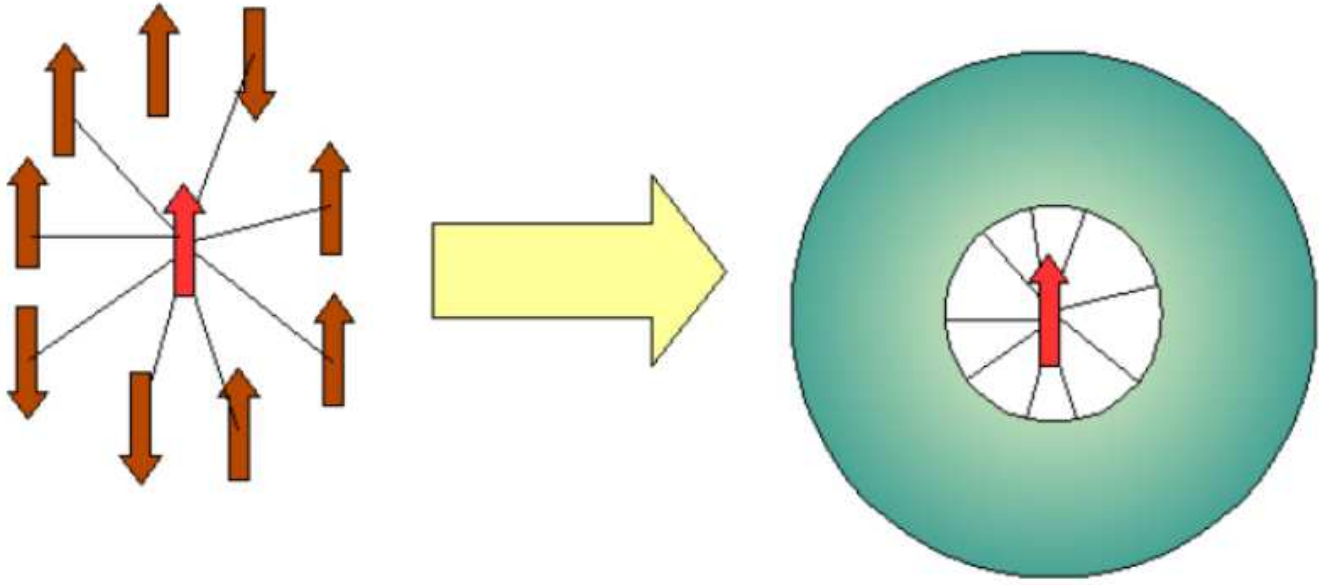
Dynamical Mean Field Theory

1 Weiss Mean Field Theory for spin systems

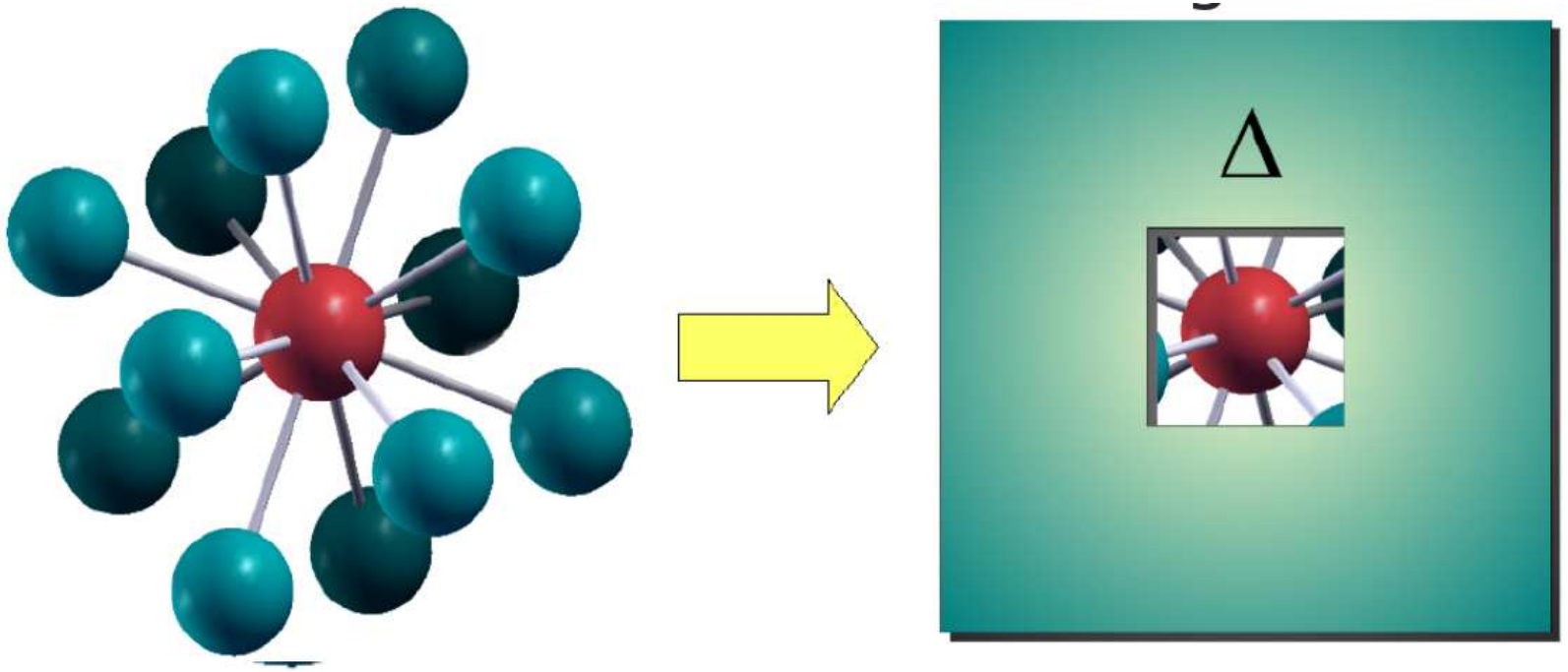


$$\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j$$

$$\sum_{i} \mathbf{B}_i\mathbf{S}_i$$

$$\mathbf{B}_i = \sum_{j\neq i} J_{ij}\langle \mathbf{S}_j \rangle$$

2 Mean Field Theory for Quantum systems (DMFT)



$$Z = \int \mathcal{D}[\psi^\dagger \psi] e^{-\sum_i S_{atom}(i) - \sum_{ij} \int d\tau \psi_i^\dagger(\tau) \hat{H}_{ij} \psi_j(\tau)}$$

$$Z = \int \mathcal{D}[\psi^\dagger \psi] e^{-\sum_i S_{atom}(i) - \sum_i \int d\tau d\tau' \psi_i^\dagger(\tau) \hat{\Delta}(\tau,\tau') \psi_i(\tau')}$$

3 Diagrammatic derivation of the Dynamical Mean Field Theory

To understand the scaling of potential and kinetic energy in large dimensions, let's consider the Hubbard Hamiltonian,

$$H = -\sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} \tag{1}$$

although the conclusion is quite general. Potential energy is purely local, hence it is of the order of unity per-site. The kinetic energy has to be of the same order of magnitude (for meaningful model in large dimensions), hence $\frac{1}{N}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}$ has to be of the order of unity. In the simplest cubic lattice we have

$$\varepsilon_{\mathbf{k}} = -2t(\cos(k_1) + \cos(k_2) + \cos(k_3) + \cdots) \tag{2}$$

