HP-SEE User Forum 2012, Belgrade

Iterative Perturbative Method for a Study of Disordered Strongly Correlated Systems

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Theory of strongly correlated materials

- Introduction
- Dynmical mean field theory

Iterative Perturbative Method

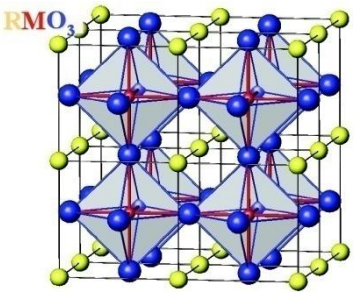
- Theory
- Hybrid parallel C++ implemetantion
  - Numerical issues
  - Optimization
  - Parallelization
- Applications
  - TMT
  - StatDMFT
- Examples of results

```
//========================= RUN SIAM With FIXED n ============================//
// applicable ONLY in solving Clean Hubbard Model which implies epsilon = 0 and NIDOS is needed on input.
//NOTE that MPT Bs will ALWAYS be one iteration late. They will converge to their real values
//when the DMFT loop converges. First DMFT Iteration is ALWAYS solved WITHOUT MPT Bs.

//TODO in case of asym NIDOS, mu and mu0 are not known EVEN FOR n=0.5 !!!!

bool SIAM::Run_CHM(Result* r) //output
{
  this->r = r;
  N = r->grid->get_N();
  grid = r->grid;
  get_fermi();

  Clipped = false;

  epsilon = 0;

  if (r->n==0.5) HalfFilling = true;
  else HalfFilling = false;

  printf("    ------- SIAM for CHM: n=%.3f, U=%.3f, T=%.3f, epsilon=%.3f -------\n", r->n, U, T, epsilon);

  if (HalfFilling)
  {
    r->mu = 0.5*U;
    mu0 = 0.0;
    MPT_B = 0.0;
    MPT_B0 = 0.0;
    SymmetricCase = true;
  }

  //------initial guess---------//
  complex<double>* V = new complex<double>[1];
  V[0] = mu0; //initial guess is always the last mu0. in first DMFT iteration it is 0
  //---------------------------//

  printf("     MPT: B = %fe, B0 = %fe\n", MPT_B, MPT_B0);

  //---------------- CALCULATION ----------------------//
  if (HalfFilling)//and (SymmetricCase))
    get_G0();
  else
    UseBroyden<SIAM>(1, MAX_ITS, Accr, &SIAM::get_G0, this, V);

  printf("    mu0 = %f\n", mu0);

  get_As();
  get_Ps();
  get_SOCSigma();

  V[0] = r->mu;

  if (HalfFilling)//and (SymmetricCase))
  { if (isBethe)
    {
      get_Sigma();
```

```
  IW   params

#---------------   GRID params   ----------------#
0               |       GRID::GridType          // type of the omega-grid: 0-LogLin. Nothing else should be use for now
2000            |       GRID::Nlog              // number of points in the logarithmic part of the grid (should be even)
2000            |       GRID::Nlin              // number of points in the linear part of the grid (should be even)

6.0             |       GRID::omega_lin_max     // the extension of the grid (it is always symmetric around 0)
0.3             |       GRID::omega_max         // the extension of the logarithmic part of the grid (it is always symmetric around 0)
1e-10           |       GRID::omega_min         // the value of points closest to 0 (0.0 is not present in the grid)

#---------------   SIAM params   ----------------#
0.0             |       SIAM::U                 // on-impurity interaction
0.01            |       SIAM::T                 // temperature
0               |       SIAM::epsilon           // impurity orbital energy

100             |       SIAM::MAX_ITS           // maximum number of iterations for the Broyden solver that solves the system of 2 equations
1e-9            |       SIAM::Accr              // desired accuracy for the above process

5e-5            |       SIAM::eta               // bradening that is included in calculation of G0

F               |       SIAM::CheckSpectralWeight       // if this is set to true n and n0 are printed
F               |       SIAM::UseMPT_Bs                 // if this is set to true MPT corrections are used
F               |       SIAM::isBethe                   // this determines the way G is calculated. when just solving siam, should be set to false

#---------------   Loop params   ----------------#
T               |       Loop::UseBroyden                // use broyden for aiding DMFT loop convergence
F               |       Loop::ForceBroyden              // use broyden even if errors accur in SIAM
5e-4            |       Loop::BroydenStartDiff          // set this to the level of convergence after reaching of which Loop starts using broyden

2               |       Loop::NtoMix                    // number of consecutive solutions to mix (ALWAYS >= 2)
1 0             |       Loop::Coefs                     // the linear coefficients for mixing solutions (newer to older)

800             |       Loop::MAX_ITS                   // maximum number of DMFT loop iterations
1e-8            |       Loop::Accr                      // desired accuracy

F               |       Loop::PrintIntermediate         // if this is set to true, after each iteration current result gets printed to a file named "intermediate.<i
F               |       Loop::HaltOnIterations          // a debugging option that halts the execution after the first iteration and proms the user for the ordinal
T               |       Loop::ForceSymmetry

#---------------  CHM params     ----------------#
2.00            |       CHM::U (overrides SIAM :: U)    // hubbard on-site interaction
0.03            |       CHM::T (overrides SIAM :: T)    // temperature
0.5             |       CHM::t                          // hopping amplitude

F               |       CHM::UseBethe (overrides SIAM :: isBethe)       // if set to true, Delta = t^2 G bethe-specific self-consistency realtion is used
0.0             |       CHM::SIAMeta (overrides SIAM :: eta)            // sets the broadening for the SIAM object used

F               |       CHM::SIAMUseLatticeSpecificG
0               |       CHM::LatticeType
6               |       CHM::SiamNt


#---------------  TMT params  ----------------#
0.3             |       TMT::W                  // disorder (orbital eneries are spread through -W, W
0               |       TMT::Distribution       // the distribution kind: 0-Uniform, 1-Gaussian (for now, only uniform is implemented)
20              |       TMT::Nimp               // number of impurities used (orbital energies are equally spaced on -W,W

8               |       TMT::AverageNt          // the number of threads to be used for averaging (should be set to the number of processors on the master m
8               |       TMT::SiamNt             // the number of threads to be used for SIAM solving (should be set to <the number of processors per machine
8               |       TMT::KramarsKronigNt    // the number of threads to be used for Hilbert transform (should be set to the number of processors on the
```

- Theoretical solid state physics
  - Modeling materials with crystal structure

$N \sim 10^{23}$

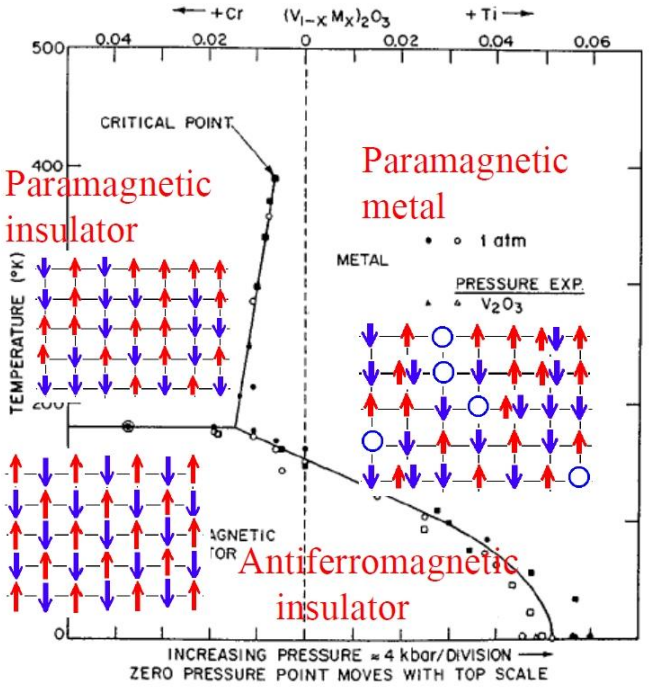


$$\hat{H} = -\frac{1}{2}\sum_{i}^{N_e}\nabla_i^2 - \sum_{i}^{N_e}\sum_{I}^{N_n}\frac{Z_I}{|\vec{r}_i - \vec{R}_I|} + \frac{1}{2}\sum_{i}^{N_e}\sum_{j\neq i}^{N_e}\frac{1}{|\vec{r}_i - \vec{r}_j|} + \frac{1}{2}\sum_{I}^{N_n}\sum_{J\neq I}^{N_n}\frac{Z_I Z_J}{|\vec{R}_I - \vec{R}_J|}$$

- Weakly correlated materials
  - Conventional metals
  - Band-insulators
  - Semi-conductors
  - Described well by effective single-particle theories (e.g. DFT+LDA)

- Strongly correlated materials
  - High Tc Superconductors (Cuprates and Fe based)
  - Numerous Transition metal oxides exhibiting metal-insulator transition
  - Rare-earth and actinide intermetallics
  - Kapa-organics
  - Still lack theories with predictive power

