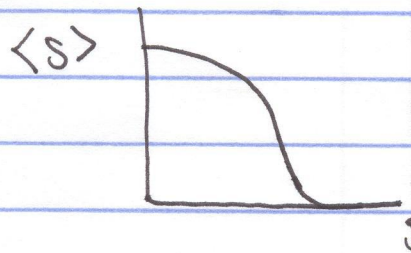
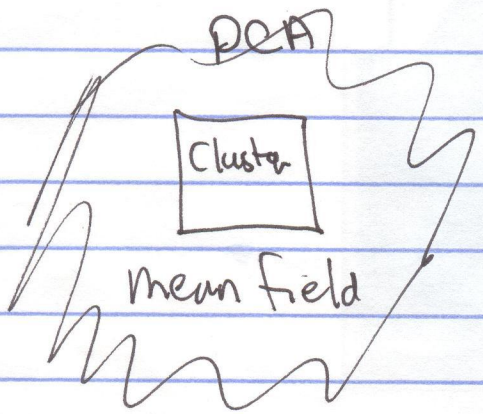
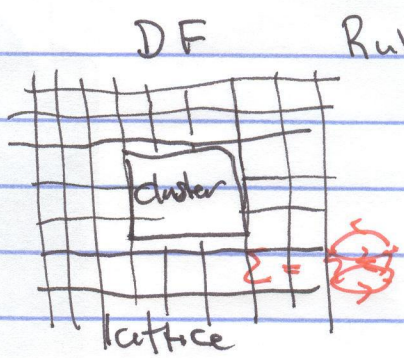
Nonlocal extensions to DMFT

Several attempts have been made to develop systematic extensions to DMFT. These include quantum cluster methods such as the DCA and CDMFT. These methods map the lattice onto a self consistently embedded periodic and open cluster, respectively. However these methods suffer from the minus sign problem or other exponential scaling of the cluster solver.



Several attempts, including V. Janis' cumulant method, the DTA, the MSMB, and the dual fermion method have been proposed. They differ from the DCA





In that while DCA projects the lattice onto a periodic "impurity" embedded in a mean field, the DF method

Maps the lattice onto an impurity embedded in a correlated lattice which is treated with Feynman diagram methods.

To derive the DF formalism we start with an action with a local interaction

$$S(c^* c) = \sum_{\omega k \sigma} (\epsilon_k - \mu - i\omega) c^*_{\omega k \sigma} c_{\omega k \sigma} + \sum_i S_{loc}(c_i^*, c_i)$$

where, e.g.,

$$S_{loc}(c_i^*, c_i) = U \int_0^\beta n_{i\uparrow\tau} n_{i\downarrow\tau} \, d\tau$$

for a Hubbard interaction, and ϵ_k is the bare dispersion of the model.

Our goal is to express S in terms of the DMFT action, so we will introduce an arbitrary (as yet) hybridization function $\Delta(\omega)$ and a corresponding impurity action

$$S_{imp} = -\sum_{\omega\sigma} (\Delta_\omega - \mu - i\omega) c^*_{i\omega\sigma} c_{i\omega\sigma} + \sum_i S_{loc}(c_i^* c_i)$$

where now $c_{i\sigma}^*, c_i$ are the impurity operators or grassmann numbers. We assume that the impurity problem is fully solvable for the one and 2 particle Green functions and vertices.

