Notes on an operator set for QITE

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In the original QITE, the imaginary time step with a Pauli operation $\hat{P}_\mu$ to the state $|\Phi\rangle$ is approximated by a unitary operation,

$$\frac{e^{-\Delta\beta\hat{P}_\mu}|\Phi\rangle}{\langle\Phi|e^{-2\Delta\beta\hat{P}_\mu}|\Phi\rangle} \approx e^{-i\Delta\beta\hat{A}_\mu}|\Phi\rangle \tag{1}$$

The Hermitian operator $\hat{A}_\mu$ is expanded as a linear combination of Pauli operators applied to N qubits,

$$\hat{A}_\mu = \sum_{i\in\{I,X,Y,Z\}^{\otimes N}}^{4^N} a_i^{[\mu]}\hat{P}_i \tag{2}$$

Therefore, with the number of qubits N, the size of $\mathbf{a}^{[\mu]}$ increases exponentially. To ameliorate this prohibitive scaling, it was first proposed to introduce the domain $D < N$ as a cut-off parameter. The previous work showed such a local treatment can produce reasonable accuracy if the Hamiltonian is local. However, when it comes to chemical systems, where the Coulomb interaction is long range. Chemical Hamiltonian is usually very sparse, and most $\{\hat{P}_i\}$ is

In this note, we work out the derivation for approximation in terms of fermion operator, but not Pauli operator. We begin by writing a Hamiltonian as a linear combination of fermion operators,

$$\hat{H} = \sum_J h_J \left(\hat{E}_J + \hat{E}_J^\dagger\right) \tag{3}$$

where $\hat{E}_J$ are generally described as

$$\hat{E}_J = a_p^\dagger a_q^\dagger \cdots a_s a_r \tag{4}$$

Note that, in chemistry, E_J contains up to two-electron operators. We propose fermion-based QITE as

$$\frac{e^{-\Delta\beta(\hat{E}_J+\hat{E}_J^\dagger)}|\Phi\rangle}{\langle\Phi|e^{-2\Delta\beta(\hat{E}_J+\hat{E}_J^\dagger)}|\Phi\rangle} \approx e^{-\Delta\beta\hat{T}_J}|\Phi\rangle \tag{5}$$

where $\hat{T}_J$ is an anti-hermitian operator,

$$\hat{T}_J = \sum_K f_K^{[J]}(\hat{F}_K - \hat{F}_K^\dagger) \tag{6}$$

Here, $\hat{F}_K$ generally takes one-, two-, ..., N_e-body fermion operators,

$$\hat{F}_K = \begin{cases} a_p^\dagger a_q \\ a_p^\dagger a_q^\dagger a_s a_r \\ a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s \\ \cdots \end{cases} \tag{7}$$

and therefore the dimention of $\hat{T}_J$ still scales exponentially; however, the number-conserving operators eliminate Pauli operators that change electron numbers. Similarly to the original QITE, we determine parameters $f_K^{[J]}$ by minimizing

the following function to first order,

$$\left\| \underbrace{\frac{\frac{e^{-\Delta\beta h_J(\hat{E}_J+\hat{E}_J^\dagger)}}{\sqrt{c_J}}|\Phi\rangle - |\Phi\rangle}{\Delta\beta}}_{|\Delta_0\rangle} - \underbrace{\hat{T}|\Phi\rangle}_{|\Delta\rangle} \right\|^2 = \underbrace{\langle\Delta_0|\Delta_0\rangle}_{const} + \langle\Phi|\hat{T}^\dagger\hat{T}|\Phi\rangle$$

$$- \frac{1}{\Delta\beta\sqrt{c_J}}\left(\langle\Phi|e^{-\Delta\beta h_J(\hat{E}_J+\hat{E}_J^\dagger)}\hat{T}|\Phi\rangle + \langle\Phi|\hat{T}^\dagger e^{-\Delta\beta h_J(\hat{E}_J+\hat{E}_J^\dagger)}|\Phi\rangle\right)$$

$$+ \frac{1}{\Delta\beta}\underbrace{\langle\Phi|(\hat{T}+\hat{T}^\dagger)|\Phi\rangle}_{0}$$

$$= const + \langle\Phi|\hat{T}^\dagger\hat{T}|\Phi\rangle$$

$$- \frac{1}{\Delta\beta\sqrt{c_J}}\Big(\langle\Phi|\hat{T}|\Phi\rangle + \Delta\beta h_J\langle\Phi|(\hat{E}_J+\hat{E}_J^\dagger)\hat{T}|\Phi\rangle$$

