

Interaction

Bath

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

- CT-INT: Expansion in power of the interactions
- CT-HYB : Expansion in power of hybridization (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 :

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

- With TRIQS (&Hands on) package : a demo CT-INT code, 1 band.

Expansion in hybridization

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

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

a,b = 1,N

- Expansion in hybridization :

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

- w is positive in single impurity problem.
- Hlocal can be anything (but we need to compute the Trace …)

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 :

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

- Green function computation (or higher order correlations functions):

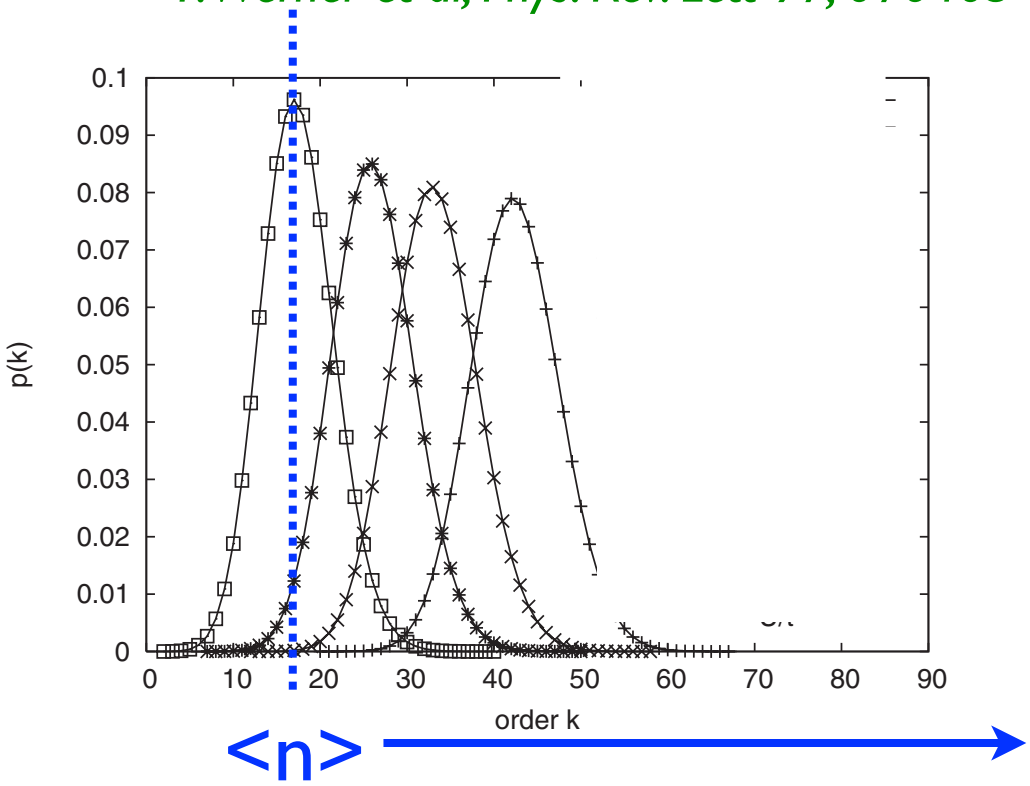
$$G_{ab}(\tau) = \frac{1}{Z}\frac{\delta Z}{\delta \Delta_{ba}(-\tau)}$$

$$G_{ab}(\tau) = \sum_{n\geq 0} \int_< \prod_{i=1}^n d\tau_i d\tau_i' \sum_{a_i,b_i=1,N} [\Delta]^{-1}_{a_i,b_j}(\tau_i-\tau_j')\delta(\tau_i-\tau_j'=\tau)\delta_{a_i=a}\delta_{b_j=b} w(\{\tau_i\})/Z$$