- To understand emergent phenomena like macropscopic quantum phases of matter, one must tackle a true many-body QM problem

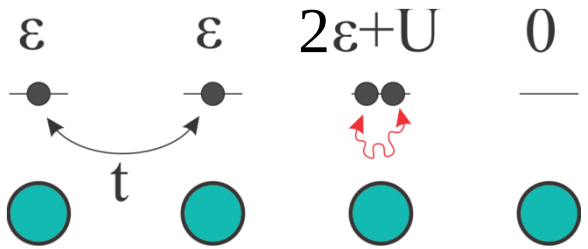


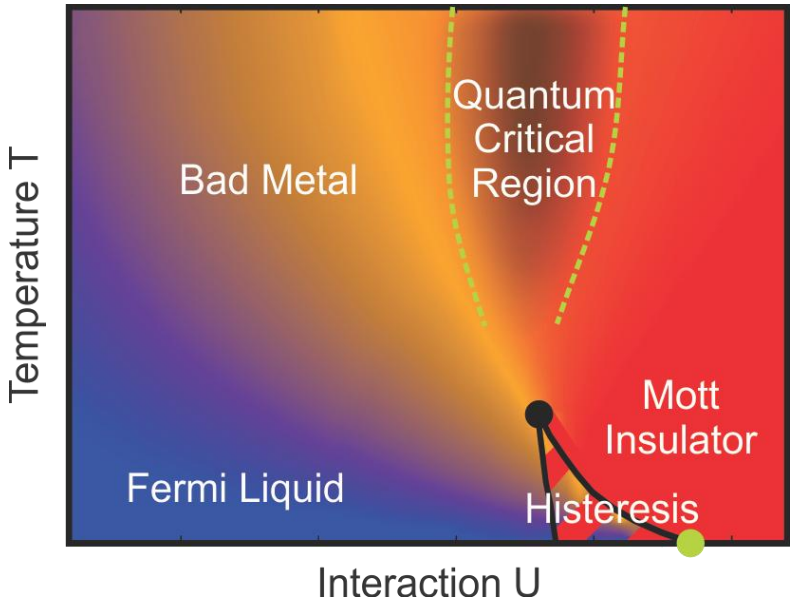
V_2O_3 phase diagram

- Hubbard Model

$$\hat{H} = -t \sum_{\langle \vec{i},\vec{j} \rangle, \sigma} \left(c^{\dagger}_{\vec{i},\sigma} c_{\vec{j},\sigma} + \text{h.c.} \right) + U \sum_{\vec{i}} \hat{n}_{\vec{i},\uparrow} \hat{n}_{\vec{i},\downarrow} - \varepsilon \sum_{\vec{i},\sigma} \hat{n}_{\vec{i},\sigma}$$

- A very simplified model:
  - No details of atomic structure
  - No lattice dynamics (phonons)
  - No long-range interactions
  - No disorder



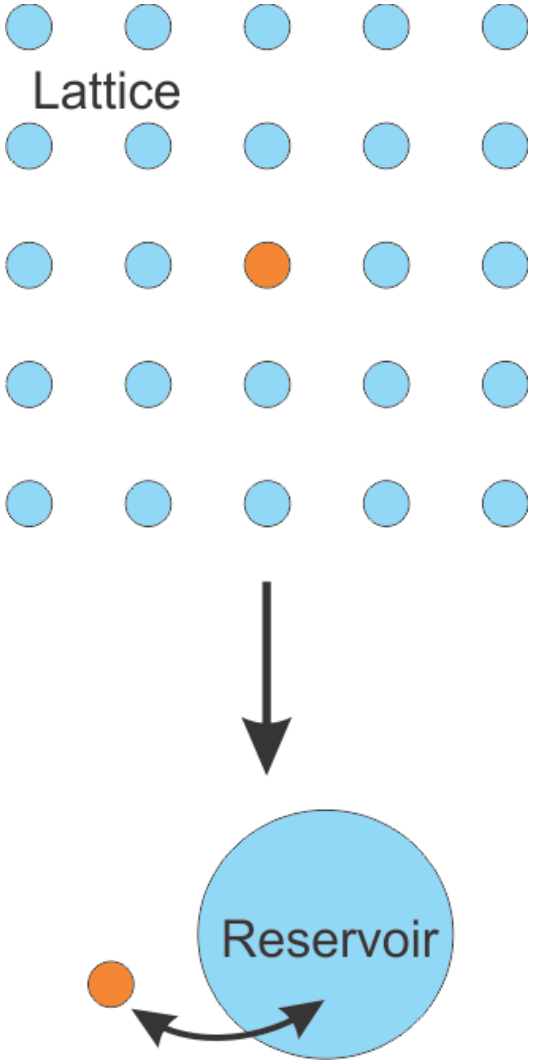


- Exactly soluble only in
  - d=1
  - d=∞ (Dynamical Mean Field Theory)

H. Terletska, J. Vucicevic, D. Tanaskovic, V. Dobrosavljevic
Phys. Rev. Lett. 107, 026401 (2011)

- DMFT solution of the Hubbard Model

A. Georges, Rev. Mod. Phys., Vol. 68, No. 1, (1996)



IT'S A MEAN-FIELD THEORY

The approach is simillar to the Weiss-Curie mean-field theory of magnetism

• The environment of a site is replaced by an effective bath of electronic states described by the self-consistently determined Hybridization function

IT IS DYNAMICAL

The effective fermionic field is frequency dependent so that the temporal fluctuations are fully taken into account

• Electrons are allowed to hop in and out from the bath

- DMFT solution of Hubbard Model

DMFT method assumes that the self-energy is purely local

$$\Sigma(\mathbf{k}, \omega)$$

In finite dimensions, it neglects spatial fluctuations

Exact only in infinite dimensions

Works particurarly well in cases when self-energy locality is a reasonable approximation

- Lattice has a large coordination number
- Long range order is geometrically frustrated
- Temperature is high as compared to the Fermi liquid coherence temperature
- Away from near vicinity of critical points

- # Numerical solution: The DMFT Loop

Step 0:
Pick an arbitrary Hybridazation fucntion

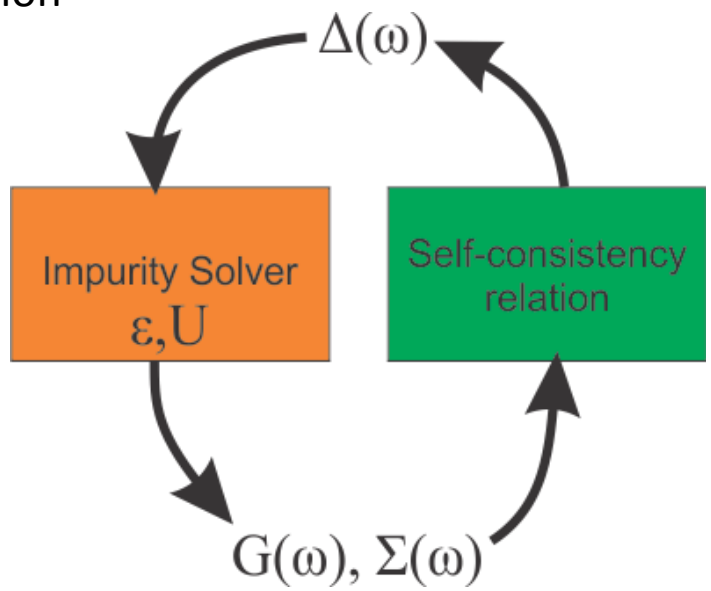
Step 1:
Solve the Single Impurity Anderson Model (SIAM)

$$\hat{H} = -\sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} \left(c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + \text{h.c.} \right) - V \sum_{\vec{k},\sigma} \left(f^{\dagger}_{\sigma} c_{\vec{k},\sigma} + \text{h.c.} \right) - \varepsilon_f \sum_{\sigma} \left(f^{\dagger}_{\sigma} f_{\sigma} + \text{h.c.} \right) + U f^{\dagger}_{\uparrow} f^{\dagger}_{\downarrow} f_{\uparrow} f_{\downarrow}$$

Step 2:
Use the solution of SIAM (Green's function and Self-energy) to Calculate a Hybridization function using the Self consistency relation

$$\Delta(\omega) = \omega + \mu - \Sigma(\omega) - G^{-1}(\omega)$$

Step 3:
GOTO Step 1



• Single Impurity Anderson Model solvers

– Exact
  - CTQMC (Continuous Time Quantum Monte Carlo)

    N.V. Prokof'ev, JETP Lett. 64, 911 (1996), P. Werner, Phys. Rev. Lett. 97, 076405 (2006), K. Haule, Phys. Rev. B 75, 155113 (2007)

    – Noisy
    – Computationally intensive
    – Formulated on the imaginary axis

$$G(i\omega_n) \rightarrow G(\omega) \rightarrow \rho(\omega)$$

Not an easy task!