$$+ \langle\Phi|\hat{T}^\dagger|\Phi\rangle + \Delta\beta h_J\langle\Phi|\hat{T}^\dagger(\hat{E}_J+\hat{E}_J^\dagger)|\Phi\rangle + \mathcal{O}(\Delta\beta^2)\Big)$$

$$= const + \sum_{KL} f_K^{[J]} f_L^{[J]} \langle\Phi|\left(\hat{F}_L^\dagger - \hat{F}_L\right)\left(\hat{F}_K - \hat{F}_K^\dagger\right)|\Phi\rangle$$

$$+ \sum_K f_K^{[J]}\langle\Phi|\left[(\hat{E}_J+\hat{E}_J^\dagger),(\hat{F}_K-\hat{F}_K^\dagger)\right]|\Phi\rangle + \mathcal{O}(\Delta\beta) \tag{8}$$

Taking the derivative with respect to $f_K^{[J]}$ and setting to zero, we finally find the linear system,

$$\sum_L S_{KL}^{[J]} f_L^{[J]} + b_K^{[J]} = 0 \tag{9}$$

with

$$S_{KL}^{[J]} = \langle\Phi|\left(\hat{F}_L^\dagger - \hat{F}_L\right)\left(\hat{F}_K - \hat{F}_K^\dagger\right)|\Phi\rangle \tag{10}$$

$$b_K^{[J]} = \frac{1}{2}\langle\Phi|\left[(\hat{E}_J+\hat{E}_J^\dagger),(\hat{F}_K-\hat{F}_K^\dagger)\right]|\Phi\rangle \tag{11}$$

Now, what kind of subset of $\hat{F}_K$ can produce a good approximation for Eq. (5)? To find such $f_K^{[J]}$ with large contribution to $\hat{F}_K$, we simply require those K with large $b_K^{[J]}$. Suppose we choose $\hat{F}_K = a_t^\dagger a_u^\dagger a_w a_v$ for $\hat{E}_J = a_p^\dagger a_q^\dagger a_s a_r$, we find

$$\langle\Phi|\left[\hat{E}_J,\hat{F}_K\right]|\Phi\rangle = \langle\Phi|\Big((\delta_{rt}\delta_{su}-\delta_{st}\delta_{ru})a_p^\dagger a_q^\dagger a_w a_v + (\delta_{qv}\delta_{pw}-\delta_{pv}\delta_{qw})a_t^\dagger a_u^\dagger a_s a_r$$

$$+ \mathcal{P}(r,s)\mathcal{P}(t,u)\delta_{st}a_p^\dagger a_q^\dagger a_u^\dagger a_r a_w a_v + \mathcal{P}(p,q)\mathcal{P}(v,w)\delta_{qw}a_t^\dagger a_u^\dagger a_p^\dagger a_v a_s a_r\Big)|\Phi\rangle \tag{12}$$

and other terms needed for $b_K^{[J]}$ can be similarly obtained. Here, $\mathcal{P}(p,q)$ is a permutation operator, i.e., $\mathcal{P}(p,q)X(p,q) = X(p,q) - X(q,p)$. Therefore, if $\hat{E}_J$ and $\hat{F}_K$ do not share the same orbitals, $b_K^{[J]} = 0$, and do not contribute. The most effective choice is $\hat{F}_K = \hat{E}_J$ (or $\hat{E}_J^\dagger$), in which case $b_J^{[J]}$ is composed of the diagonal elements of n-PDM, where n is the order of $\hat{E}_J$. In particular, for $n = 2$, using the result Eq. (12),

$$b_J^{[J]} = \langle\Phi|\left(a_p^\dagger a_p a_q^\dagger a_q(1-a_r^\dagger a_r - a_s^\dagger a_s) - (1-a_p^\dagger a_p - a_q^\dagger a_q)a_r^\dagger a_r a_s^\dagger a_s\right)|\Phi\rangle \tag{13}$$

For strongly correlated systems, n-PDMs may have significantly large elements in the off-diagonal. However, their structure is governed by $\hat{H}$ ($\{\hat{E}_J\}$), and therefore the use of the set $\hat{F}_K \in \{\hat{E}_J\}$ can efficiently include such transitions.