Continuous-time auxiliary-field quantum Monte Carlo (CT-AUX)

It is the "state of the art" method to solve the effective cluster problem in DCA & DCA$^+$ calculations.

Really useful for large cluster calculations of single-band Hubbard model.

Consider a generalized Hubbard model given by:

$$H = \underbrace{\sum_{ij,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - \mu \sum_{\mu} n_{\mu} + \frac{1}{2} \sum_{\mu\nu} U_{\mu\nu}(n_{\mu}+n_{\nu})}_{H_0 \text{ (non-interacting)}} + \underbrace{\sum_{\mu\nu} U_{\mu\nu}\left[n_{\mu}n_{\nu} - \frac{1}{2}(n_{\mu}+n_{\nu})\right]}_{H_{int} \text{ (interacting)}}$$

where i,j span all sites & orbitals

μ,ν are combined indices of spin, orbital, & site — i.e, two spin-orbitals that do interact?

the sum $\sum_{\mu\nu}$ is carried over all pairs of correlated spin-orbitals ($U_{\mu\nu} \neq 0$)

N_{corr} is the number of correlated spin-orbital pairs

For the single-band Hubbard model, $N_{corr} = N_c$, where N_c is the number of sites.

In the interaction picture: $H = H_0 + H_{int}$, & the partition fn. becomes:

$$Z = \mathrm{Tr}\, e^{-\beta H}$$

$$= \mathrm{Tr}\left[e^{-\beta H_0} e^{-\beta H_{int}}\right] \quad \rightarrow \text{try understanding this.}$$

$$Z = e^{-K} \mathrm{Tr}\left[e^{-\beta H_0} T_{\tau}\, e^{-\int_0^{\beta} d\tau \left(H_{int} - \frac{K}{\beta}\right)}\right.$$

where K is a parameter controlling the expansion order.

Thesis

The Hubbard Hamiltonian, shifted such that $\mu = 0$ denotes half-filling is:

zero or one

$$H = -t\sum_{\langle i,j\rangle}\left(c_i^{\dagger}c_j + c_j^{\dagger}c_i\right) + \underbrace{U\sum_i\left(n_{i\uparrow}n_{i\downarrow} - \frac{n_{i\uparrow}+n_{i\downarrow}}{2}\right)}_{H_U \text{ (interaction part)}} - \mu\sum_i\left(n_{i\uparrow}+n_{i\downarrow}\right)$$

H_0 (non-interacting)

Can add / subtract constant to the Hamiltonian such that the int/non-int parts give:

$$H_U = U\sum_i\left(n_{i\uparrow}n_{i\downarrow} + \frac{n_{i\uparrow}+n_{i\downarrow}}{2}\right) - \frac{K}{\beta} \quad ; \quad K > 0 \in \mathbb{R}$$

$$H_0 = -t\sum_{\langle i,j\rangle}\left(c_i^{\dagger}c_j + c_j c_i^{\dagger}\right) + \frac{K}{\beta} - \mu\sum_i\left(n_{i\uparrow}+n_{i\downarrow}\right)$$

They claim that:

$$1 - \frac{\beta U}{K}\left(n_{i\uparrow}n_{i\downarrow} - \frac{n_{i\uparrow}+n_{i\downarrow}}{2}\right) = \frac{1}{2}\sum_{s=\pm 1} e^{\gamma s\left(n_{i\uparrow}-n_{i\downarrow}\right)}$$

where $\gamma = \cosh^{-1}\left(1 + \frac{U\beta}{2K}\right)$ (Auxiliary-Field Decomposition)

↳ derivation in two of their references. Will trust them for now.

Substituting $\star$ into H_U:

$$H_U = U \sum_i \left[\frac{-K}{2\beta U} \sum_{s=\pm 1} e^{\gamma s (n_{i\uparrow} - n_{i\downarrow})} + \frac{K}{\beta U} \right] - \frac{K}{\beta}$$

Not sure what's going on now, but I also don't think it's important for us at the moment. What is important is that the partition fn expansion is:

$$Z = \mathrm{Tr}\, e^{-\beta H}$$

$$= e^{-K} \mathrm{Tr}\, e^{-\beta H_0} \mathrm{T_r} T_\tau e^{\int_0^\beta d\tau \left(\frac{K}{\beta} - U\left(n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) - \frac{n_{i\uparrow}(\tau) - n_{i\downarrow}(\tau)}{2} \right) \right)}$$

↳ "irrelevant", can drop... apparently.

Applying Aux-field decomposition:

$$Z = \mathrm{Tr}\, e^{-\beta H_0} T_\tau e^{\int_0^\beta d\tau \frac{K}{2\beta} \sum_{s=\pm 1} e^{\gamma s (n_{i\uparrow}(\tau) - n_{i\downarrow}(\tau))}}$$

Summands are always positive. This allows avoiding the sign-problem.

