Quantum impurity models
Algorithms and applications

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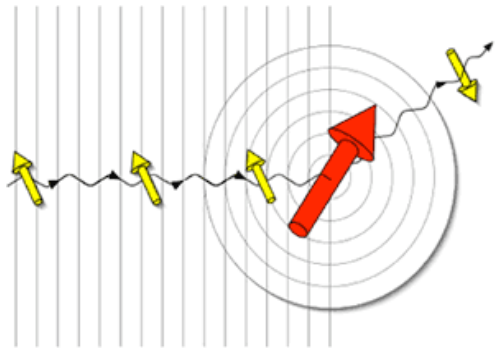
- Motivations : why do we need specific algorithms ?
- A few algorithms and examples of applications
- Out of equilibrium physics. Open problems.

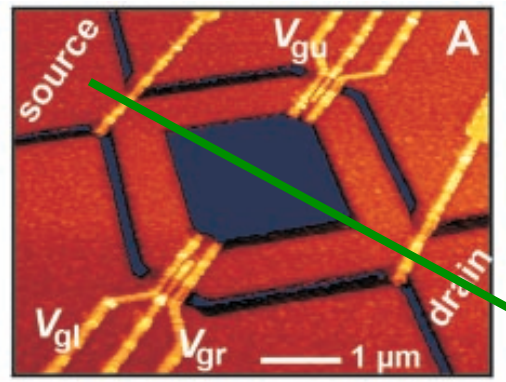
Quantum impurity models

"Standard" case

- Magnetic impurity in a metallic host
- Thermodynamics : C, χ, transport : ρ ?



Nanostructures



I(V)

- Quantum dots. Non-equilibrium
- Current : I(V), conductance, noise ?

Dynamical Mean Field Methods (DMFT)

- Approximations of a lattice model or a solid by an impurity model in a self-consistent bath
- Requires computing Local Green function G(ω)

How to solve quantum impurity models ?

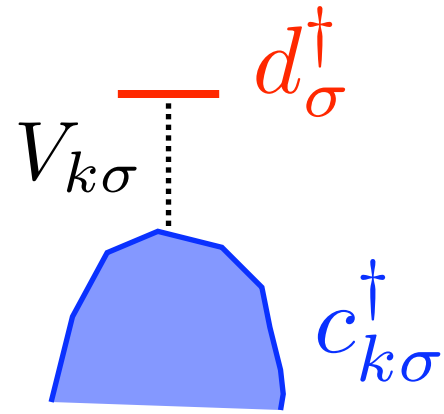
Impurity solvers : a rich toolbox

- Exact analytic methods (e.g. Bethe Ansatz, BCFT)
- Controllable algorithms :
  - *Exact diagonalization* (ED)
  - *Numerical Renormalization group* (NRG)
  - *Density Matrix Renormalization group* (DMRG).
  - *Continuous Time Quantum Monte Carlo family* (CT-QMC)
- Approximate solvers (e.g. NCA).

Anderson model : Hamiltonian vs Action

$$H = \underbrace{\epsilon_0 \sum_{\sigma=\uparrow,\downarrow} d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow}}_{\text{Local site with interaction}} + \underbrace{\sum_{k,\sigma=\uparrow,\downarrow} V_{k\sigma} c^\dagger_{k\sigma} d_\sigma + h.c.}_{\text{Hybridization}} + \underbrace{\sum_{k,\sigma=\uparrow,\downarrow} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}}_{\text{Free electronic band}}$$

Integrate the fermionic bath



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

Hybridization function $\longrightarrow$ $\Delta_\sigma(i\omega_n) \equiv \sum_{\vec{k}} \frac{|V_{\vec{k}\sigma}|^2}{i\omega_n - \epsilon_{\vec{k}\sigma}}$

$$G^{-1}_{0\sigma}(i\omega_n) \equiv i\omega_n + \epsilon_0 - \Delta_\sigma(i\omega_n)$$

General quantum impurity model

- A local problem coupled to a free fermionic bath

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

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

(Local) Interaction

Bath

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

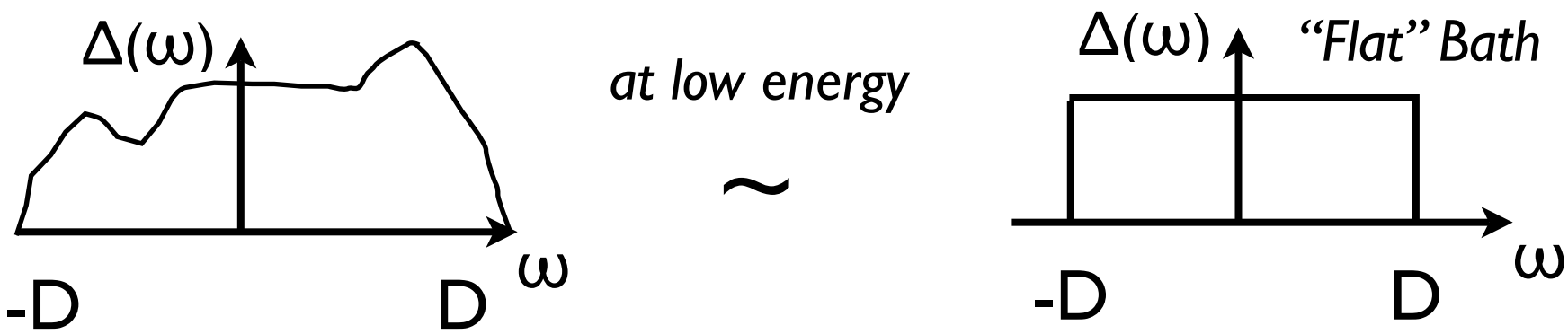
Challenges for the impurity solvers

Why do we need specific algorithms ?

Universal regime

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

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



How to handle the large separation of scales numerically ?

Baths can have a low-energy structure

- Gapped bath (insulator, superconductor) : no Kondo effect.
- The bath can be pseudo-gapped *Withoff-Fradkin PRL 64,1835 (1990)*

$$\Delta(\omega) \sim \Delta_0 |\omega|^r$$

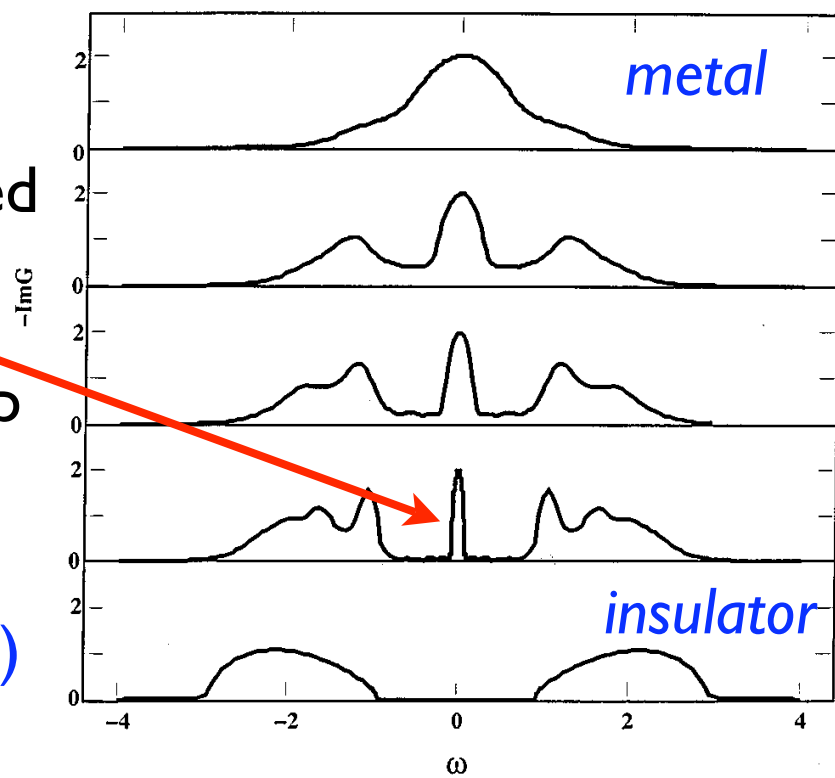
(screening transition when r varies)

- DMFT bath is self-consistently determined and has a structure at low energy
- Cluster DMFT : bath can have pseudo-gap

  Ferrero et al. EPL and PRB 2009

- Analytical methods (Bethe Ansatz & CFT) can not handle this.

DMFT bath evolution close to Mott transition



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

How to solve an impurity model in such a bath ?

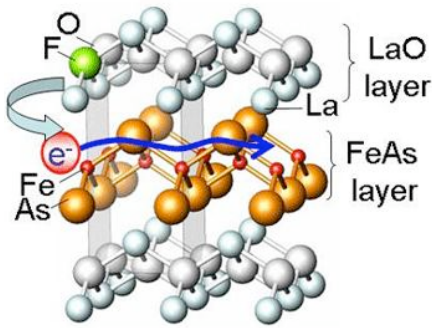
Multiorbital models

- Realistic electronic structure calculations for correlated systems
  e.g. LDA + DMFT.
- The impurity is *d* or *f* shell : 5, 7 bands (3 with crystal-field splitting)
- Local interaction can be complex : not only density-density
  (e.g. spin-spin, Hund's coupling)
- Example : Iron-based superconductors : 5 bands at Fermi level.
  Need to treat 5 orbitals.

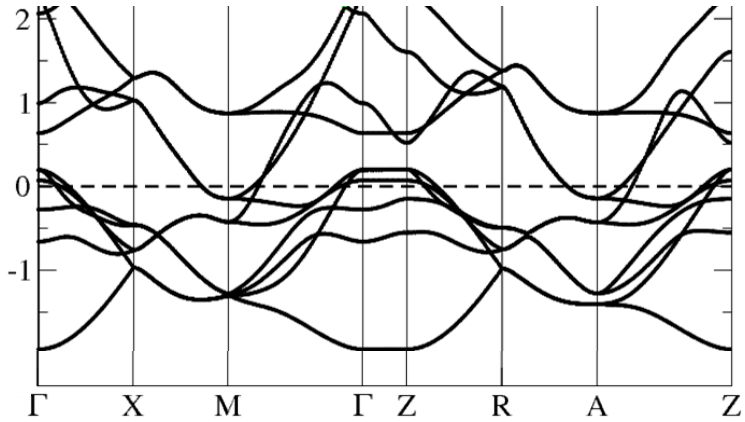
How correlated are those materials ?

