1 Review of DCA

Big picture goal is to calculate interacting Green's function for some Hamiltonian

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

$$\begin{aligned} G_\sigma(\tau) &= -\left\langle \mathcal{T} c_\sigma(\tau) c^\dagger_\sigma(0) \right\rangle \\ &= -\frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} c_\sigma(\tau) c^\dagger_\sigma(0) \right] \quad \tau > 0 \end{aligned}$$

Diagonalize matrix t_{ij} to get kinetic energy eigenvalues ϵ_k. Originally,

$$\begin{aligned} G_{\mathrm{loc}}(i\omega_n) &= \frac{1}{N} \sum_k G(k, \omega_n) \\ &= \frac{1}{N} \sum_k \frac{1}{i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon_k} \end{aligned} \tag{1}$$

where

$$\omega_n = (2n+1)\pi T.$$

Suppose hopping $t = 1$ and $T = 0.05 = 1/20$. Roughly $n \sim 10^2$ to 10^3 (in DMFT!). In DCA G_0 also depends on the k-mode (as many k modes as sites in the cluster, N_{sites}), so could be another factor of $N_{\mathrm{sites}} \sim 32$ maybe.

In terms of a density of states,

$$G_{\mathrm{loc}}(i\omega_n) = \int_{-\infty}^{+\infty} d\epsilon \, \frac{\rho_0(\epsilon)}{i\omega_n + \mu - \Sigma(i\omega_n) - \epsilon}.$$

Define free cluster noninteracting Green's function

$$G_0^{-1}(i\omega_n) = G_{\mathrm{loc}}^{-1}(i\omega_n) + \Sigma(i\omega_n) \tag{2}$$

$$G_0(\tau) = \frac{1}{\beta} \sum_n e^{i\omega_n \tau} G_0(i\omega_n) \tag{3}$$

Workflow. Phase one, DCA self-consistency loop, which converges interacting $G(i\omega_n)$

1. CT-AUX maps $G_0(i\omega_n), U$ to $G_{\mathrm{imp}}(i\omega_n)$ [Simplification here, we are neglecting k-dependence]. At self-consistency we will find $G_{\mathrm{loc}} = G_{\mathrm{imp}}$.
2. Given G and G_0, solve the Dyson equation (2) for $\Sigma(i\omega_n) = G_0^{-1}(i\omega_n) - G_{\mathrm{imp}}^{-1}(i\omega_n)$ (definition for Σ *if* $G_{\mathrm{loc}} = G_{\mathrm{imp}}$).
3. Given Σ can calculate G_{loc} from (1) and then G_0 from (2).

Phase two: Analytically continue to real time, $G(\tau) \to G(t)$, to connect with time-dependent observables.

2 SLMC

We have

$$N_{i,j}^{-1} = N^{-1}(\tau_i, \tau_j)$$

Note that N^{-1} is *not* generally a function of $\tau_i - \tau_j$ because the vertex interactions $e^{V_\sigma\{s\}}$ couple locally to the vertices in a "local" way (local in imaginary time.)

It will be interesting to construct Fourier transform and plot magnitude of matrix elements. Do we find the diagonal elements to be much larger than off-diagonal ones? If so, it would perhaps justify the translation invariant ansatz of Nagai et al and suggest a starting point for a perturbation expansion. Here is the necessary formula

$$N_{\omega_n,\omega_m}^{-1} = \sum_{i,j} e^{-\iota(\omega_n \tau_i - \omega_m \tau_j)} N^{-1}(\tau_i, \tau_j)$$

If $N_{\omega_n,\omega_m}^{-1}$ were perfectly diagonal then we would be done. The diagonal elements would be the eigenvalues, and we could multiply them all together to get the determinant. It probably won't be that easy.

3 Perturbation expansion

What about trying to construct a perturbation expansion. Let $N^{-1} = A + B$ where A denotes the diagonal part and B is whatever is left over (hopefully small). To first approximation, presumably

$$\det N^{-1} = \det(A + B) \approx \det A.$$

Now let's try to get a correction.

Might be useful to work with an action

$$\det N^{-1} = e^{-S}$$

where

$$S = -\mathrm{Tr}\, \ln N^{-1} = -\mathrm{Tr}\, \ln\left(A + B\right).$$

Assuming A is invertible, we can write

$$A + B = A(I + A^{-1}B),$$

such that

$$S = -\mathrm{Tr}\, \ln A - \mathrm{Tr}\, \ln\left(I + A^{-1}B\right).$$

If indeed $A^{-1}B$ is small (and this could likely be a bad assumption!) then we can Taylor expand in powers of this matrix. At the scalar level,

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \ldots$$

This should also work for matrices,

$$\ln\left(I + A^{-1}B\right) \approx A^{-1}B - \frac{\left(A^{-1}B\right)^2}{2} + \ldots,$$

This gives

$$S = -\mathrm{Tr}\,\ln A - \mathrm{Tr}\left(A^{-1}B - \frac{\left(A^{-1}B\right)^2}{2} + \ldots\right).$$

Since A was constructed to be diagonal, we get some simplifications. We can immediately calculate A^{-1} which is also diagonal. Then note that

$$\mathrm{Tr}\,A^{-1}B = \sum_{ij} A^{-1}_{ij} B_{ji},$$

where matrix indices ij presumably represent Matsubara modes?

If B has *no* diagonal part (again, by construction) then this term is identically zero. So we are left with

$$S = -\mathrm{Tr}\,\ln A + \mathrm{Tr}\,\frac{\left(A^{-1}B\right)^2}{2} + \mathcal{O}(B^3).$$

The second term can be efficiently calculated since A^{-1} is assumed to be diagonal.