We now add and subtract Δ from terms in S so that we may write

$$S(c^*,c) = \sum_i S_{imp}(c_i^* c_i) - \sum_{wk\sigma} (\Delta_w - \epsilon_k) c^*_{wk\sigma} c_{wk\sigma}$$

Now the dual variables are introduced via the Gaussian identity

$$\int_{f^*f} \exp\left\{ -f^*_\alpha a_{\alpha\beta} f_\beta - f^*_\alpha b_{\alpha\beta} c_\beta - c^*_\alpha b_{\alpha\beta} f_\beta \right\}$$

$$= \det a \exp\left\{ c^*_\alpha (b a^{-1} b)_{\alpha\beta} c_\beta \right\}$$

We apply this to the partition function

$$Z = \int_{c^*c} \exp\left\{ -S(c^*,c) \right\}$$

Specifically, we choose a & b to be diagonal

$$a_{wk\sigma} = \bar{g}^{-2}(iw)\left[\Delta(iw) - \epsilon_k\right]^{-1}$$

$$b_{wk\sigma} = \bar{g}^{-1}(iw) = iw + \mu - \Sigma_{imp}(iw) - \Delta(iw)$$

where $\bar{g}(iw)$ is the impurity single particle Green function. Now S takes the form

$$S(c^*c f^*f) = \sum_k S_{rest}(c^*c\, f^*f) + \sum_{wk\sigma} \frac{f^*_{wk\sigma} f_{wk\sigma}}{\bar{g}^2(iw)\left[\Delta(iw) - \epsilon_k\right]}$$

where now

$$Z = \int_{\substack{c^*c \\ f^*f}} \exp\left\{S(c^*c\, f^*f)\right\}^*$$

and S_{rest} is the part of the action restricted to the cluster or impurity

$$S_{rest}(c^*c\, f^*f) = S_{imp}(c_i^* c_i) + \sum_{\omega\sigma} f^*_{\omega\sigma i}\, \tilde{g}^{-1}(i\omega)\, c_{\omega\sigma i} + h.c.$$

The mapping to the dual degrees of freedom is completed by integrating out the impurity degrees of freedom. Since S_{rest} is independent of k, this may be done individually for each site i, i.e., each "impurity"

Let's just perform this part of the path integral above*

$$\frac{1}{Z_{imp}} \int_{c^*c} \exp\left\{-S_{rest}(c^*c)\right\} = \exp\left\{-\sum_{\omega\sigma} f^*_{\omega\sigma}\, \tilde{g}^{-1}(i\omega)\, f_{\omega\sigma} - V(f^*f)\right\}$$

which defines a dual potential V.

V may be calculated by expanding this part of the action and comparing terms on the left & right hand sides order by order. It is given by

$$V(f^* f) = \frac{1}{4} \sum_{\substack{\omega \omega' \nu \\ \sigma_1 \cdots \sigma_4}} \Gamma^{\sigma_1 \sigma_2 \sigma_3 \sigma_4}(i\omega\, i\omega'\, i\nu) \times f^*_{\omega+\nu\,\sigma_1} f_{\omega \sigma_2} f^*_{\omega' \sigma_3'} f_{\omega'+\nu\,\sigma_4}$$

(impurity full (2pi) vertex)

$$+ \cdots$$

where n-body terms, for $n > 2$, have been neglected.

Now the partition function

$$Z = Z_{imp} \int_{f^* f} \exp\left\{ - S_d(f^* f) \right\}$$

where

$$S_d(f^* f) = - \sum_{k \omega \sigma} f_{\omega k \sigma} G_d^{\circ\,-1}(k, i\omega) f_{\omega k \sigma} + \sum_i V_i (f^* f)$$

and

$$G_d^{\circ}(k, i\omega) = \frac{\bar{g}^2(i\omega)}{\bar{g}(i\omega) + (\Delta(i\omega) - \epsilon_k)^4}$$