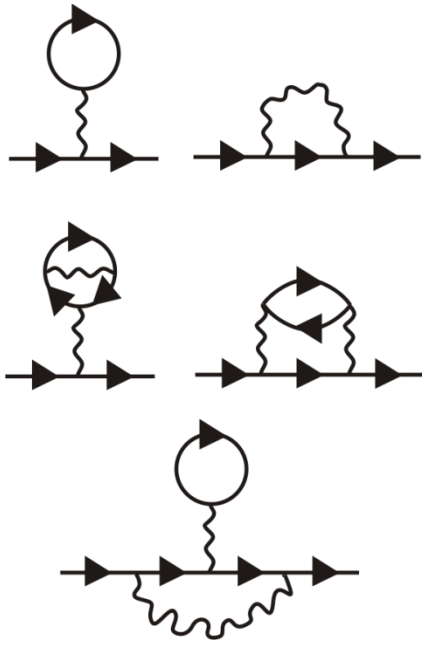
  - ED (Exact Diagonalization)
    – Unfeasible unless Hybridization bath is approxiated with only a small number of orbitals
  - NRG (Numerical Renormalization Group)
    – Works well only at zero termperature

– Approximate
  - NCA (Non-crossing approximation)
  - SB (Slave boson)
  - SOP (Second order perturbative solution)

- The DMFT with SOP impurity solver a.k.a.

The iterative perturbation theory (IPT)

- Approximate
  - Takes into account the Feynman diagrams of only up to the second order
- Computationally not very demanding
- Can be formulated on both real and imaginary axes
- In good qualitative and even quantitative agreement with CTQMC



H.Kajueter, Phys. Rev. Lett. 77, 131–134 (1996)
M. Potthoff, Phys. Rev. B 55, 16132–16142 (1997)

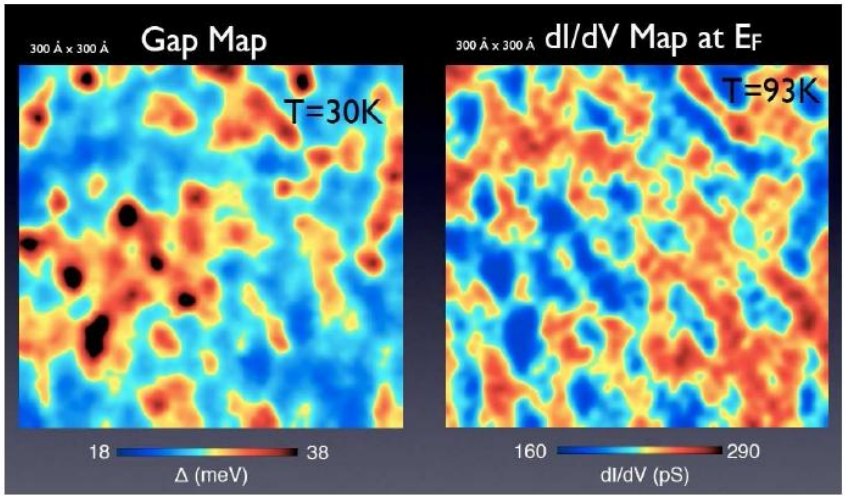
- # Disordered systems

Crystal lattices are usually not perfect…

- Structural defects
  - Interstitial atoms
  - Vacancies
  - Deviations from the perfect translational symmetry
- Impurities

… but highly doped systems are usually very disordered, with many dopants distributed randomly across the lattice.

DMFT for disordered systems:
each lattice site has different properties and a different environment and must be treated as an independent impurity problem!



STM images of the spatial distribution of the superconducting gap and normal phase conductivity of the doped $Bi_2Sr_2CaCu_2O_{8+x}$

The efficiency of IPT is of great importance.

$$
\begin{aligned}
G_0(\omega) &= \frac{1}{\omega + \mu_0 - \Delta(\omega)} \\
n_d &= -\frac{1}{\pi}\int G_0(\omega) f(\omega) d\omega \\
A^{\pm}(\omega) &= -\frac{1}{\pi} G_0''(\omega) f(\pm\omega) \\
P_1(\omega) &= \pi \int A^-(\omega') A^+(\omega' - \omega) d\omega' \\
P_2(\omega) &= \pi \int A^+(\omega') A^-(\omega' - \omega) d\omega' \\
\mathrm{Im}\Sigma^{(2)}(\omega) &= -U^2 \int \left[A^+(\omega - \omega') P_2(\omega') \right. \\
&\qquad \left. + A^-(\omega - \omega') P_1(\omega') \right] d\omega' \\
\mathrm{Re}\Sigma^{(2)}(\omega) &= -\frac{1}{\pi}\int \frac{\mathrm{Im}\Sigma^{(2)}(\omega')}{\omega - \omega'} d\omega' \\
B_0 &= \epsilon_d - \frac{1}{\pi} \frac{2n_d - 1}{n_d(1-n_d)} \mathrm{Im} \int f(\omega')\Delta(\omega') G_0(\omega') d\omega' \\
b &= \frac{(1-2n_d)U - \mu + (\mu_0 + \epsilon_d + U n_d) - B + B_0}{n_d(1-n_d)U^2} \\
\Sigma(\omega) &= U n_d + \frac{\Sigma^{(2)}(\omega)}{1 - b\Sigma^{(2)}(\omega)} \\
G(\omega) &= \int \frac{\rho(\varepsilon) d\varepsilon}{\omega + \mu - \varepsilon - \Sigma(\omega)}
\end{aligned}
$$

$\Delta(\omega)$

$$\Delta(\omega) = \omega + \mu - \Sigma(\omega) - G^{-1}(\omega)$$

μ_0,B

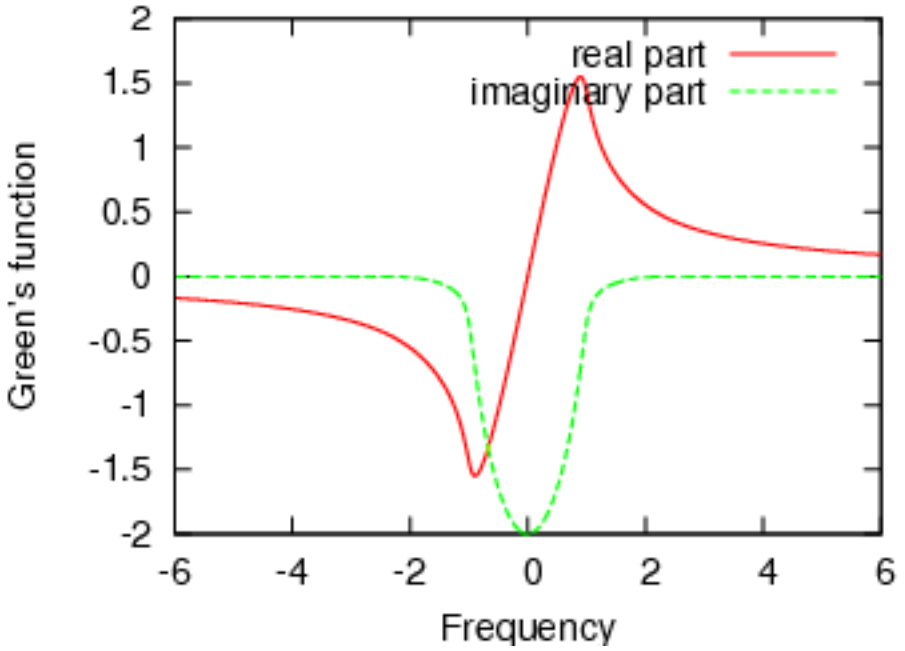
$$
\begin{aligned}
n_d &= -\frac{1}{\pi}\int G(\omega) f(\omega) d\omega \\
B &= \epsilon_d - \frac{1}{\pi}\frac{1}{n_d(1-n_d)} \times \\
&\qquad \times \mathrm{Im} \int f(\omega)\Delta(\omega) \left(\frac{2}{U}\Sigma(\omega) - 1 \right) G(\omega) d\omega
\end{aligned}
$$

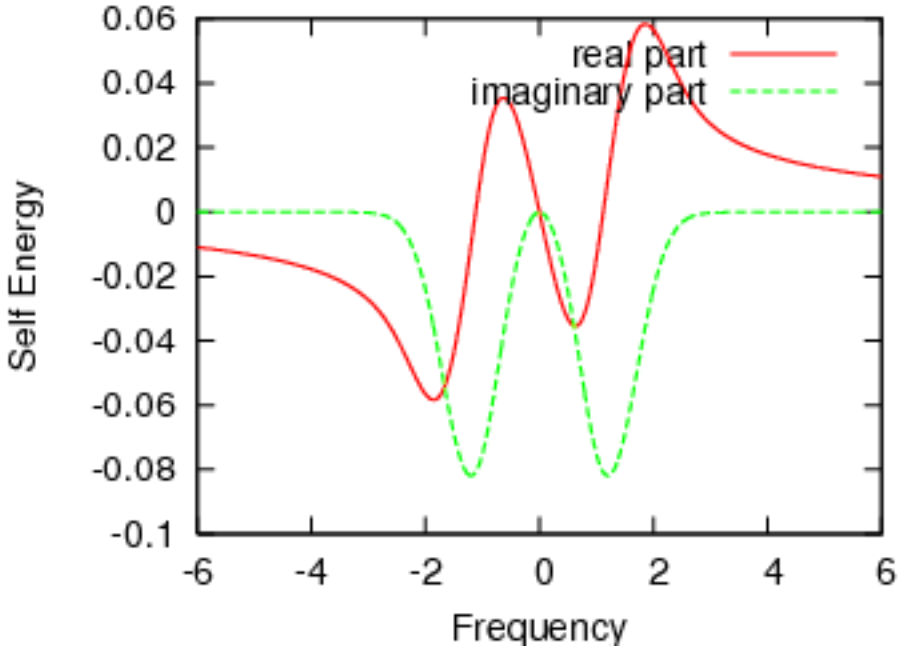
$\Sigma(\omega)$,$G(\omega)$

- General numerical issues

Function discretization grid $G(\omega) \longrightarrow G(\omega_i)$

A uniform but dense grid can be good enough…

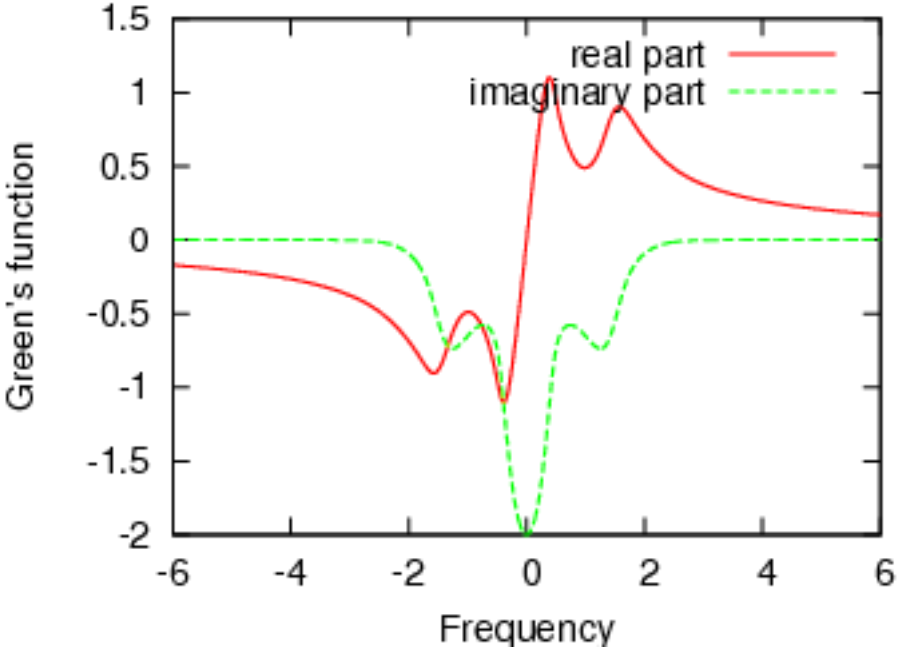


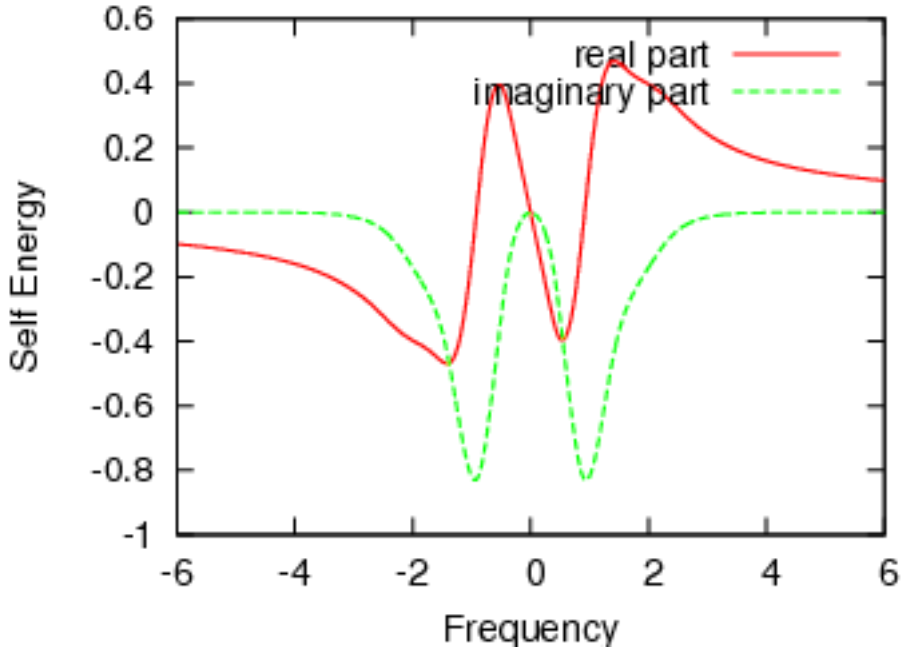


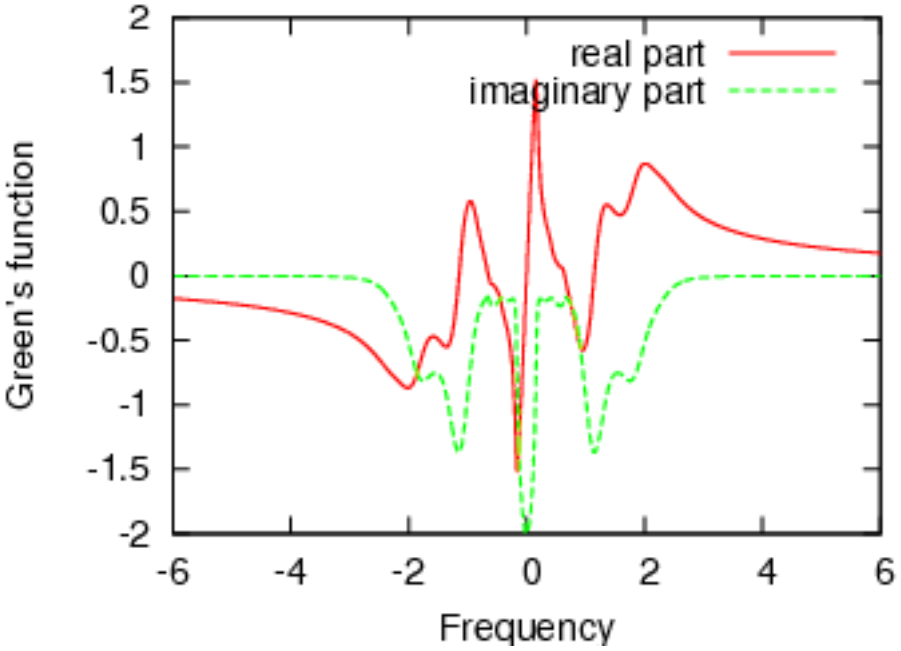
Weak to medium interaction

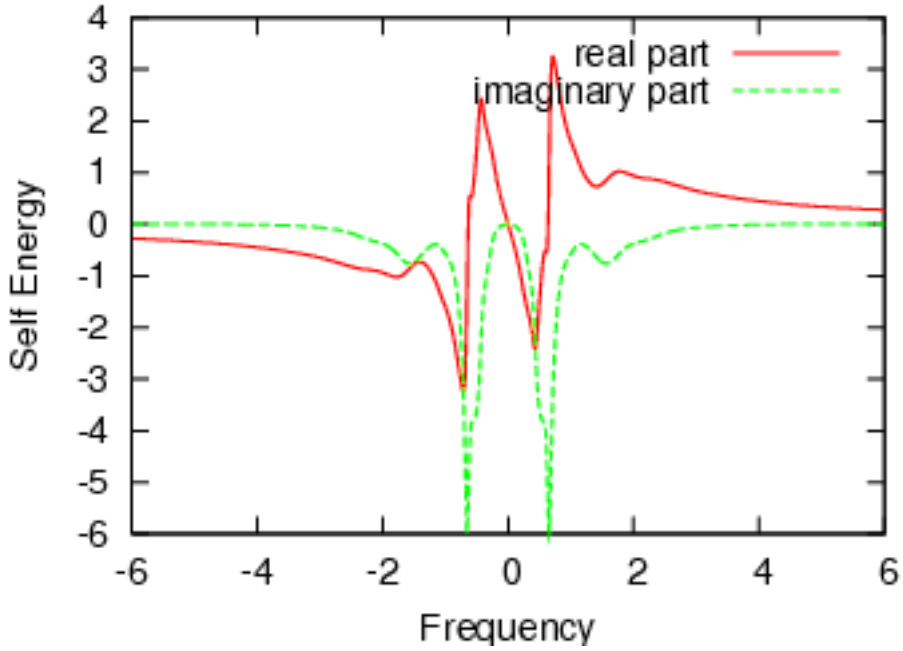
Metallic solution

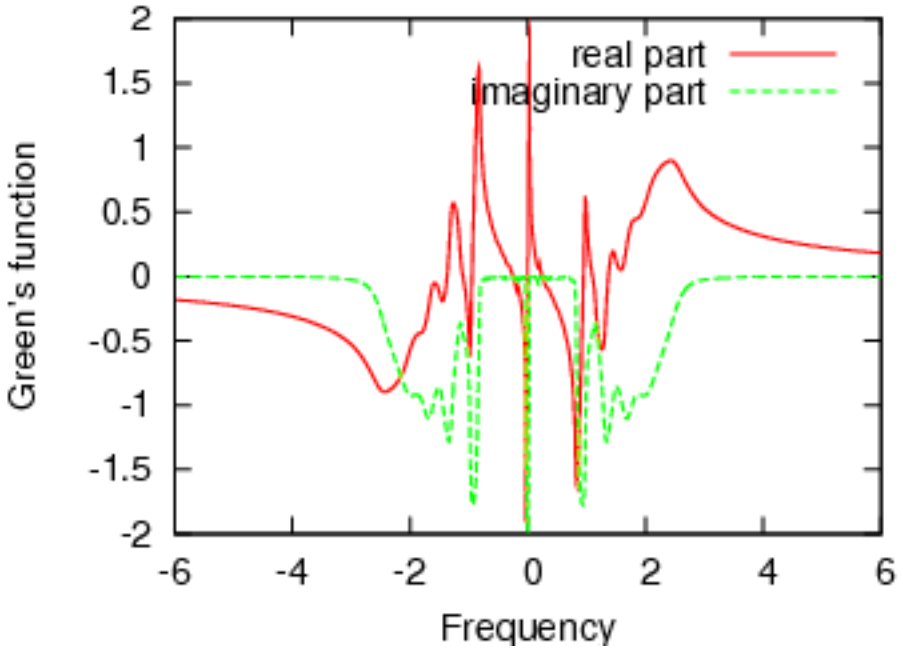
Relatively featureless Green's function and self-energy

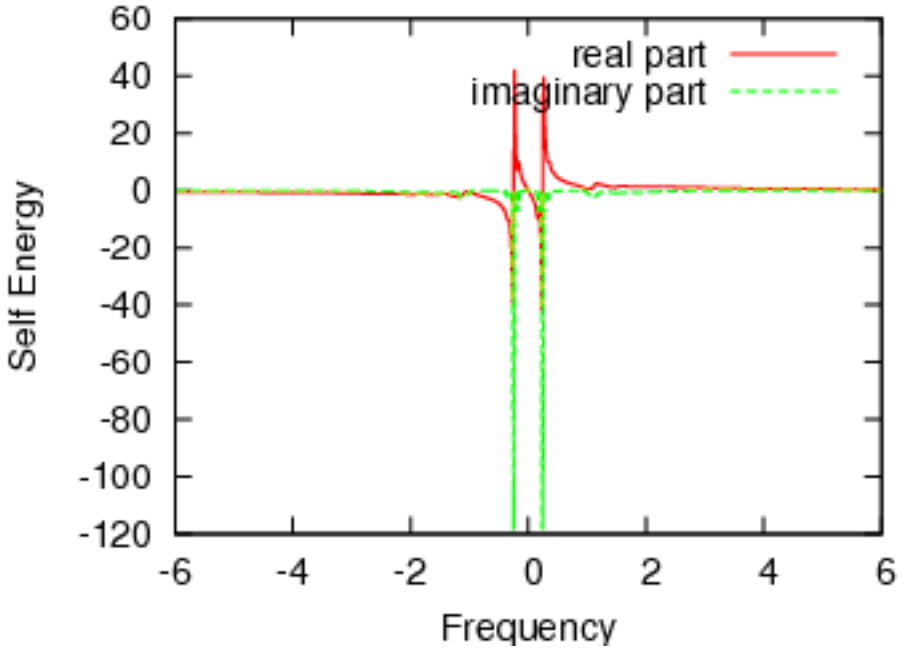

real part
imaginary part
Green's function
Frequency
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-6