DMFT computation :

Aichhorn et al. (2009),
Haule et al. (2008)



Fe-d LDA band structure of LaFeAsO



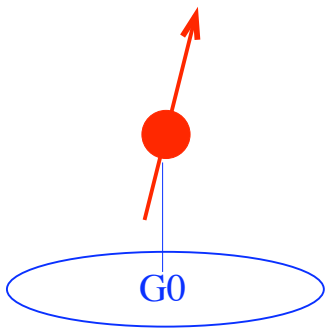
How to handle N=5,7,... and a general (local) interaction ?

Multiple impurity models

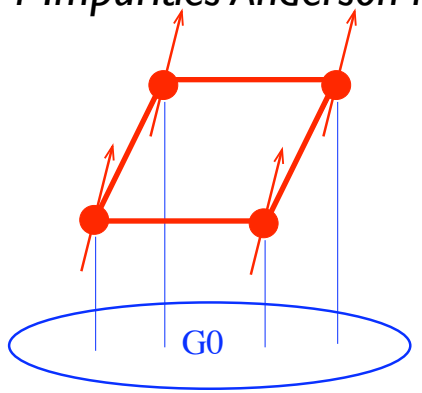
- A few impurities, interacting with a free fermionic bath
- Richer physics than single impurity (Kondo effect vs singlets)
  Review : M. Ferrero et al., J. Phys.Cond. Mat (2007)
- Cluster DMFT : systematic interpolation between DMFT and lattice. Overcome important limitations of DMFT (short range AF fluctuations, singlet nature of the insulator, d-SC order, ...)

Real space point of view

Single Impurity Model

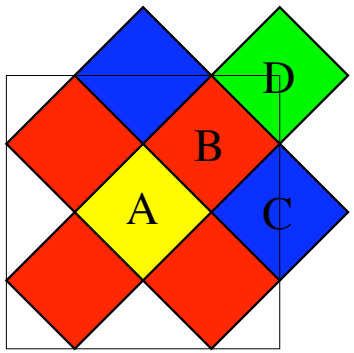


4 Impurities Anderson model



k-space point of view

Brillouin zone patching



8 sites cluster

Cluster size = momentum resolution of the self-energy.

How to solve 8, 16 coupled impurity models in a self-consistent bath ?

Exact Diagonalisation

Hamiltonian representation of the Bath

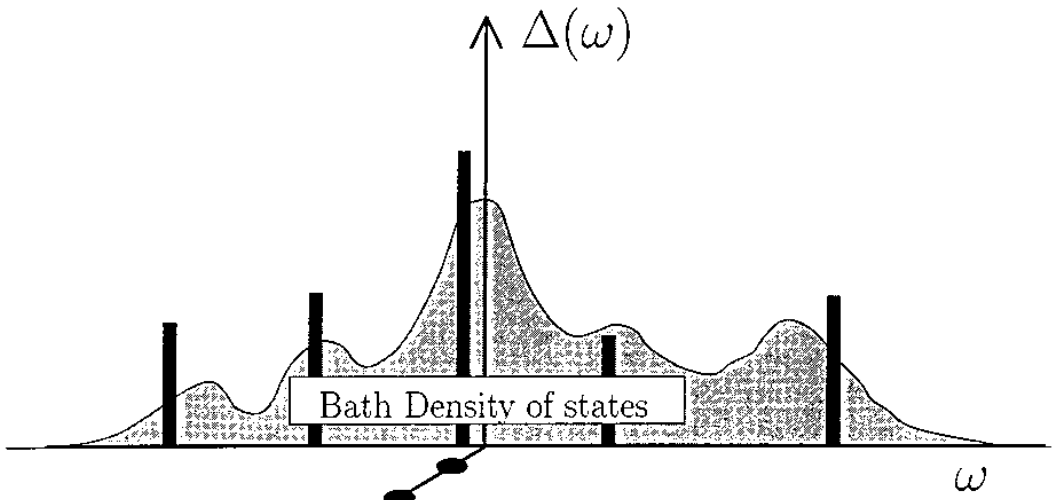
- Represent the bath with a finite number of auxiliary sites
  Necessary step for all Hamiltonian methods (ED, NRG, DMRG...)

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

$$\downarrow$$

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

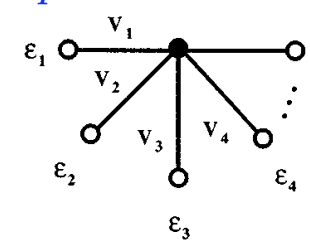
Approximation of Im Δ(ω) by a finite set of Dirac peaks.



Different possible shapes for the bath

$$\Delta_\sigma(i\omega_n) \equiv \sum_p \frac{|\tilde{V}_{p\sigma}|^2}{i\omega - \tilde{\epsilon}_{p\sigma}}$$

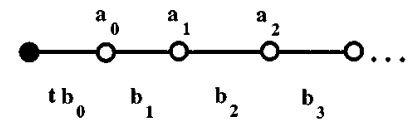
Star



Δ(ω) = continuous fraction

The energy and hoppings of the bath are effective

Chain



Exact Diagonalization

Caffarel-Krauth, 1994

- Principle :

  1. Represent the bath with a finite number of sites (fit V and ε)
  2. Compute the ground state of H (Lanczos) and physical quantities : thermodynamics, G(ω),...

- Examples :
  - Anderson impurity (DMFT bath), ok with only a few sites (5-10).
  - Cluster DMFT of 2d-Hubbard (normal and superconducting phases)
    e.g. *Civelli et al PRL. 100, 046402 (2008).*

- Limitations
  - Scaling with size of cluster/number of orbitals is exponential !
  - Small bath → ω resolution is poor
    → impossible to resolve low energy scales like Tk

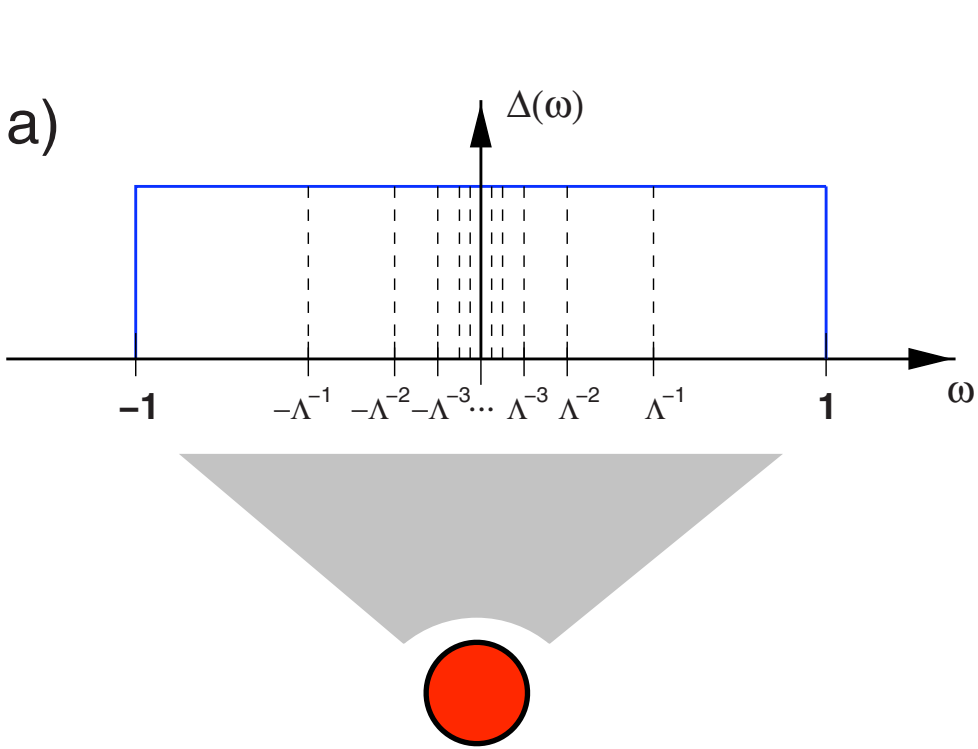
⇒ Numerical Renormalization Group

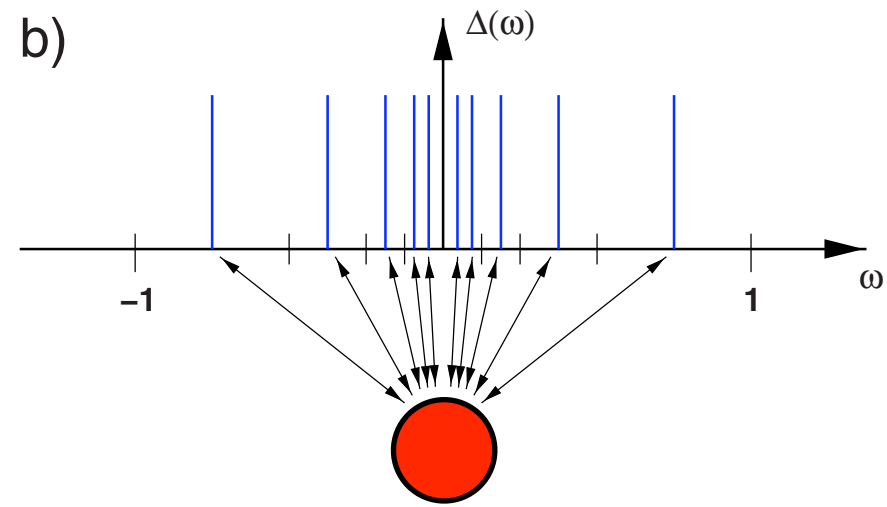
Numerical Renormalization Group

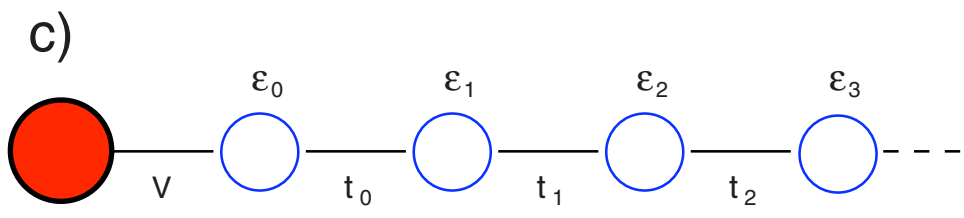
Numerical Renormalization Group : principle

K. Wilson, Rev. Mod. Phys. 47, 773, (1975); R. Bulla et al., Rev. Mod. Phys 80, 395 (2008)

1. Use a better representation of the bath, adapted to low energy physics.
   a. Divide the bath spectral function into <u>logarithmic</u> intervals with parameter $\Lambda > 1$
   b. Reduce to a discrete spectrum by associating 1 site to each slice.
   c. Transform the bath structure into a semi-infinite chain.