CT-QMC : efficient algorithms

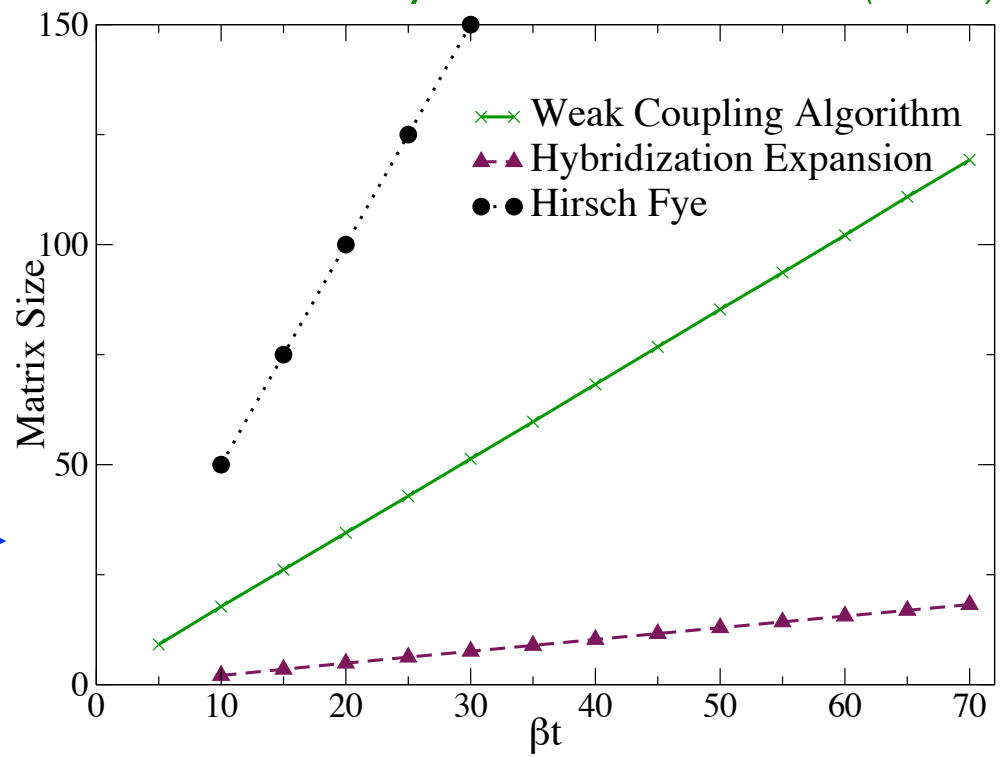
Histogram of expansion order
(CT-HYB, DMFT, βt=100, δ=0, various U)

P. Werner et al, Phys. Rev. Lett 97, 076405 (2006)



Typical matrix size vs β
(DMFT, U/t=1)

E. Gull et al, Phys. Rev. B 76, 235123 (2007)



- Complexity ≈ <n>^3
- All diverge like 1/T (singular at T=0), but huge prefactor differences

CT-QMC is much more efficient than previous algorithm

Expansion in hybridization

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

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

a,b = 1,N

- Expansion in hybridization :

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

- Tr are correlators of the atomic problem
- Algorithmic issue : how to compute quickly atomic correlators ?

Atomic correlators

$$\mathrm{Tr}\left(\mathcal{T}e^{-\beta H_{\mathrm{local}}}\prod_{i=1}^{n}c^{\dagger}_{a_i}(\tau_i)c_{b_i}(\tau'_i)\right)$$