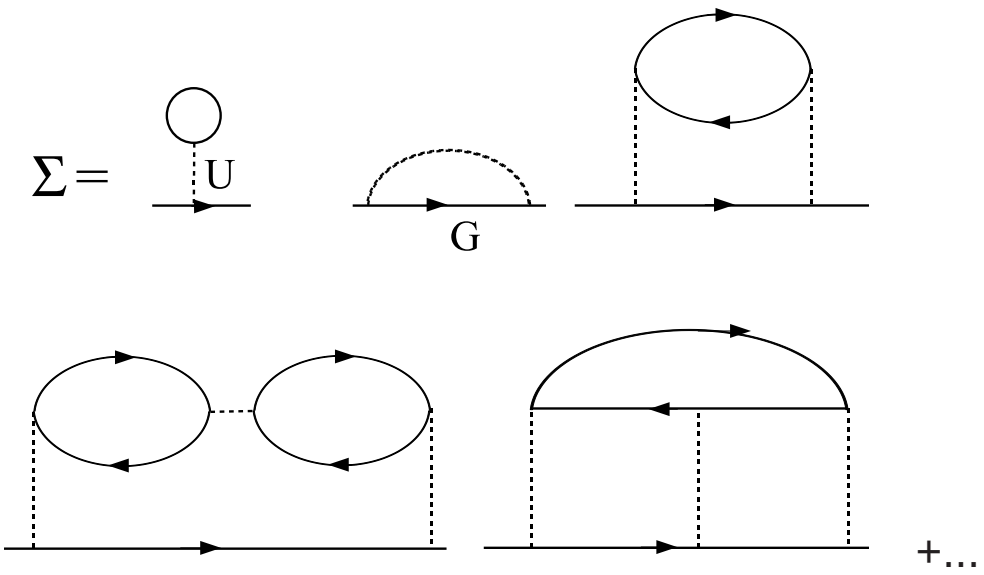
For a generic $\mathbf{k}$-point, the sign of $\cos$ terms is arbitrary and the sum of $\cos$ terms does not become of the order of d for large d. It rather scales as the length of the random walk, namely, as $\sqrt{d}$. For the kinetic energy to be of the order of unity, hopping matrix elements has to scale as $t \propto 1/\sqrt{d}$.

The non-local Green's function scales as $G_{ij} \propto t^{|i-j|}$, where $|i-j|$ is the distance between the two points in Manhattan matrix. Hence the local Green's function is of the order of unity, the nearest neighbor Green's function is of the order of $1/\sqrt{d}$, the next-nearest neighbor Green's function is of the order of $1/d$, etc.

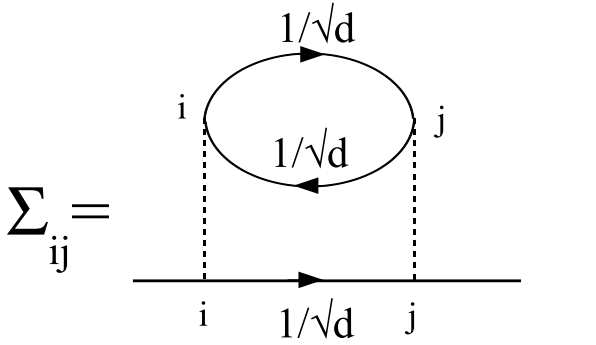
Let's consider the interacting problem on a lattice. For simplicity, we take only local interaction U, which leads to a Hubbard-like action

$$Z = \int \mathcal{D}[\psi^\dagger \psi] e^{-\sum_{i\sigma} \int_0^\beta d\tau \psi^\dagger_{i\sigma} (\frac{\partial}{\partial \tau} - \mu + H^0_{\mathbf{k}}) \psi_{i\sigma} - \sum_{i\sigma\sigma'} \int_0^\beta d\tau U_{iiii} \psi^\dagger_{i\sigma} \psi^\dagger_{i\sigma'} \psi_{i\sigma'} \psi_{i\sigma}} \quad (3)$$

and we consider all skeleton diagrams in the perturbation theory with respect to U. We consider the perturbation theory with fully dressed propagators G, where only skeleton diagrams enter. We obtain the following series



It turns out that all non-local contributions to the self-energy vanish at least as $1/\sqrt{d}$ in the limit of large d. Consider for example the lowest order non-local contribution, the second order diagram.