-4
-2
0
2
4
6


real part
imaginary part
Self Energy
Frequency
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-6
-4
-2
0
2
4
6


real part
imaginary part
Green's function
Frequency
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-6
-4
-2
0
2
4
6


real part
imaginary part
Self Energy
Frequency
4
3
2
1
0
-1
-2
-3
-4
-5
-6
-6
-4
-2
0
2
4
6

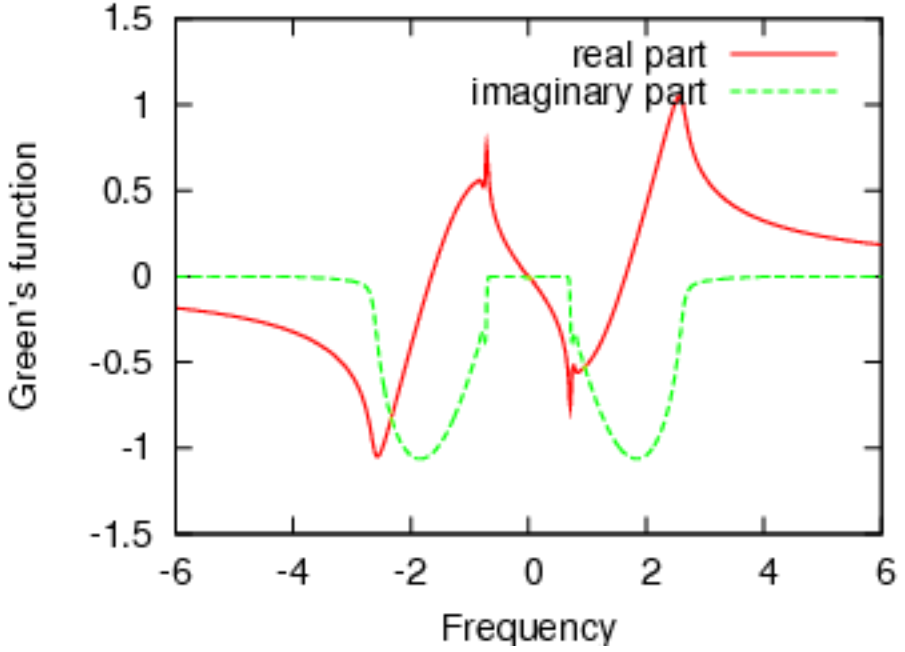

real part
imaginary part
Green's function
Frequency
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-6
-4
-2
0
2
4
6

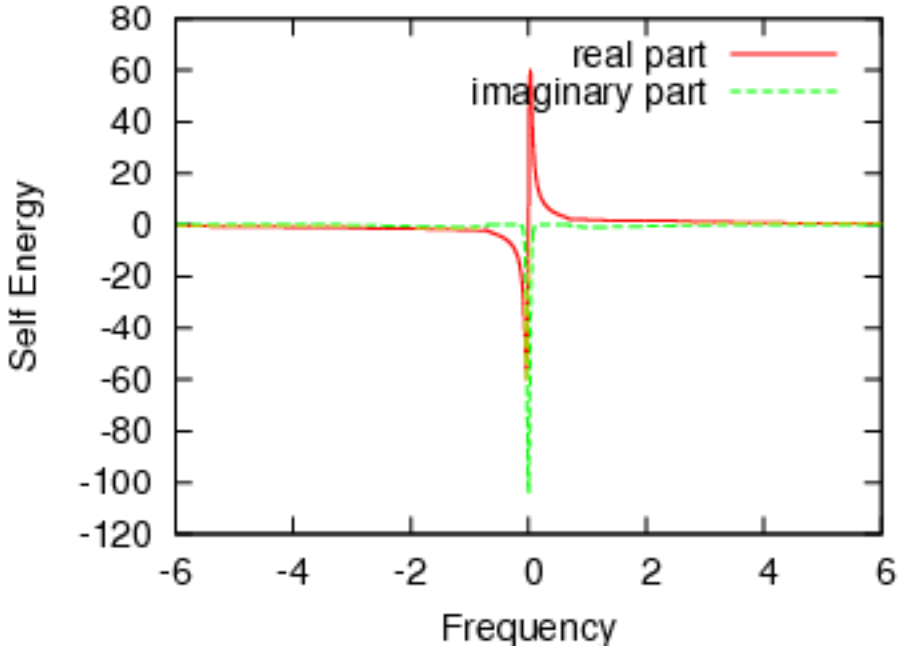

real part
imaginary part
Self Energy
Frequency
60
40
20
0
-20
-40
-60
-80
-100
-120
-6
-4
-2
0
2
4
6