- For density-density interaction

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

- Take one of these correlators

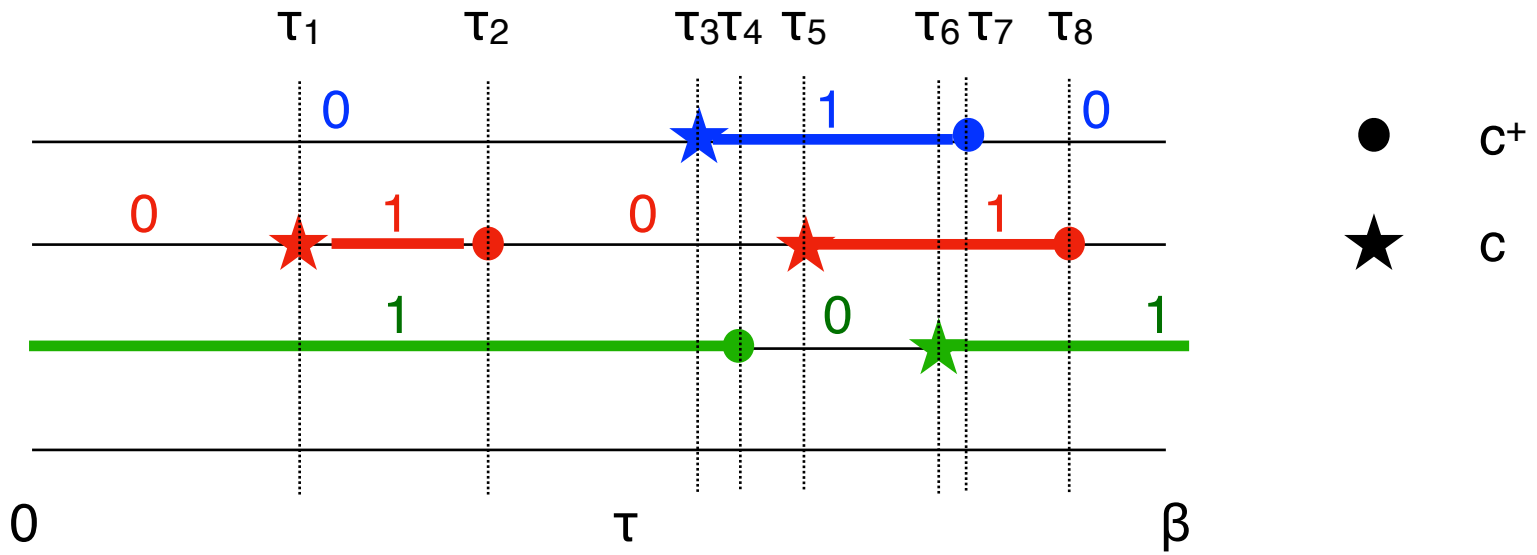
$$\mathrm{Tr}\left(\mathcal{T}e^{-\beta H_{\mathrm{local}}}c^{\dagger}_{2}(\tau_8)c^{\dagger}_{1}(\tau_7)c_{3}(\tau_6)c_{2}(\tau_5)c^{\dagger}_{3}(\tau_4)c_{1}(\tau_3)c^{\dagger}_{2}(\tau_2)c_{2}(\tau_1)\right)$$

Atomic correlators

- For density-density interaction
  The trace can be represented by overlapping "segments"

$$\mathrm{Tr}\left(\mathcal{T} e^{-\beta H_{\mathrm{local}}} c_2^\dagger(\tau_8) c_1^\dagger(\tau_7) c_3(\tau_6) c_2(\tau_5) c_3^\dagger(\tau_4) c_1(\tau_3) c_2^\dagger(\tau_2) c_2(\tau_1)\right)$$

$$\mathrm{Tr}\,(\mathcal{T}\; e^{-H(\beta-\tau_8)} c_2^\dagger e^{-H(\tau_8-\tau_7)} c_1^\dagger e^{-H(\tau_7-\tau_6)} c_3 e^{-H(\tau_6-\tau_5)} c_2 e^{-H(\tau_5-\tau_4)} c_3^\dagger \times$$
$$e^{-H(\tau_4-\tau_3)} c_1 e^{-H(\tau_3-\tau_2)} c_2^\dagger e^{-H(\tau_2-\tau_1)} c_2 e^{-H(\tau_1-0)}\Big)$$



- Density-density interaction, "segment picture" CT-HYB a lot faster

Atomic correlators

- General case.

$$\mathrm{Tr}\left(\mathcal{T} e^{-\beta H_{\mathrm{local}}} \prod_{i=1}^{n} c^{\dagger}_{a_i}(\tau_i) c_{b_i}(\tau'_i)\right)$$

