Introduction to DMFT

Lecture 2 : DMFT formalism

Toulouse, May 25th 2007

O. Parcollet

1. Derivation of the DMFT equations
2. Impurity solvers.

Derivation of DMFT equations

- Cavity method. Large dimension limit.
- Approximation of the Luttinger-Ward Functionnal.

[Derivation done on the board : no slide for this part]

DMFT equations (general lattice)

$$H = -J \sum_{ij} \sigma_i \sigma_j$$

$$m = \langle \sigma \rangle$$

$$H_{\text{eff}} = -J h_{\text{eff}} \sigma$$

$$m = \tanh(\beta h_{\text{eff}})$$

$$h_{\text{eff}} = z J m$$

$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

$$G_c(\tau) = -\langle T c(\tau) c^\dagger(0) \rangle_{S_{eff}}$$

$$S_{\text{eff}} = -\int_0^\beta c^\dagger_\sigma(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$\Sigma = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left(\sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n)$$

Thermodynamics

- On the lattice :

$$\Omega = \Phi + T \sum_{n,\mathbf{k},\sigma} [\ln G_\sigma(\mathbf{k}, i\omega_n) - \Sigma_\sigma(i\omega_n) G_\sigma(\mathbf{k}, i\omega_n)],$$

- For the impurity :

$$\Omega_{\text{imp}} = \phi[G] + T \sum_{n\sigma} [\ln G_\sigma(i\omega_n) - \Sigma_\sigma(i\omega_n) G_\sigma(i\omega_n)].$$

- Therefore :

$$\frac{\Omega}{N} = \Omega_{\text{imp}} - T \sum_{n\sigma} \left(\int_{-\infty}^{+\infty} d\epsilon \; D(\epsilon) \right.$$

$$\left. \times \ln[i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon] + \ln \; G_\sigma(i\omega_n) \right),$$

Thermodynamics (2)

- Internal energy :

$$\frac{E}{N} = T\sum_{n,\sigma} \int_{-\infty}^{+\infty} d\epsilon \, \frac{\epsilon D(\epsilon)}{i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon}$$

$$+ \frac{1}{2} T\sum_{n,\sigma} \Sigma_\sigma(i\omega_n) G_\sigma(i\omega_n).$$

DMFT : Spectral Density Functional Theory

- Functional formulation of DMFT

$$\Gamma_{BK}[G_{ij}] = \mathrm{Tr}\ln G_{ij} - \mathrm{Tr}(g_{0ij}^{-1}G_{ij}) + \Phi_{BKLW}[G_{ij}]$$

$$G_{ij}(t) \equiv -\left\langle Tc_i(t)c_j^\dagger(0)\right\rangle \qquad \Sigma_{ij} = \frac{\delta\Phi_{BKLW}}{\delta G_{ij}}$$

Dynamical Mean Field Theory (DMFT) : $\Phi_{BKLW}[G_{ij}] \approx \phi[G_{ii}]$

- Density Functional Theory :

  Approximation for electronic density n(x)

$$\Gamma_{DFT}[n(x)] = \Gamma_{DFT}[n(x), e^2 = 0] + \Delta\Gamma_{DFT}[n(x)]$$

→ Realistic calculations for Strongly correlated materials.

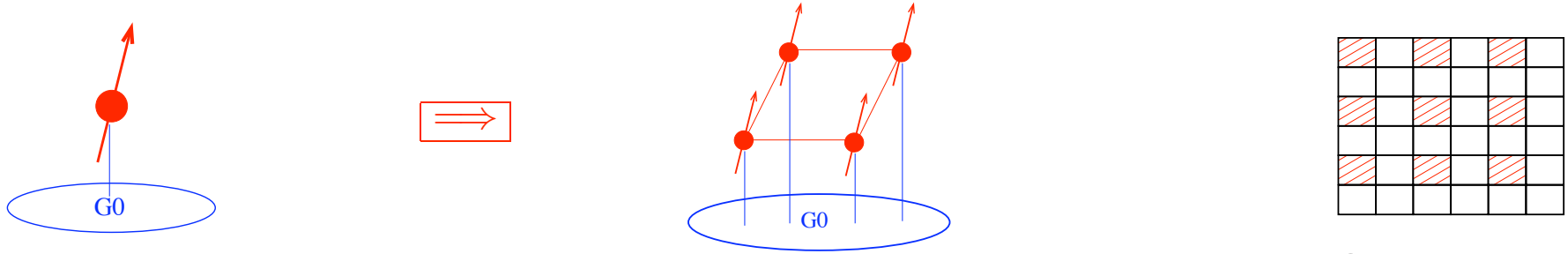
Rev. Mod. Phys. 2006 and Lecture 4.