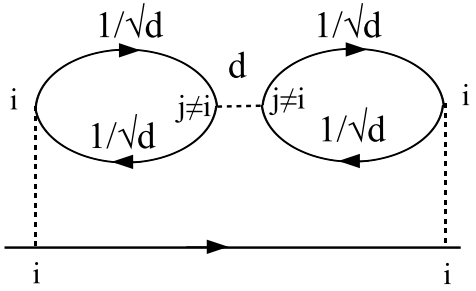


Total contribution: $d/d^{3/2}=1/\sqrt{d}$

Even for the nearest neighbors, the self-energy scales as $1/\sqrt{d}$, and vanishes in the large d limit.

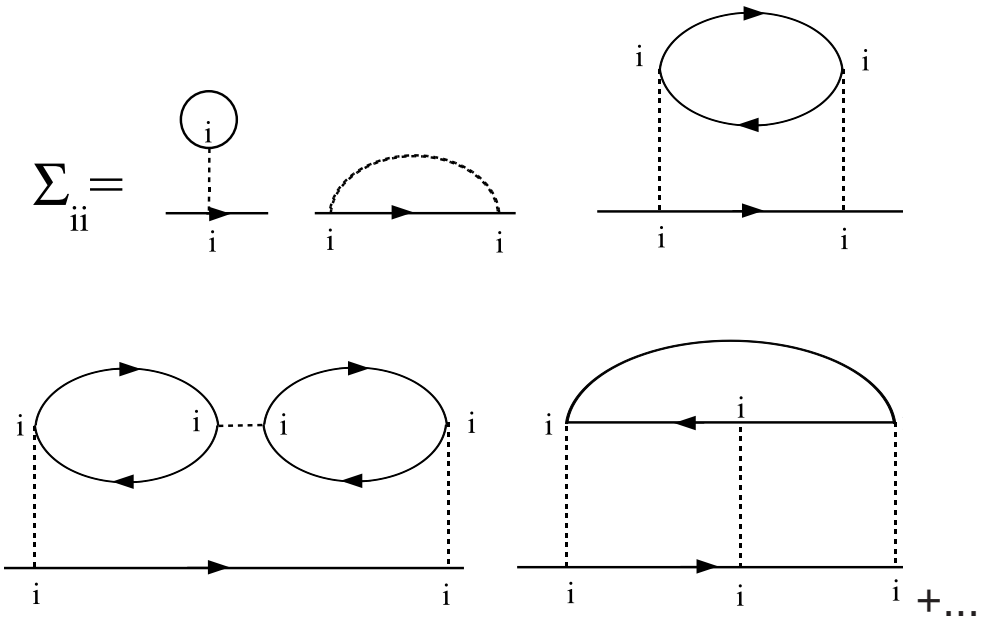
The local self-energy in the infinite d limit contain only local propagators. For example, the contribution to the local self-energy with non-local propagators vanishes at least as $1/\sqrt{d}$:

$\Sigma_{ii} =$



Total contribution: $d/d^2=1/d$

Hence, in the infinite-d limit, the self-energy contains all possible skeleteon diagrams, and the propagators are only the local propagators:



If the interaction is non-local, one can show that similarly all diagrams but the Hartree-Fock (first order term in U) become local in the large d limit, and those diagrams can be computed from the local propagator only.

There are infinite number of diagrams even in the large d limit, and they can not be evaluated order by order. In the Mott insulating state, even very high order diagrams diverge, hence the perturbation series can not be truncated.