If we take the lattice and impurity Green functions of the form

$$G_{\mathbf{k}} = \frac{1}{i\omega - \epsilon_{\mathbf{k}} + \mu - \Sigma(i\omega)}$$

$$G_{imp} = \frac{1}{i\omega + \mu - \Delta(i\omega) - \Sigma(i\omega)} \equiv \bar{g}(i\omega)$$

where $\Sigma(i\omega)$ is the impurity self energy, then

$$G_{\mathbf{k}}^{0} = G_{\mathbf{k}} - \bar{g}$$

Thus far Δ is unknown. We will fix it by requiring that

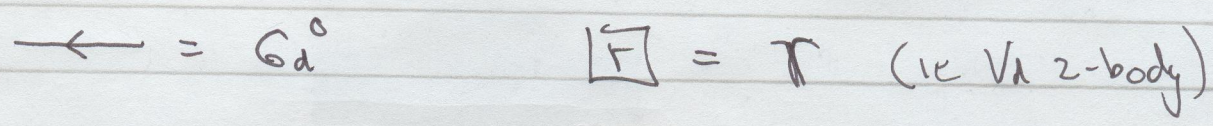
$$G_{\mathbf{k}}^{0}(i\omega) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}^{0}(\mathbf{k}, i\omega) = 0$$

which is the course graining identity for DMFT. I.e. when self consistency is obtained in the DMFT

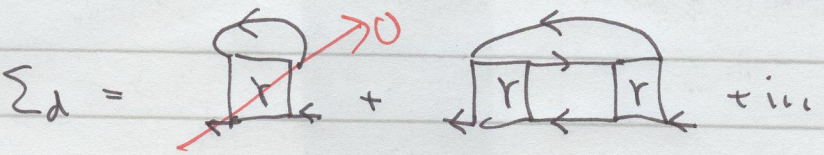
$$\frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{i\omega - \epsilon_{\mathbf{k}} + \mu - \Sigma(i\omega)} = \frac{1}{i\omega + \mu - \Delta(i\omega) - \Sigma(i\omega)}$$

$$= \bar{g}(i\omega)$$

This has important consequences for the dual fermion diagrammatics. For example, if



Then for the Hubbard model



The first, Hartree, term is zero since Γ is k independent (its local!) and so it involves a free sum on k of G_d^0 which is zero. As is $\Sigma^{(1)}$ etc.

Another consequence is that since G_d^0 is the difference of two proper Green function the dual variables have a Grassmann algebra but they are not fermions! For fermions, we have shown that

$$G(k,\omega) \sim \frac{\{c_k c_k^\dagger\}}{\omega} \sim \frac{1}{\omega}$$

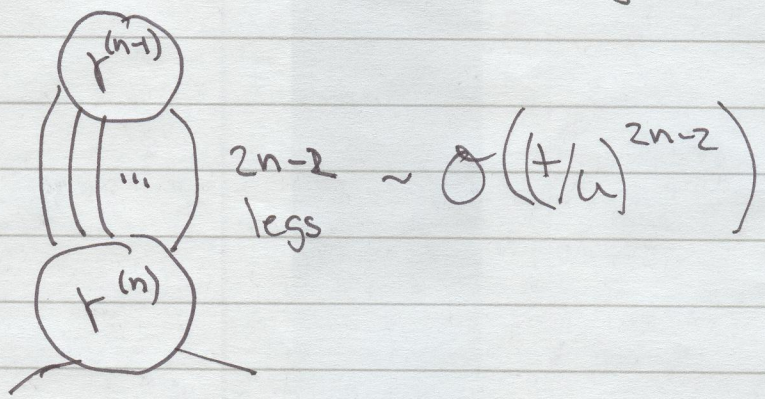
But G_d^0 is the difference of two terms each $\sim 1/\omega$, a property which is inherited by the dressed G_d

One consequence of this is that, in the strong coupling limit $t/u \to 0$ (or high D)

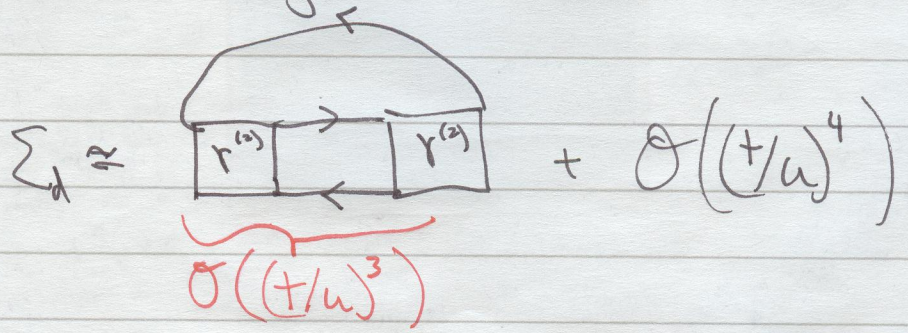
$$G_d^\circ = G(k,\omega) - \bar{g} \sim t/u$$