1. Derivation of the DMFT equations
2. Impurity solvers.

What do we need to solve ? e.g. CDMFT

- 4 Anderson impurities coupled to an effective bath

DMFT **Cluster DMFT**



Superlattice

$$S_{\rm eff} = -\int\int_0^\beta d\tau d\tau' c^\dagger_\mu(\tau) G^{-1}_{0,\mu\nu}(\tau,\tau') c_\nu(\tau') + \int_0^\beta d\tau U(n_{i\uparrow}n_{i\downarrow})(\tau)$$

$$G_{c\mu\nu}(\tau) = -\langle T c_\mu(\tau) c^\dagger_\nu(0)\rangle_{S_{\rm eff}} \qquad 1 \le \mu,\nu \le 4$$

$$\Sigma_c = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left[\sum_{K \in R.B.Z.}{}' \left(i\omega_n + \mu - \hat{t}(K) - \Sigma_c(i\omega_n) \right)^{-1} \right]^{-1} + \Sigma_c(i\omega_n)$$

CDMFT equations

How to solve a quantum impurity model ?

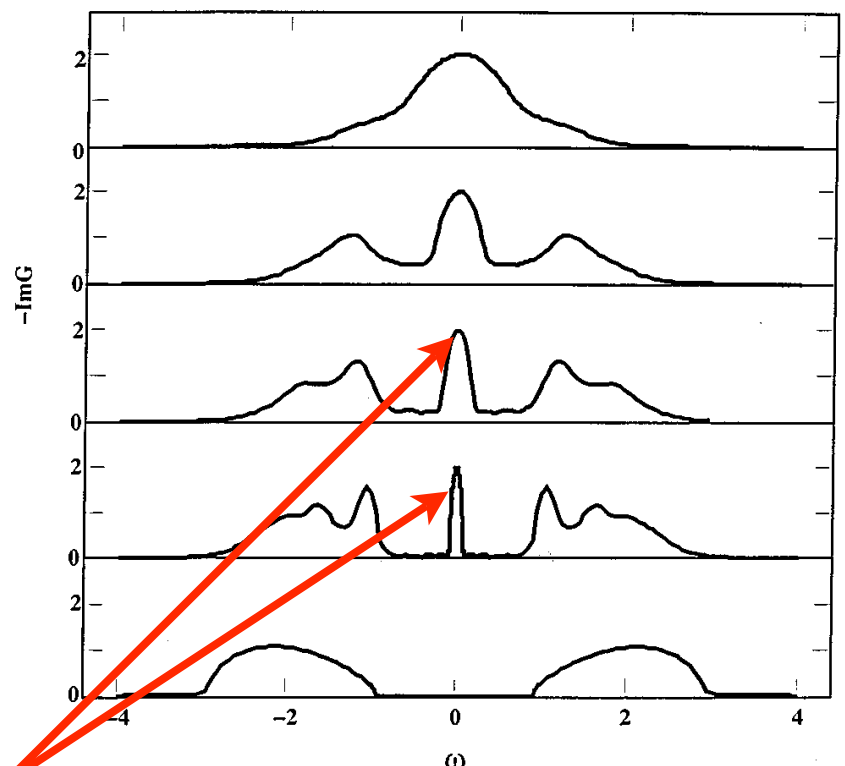
- *Numerical methods :*
  - Quantum Monte-Carlo (Hirsch-Fye, CTQMC).
  - Exact diagonalisation (ED).
  - Renormalization group methods : NRG, DMRG.
- *Analytic methods :*
  - Low energy theories : bosonisation, boundary CFT.
  - Integrability by Bethe Ansatz.
  - Projective method.
- *Approximate methods (fast) :*
  - Iterated Perturbation Theory (IPT)
  - NCA familly (NCA, large-N, SUNCA).