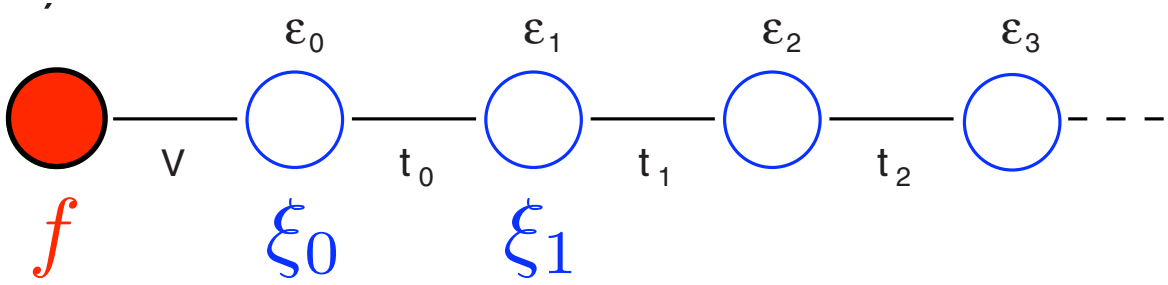


Numerical Renormalization Group : principle

K. Wilson, Rev. Mod. Phys. 47, 773, (1975); R. Bulla et al., Rev. Mod. Phys 80, 395 (2008)

- The effective hopping decays exponentially with n

$$H = H_{\rm imp}(f, f^\dagger) + \alpha \sum_\sigma (f_\sigma^\dagger \xi_{0\sigma} + \xi_{0\sigma}^\dagger f_\sigma) + \sum_{\sigma n \geq 0} \left(\varepsilon_n \xi_{n\sigma}^\dagger \xi_{n\sigma} + t_n (\xi_{n\sigma}^\dagger \xi_{n+1\sigma} + h.c.) \right)$$



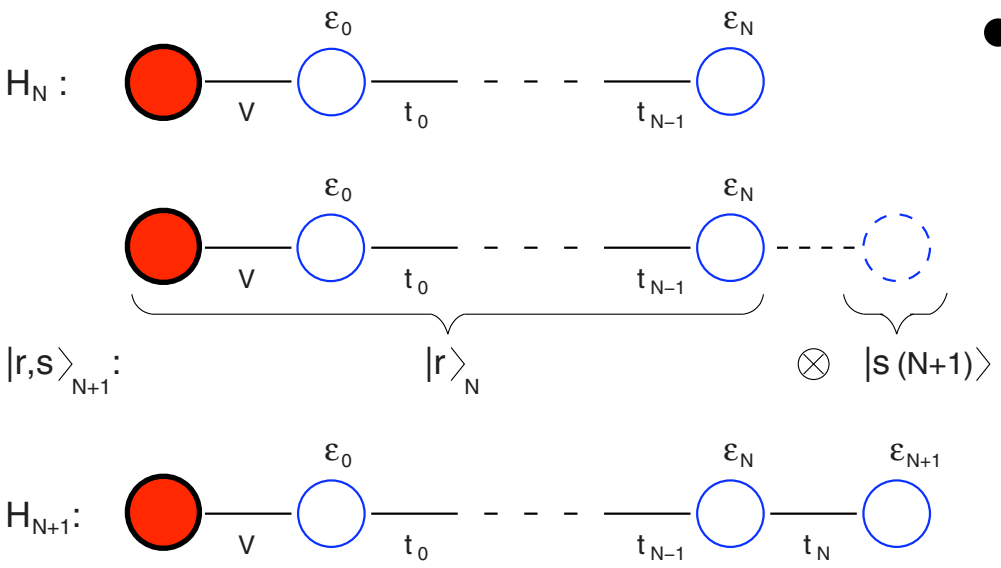
$$t_n \sim \Lambda^{-n/2}$$

- Approach the chain by successive finite size Hamiltonians

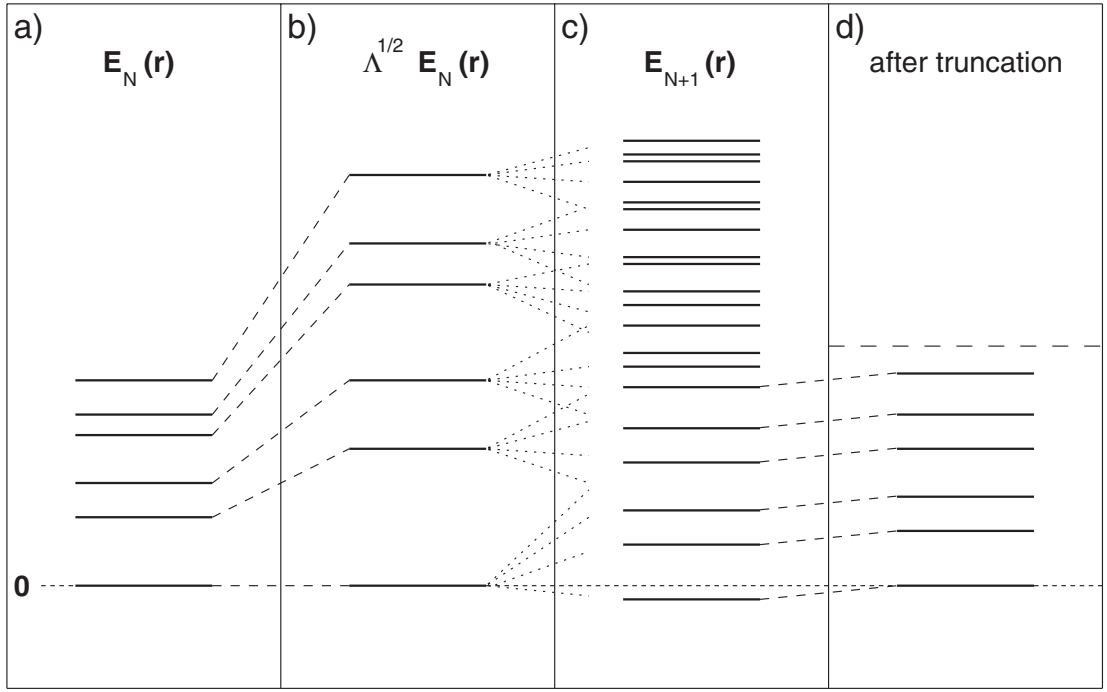
$$H_N = \Lambda^{(N-1)/2} \left[H_{\rm imp}(f, f^\dagger) + \alpha \sum_\sigma (f_\sigma^\dagger \xi_{0\sigma} + \xi_{0\sigma}^\dagger f_\sigma) + \sum_{\sigma n \geq 0}^{\mathbf{N}} \left(\varepsilon_n \xi_{n\sigma}^\dagger \xi_{n\sigma} + t_n (\xi_{n\sigma}^\dagger \xi_{n+1\sigma} + h.c.) \right) \right]$$

$$H_{N+1} = \sqrt{\Lambda} H_N + \Lambda^{N/2} \sum_\sigma \left(\varepsilon_{N+1} \xi_{N+1\sigma}^\dagger \xi_{N+1\sigma} + t_n (\xi_{N\sigma}^\dagger \xi_{N+1\sigma} + h.c.) \right)$$

Numerical Renormalization Group : principle



- Iterative diagonalization of H_N, with truncation to Ns lowest states



- Evolution of low energy spectrum of H_N

- Allows also computation of thermodynamics, spectral function, at finite T.

R. Bulla et al., Rev. Mod. Phys 80, 395 (2008)

NRG describe the RG flow to the I.R. fixed point

NRG : applications

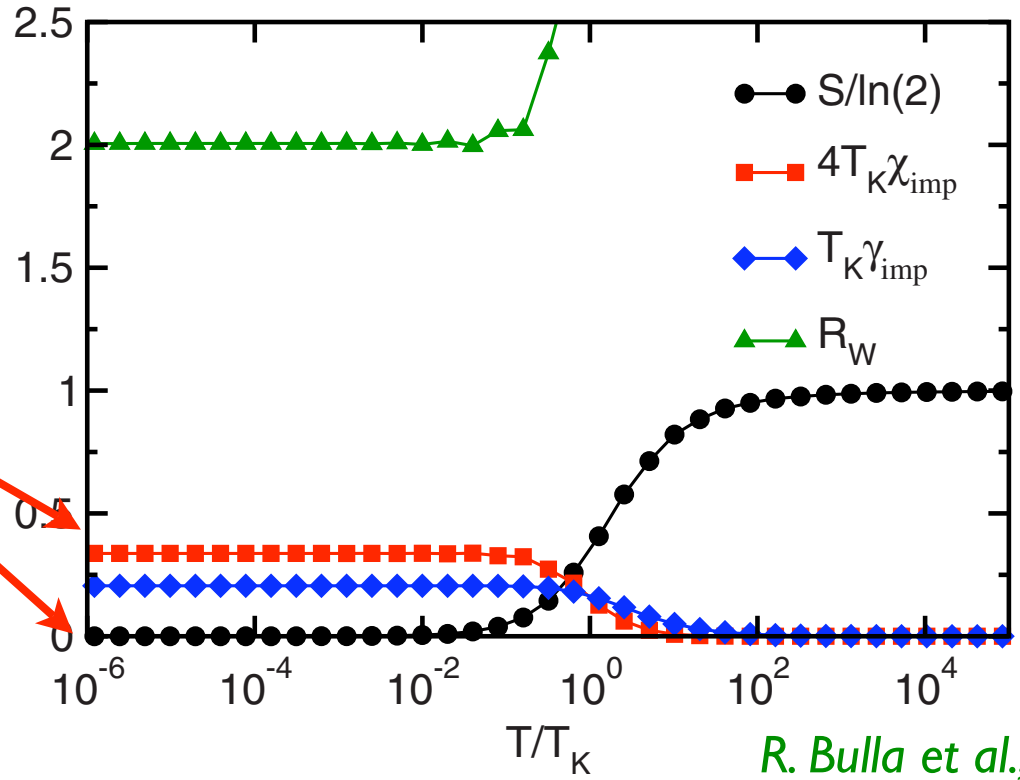
- Solution of the Kondo model (1 band, S=1/2) *Wilson (1975)*