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

- Complex atom : this trace is the bottleneck

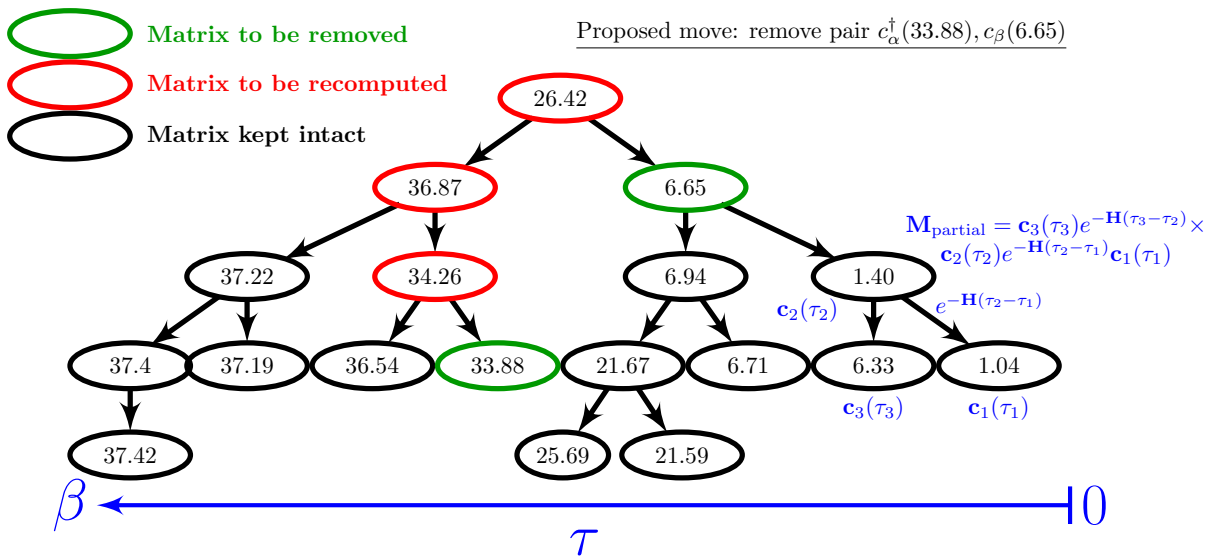
- Monte Carlo move. Insert or remove a pair of c^{+}, c at any place…

Atomic correlators

- Monte Carlo move. Insert or remove a pair of c^+, c at any place
- Algorithm question :
  - I have a trace of a product of n matrices.
    I insert/remove 2 matrices.

$$\mathrm{Tr}\left(\mathcal{T} e^{-\beta H_{\mathrm{local}}} \prod_{i=1}^{n} c^{\dagger}_{a_i}(\tau_i) c_{b_i}(\tau_i')\right)$$

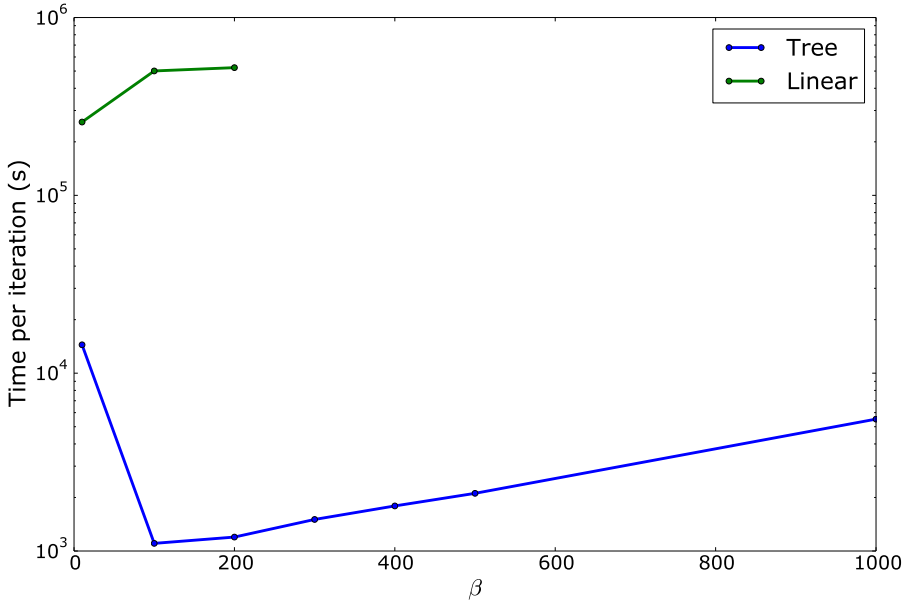
  - How long does it take to recompute the trace ?
- Log n if you use a balanced tree. *E. Gull, PhD.*