Impurity solvers : requirements

$$S_{\rm eff} = -\int\int_0^\beta d\tau d\tau' c^\dagger_\mu(\tau) G^{-1}_{0,\mu\nu}(\tau,\tau') c_\nu(\tau') + \int_0^\beta d\tau U(n_{i\uparrow} n_{i\downarrow})(\tau)$$

$$G_{c\mu\nu}(\tau) = -\langle T c_\mu(\tau) c^\dagger_\nu(0)\rangle_{S_{\rm eff}}$$

- Compute G at all frequencies.
- Quick, reliable ....
- Gapped case : perturbation in Δ is regular
- Ungapped case : Kondo problem with Δ(0)≠0.
- *Bath has a structure at low energy !*



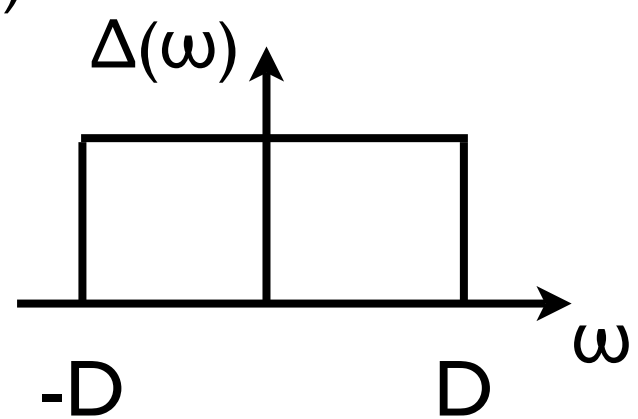
Evolution of the spectral function close to Mott transition (cf lecture 1)

Bethe Ansatz and CFT are useless for DMFT !

- Integrability in the universal regime *(A.Tsvelik, P.Wiegmann/ N.Andrei,1980) N.Andrei, K. Furuya, JH Lowentein, Rev. Mod. Phys. 55, 331 (1983); N.Andrei,Trieste lecture 1994 condmat/9408101.*
  - Thermodynamics but Green function very hard to compute.
- Boundary Conformal Field Theory *(Cardy;Affleck, Ludwig, 1991; I.Affleck,Acta Phys.Polon. B26 (1995) 1869; condmat/9512099)*
  - Description of the low-energy fixed point. Computation of the low frequency correlations (hence e.g. ρ(T)).
- BUT both methods starts from a flat band and linearize the energy close to the Fermi level (universal regime).

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

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



Not sufficient to solve DMFT

Continuous time QMCs

- *Principle* : Perform an expansion in a coupling constant and sum this expansion with Monte-Carlo technique.
  - Expansion in U : U-CTQMC
    A.N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005)
  - Expansion in $\Delta(\omega)$, around the atomic limit : Δ-CTQMC
    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)

Advantages of Δ-CTQMC

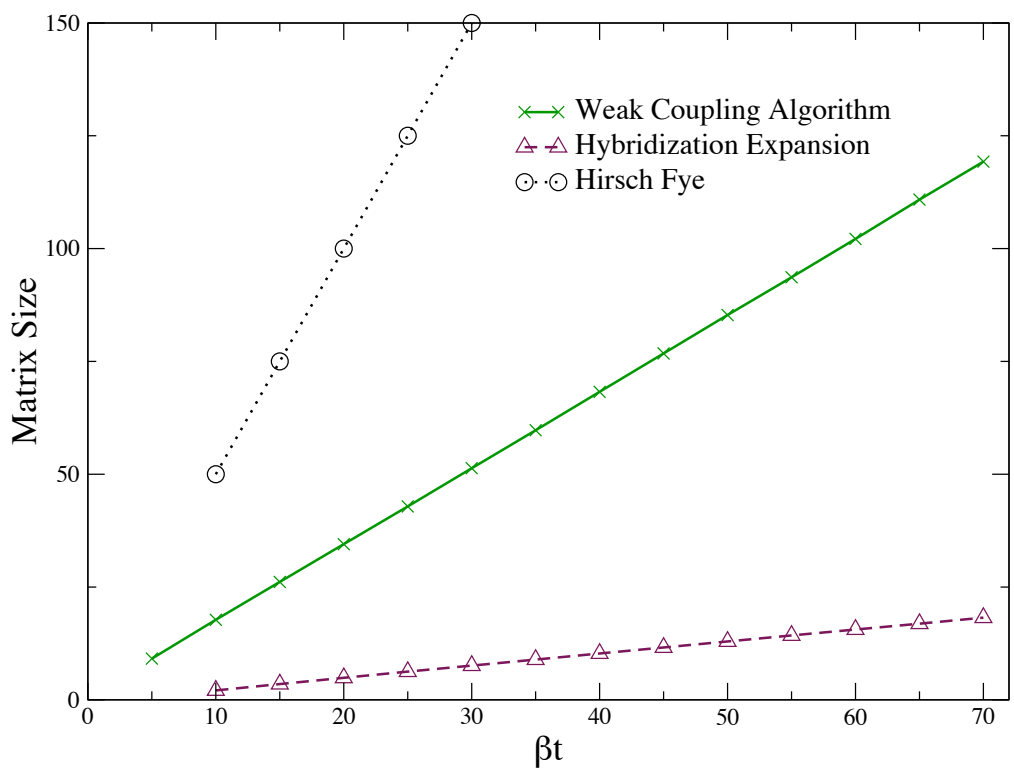
- Time is continuous !
- For frustrated clusters, sign problem does not seems important. The algorithm is a mixture of diagonalization and QMC
- Use the symmetry : diagonalize Δ !
- Size of the matrix does not increase much

<matrix size> ~ Kinetic energy (Haule, 2006)

Comparison of various QMCs

- In practice, first computation of SC phase in CDMFT with Werner's algorithm since Tc is low : *K. Haule, condmat/0612172*

- Systematic comparison of Hirsch-Fye, U-CTQMC, Δ-CTQMC
  E. Gull et al condmat/0609438
  Size of the matrix versus 1/T (Bethe lattice, 1 site, U/t = 4).



Δ-CTQMC seems to be the most efficient

Exact diagonalisation : principle

- Use the Hamiltonian form of the Anderson model (see lecture 1).

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

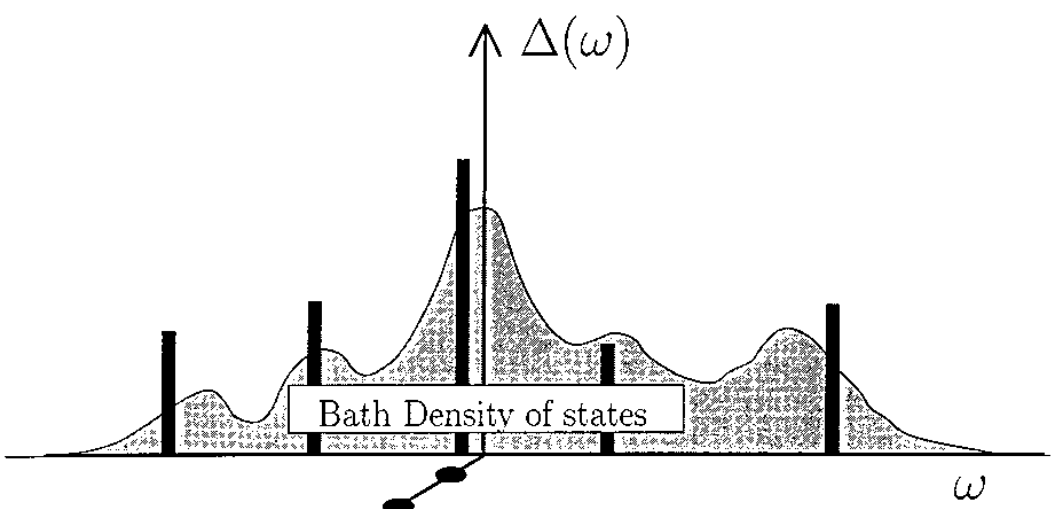
$$G_{0\sigma}^{-1}(i\omega_n) \equiv i\omega_n + \epsilon_d - \Delta_\sigma(i\omega_n) \qquad \Delta_\sigma(i\omega_n) \equiv \sum_k \frac{|V_{k\sigma}|^2}{i\omega - \epsilon_{k\sigma}}$$