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

- Entropy, susceptibility vs temperature

Screening of the impurity

$$\chi_{\rm imp} \underset{T\to 0}{\sim} \frac{a}{T_K}$$

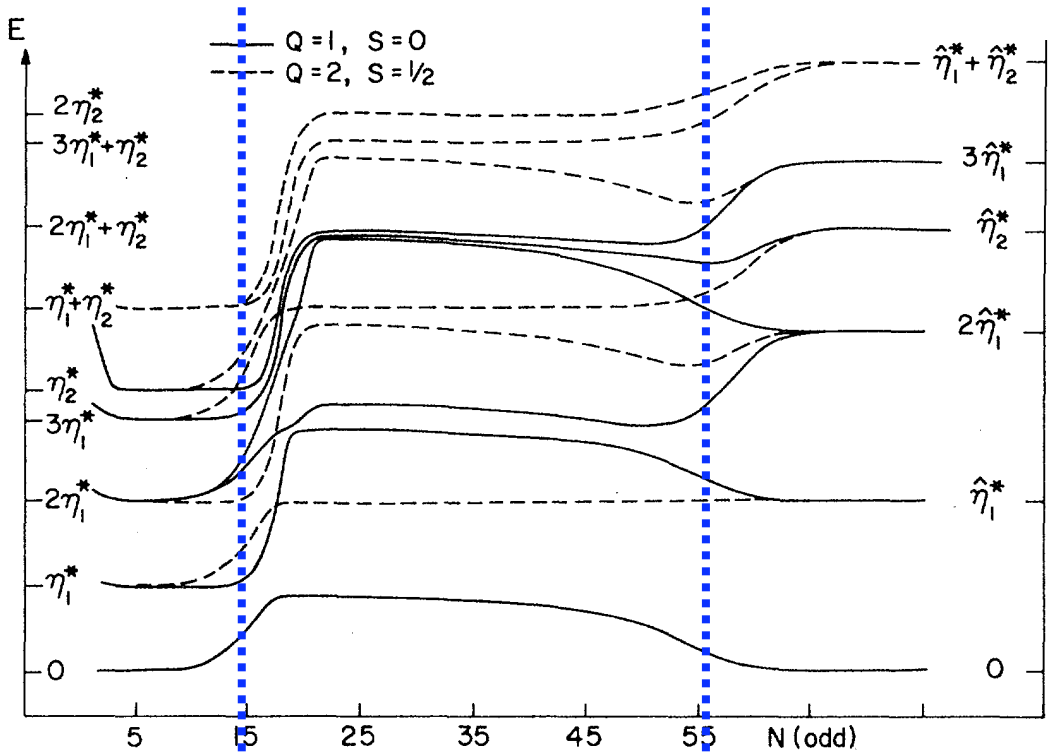


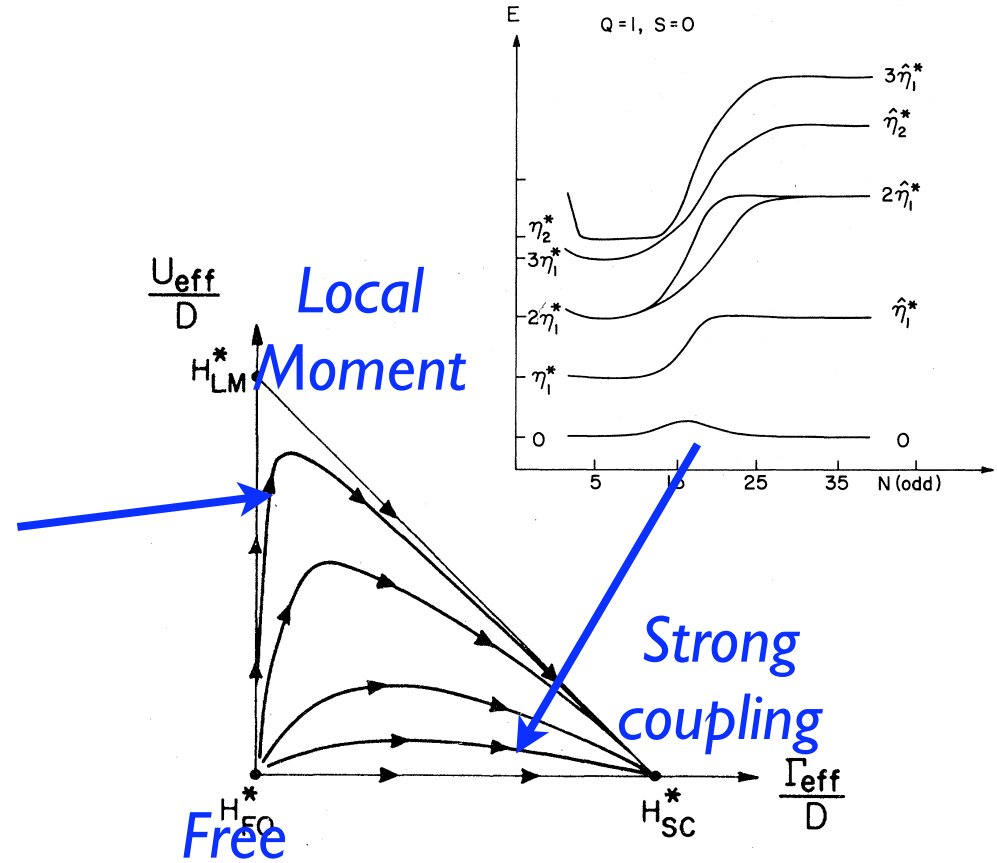
R. Bulla et al., RMP (2008)

RG evolution of the low energy spectra

- Anderson model (symmetric case), *Krishnamurthy et al, PRB 21, 1003 (1980)*

Low-lying energy levels of H_N for odd N for
$U/D = 1.e\text{-}3$, $U/\pi\Gamma = 12.6$, $\Lambda = 2.5$

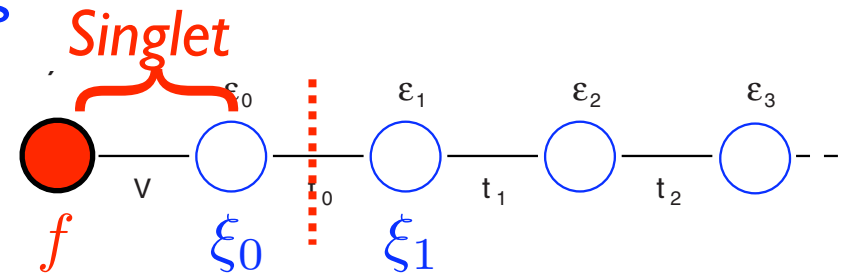




Schematic RG flow

Strong coupling = Spectrum N-1 free fermions
= π/2 phase shift

Nozières (1974)



NRG : susceptibility of the Anderson model

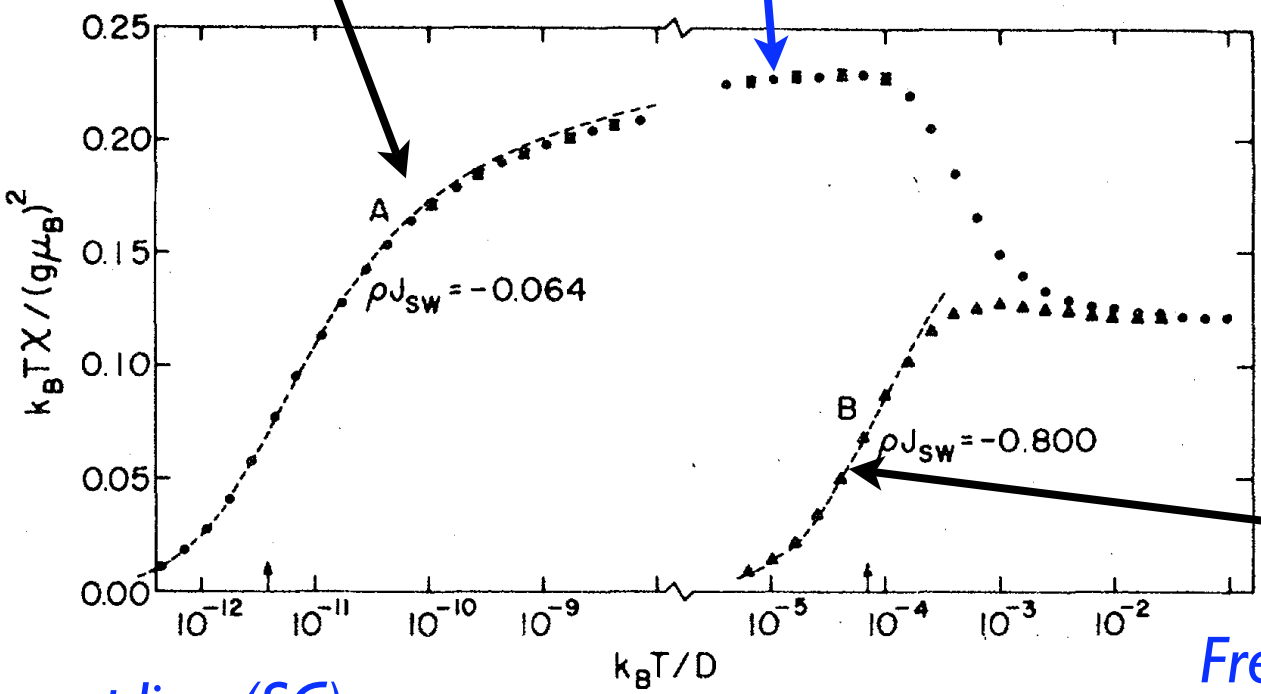
- Anderson model (symetric case), for U/D = 1.e-3, Λ=2.5
  Krishnamurthy et al, PRB 21, 1003 (1980)

Local Moment regime

U/πΓ = 12.6

Curie law $\chi_{\rm imp} \sim \dfrac{1}{4T}$

Tχ(T)