- General numerical issues

Function discretization grid $G(\omega) \longrightarrow G(\omega_i)$

… but is not good enough for a Mott-insulator

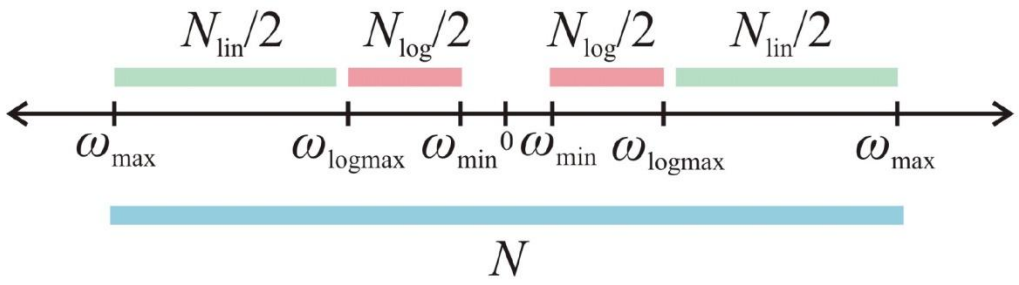




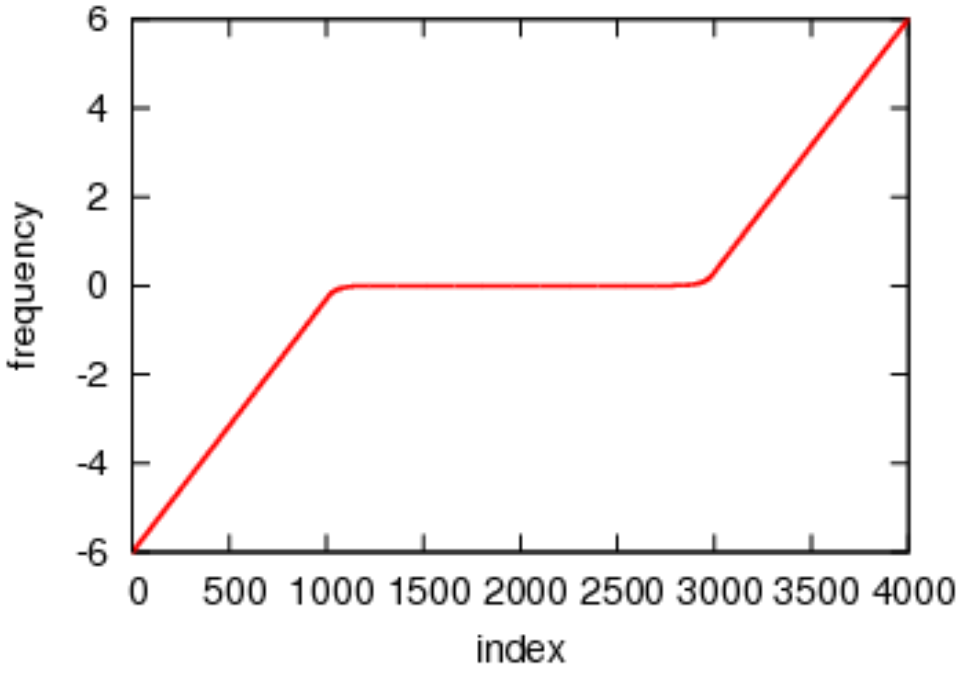
Very sharp delta-like peaks in Self-energy at zero frequency
Have to be resolved with high precision

- General numerical issues

Function discretization grid



A combination of logarithmic and uniform grids



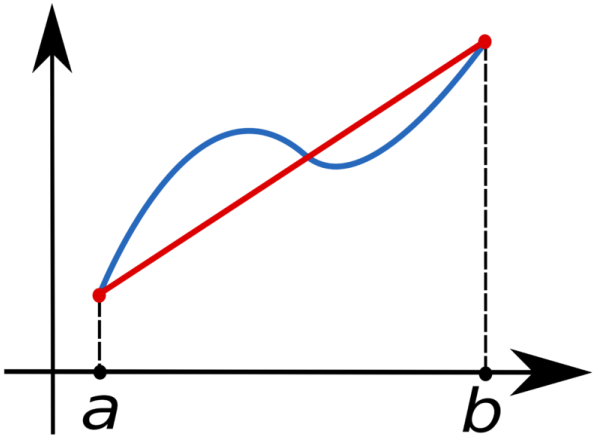
The majority of points is located around zero frequency

- General numerical issues

Integration

Trapezoidal integration is sufficient

Using adaptive grids for integrands with features away from zero frequency could in principle increase precision and efficiency



Integration of divergent integrands

$$G(\omega) = \int \frac{\rho(\varepsilon)d\varepsilon}{\omega+\mu-\varepsilon-\Sigma(\omega)}$$

Straight-forward integration fails

$$= \int \frac{\rho(\varepsilon)d\varepsilon}{\omega+\mu-\varepsilon-\Sigma(\omega)+i\eta}$$

Easy solution degrades the result

$$= \int d\varepsilon \frac{\rho(\varepsilon)-\rho(\omega+\mu-\Sigma(\omega))}{\omega+\mu-\varepsilon-\Sigma(\omega)} + \rho(\omega+\mu-\Sigma(\omega)) \int \frac{d\varepsilon}{\omega+\mu-\varepsilon-\Sigma(\omega)}$$

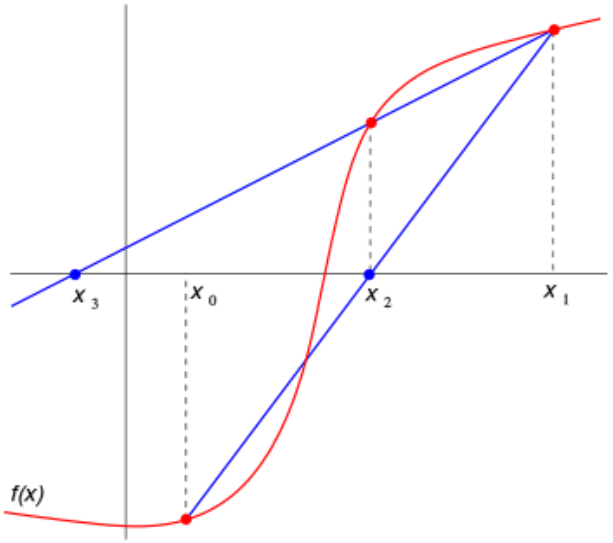
$$= \int d\varepsilon \frac{\rho(\varepsilon)-\rho(\omega+\mu-\Sigma(\omega))}{\omega+\mu-\varepsilon-\Sigma(\omega)} + \rho(\omega+\mu-\Sigma(\omega)) \log \frac{\omega+\mu-\Sigma(\omega)+\omega_{max}}{\omega+\mu-\Sigma(\omega)-\omega_{max}}$$

Smart solution works well!

- Optimization

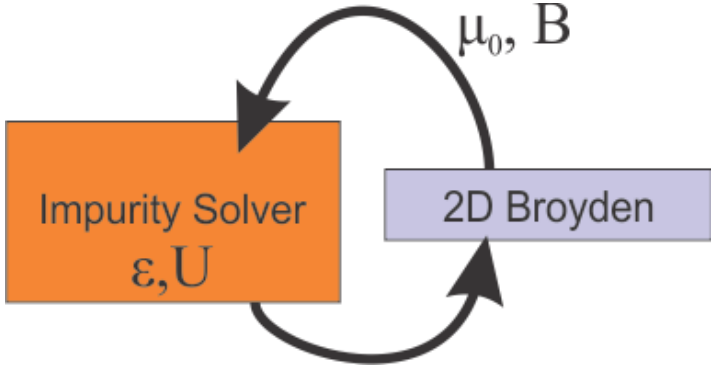
Solving systems of non-linear equations

Broyden solver – generalization of secant method in 1D



In some cases, solving SIAM = solving a system of 2 equations (2 parameters need to be fixed self-consistently)

Very fast, but can fail



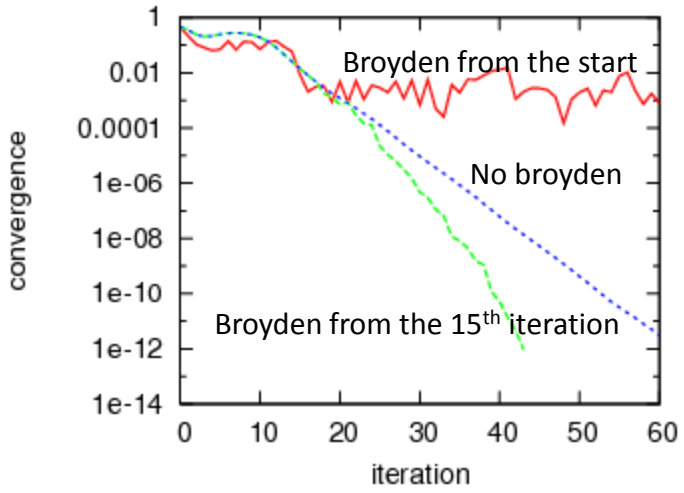
When Broyden fails, the procedure has to be restarted with another initial guess

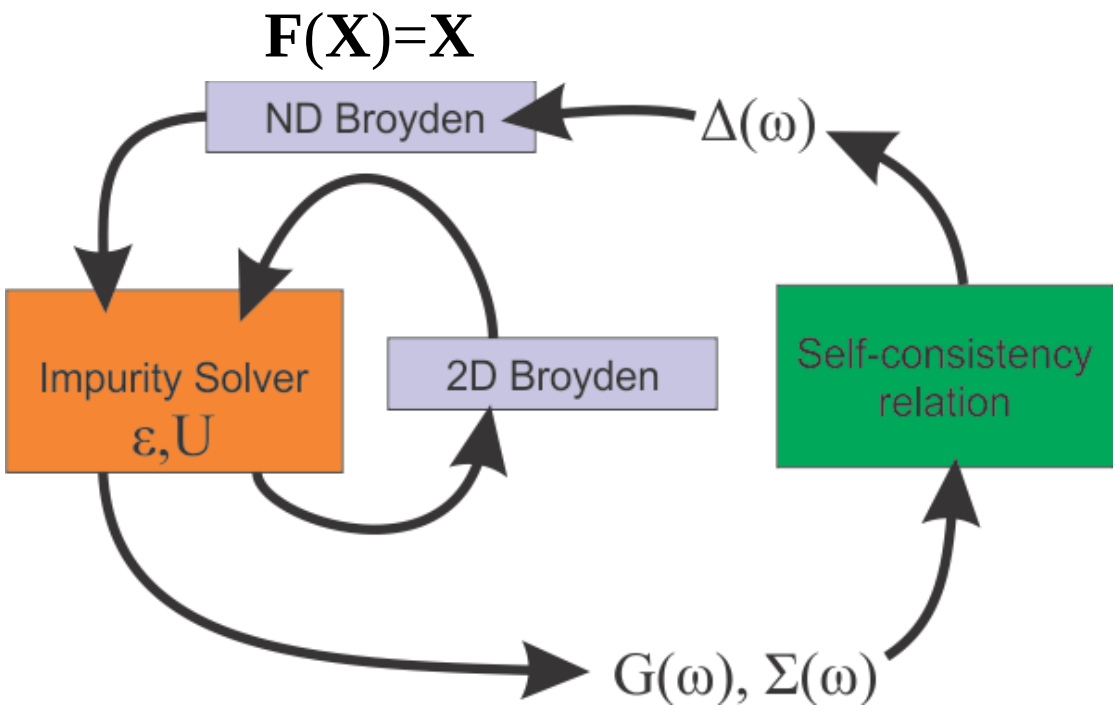
- Optimization

Speeding up the convergence of the DMFT loop

Rok Žitko, Phys. Rev. B 80, 125125 (2009)

Improved broyden –
"remembers" all previous iterations



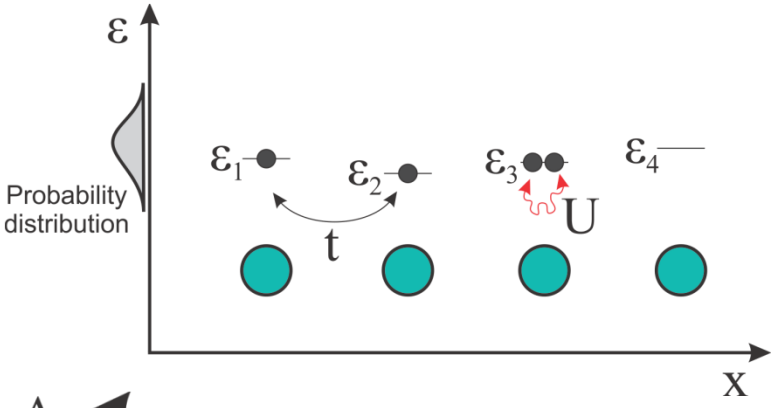


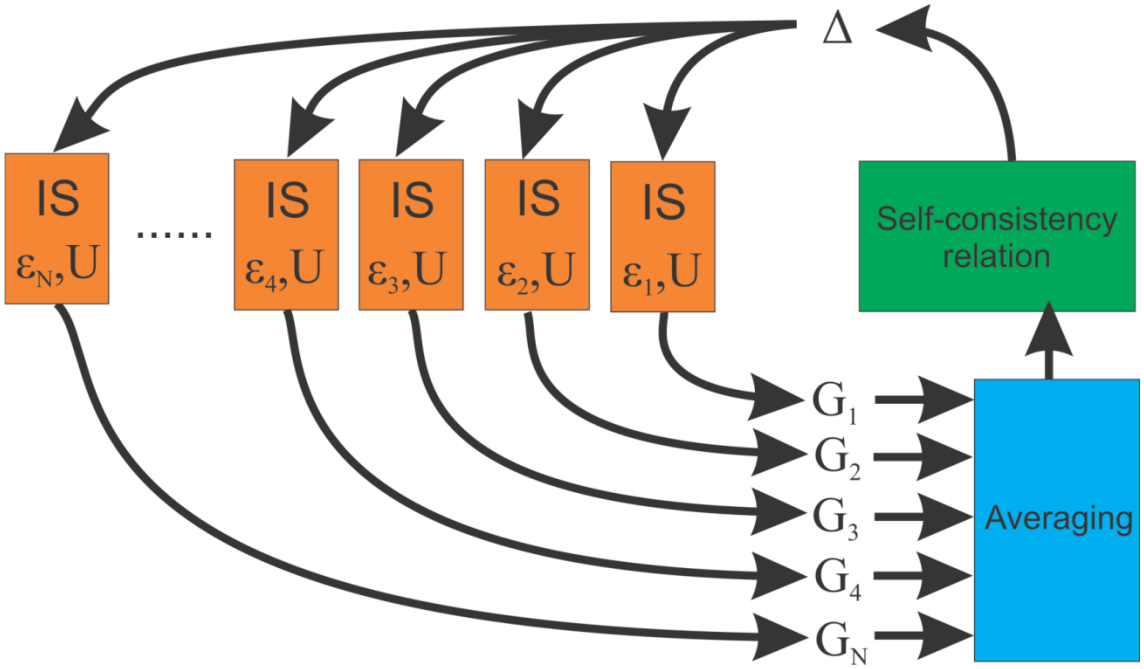
Should not be used from the start

- Application in Typical medium theory (TMT)