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} V_{k\sigma}\left(c_{k\sigma}^\dagger d_\sigma + h.c.\right)$$

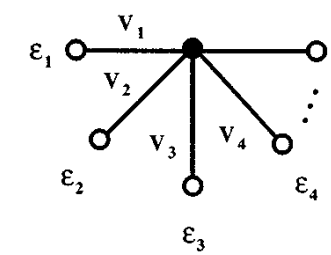
- *The energy and hoppings of the bath are effective*
- Principle : use Lanczos to compute the GS of H
  - How to find the V's and ϵ's from Δ(ω) ?
  - How to compute G ?

ED : discretisation of the bath

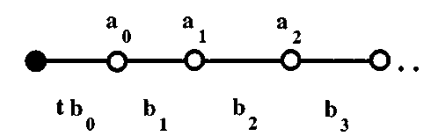
- Approximation of Im Δ(ω) by a finite set of Dirac peaks.
- The bath can take different shapes.



Star



Chain



- V and ϵ computed by minimizing a distance *(Caffarel-Krauth, 1994)*

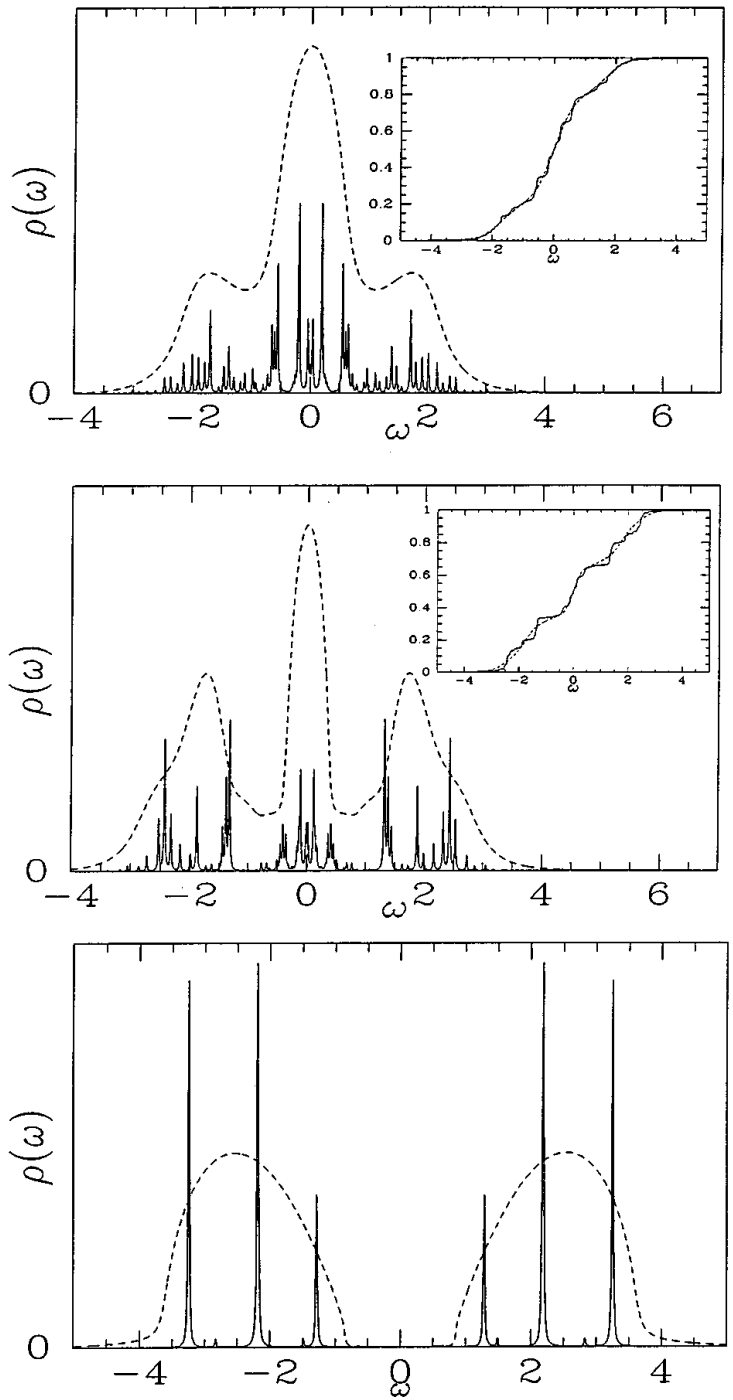
$$d = \frac{1}{n_{\max}+1} \sum_{n=0}^{n_{\max}} \left| \mathcal{G}_0(i\omega_n)^{-1} - \mathcal{G}_0^{n_s}(i\omega_n)^{-1} \right|^2$$