Might still get negative signs from H_0 part.

$$Z = \mathrm{Tr}\, e^{-\beta H_0} \sum_{K=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{K-1}}^\beta d\tau_K \left(\frac{K}{2\beta} \right)^K \times$$

$$\left[e^{\tau_K H_0} \left(\sum_{s_K} e^{\gamma s_K (n_\uparrow - n_\downarrow)} \right) \cdots e^{-(\tau_2 - \tau_1) H_0} \left(\sum_{s_1} e^{\gamma s_1 (n_\uparrow - n_\downarrow)} \right) e^{-\tau_1 H_0} \right]$$

Pulling out all the summations:

$$Z = \sum_{K=0}^{\infty} \sum_{s_1,\dots,s_K=\pm 1} \int_0^{\beta} d\tau_1 \cdots \int_{\tau_{K-1}}^{\beta} d\tau_K \left(\frac{K}{2\beta}\right)^K \times$$

$$\underbrace{\mathrm{Tr}\left[e^{-\beta H_0} e^{\tau_K H_0} \left(\sum_{s_K} e^{\gamma s_K (n_\uparrow - n_\downarrow)}\right) \cdots e^{-(\tau_2-\tau_1)H_0} \left(\sum_{s_1} e^{\gamma s_1 (n_\uparrow - n_\downarrow)}\right) e^{-\tau_1 H_0}\right]}$$

$$= \mathrm{Tr} \prod_{i=K}^{1} e^{-\Delta\tau_i H_0} e^{\gamma s_i (n_\uparrow - n_\downarrow)} \equiv Z_K(\{s_K, \tau_K\})$$

where $\Delta\tau_i = \begin{cases} \tau_{i+1} - \tau_i & \text{if } i < K \\ \beta - \tau_K + \tau_1 & \text{if } i = K \end{cases}$

Types of updates: - insert/remove auxiliary spin
- spinflip

Exercise: try to reproduce log-weights from data, by substituting configuration data into $Z_K(\{s_K, \tau_K\})$.

& try $\boxed{K=1}$

$$\boxed{U_{\mu\nu} = 4 \quad t_{ij} = 1 \quad \mu = 0 \quad \beta = 5 \quad N_{corr} = 4 = N}$$

2x2 lattice:

0	1
2	3

Use these parameters when trying to calculate weights.

$$\gamma = \cosh^{-1}\left(1 + \frac{U\beta}{2K}\right)$$

$$Z_K(\{s_K, \tau_K\}) = \mathrm{Tr} \prod_{i=K}^{1} e^{-\Delta\tau_i H_0} e^{\gamma s_i (n_\uparrow - n_\downarrow)}$$

$$H_0 = -t \sum_{\langle i,j \rangle} \left(c_i^{+} c_j + c_j c_i^{+} \right) + \frac{K}{\beta} - \mu \sum_i \cancel{\left(n_{i\uparrow} + n_{i\downarrow} \right)} \qquad \mu = 0$$

$\frac{K}{\beta} \hat{\mathbb{1}}$ (I think)

Strategy

I. Build H_0 (stays fixed)

~~- Might actually only need the diagonal elements since Z_K only depends on the trace.~~

II. Compute γ (stays fixed)

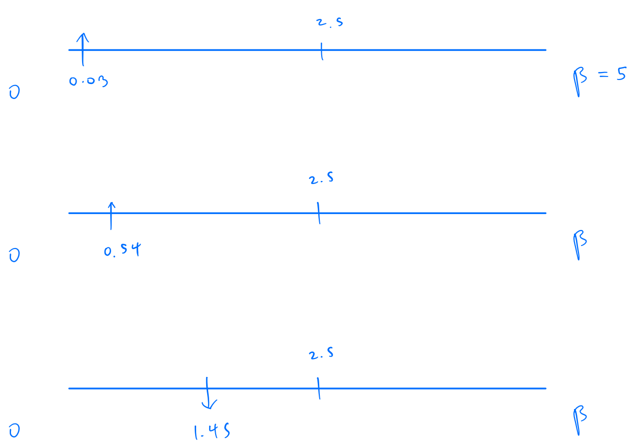
III. Loop over vertices $i = [1, K]$

1. compute matrix $e^{\gamma s_i (n_\uparrow - n_\downarrow)} \, e^{-\Delta \tau_i H_0}$

2. Accumulate matrix product

IV. Take trace of accumulated matrix product.

site 1:



How are removed spins tracked in config file?

$L = 2$

$N_{spins} = 2$

$\underline{\uparrow} \quad \underline{\uparrow}$

$\underline{\uparrow\downarrow} \quad \underline{\ \ }$

$\underline{\ \ } \quad \underline{\uparrow\downarrow}$

$\underline{\downarrow} \quad \underline{\downarrow}$

$\underline{\uparrow} \quad \underline{\downarrow}$

$\underline{\downarrow} \quad \underline{\uparrow}$

$\uparrow$ 1 2 $\qquad$ $\downarrow$ 1 2

$$\boxed{\frac{L^2!}{N_{spins}!\,(L^2-N_{spins})!}} = \frac{12}{2} = 6 \quad \checkmark$$

Could've chosen:

1 $\quad$ 2

or

2 $\quad$ 1

(which are the same

The number of combinations of N spins on $M = L^d$ lattice sites at half-filling is:

$$\boxed{\# = \frac{M^2!}{N!\,(M^2-N)!}}$$

Check: