Exploring Hilbert space on a budget II

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This work explores the ability of quantum computational algorithms to represent the information content of Full Configuration Interaction (FCI) wave functions.

I. INTRODUCTION

This is an introduction. It should include the following subtopics:

1. A review of the strong correlation problem (relevance, and difficulty for classical methods, discuss findings from EHS-1).
2. A discussion of the relevance of quantum algorithms to combat this problem, inherent circumvention of storage.
3. A discussion of the outstanding need for intercomparison between the now wide variety of quantum algorithm classes that exist, resource estimation and accuracy, and comparison to classical methods. Investigate the quantum advantage boundary.
4. Also a need to compare the border of near-term and fault tolerant algorithms (not done often or at all).
5. Overview of previous quantum benchmark students, overview of the quantum algorithms we implemented, and classical algorithms from EHS-1,
6. Summary of findings (obviously later).

This is a citation:[1]

II. THEORY

A. FCI wave functions and strong correlation

Given a basis of K spin orbitals $\{\psi_p\}$ with $p = 1, \ldots, K$, we indicate a generic N-electron determinant $|\psi_{i_1} \cdots \psi_{i_N}\rangle$ using the notation $|\Phi_I\rangle$ where the multindex $I = (i_1, \ldots, i_N)$ represents an ordered list of indices ($i_1 < i_2 < \ldots < i_N$). The set of N-electron determinants ($\mathcal{H}_N$) forms a Hilbert space of dimension $|\mathcal{H}_N| = N_\mathcal{H}$. Using this notation, the FCI wave function is written as a linear combination of determinants, each parameterized by a coefficient ($C_{i_1,\ldots,i_N} \equiv C_I$)

$$|\Psi_{\text{FCI}}\rangle = \sum_{i_1<i_2<\ldots<i_N}^{K} C_{i_1\cdots i_N} |\Phi_{i_1\cdots i_N}\rangle = \sum_{I}^{N_\mathcal{H}} C_I |\Phi_I\rangle . \quad (1)$$

An equivalent way to express the FCI wave function employs occupation vectors. In this representation, each determinant $|\Phi_I\rangle$ is associated with a vector of length K, $|\mathbf{n}\rangle = |n_1, n_2, \ldots, n_K\rangle$, where $n_i \in \{0, 1\}$ is the occupation number of spin orbital ψ_i. The FCI wave function represented in the occupation vector form is given by

$$|\Psi_{\text{FCI}}\rangle = \sum_{\{n_i\}} C_{n_1\ldots n_K} |n_1 \ldots n_K\rangle = \sum_{\mathbf{n}} C_\mathbf{n} |\mathbf{n}\rangle \quad (2)$$

where the sum over all occupation vectors ($\{n_i\} \equiv \mathbf{n}$) is restricted to N-electron determinants ($\sum_i n_j = N$) of given spin and spatial symmetry.

B. Resources for Quantum Algorithms

Overview of what contributes to runtime and accuracy.

1. Classical Parameter Optimization

Can probably keep some of this, will likely use here. For a systematically improvable method X we indicate the energy computed using N_{par} parameters as $E_X(N_{\text{par}})$. We then define the accuracy volume, $\mathcal{V}_X(\alpha)$, to be the smallest number of parameters such that the error per electron with respect to the FCI energy (E_{FCI}) is less than or equal to $10^{-\alpha}$:

$$\mathcal{V}_X(\alpha) = N_{\text{par}} : \frac{|E_X(N_{\text{par}}) - E_{\text{FCI}}|}{N} \leq 10^{-\alpha}\ E_{\text{h}}. \quad (3)$$

2. Circuit Depth (NISQ and FT)

3. Measurement

4. Hamiltonian Factorization

C. Quantum Eigensolvers

General ideal of optimized unitary, discuss discrepancy between PQE and VQE

Now list Ansatz

1. dUCC

particle hole dUCC, k-upG-UCCSD, AGP, symmetry adaptation. Mention that some are introduced in layers

2. Orbital Fabric

3. Tensor Network

4. Qubit CC

5. Hardware Efficient Ansatz

6. LDCA

7. Selected QE

S-PQE, ADAPT, Iterative Qubit CC

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D. Quantum Imaginary Time Evolution

1. Fermionic 1st order QITE

2. Fermionic 1st order MVP QITE

E. Quantum Subspace Diagonalization

1. QSE

2. NO-VQE

3. MC-VQE

4. QLanczos

5. QKrylov

6. QDavidson

F. Quantum Phase Estimation

III. HYDROGEN MODEL SYSTEMS

IV. COMPUTATIONAL CONSIDERATIONS

V. RESULTS

VI. CONCLUSIONS

[1] J. B. Schriber and F. A. Evangelista, J. Chem. Phys. **144**, 161106 (2016).