- In Matsubara, with an effective temperature T_{eff}

ED : Computation of the Green function

- Start another Lanczos from $c^\dagger|0\rangle$
- Gives G(ω) as a continuous fraction expansion.
- Finite-Bath ⇒ any structure is replaced

  by a set of finite δ peak (with some broadening).



ED : Limitations of the method

- The bath is effective ⇒ H has less symmetry than a finite-size model
- Size of the bath (hence ω-resolution) is limited.
- Always pay attention to the effective temperature !
- If the bath is too small, spurious solutions of the DMFT loop appear.
- The result may depend on distance : in clusters, more weight to small frequencies.

Which impurity solver should I choose ?

There is no universal answer !

Monte-Carlo (i.e. Δ-CTQMC)

Principle

- Compute G(iomega_n) by some Monte-Carlo sum.

Advantages

- Numerically "exact", reliable.
- Can compute vertex, response (e.g. Jarrell 1992, Hirsch-Fye).
- Finite temperature method
- Modern CTQMC very flexible (various interactions)

Drawbacks

- Only imaginary time : need for hazardous analytic continuation methods (e.g. Maxent).
- Limited at low temperature (?)
- Sign problem largely uncontrolled. Was problematic in Hirsch-Fye for cluster in frustrated models.
- Speed ? Noise ?

Exact diagonalisation

Principle

- Use Hamiltonian form of the Anderson model, discretize the bath and use Lanczos to find the ground state and G

Advantages

- Computes for real ω
- Insensitive to frustration.

Drawbacks

- (Almost) limited to T=0.
- Size of bath is limited, hence ω resolution can be quite poor, specially for 4 orbital or 2x2 cluster.
- Scaling with size of cluster or number of orbital is exponential !!

Numerical Renormalisation Group (NRG)

Principle

- Use Wilson algorithm.
- Used e.g. in the resistivity calculation (see lecture 1).