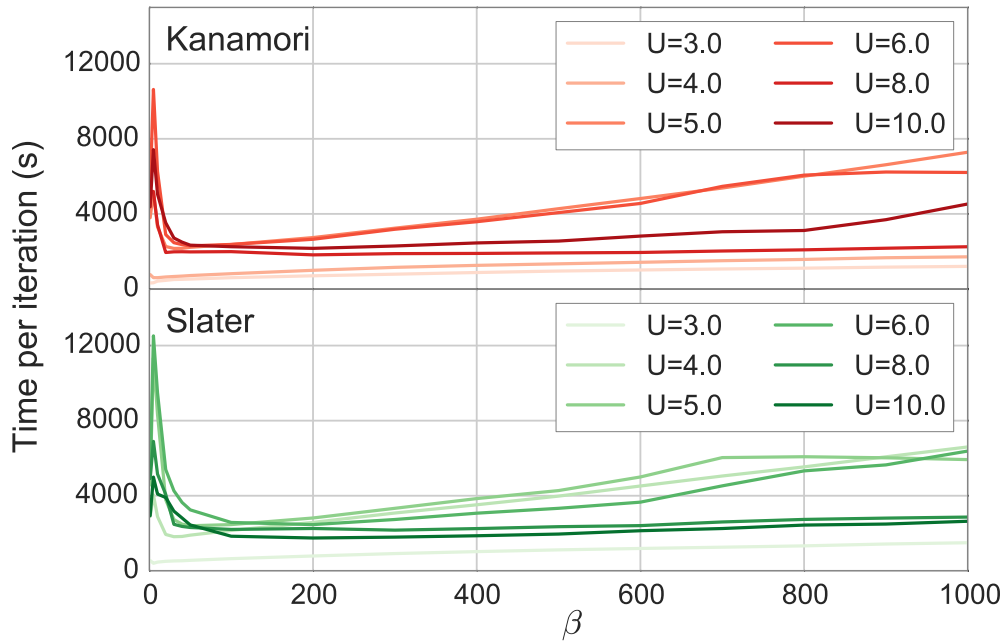


TRIQS/CTHYB P. Seth et al. (2015)

Atomic correlators

- In addition, controlled truncations on the tree
  (Yee et al., Sémon et al. 2014)
- Huge speed up, in particular at low temperatures
- Make calculation for 3, 5 bands feasible, with a general interaction.





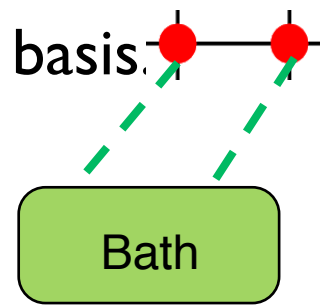
TRIQS/CTHYB P. Seth et al. (2015)

Limitations of CT-QMC

- Sign problem
- Imaginary time. Analytic continuation.
- Inherently slow. Noise $\sim 1/\sqrt{\text{Computing Time}}$
- Scaling with # orbitals, # sites.

Sign problem in QMC

- In some cases, there is no sign problem, i.e. ***s = 1***
  - Single band DMFT.
- Large clusters, more bands, spin-orbit : $s \sim e^{-\beta L}$
  - Example : large cluster $\wr$ lattice problem
- Sign problem :
  - can not really be predicted a priori
  - is not physical
  - depends on the basis, e.g.
    dimer studied above. Need to use the odd even basis.



Need of analytic continuation

- Usual QMC work in imaginary time/frequencies.
- Spectral representation

$$G(i\omega_n) = \int d\epsilon \frac{A(\epsilon)}{i\omega_n - \epsilon} \qquad A(\omega) \equiv -\frac{1}{\pi} Im\, G^R(\omega + i0^+)$$

$$G(\tau) = -\int d\epsilon A(\epsilon) \frac{e^{-\epsilon\tau}}{1 + e^{-\beta\epsilon}}$$

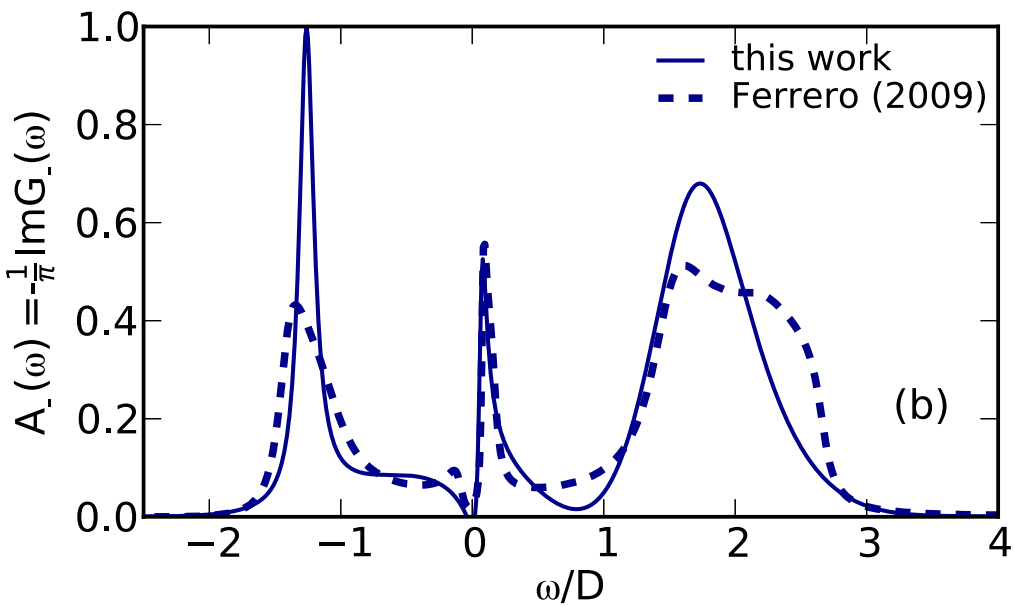
- Transport, response functions : need the real time A, not simply G, e.g. Cf example of lecture 2 for optical c-axis conductivity