U/πΓ ≈ 1

Free

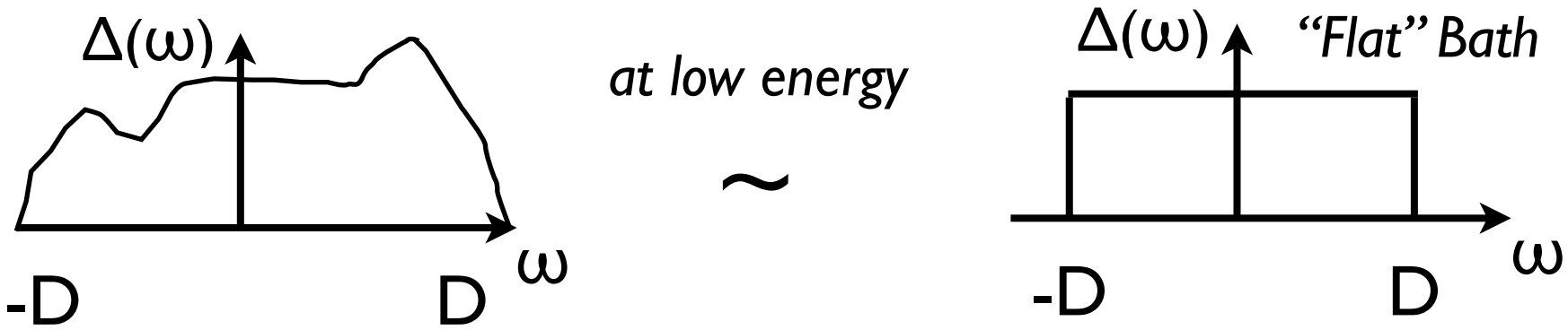
Strong coupling (SC)

$$\chi_{\rm imp} \underset{T\to 0}{\sim} \frac{a}{T_K}$$

NRG & Conformal symmetry

(Cardy; Affleck, Ludwig, 1991; I. Affleck, Acta Phys.Polon. B26 (1995) 1869; condmat/9512099)

- NRG give the finite size spectra of the I.R. fixed point



$$\varepsilon_k = \varepsilon_{k_F} + \alpha(k - k_F)$$

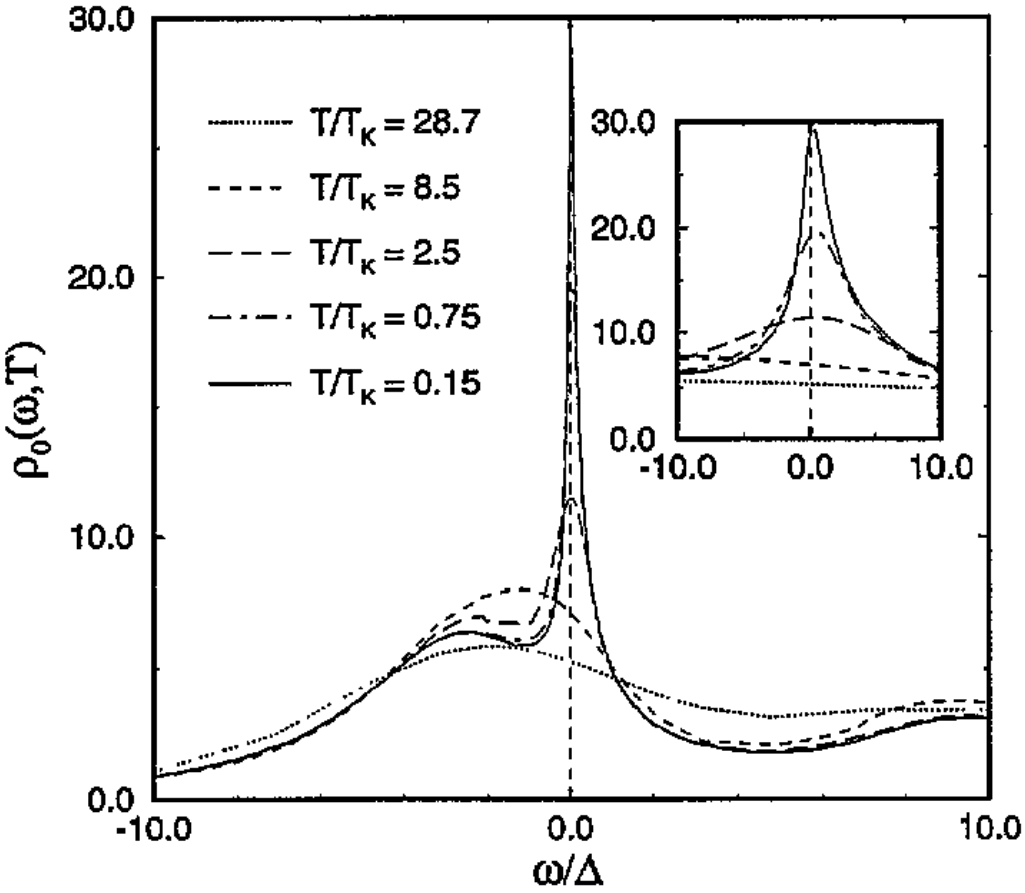
$$E(k_1, k_2) = \varepsilon_{k_1} + \varepsilon_{k_2} = \varepsilon_{k_1 - q} + \varepsilon_{k_2 + q} = E(k_1 - q, k_2 + q)$$

- Huge degeneracies → powerful symmetries of free fermions & IR fixed point (Conformal, Kac-Moody,...)
- H is part of the symmetry algebra !
- With finite spectra, identify the representation at the fixed point
- Then use CFT to compute various low energy properties.

NRG : applications

- Abrikosov-Suhl-Kondo Resonance in the spectral function (Anderson model)

Costi et al.. J. Cond. Mat (1994)



Asymmetric case, varying T

- Resolution of NRG is much better at low energy than high energy

NRG : scaling property

- Scaling property of the resistivity as a function of T/Tk in the universal regime

Costi et al.. J. Cond. Mat (1994)

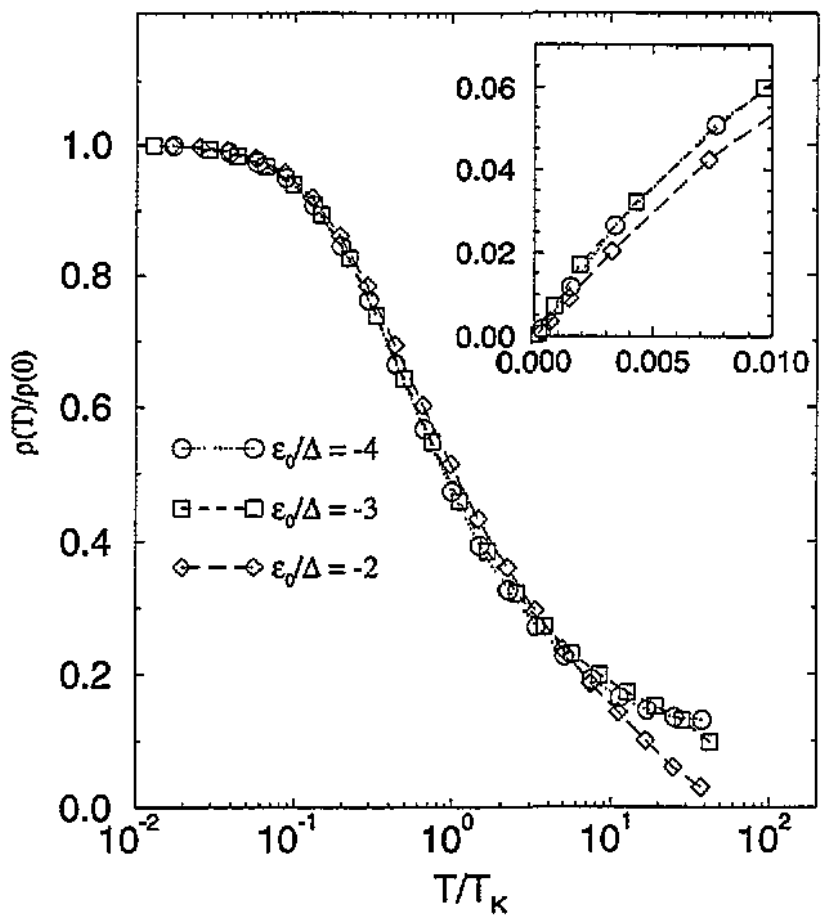
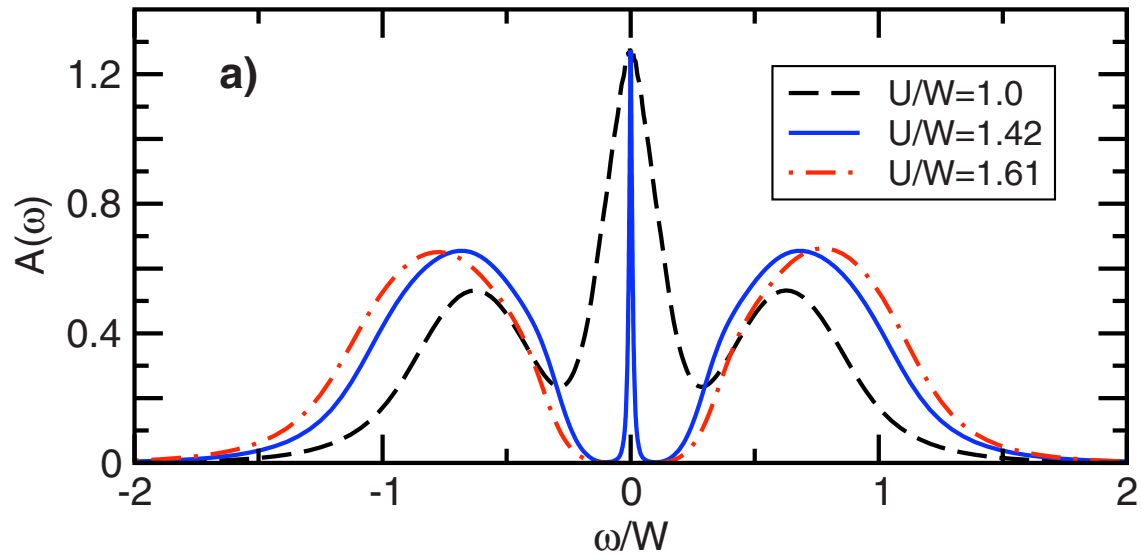


Figure 12. The scaled resistivity in the Kondo regime showing the universal behaviour at low temperature up to approximately $5T_K$. The inset for $1 - (\rho(T)/\rho(0))$ versus $(T/T_K)^2$ shows the expected Fermi liquid behaviour for the resistivity at low temperature $T < 0.1T_K$. The

NRG & DMFT

- NRG can also solve DMFT (1 band)



R. Bulla et al. (1999)

- Specially useful to compute transport (e.g. resistivity), e.g. Transport in organics compound κ-$(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu}[\mathrm{N}(\mathrm{CN})_2]\mathrm{Cl}$

  P. Limelette, P. Wzietek, S. Florens, A. Georges, T.A. Costi, C. Pasquier, D. Jérome, C. Meziere, P. Batail

  PRL 91, 016401 (2003)

- But :
  - difficult away from half-filling.
  - CT-QMC is a now a serious competitor (see later)

NRG : strengths & limitations

- Strengths :
  - Energy scale separation built in.
  - Low energy fixed points, crossover towards low temperature.
  - Solve directly in real frequency (≠ QMC)
- Limitations :
  - Not precise at high energy (e.g. details in the Hubbard bands)
  - Does not scale well with the size of the impurity problem
    - Flat bath, no spectral function : 3-4 maximum
    - DMFT : 1 band, undoped only.