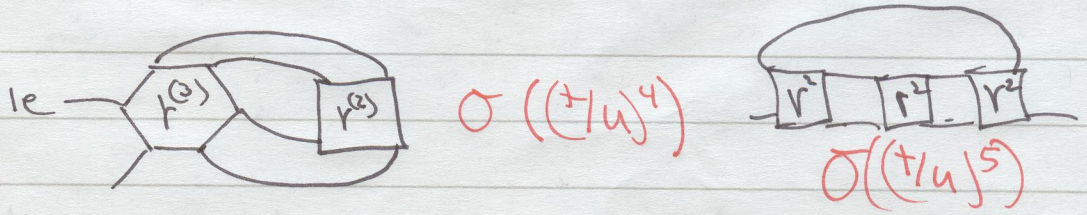
As a result the dual "fermion" pertubation theory converges quickly.

First n-body corrections are negligible in the strong coupling limit. Consider the leading n-body correction to Σ_d



Second low order perturbation theory should be good as well

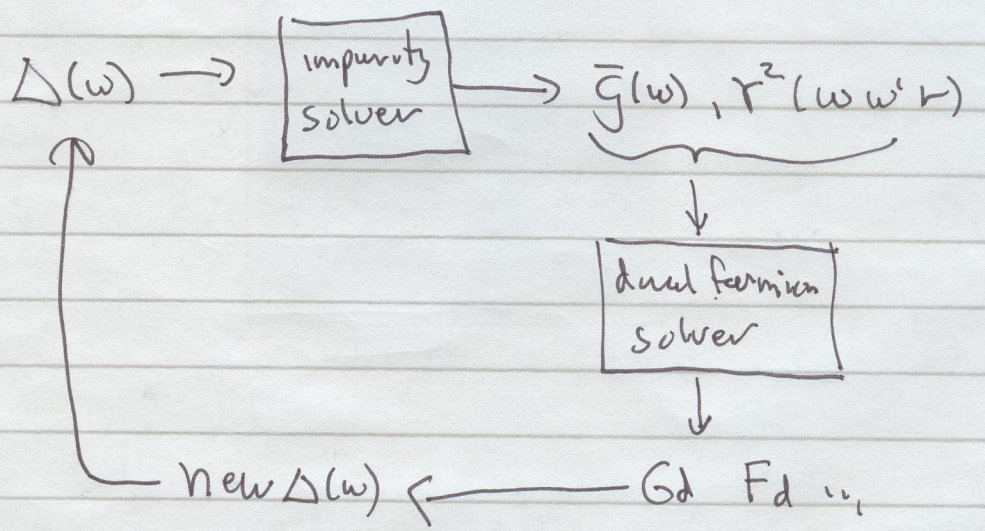




To map back to the real fermion lattice problem we take functional derivatives of Σ to get G and find that

$$F^{KK'q}_{\omega\omega'\nu} = T(k+q, i\omega+i\nu)\, T(k, i\omega) \times F^{d\,KK'q}_{\omega\omega'\nu} \times T(k', i\omega')\, T(k'+q, i\omega'+i\nu)$$

where $$T(k i\omega) = -\left\{1 + \bar{g}(i\omega)\, \Sigma_d(k, i\omega)\right\}^{-1}$$

$$G(k i\omega) = T(k i\omega)\, G_d(k i\omega)$$

So the Rubtsov dual fermion algorithm is