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

- Going from A to G is easy
- Going from G to A is very hard : ill-posed problem

Continuation methods

- Padé approximants
- Maximum entropy methods (MAXENT). Several variants
  - Yield the most probable A(ω) given the G(τ), error bar and correlations.
- Only one true solution to this problem :
  develop/use other solvers which work directly in real time.
- Example. Cf lecture 2, 2 patch DCA. High quality comparison.



Padé vs DMRG solver
A. Wolf et al. 2014

Impurity solvers in the Hamiltonian form:

Exact diagonalization, NRG, DMRG

Hamiltonian representation of the Bath

- Represent the bath with a finite number of auxiliary sites

$$S = -\int_0^\beta d_\sigma^\dagger(\tau) G_{0\sigma}^{-1}(\tau-\tau') d_\sigma(\tau') + \int_0^\beta d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

$$\downarrow$$

$$H = \sum_{p\sigma} \tilde{\epsilon}_{p\sigma} \xi_{p\sigma}^\dagger \xi_{p\sigma} + \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{p\sigma} \tilde{V}_{p\sigma} \left(\xi_{p\sigma}^\dagger d_\sigma + h.c. \right)$$

- Exact Diagonalization (ED), NRG, DMRG.

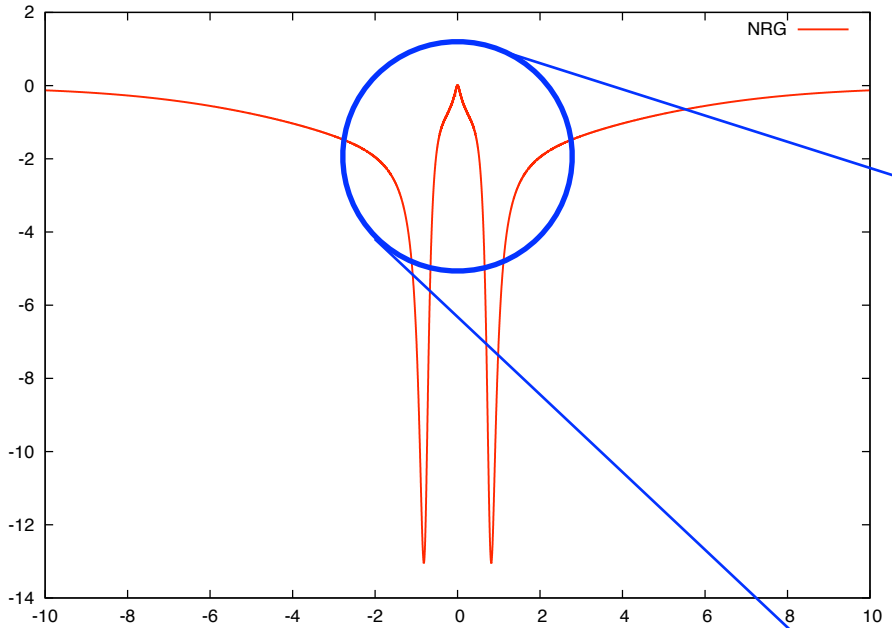
Example: NRG vs CTQMC

M. Ferrero & P. Cornaglia

- Im Σ(ω) by CTQMC (Werner's algorithm) and NRG for DMFT, 1 band, Bethe Lattice, Beta=400, U = 5.2 et D = 1.