Advantages

- Good description of the Kondo peak
- Fast

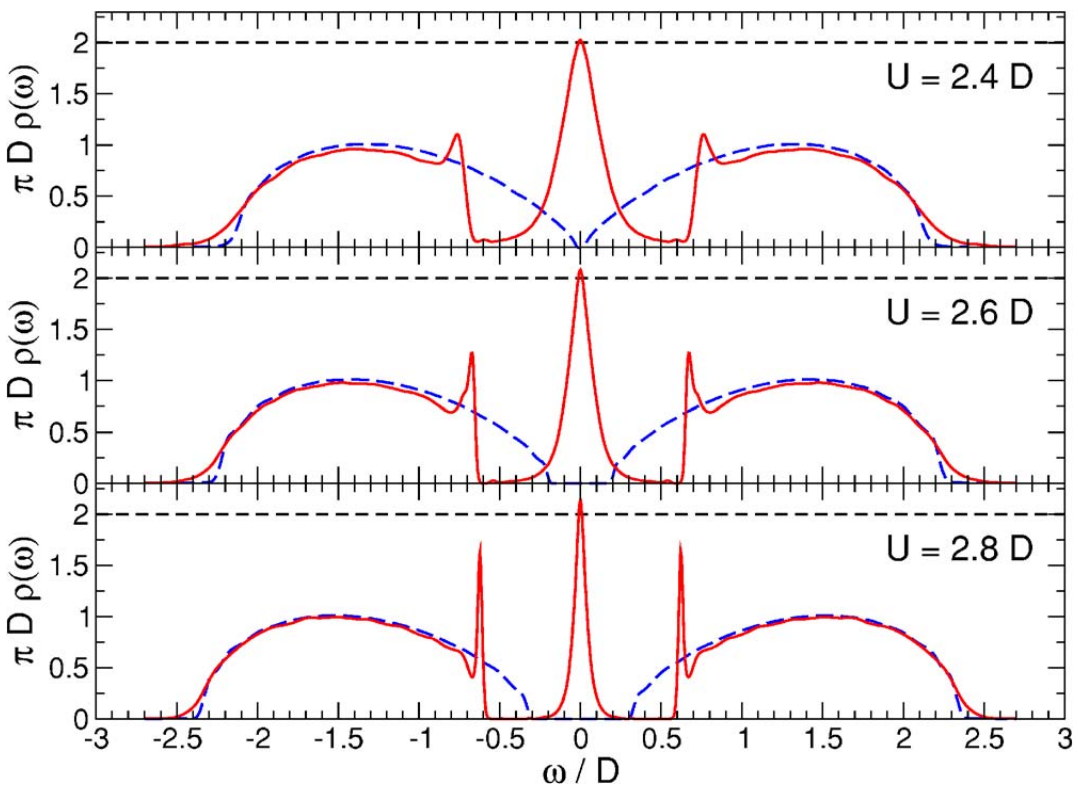
Drawbacks

- Rough for the Hubbard bands.

Density Matrix Renormalization Group (DMRG)

Principle

- Use the quasi-1d formulation of the bath (as a chain).
- Calculation of the Green function must be done by correction vector method.



M. Karski et al PRB 72, 113110, 2005

Advantages

- Computes for real ω, with good resolution
- Kondo peak like NRG, but good resolution for Hubbard bands.
- Satellite peaks in the Hubbard bands.

Drawbacks

- Slow (?)

Iterated Perturbation Theory (IPT)

Principle

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

$$\Sigma(i\omega_n) \simeq \frac{U}{2} + U^2 \int_0^\beta d\tau \; e^{i\omega_n \tau} \hat{\mathcal{G}}_0(\tau)^3$$

Advantages

- Quick and relatively simple.
- U=0 and U=∞ limit correct !
- Reproduce the main feature of the solution of the Mott transition (see lecture 1).

Drawbacks

- Largely uncontrolled
- Extension beyond 1/2 filling or for clustrer do not interpolate well between U=0 and U=∞ *(see however Kajueter-Kotliar, condmat/9509152).*

NCA family

Principle

- Large-N methods or resummation of diagrams.
- Lowest order diagram in the Luttinger-Ward functional.
  See G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. 78, 865 (2006)

Advantages

- Well studied in impurity models.
- Simple enough to do complex materials.

Drawbacks

- Controlled by large N limits.
- Simple NCA has trouble to capture local Fermi liquid (it corresponds to overscreened Kondo, see O.P. PhD 1998).

Conclusion of lecture 2

- Derived DMFT equations.
- Impurity solvers : work still in progress

- Next time : clusters !