Approximate Fermionic Hamiltonian Simulation for H-chains

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1 Introduction

One of the most promising applications of quantum computing is in the field of quantum computational chemistry, which aims to efficiently simulate the behavior (i.e. Hamiltonian evolution) of chemical systems that are too complex for classical computers. The ability to computationally predict behavior of molecular systems would significantly benefit drug discovery efforts. This paper presents a sub-quadratic (in n) quantum algorithm to simulate the Hamiltonian evolution of the hydrogen chain, a benchmark chemical system in this field.

2 Algorithm

Denote n as the number of hydrogen atoms. Since we're only dealing with 1s orbitals, this is also the number of orbitals. The electronic Hamiltonian has a form that can be separated into one-electron and two-electron components.

$$H = H_1 + H_2 = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{i,j,k,l} a_i^\dagger a_j^\dagger a_k a_l \tag{1}$$

It is always the case that H is symmetric between i and j, between k and l, and between ij and kl. This means that the matrix $h_{i,j,k,l}$ can be eigendecomposed with eigenvalues $\{\lambda_r\}_{r\in[n^2]}$ (in descending order) and orthonormal eigenvectors $\{|r\rangle\}_{r\in[n^2]}$. Denote $L^r = \lambda_r |r\rangle \langle r|$, which is symmetric.

$$H_2 = \frac{1}{2} \sum_{r\in[n^2]} \Big(\sum_{i,j\in[n]} L_{ij}^r a_i^\dagger a_j \Big)^2 \tag{2}$$

In the case of the H-chain, numerical results show that there is a significant drop between the λ_n and λ_{n+1}. That is, eigenvalues $n+1$ and above are significantly smaller than the first n eigenvalues. In addition, for the H-chain, the $L^1, ..., L^r$ are all approximately diagonal.

$$H_2 \approx \frac{1}{2} \sum_{r\in[n]} \Big(\sum_{i\in[n]} L_{ii}^r a_i^\dagger a_i \Big)^2 = \frac{1}{2} \sum_{r\in[n]} \Big(\sum_{i\in[n]} L_{ii}^r n_i \Big)^2 \tag{3}$$