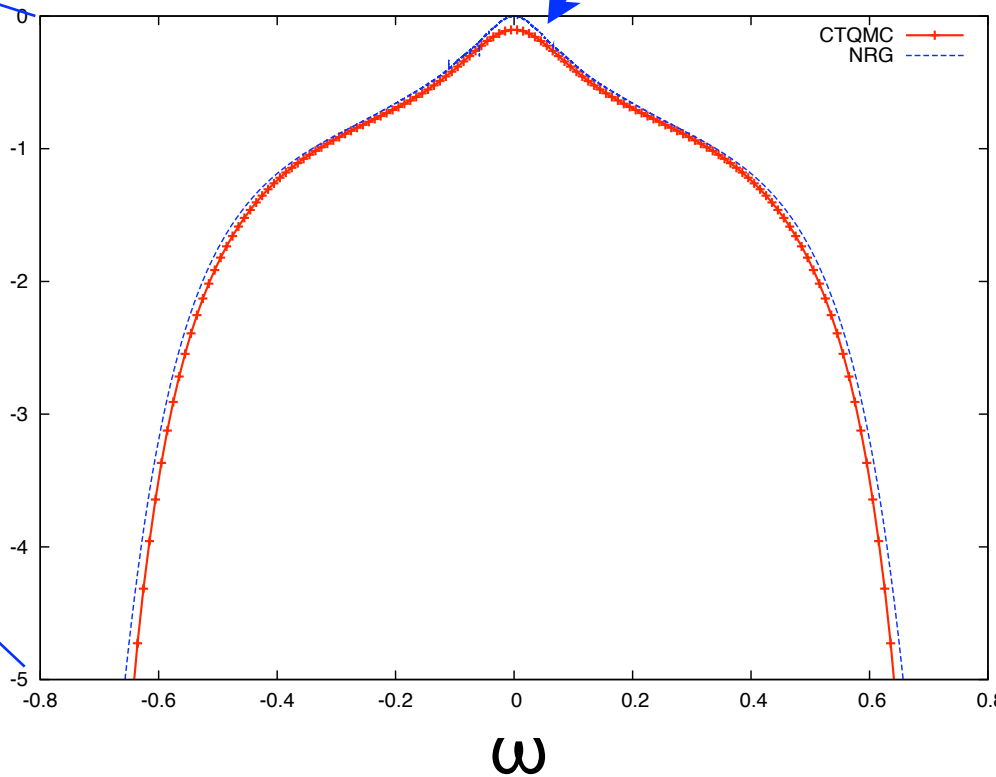
- Continued by Padé method to real axis from Matsubara

Im Σ(ω)



Little finite temperature effect

Im Σ(ω)

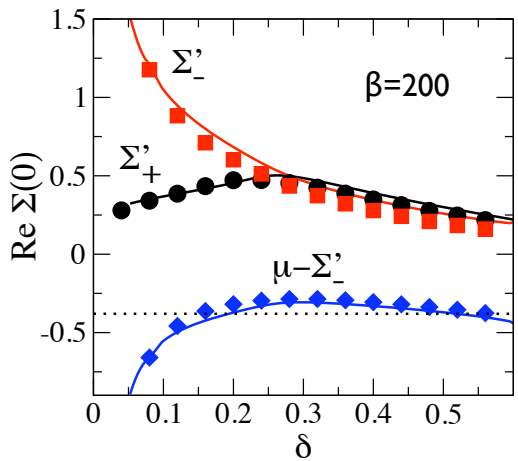


Approximated solvers

- Iterated Perturbation Theory (IPT)
  - Anderson model : perturbation in U is regular *(Yosida, Yamada, 70's.)*.
  - Use first non-trivial order *(Kotliar-Georges, 1992)*.

$$\Sigma(i\omega_n) \simeq \frac{U}{2} + U^2 \int_0^\beta d\tau \, e^{i\omega_n \tau} \hat{\mathcal{G}}(\tau)^3$$

- NCA, OCA
  - First/second bold diagram in the hybridisation expansion.
  - Best close to the atomic limit
- Rotationally invariant slave bosons
  - Generalization of slave bosons for multiorbital systems



Which solver should I use ?

- CTQMC :
  - Finite temperature. Flexible
  - Potential sign problem. Imaginary time. "Slow"
- DMRG, NRG :
  - Real time
  - Low T only, limited to 2/3 bands ?
- Approximate solvers : IPT, NCA, Slave Bosons
  - Very fast. To e.g. explore phase diagram.
  - Not exact.

Thank you for your attention