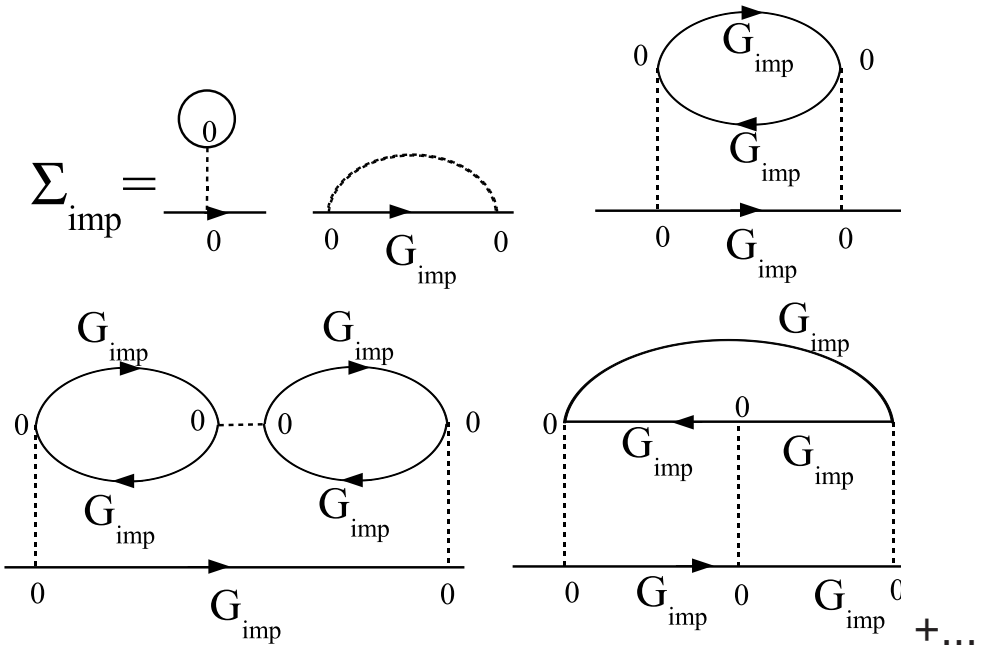
The trick is to find a quantum mechanical problem, which is (numerically) tractable, and in its solution, becomes equivalent to our original infinite d lattice problem. It turns out that the

equivalent problem is the quantum impurity problem.

Let's consider the quantum impurity problem

$$Z = \int \mathcal{D}[\psi^\dagger \psi] e^{-\sum_{i\sigma} \int_0^\beta d\tau \psi^\dagger_{i\sigma}(-G^{-1}_{0,imp})\psi_{i\sigma} - \sum_{i\sigma\sigma'} \int_0^\beta d\tau U_{iiii} \psi^\dagger_{i\sigma} \psi^\dagger_{i\sigma'} \psi_{i\sigma'} \psi_{i\sigma}} \quad (4)$$

The skeleton perturbation theory in interaction U leads to the following set of diagrams



Since we expand in terms of fully dressed propagators G_{imp} (and consider only skeleton diagrams), the propagator is

$$G^{-1}_{imp} = G^{-1}_{0,imp} - \Sigma \quad (5)$$

If we make sure that G_{imp} is the same as the local Green's function G_{ii} above, the resulting impurity self-energy is obviously equal to our desired local self-energy of the original lattice problem. If we have a method to solve the quantum impurity problem with arbitrary propagator, we can obviously solve lattice problem in the infinite d limit.

We just explained the basic DMFT equation

$$\Sigma_{ii}^{DMFT} = \Sigma_{imp}[G_{imp} \leftarrow G_{ii}] \tag{6}$$

In a translational invariant case, the DMFT self-consistency condition is

$$G_{imp} \equiv \frac{1}{\omega - E_{imp} - \Sigma_{imp} - \Delta} = G_{ii} \equiv \sum_{\mathbf{k}} \frac{1}{\omega + \mu - H^0_{\mathbf{k}} - \Sigma_{ii}} \tag{7}$$

and $\Sigma_{ii} = \Sigma_{imp}$.

By definition, the hybridization $\Delta(\omega)$ falls off at large frequency, and hence the impurity levels can be obtained by the high frequency expansion of both sides of the equation:

$$\frac{1}{\omega} + \frac{E_{imp} + \Sigma_\infty}{\omega^2} + \cdots = \sum_{\mathbf{k}} \frac{1}{\omega} + \frac{-\mu + H^0_{\mathbf{k}} + \Sigma_\infty}{\omega^2} + \cdots \tag{8}$$

hence $E_{imp} = -\mu + \sum_{\mathbf{k}} H^0_{\mathbf{k}}$.