Quantum Monte Carlo

Monte Carlo sampling

Cf e.g. Werner Krauth's book "Statistical Mechanics : algorithms & computations"

- 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)

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

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

A textbook example : the Ising model

- Ising model :

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \qquad \sigma_i = \pm 1$$

- Configuration : the value of all the Ising spins.

$$p(\{\sigma_i\}) \propto e^{-\beta H[\{\sigma_i\}]}$$

- MC Move (simplest) : flip spin k chosen at random
  - The probability ratio is easy to compute since H is local

The sign problem

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

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

- But generically, the denominator (average of sign (p(x)) decays 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 pb is not intrinsic : it depends on the basis/rewriting of Z ! We can hope to find "better" expression for 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 !

Quantum Monte Carlo for impurity models

- *Hirsch-Fye algorithm* : *Hirsch-Fye PRL (1986)*
  The historical algorithm: uses a fixed time grid, is limited to density-density interaction.

- *The Continuous Time "Revolution" (CT-QMC)* :
  Expansion in interactions (CT-Int): *A.N. Rubtsov et al., PRB (2005)*
  Expansion around atomic limit (CT-Hyb): *P. Werner et al, PRL (2006)*
  Auxiliary field (CT-AUX): similar to Hirsch-Fye, but in continuous time) : *E.Gull et al., EPL (2008)*

- Work in imaginary time (Matsubara formalism)

- No sign problem for single impurity (and some N orbital cases).
  Sign problem reappears for large cluster of impurities

- CT-QMC are several orders of magnitude faster than Hirsch-Fye
  and exact (up to Monte Carlo error bars) : no time discretization.

Continuous time QMC : principle

- Write a perturbative expansion of the partition function :

$$H = H_a + H_b$$

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

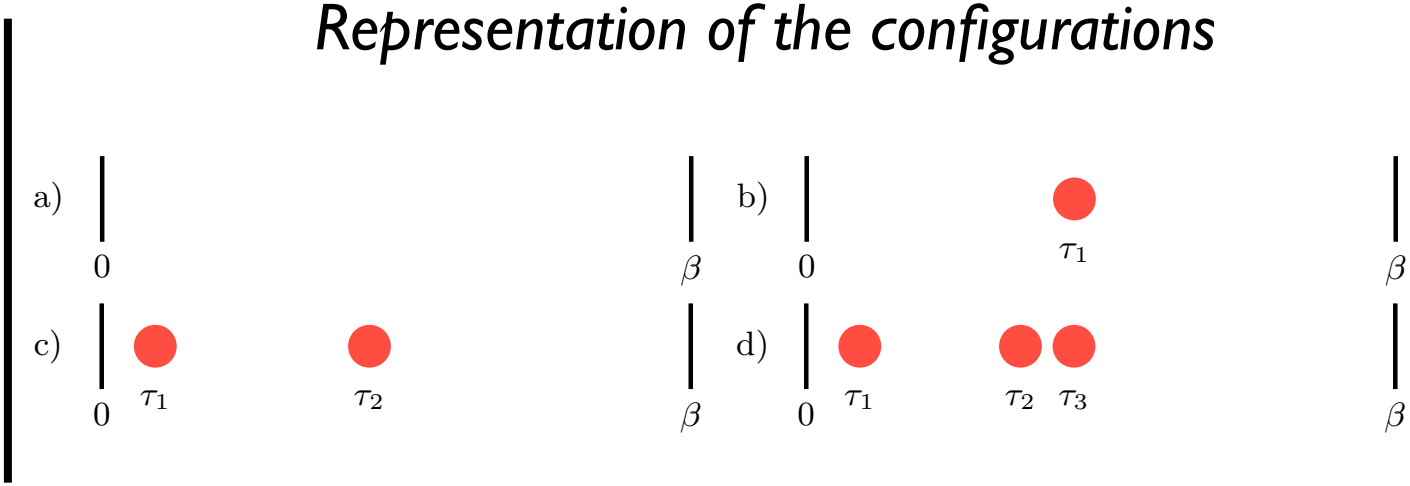
$$= \sum_{n\geq 0}(-1)^n \int_0^\beta d\tau_1 \ldots \int_{\tau_{n-1}}^\beta d\tau_n \,\mathrm{Tr}\left[e^{-\beta H_a} H_b(\tau_n) H_b(\tau_{n-1}) \ldots H_b(\tau_1)\right]$$

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

Configurations

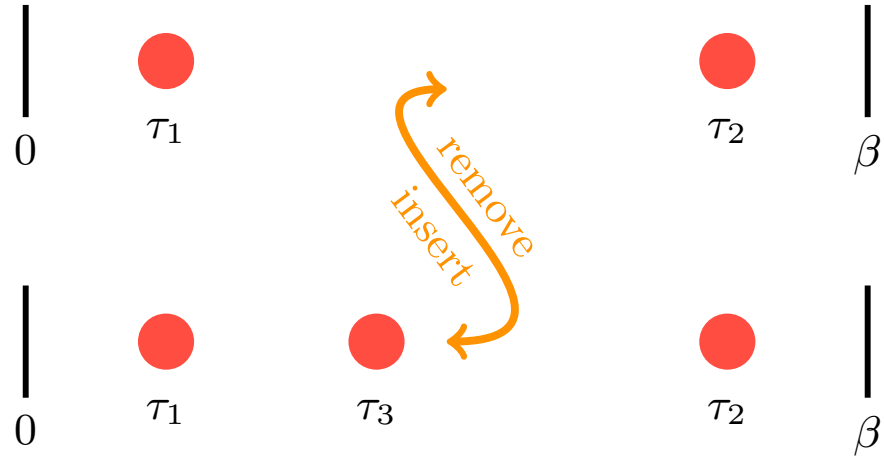
$$x = (n, \gamma, \tau_1, \tau_2, \ldots \tau_n)$$

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, ...)

- Expansion in power of the interactions :
  A.N. Rubtsov et al., Phys. Rev. B 72, 035122 (2005)
- Expansion in power of hybridization (around atomic limit) :
  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)

Expansion in interaction

- Standard perturbative technique at finite temperature.

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

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

- Using Wick Theorem :

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

Expansion in hybridization

P. Werner et al, PRL (2006)

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

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

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 exponential scaling in N !)
- Green function computation (or higher order correlations functions):

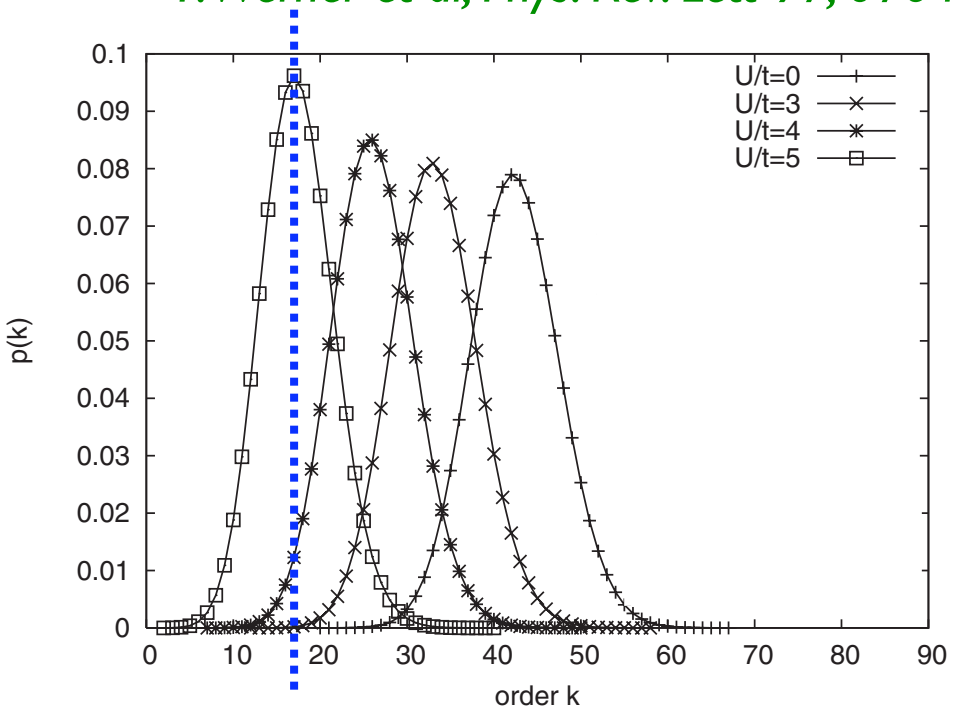
$$G_{ab}(\tau) = \frac{1}{Z}\frac{\delta Z}{\delta \Delta_{ba}(-\tau)}$$

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

CT-QMC : efficient algorithms

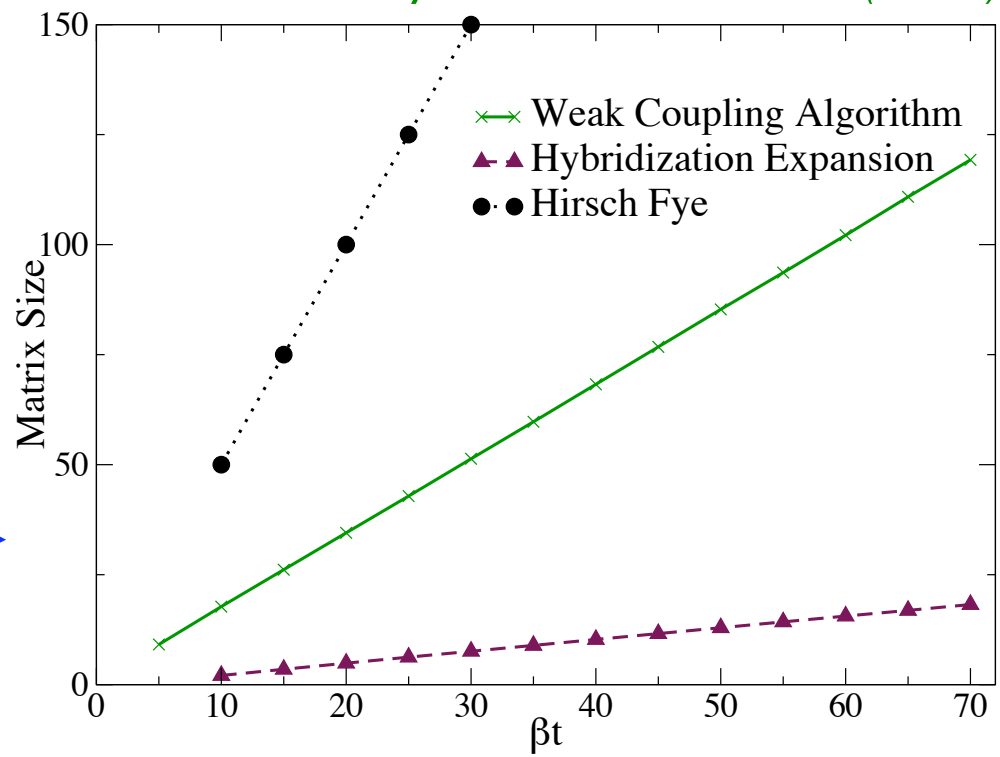
Histogram of expansion order
(Werners' algo, DMFT, βt=100, δ=0, various U)

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

CT-QMC : some applications

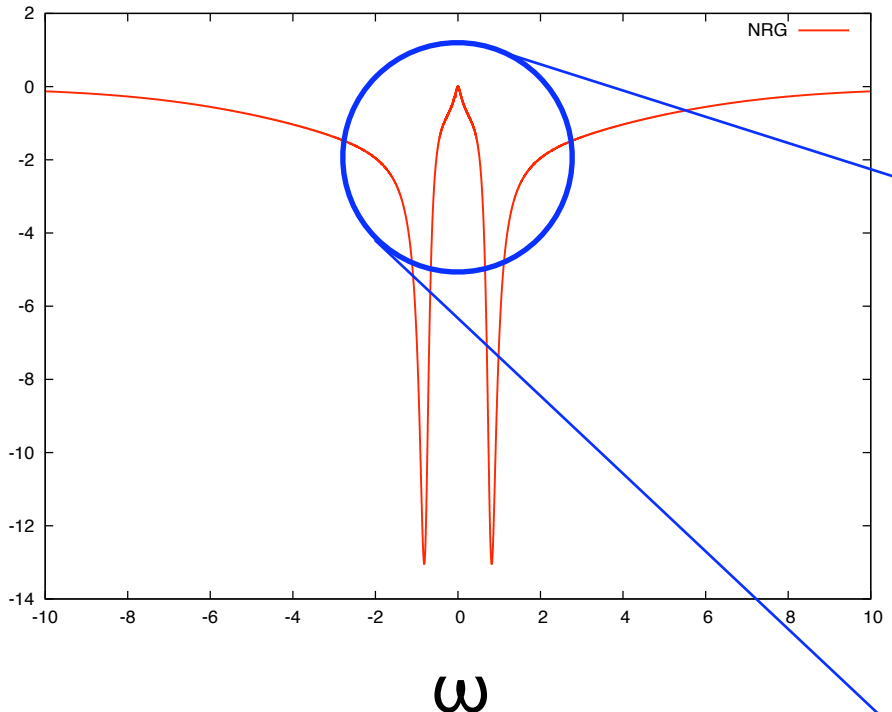
Comparison NRG-CTQMC

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.

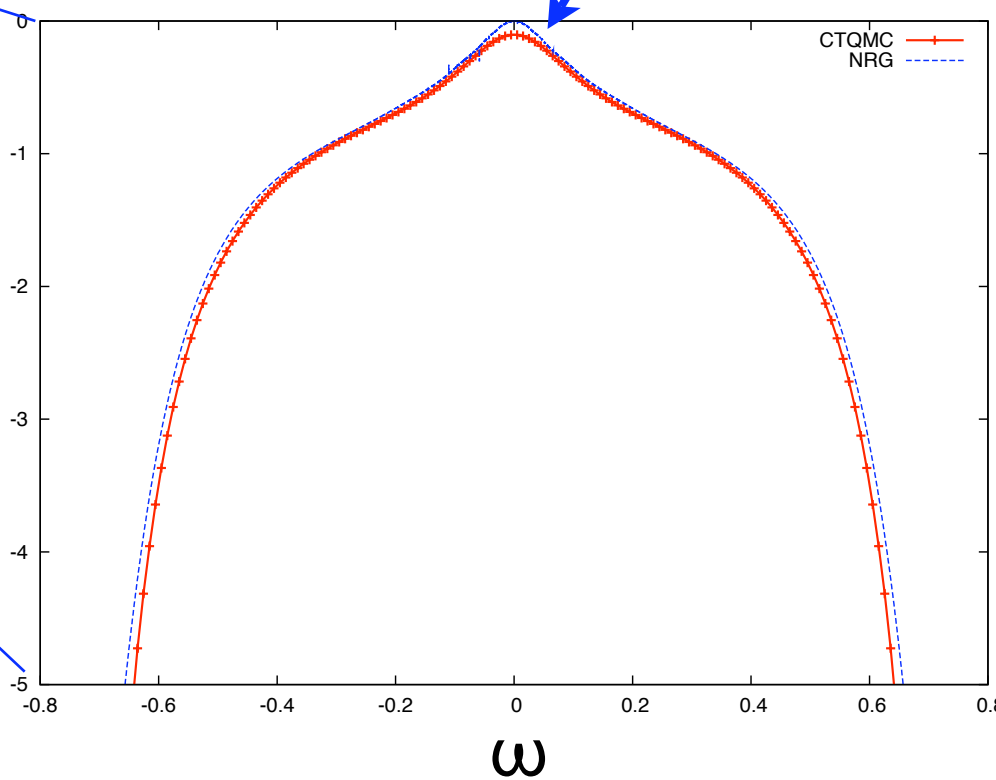
- Continued by Padé method to real axis from Matsubara

Im Σ(ω)



Little finite temperature effect

Im Σ(ω)

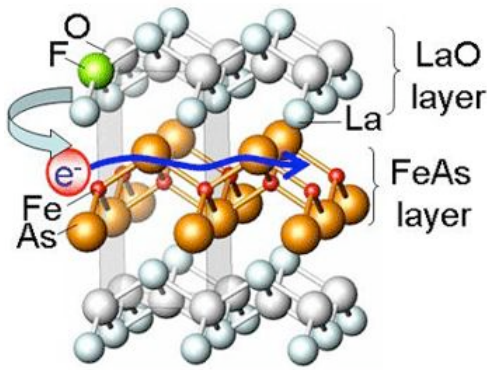


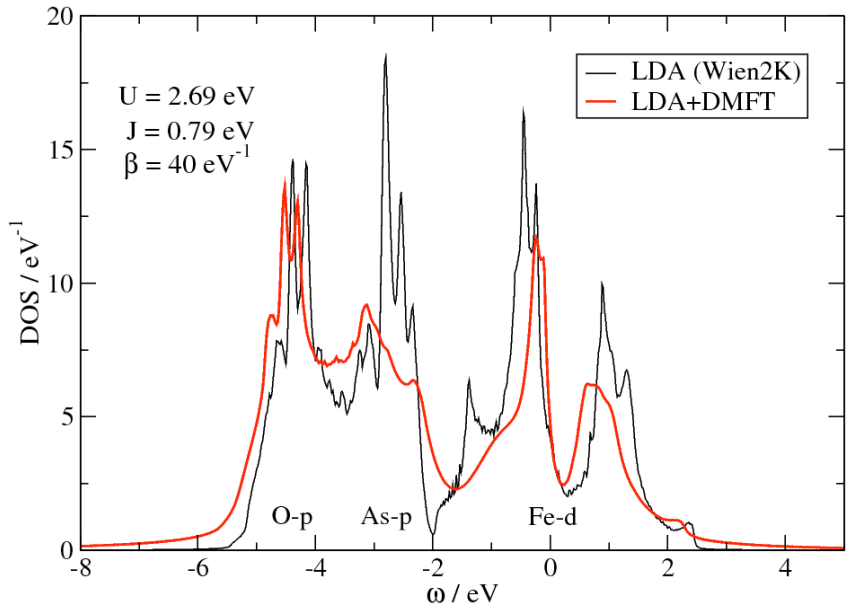
Back to multiorbital models

- Example : Iron-based superconductors LaFeAsO, LDA +DMFT, *Aichhorn et al. (2009).*
- Possible to solve the 5-band impurity model with Werner's algorithm.
- Degree of correlations of those materials ? Moderate.
  - Extract quasi-particle residue Z /effective mass m* from Matsubara self-energy (Z ≈ 0.62, m* ≈ 1.62)

$$Im\Sigma(i\omega_n) \sim \omega_n \left(1 - \frac{1}{Z}\right)$$

  - Using analytic continuation method, spectral function....



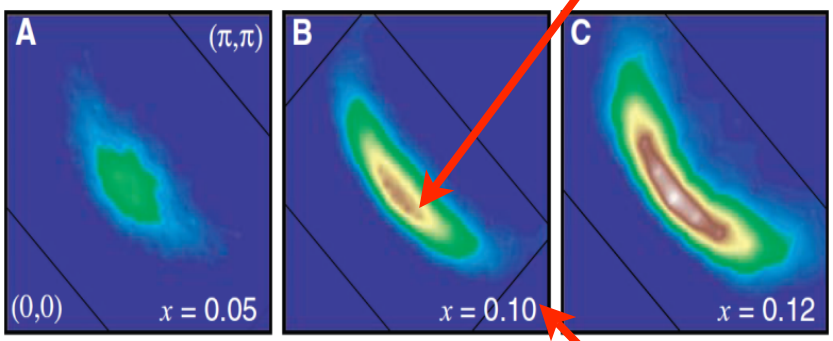


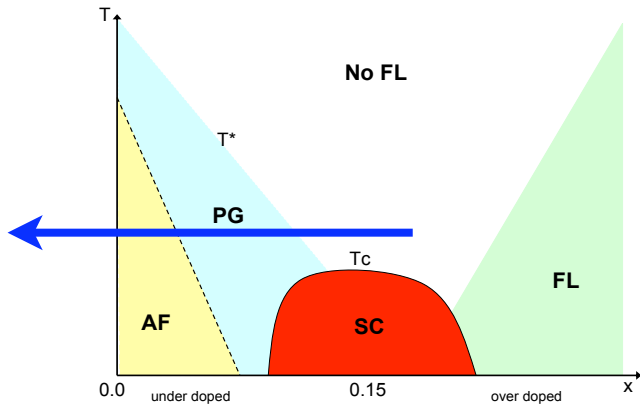
Cluster DMFT & cuprates

- ***Experiments*** : Nodal-antinodal dichotomy in cuprates.

Nodal region : Quasi-Particle

$A(k, \omega = 0)$ ARPES

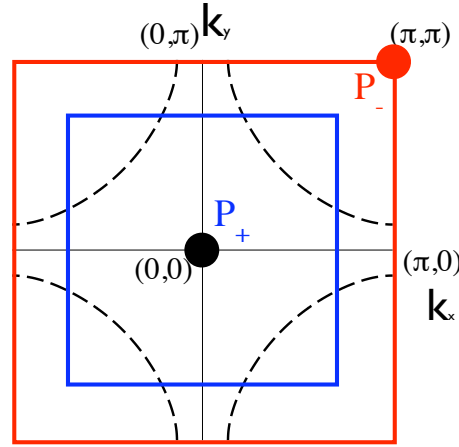




Shen et al. Science 307, 901 (2005)

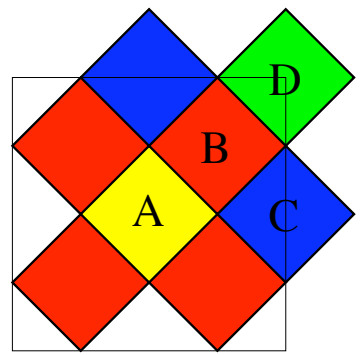
Antinodal region: No Quasi-Particle

Brillouin zone patchings



- ***Theory*** : sector selective Mott transition
  Some sector of the Brillouin Zone (C) become insulating first.

2 sites cluster



Gull, OP, Werner, Millis PRB 80 245102 (2009)
Werner, Gull, OP , Millis PRB 80 045120 (2009)
Ferrero, Cornaglia, De Leo, OP, Kotliar, Georges, EPL and PRB 2009

Only possible with CT-QMC (various flavours)

8 sites cluster

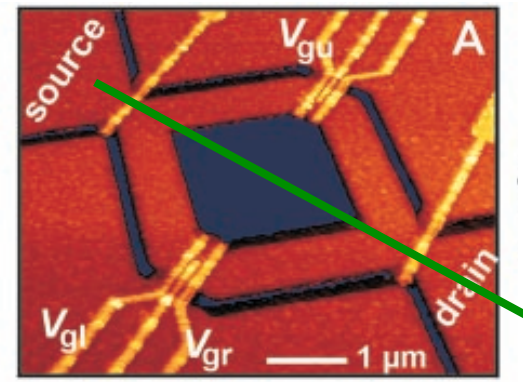
CTQMC : strengths & limitations

- Strengths :
  - A lot faster than before.
  - Solve more general interactions (except CT-AUX)
  - Some have good scaling with number of orbitals/sites
- Limitations :
  - Works in Matsubara : analytical continuation is an ill-posed pb.
  - Still long for complex interactions & low symmetry ...
  - Werner's algorithm scales exponentially with size of the local pb.
- Open question :
  - Even faster/more precise algorithms, other rewriting of Z....

Out of equilibrium physics

Motivations

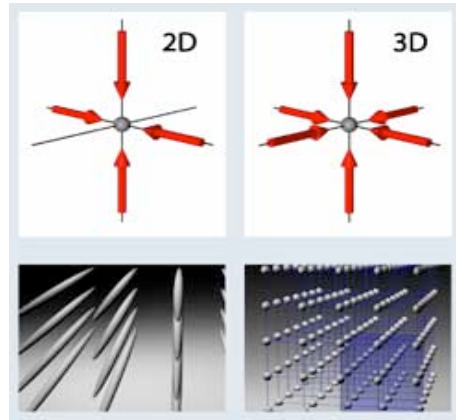
Nanostructures



I(V)

- Quantum dots. Current : I(V).
- Steady state computations

Quenches in cold atoms



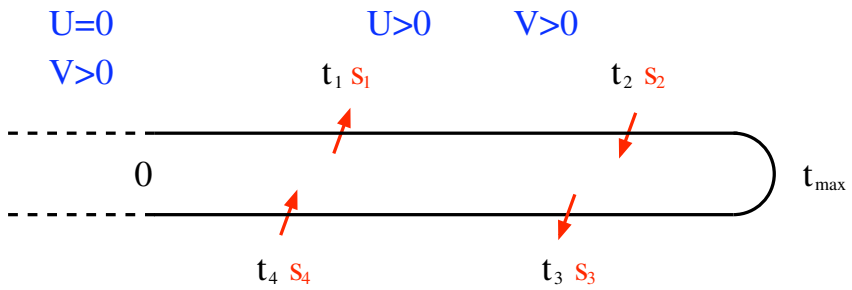
- Lattice to impurity via DMFT
- e.g. Change interaction at t=0, study relaxation, etc...

- Methods, e.g. :
  - Time dependent NRG *F. Anders et al. Phys. Rev. Lett. 100, 086809 (2008)*
  - Real time QMC ....

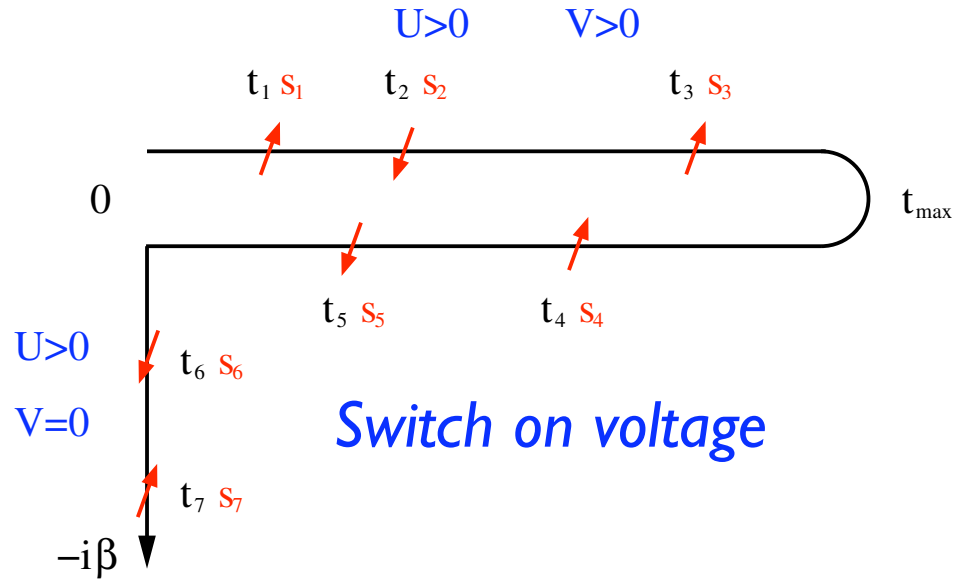
Real Time Quantum Monte Carlo

- Diagrammatic Monte Carlo : use the Keldysh contour !
- Start non-equilibrium at t=0, and
  - try to relax to steady state
  - study quench

Mühlbacher, Rabani (2008)
Werner et al (2009)
Schiro and Fabrizio (2009)



Switch on interaction

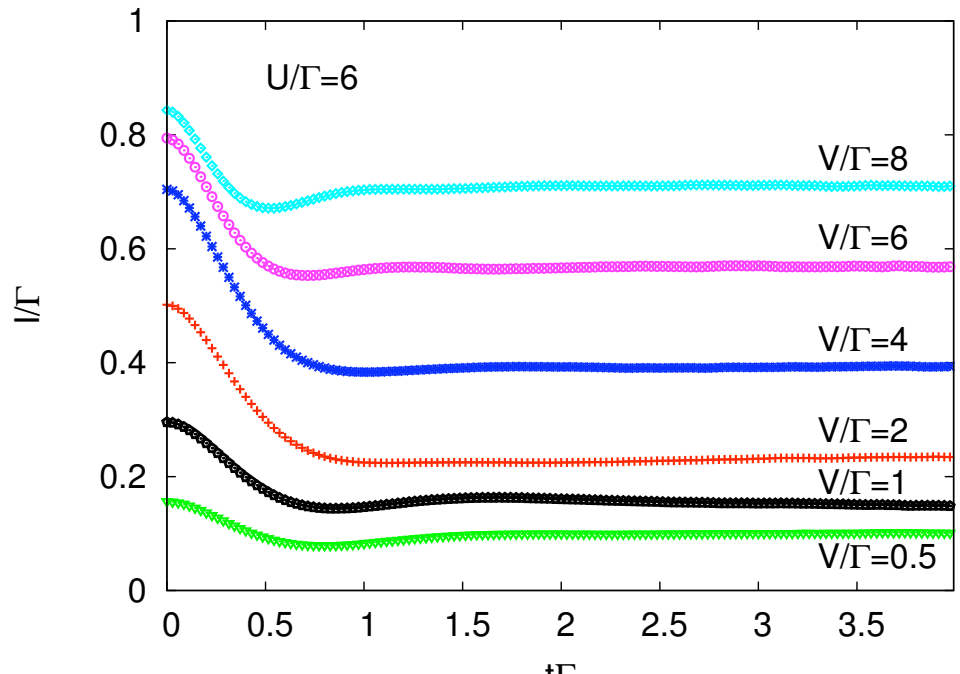


Switch on voltage

- Sign problem due to real time (i factor in time evolution)
- Computation limited in time (does not reach the Kondo time)

Real Time QMC : applications

- Quench in Hubbard model *M. Eckstein et al, ArXiv:0904.0976*
  - DMFT, change U at t=0. Dynamical phase transition at U = 3.2 (?)
- Solution of a quantum dots (in some regimes) *Werner et al. (2010)*



Time evolution of the current for different voltage biases (U/Γ=6,T=0). In the initial state, the current is given by the steady state current through the non-interacting dot. Interaction turned on at t=0

Conclusion

- A lot of progress recently on Continuous Time QMC
- Enable us to solve more complex/realistic models.

- Open issues :
  - Faster QMC for low symmetry realistic atoms ?
  - Real frequency QMC solution ?
  - (t-)DMRG for small cluster ?
  - Use other diagrammatics ? e.g. NCA, cf *Gull et al. arXiv:1004.0724*
  - Better methods out of equilibrium ?