1 Exact diagonalization

We need to evaluate the trace of this term:

$$e^{-H*(\beta-t_n)}F_{t_n}e^{-H*(t_n-t_{n-1})}F_{t_{n-1}}\dots F_{t_0}e^{-Ht_0} \tag{1}$$

We diagonalize the Hamiltonian with

$$H = UVU^T$$

where V is diagonal matrix with eigenvalues of H, each column of U is a eigenvector of H. Using

$$UU^T = I$$

we have

$$e^{-Ht} = e^{-UVU^T t} = Ue^{-Vt}U^T$$

the term becomes

$$Ue^{-V*(\beta-t_n)}U^T F_{t_n} Ue^{-V*(t_n-t_{n-1})}\dots F_{t_0}Ue^{-Vt_0}U^T$$

define

$$D_t = U^T F_t U$$

The term is then

$$Ue^{-V*(\beta-t_n)}D_{t_n}e^{-V*(t_n-t_{n-1})}\dots D_{t_0}e^{-Vt_0}U^T \tag{2}$$

We can then evaluate the full trace of the matrix above.

2 Krylov method

The complexity of the above method is $O(m^3 n)$, where m is the size of the matrix, and n is the number of fermion operators in the series. Since m scales exponentially with the number of orbitals, this can be very expensive even for a moderate number of orbitals (say 5). Instead, we can use the Krylov method to find the trace.

First, we find the few lowest eigenstates of the Hamiltonian $|i\rangle$, since they are usually more relevant at low temperatures. Then the trace is approximately

$$\sum_i \langle i|e^{-H*(\beta-t_n)}F_{t_n}e^{-H*(t_n-t_{n-1})}F_{t_{n-1}}\dots F_{t_0}e^{-Ht_0}|i\rangle$$

Then each of the term in the summation become of a series of the following operations:

- $e^{-Ht}|v\rangle$
- $F|v\rangle$

The second operation is $O(m^2)$, so we'll ignore it for now. For the first term, we can generate a Krylov space using the following method: [1]

1. $v_1 = v/||v||$,
2. Iteration: do $j = 1, 2, \ldots, k$
   (a) $w = Hv_j$
   (b) Iteration: do $i = 1, 2..., j$
      i. $h_{i,j} = w \cdot v_i$
      ii. $w = w - h_{i,j} v_i$
   (c) $h_{j+1,j} = ||w||$, $v_{j+1} = w/h_{j+1,j}$

With these iteration, we generate a orthonormal basis $V_k = [v_1, v_2, \ldots, v_k]$ and a $k \times k$ matrix H_k, where $H_k(i,j) = h_{i,j}$.

The exponential term can be just evaluated by:

$$e^{-Ht} v \approx ||v|| V_m e^{-H_k t} e_1$$

where $e_1 = [1, 0, 0, \ldots 0]^T$.

The complexity of this operation is $O(k^3 + mk^2 + m^2 k)$. Usually a small value (~ 3) of k is needed, thus the complexity of the computation is reduced. Overall the complexity scales as $O(m^2 kn)$.

[1] ANALYSIS OF SOME KRYLOV SUBSPACE APPROXIMATIONS TO THE MATRIX EXPONENTIAL OPERATOR, Y. SAAD , section 2.1