4 General formulation

For a most general formulation of the DMFT problem, it is convenient to introduce the concept of the Luttinger-Ward functional. The Luttinger-Ward functional $\Gamma[G]$ is a functional of the fully dressed Green's function, and is extremized when G is the exact solution of the problem. When Γ is evaluated on the exact G, it gives the free energy of the system.

The Luttinger-Ward functional takes the form

$$\Gamma[G] = \mathrm{Tr}\log G - \mathrm{Tr}(\Sigma G) + \Phi[G] \tag{9}$$

where $\Phi[G]$ is the sum of all possible two particle irreducible skeleton diagrams obtained by the bare Coulomb interaction U and fully dressed propagator G.

The variation of functional Γ with respect to G is

$$\frac{\delta\Gamma}{\delta G} = \delta G G^{-1} - \Sigma\delta G - \delta G\frac{\delta\Sigma}{\delta G}G + \frac{\delta\Phi[G]}{\delta G}\delta G. \tag{10}$$

Here G obeys the Dyson equation $G^{-1} = G_0^{-1} - \Sigma$, hence

$$\delta G G^{-2} = -\delta G\frac{\delta\Sigma}{\delta G} \tag{11}$$

since G_0 is the non-interacting propagator and does not depend on Σ and does not vary with G.

Inserting above, we obtain

$$\frac{\delta\Gamma}{\delta G} = (-\Sigma + \frac{\delta\Phi[G]}{\delta G})\delta G \tag{12}$$

which requires that

$$\Sigma = \frac{\delta\Phi[G]}{\delta G}. \tag{13}$$

Since the functional derivative of $\delta\Phi[G]/\delta G$ amounts to cutting a propagator in Φ in all possible ways, the resulting self-energy is the sum of all possible skeleton graphs constructed from the fully dressed green's function G and bare interaction U. This is clearly the exact self-energy of the problem.

The DMFT is an approximation to this exact Luttinger-Ward functional $\Gamma[G]$.

The DMFT approximates the $\Phi[G]$ functional with the sum of all (skeleteon and two particle irreducible) *local diagrams* rather then *all diagrams*. We therefore have

$$\Gamma_{DMFT}[G] = \mathrm{Tr}\log G - \mathrm{Tr}(\Sigma G) + \Phi[G_{ii}] \tag{14}$$

Self-energy is obviously

$$\Sigma_{ij} = \delta_{i=j} \frac{\delta \Phi[G_{ii}]}{\delta G_{ii}}, \tag{15}$$

and can be computed from the corresponding impurity problem, which has a functional

$$\Gamma_{imp}[G_{imp}] = \mathrm{Tr} \log G_{imp} - \mathrm{Tr}(\Sigma_{imp} G_{imp}) + \Phi[G_{imp}] \tag{16}$$

and obeys the relation

$$\Sigma_{imp} = \frac{\delta \Phi[G_{imp}]}{\delta G_{imp}} \tag{17}$$

If $G_{imp} = G_{ii}$ we have $\Sigma_{imp} = \Sigma_{ii}$, and we were able to relate the DMFT self-energy to the solution of the impurity problem.

5 One band model

In the case of a one-band model, we can express the self-consistency condition in terms of the density of states, i.e.,

$$\frac{1}{\omega - E_{imp} - \Sigma - \Delta} = \int d\epsilon \frac{D(\epsilon)}{\omega + \mu - \epsilon - \Sigma} \tag{18}$$

hence only the density of states matters in the large dimensional limit (it turns out that different lattices can have the same density of states in finite dimensions, the effect which is clearly beyond DMFT).