V. Dobrosavljević, Europhys. Lett. 62 76, (2003)

disordered Hubbard model



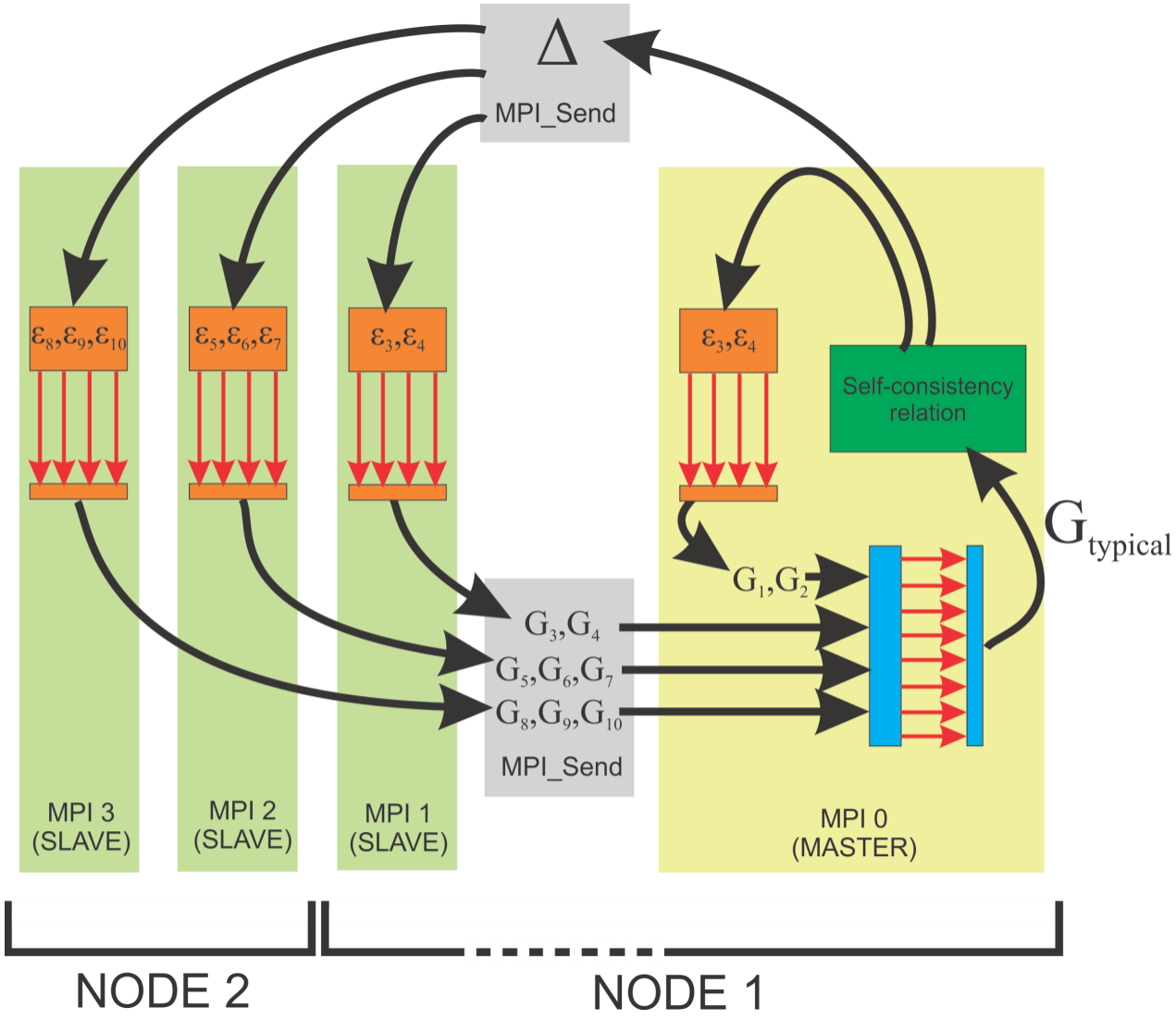


$$\mathrm{Im}G_{\mathrm{typ}}(\omega) = -\frac{1}{\pi} e^{\sum_i P(\varepsilon_i)\ln(-\pi \mathrm{Im}G_i(\omega))}$$

$$\mathrm{Re}G_{\mathrm{typ}}(\omega) = -\frac{1}{\pi}\int \frac{\mathrm{Im}G_{\mathrm{typ}}(\omega')}{\omega-\omega'}d\omega'$$

- Hybrid implementation of TMT

- This Example:
  - 4 MPI processes
  - 4 OpenMP threads per MPI process
  - solving 10 impurities



• Hybrid implementation of TMT

Tested on:
• 2 computational nodes of 8 cores (Intel Xeon E5405 @ 2.00GHz) interconnected by Infiniband
• Intel compiler (icpc)
• OpenMPI + Intel OpenMP

• This Example:
▪ 41 iterations for convergence
▪ U=0.1, T=0.1, W=0.3
▪ solving 32 impurities
▪ 2000 points in freq grid

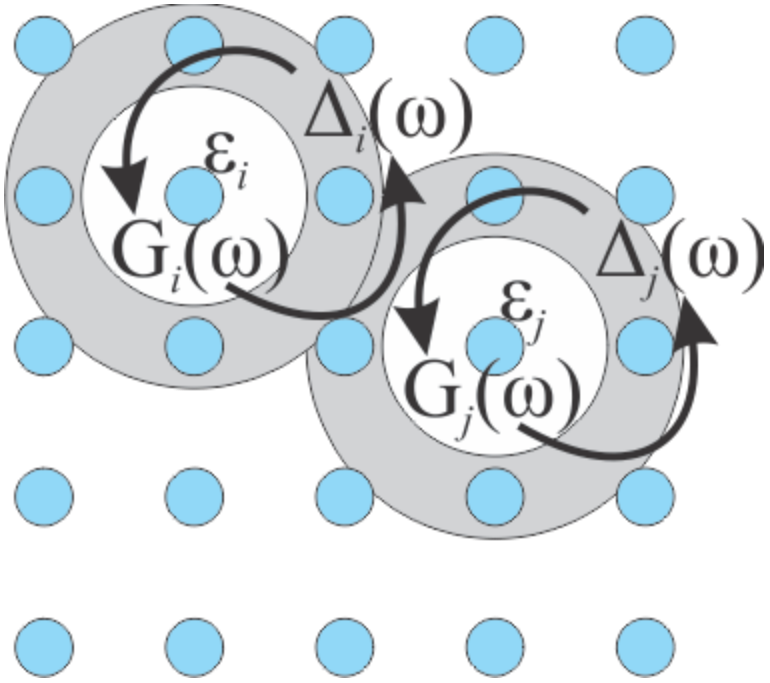
Number of MPI processes	Number of OpenMP threads per MPI process	Execution time [min:sec]
1	1	31:01
1	2	15:46
1	4	07:58
1	8	04:06
16	1	02:20
8	2	02:10
4	4	02:08
2	8	02:07

- Statistical (Inhomogeneous) DMFT

Deals with disorder in a more detailed way :

every lattice site is coupled to a different bath determined by green's functions of surrounding lattice sites

A step forward from the mean-field philosophy!

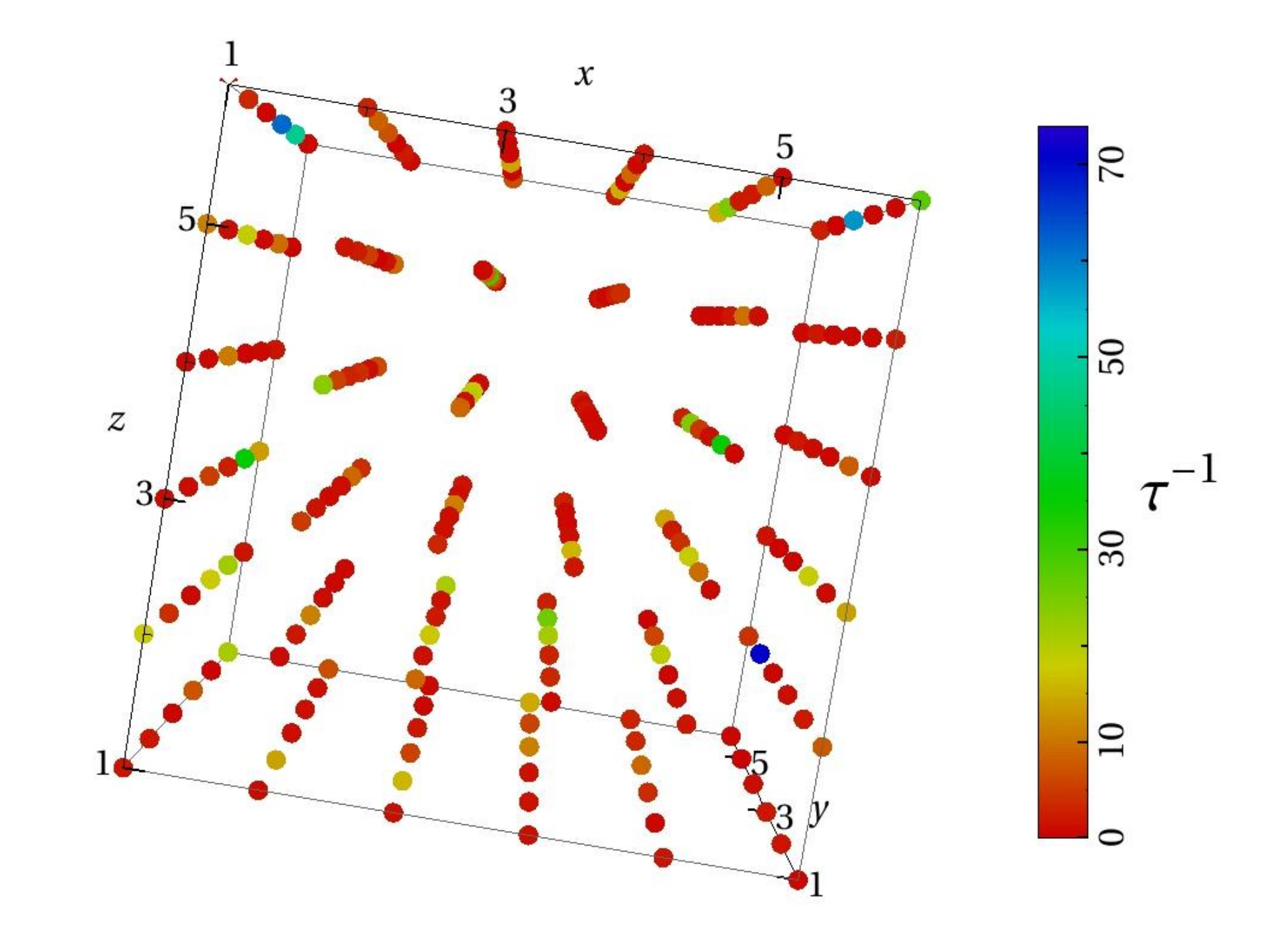


Finite dimensions and finite samples

Energies are randomized – many realizations are needed to get statistical averages

Large matrix inversion needs to be done in every iteration – MKL library routine does the job

Massive computation - would take months with CTQMC


1
3
5
x
5
3
1
z
1
5
3
y
70
50
30
10
0
τ^{-1}