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Near-term Quantum Algorithms for Quantum Many-body Systems

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Abstract. There has been a good deal of work on algorithms to simulate quantum many-body systems with fault-tolerant quantum computers- those with full error correction. Fault-tolerant quantum computers of scale requisite to achieve computational advantage for these problems are likely over a decade away. Moreover, devices that we can build in the near term, called Noisy Intermediate Scale Quantum computers (NISQ), have too much noise to implement the long circuits required by these algorithms. We review heuristic, short-depth quantum algorithms more suited to NISQ computers; specifically, their scaling properties when applied to electronic and nuclear structure calculations, including Hamiltonian complexity with particle number, ansatz state preparation, convergence, and noise. We will present examples of actual quantum structure calculations with NISQ computers, as well as a newly-developed error mitigation technique that significantly improves accuracy. We end with an outlook for “advantage” – when NISQ systems might excel conventional HPC approaches for comparable problems.

1. Introduction

Feynman’s early insight [1] was this: researchers knew that quantum many-body calculations required to describe all matter require conventional computers to grow exponentially with the problem size. However, he speculated, if a computer could be built with quantum devices, the quantum resources required would scale linearly with problem size, and could solve far larger problems that would be forever intractable for conventional computers. That early insight first inspired theorists to explore algorithms, such as Shor’s factoring algorithm or Grover’s search algorithm [2] [3]. Naturally, since little was actually known about actual quantum devices, theorists started with the assumption that quantum calculations could be performed perfectly, with no errors occurring during the manipulation or storage of the quantum states. However, we now realize that the fragility of quantum devices, qubits, will require complex coding with great hardware overhead to realize fault-tolerant quantum computers - quantum computers that perform calculations free from errors. Therefore, our team is exploring algorithms that can be performed with a quantum computer that has little or no error correction - a computational paradigm that John Preskill has named “Noisy Intermediate-Scale Quantum” computing, or NISQ [4].

2. Back to Feynman’s Insight

Quantum many-body problems seem more appropriate for NISQ systems than the mathematical tasks like Shor or Grover– for there is no such thing as an approximate prime or approximate



match! However, quantum chemistry or materials science can benefit from an approximate computation of bond length or angle if the computation can yield a sufficiently accurate result on problems intractable to conventional approximate methods. NISQ algorithms for strongly-interacting fermionic many-body problems have also been an area of theoretical work [10, 6], and only relatively recent demonstrations of one and two-qubit calculations on actual hardware [9]. In this paper we summarize the steps required to: a) transform a many-body Hamiltonian into the qubit basis, b) solve this problem on a quantum computer, and c) mitigate noise on the quantum hardware to improve the accuracy of the result. We give a summary of our new work [7] that extend computations to six qubits to model the triatomic molecule BeH_2 .

2.1. Simplifying the Hamiltonian and Transforming the Basis

To make the discussion more concrete we will describe the computational flow used to solve the electronic structure problem, though the same methods can be used to solve other many-body problems like nuclear states or fermionic-Hubbard models. In essence, these quantum algorithms use the quantum computer to represent and explore the exponentially-large Hilbert space of fermionic particles to find the eigenstate wavefunctions, and use these wavefunctions to estimate energy eigenvalues. Analysis of the ground-state eigenvalue of a chemical bond as a function of bond length then gives information about the equilibrium bond length, bond angle, and dissociation energy. The flow (Figure 1) begins with writing the first-quantization Hamiltonian using the Born-Oppenheimer approximation.

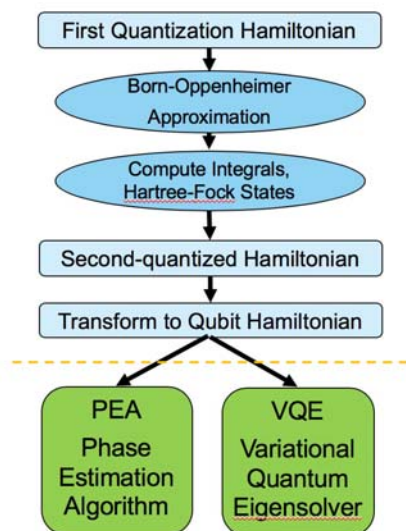


Figure 1. Flow of electronic structure computation for NISQ quantum computation. The first-quantized Hamiltonian is simplified as much as possible before computing the integrals to generate the second-quantized Hamiltonian. There are several transformations to the qubit basis states (text), allowing the transformed problem to be solved with quantum-classical algorithms (green boxes).

We do not need to make this approximation to solve the problem— we are only trying to simplify the problem to use as few qubits as possible because they are currently so precious. (Note: if the reader wishes, they can follow the computational process in this paper using IBM’s Open Source qiskit.org software and Qiskit Aqua for quantum chemistry.) Standard quantum chemistry packages can be used to compute the integrals in a chosen basis (STO3G, STO6G, etc.) for a particular molecular configuration of bond lengths and angles. With this preparation we calculate the second-quantized Hamiltonian for the problem at hand.