Among all latices, the simplest DMFT equations turn out to be for the so-called Bethe lattice, which is characterized by the semicircular density of states

$$D(\epsilon) = -2/\pi \sqrt{1 - \epsilon^2} \tag{19}$$

It is easy to obtain a close expression for the Hilbert transform of the Bethe lattice density of states:

$$w(z) = \int d\epsilon \frac{D(\epsilon)}{z - \epsilon} = 2(z - \sqrt{z^2 - 1}) \tag{20}$$

The local green's function on the Bethe lattice is thus equal to

$$G = 2(z - \sqrt{z^2 - 1}) \tag{21}$$

with $z = \omega + \mu - \Sigma$. The self-consistency condition becomes

$$2(z - \sqrt{z^2 - 1}) = \frac{1}{\omega + \mu - \Sigma - \Delta} = \frac{1}{z - \Delta} \tag{22}$$

and the expression for Δ is

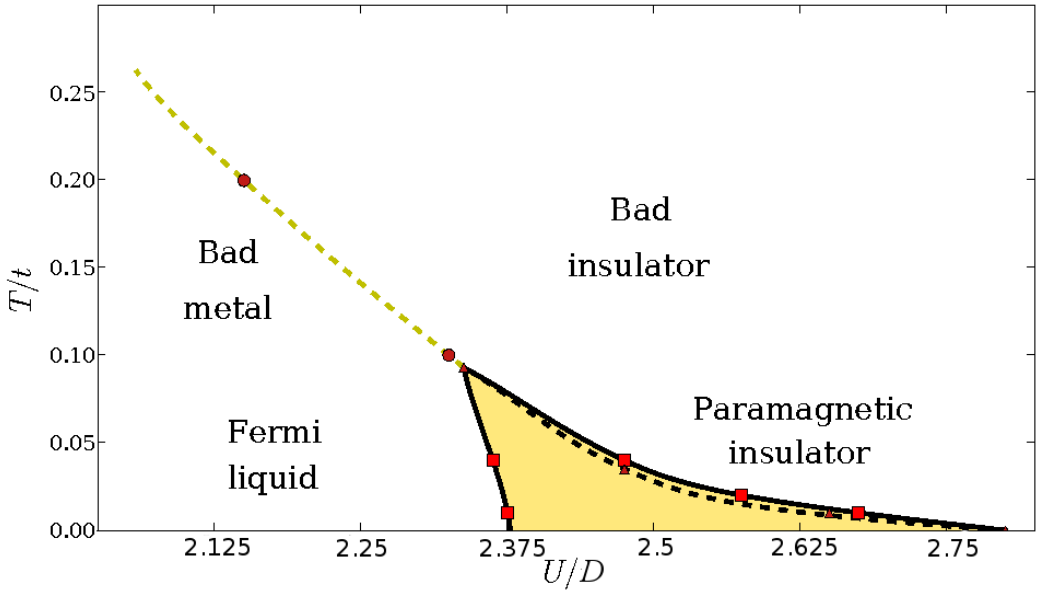
$$\Delta = \frac{1}{4} 2(z - \sqrt{z^2 - 1}) \tag{23}$$

or

$$\Delta = \frac{1}{4} G_{ii} \tag{24}$$

and $E_{imp} = -\mu$.

The phase diagram of the DMFT (here for the 2D-square lattice) is:


0.25
0.20
0.15
0.10
0.05
0.00
T/t
Bad
metal
Bad
insulator
Fermi
liquid
Paramagnetic
insulator
2.125
2.25
2.375
2.5
2.625
2.75
U/D

Homework:

- Download the code from

  `http://www.physics.rutgers.edu/~haule/681/src_CTQMC/`

- Compile the source code in subdirectory `src`
- Check the script `iterate.py` in the `run` subdirectory. The script properly runs the code creating necessary input files.
- Change parameters U and mu to sketch the phase diagram of the one band Hubbard model in $D \to \infty$ limit. Since we are interested in the phase diagram of the half-filled model, mu should be always equal to $U/2$.
  - Verify that for $U = 2.4$ and $mu = 1.2$ and $beta = 100$ two different solutions are possible (coexistance of solutions)
  - Slowly increase U and check when the metallic solution disappears.
  - Slowly decrease U and check when insulating solution dissapears.
  - Sketch the region where the two solutions coexist.
  - Increase temperature and find the coexistence region for few temperatures.