The next step is a basis transformation of the problem to encode the fermionic degrees of freedom using qubits [13]. Encoding efficiency is important to scaling: we want to use the least number of qubits possible and the least number of terms in the qubit Hamiltonian. There are a number of transformation rubrics; the Jordan-Wigner, Parity, and Binary Tree encodings. All

three formulations require N -qubits to represent N -modes; however, the locality of the operators in the Hamiltonian scales as $\mathcal{O}(N)$ for the Parity and Jordan-Wigner hamiltonians while the locality in the Binary Tree scales as $\mathcal{O}(\log(N))$. Further, if the symmetry of the Hamiltonian is analyzed, at least two qubits can be eliminated and even more based on further symmetries [13].

The result of the transformation takes the second quantized fermionic Hamiltonian and produces a qubit Hamiltonian which is a weighted sum of Pauli operators. Each term in the qubit Hamiltonian has a coefficient which depends on bond length, angle, and other desired features of the many-body problem. For example, the qubit Hamiltonian for the hydrogen atom using the Binary Tree encoding has five terms which can be expressed using only two qubits to represent the four spin orbitals [7].

For quantum chemistry, the number of terms in the mapped Hamiltonian grows as $\mathcal{O}(n^4)$, where n is the number of spin orbitals.

There are two classes of algorithms to arrive at the eigenstate of a qubit Hamiltonian: the Phase Estimation Algorithm (PEA), and a Variational Quantum Eigensolver (VQE). We next describe and contrast these two solution methods.

2.2. Phase Estimation Algorithm

The PEA starts with an approximation to the groundstate, usually chosen as the (approximate) Hartree-Fock (HF) ground state expressed in qubit states, $|\widetilde{\psi}(0)\rangle$ and evolves this in time using the Hamiltonian in the qubit basis (see equation 1) to arrive at the actual groundstate of the Hamiltonian $|\psi(t)\rangle$. This method works as long as the HF groundstate has sufficient overlap with the actual groundstate. The propagator in equation [5] can be expressed as a sum of projectors onto eigenstates of the Hamiltonian, each with different phase, ϕ_n , with phases related to eigenstate energies $E_n = \phi_n t$. [10, 11, 12].

$$|\psi(t)\rangle = e^{iHt}|\widetilde{\psi}(0)\rangle = \left(\sum_n e^{i\phi_n t} |\psi_n\rangle\langle\psi_n| \right) |\widetilde{\psi}(0)\rangle \quad (1)$$

The PEA algorithm allows one to measure the phase ϕ_n on a quantum computer. The probability for measuring the phase ϕ_0 is given by $|\langle\psi_0|\widetilde{\psi}(0)\rangle|^2$, from which the ground state energy is easily determined.

Implementing this algorithm requires Trotterization of the exponential, which for most molecules will require $\mathcal{O}(N^5)$ terms and a circuit depth which has been improved [8] to be $\mathcal{O}(N^7)$, where N is the number of spin orbitals. The depth of circuit required is beyond present NISQ capabilities except for the simplest molecules H_2 and HeH^+ . The bond distance dependence of the ground state energy has been computed using PEA with photonic and superconducting qubits [9, 10], but the results show more error and higher noise than the VQE algorithm.

2.3. Variational Quantum Eigensolver (VQE) Algorithm

The variational quantum eigensolver (VQE) approach consists in using a qubit processor to approximate the ground state eigenvector, $|\psi\rangle$, with

$$H_q|\psi\rangle = E_q|\psi\rangle, \quad (2)$$

in terms of a classically-intractable trial state. A quantum computer is used to represent the trial state $|\psi(\theta)\rangle$ in its physical memory consisting of qubits. On the quantum computer, a tentative variational eigenstate, usually called the Ansatz or guess eigenstate, $|\psi(\theta)\rangle$ is prepared using a sequence of parameterized quantum gates labeled by control variables $\vec{\theta}$. One approach to create an ansatz uses the UCCSD (Unitary Coupled Cluster Singlet and Doublet excitation) approximation which must be implemented using Trotterization and is not hardware efficient–

just like the PEA approach discussed above. Shown below is an example of an “Hardware-efficient” ansatz[7], that is constructed as an interleaved sequence of parametrized single qubit rotations and entangling blocks U_{ENT} . As long as this heuristic ansatz state overlaps sufficiently with the true ground state, optimization by varying the control variables $\vec{\theta}$ is possible.

$$|\psi(\vec{\theta}_k)\rangle = \prod_{q=1}^M \left(U^{q,0}(\vec{\theta}_k) \right) \times U_{ENT} \times \prod_{q=1}^M \left(U^{q,1}(\vec{\theta}_k) \right) \times \dots \times U_{ENT} \times \prod_{q=1}^M \left(U^{q,d}(\vec{\theta}_k) \right) |0, 0 \dots 0\rangle \quad (3)$$

Estimates of the average energy of the Hamiltonian, $E = \langle \Psi(\vec{\theta}_k) | H_q | \Psi(\vec{\theta}_k) \rangle$, are obtained by repeated quantum measurements on the qubits prepared in the state $|\Psi(\vec{\theta})\rangle$. This requires projective measurement of the prepared trial state to compute the expectation value for the $\mathcal{O}(N^4)$ terms in the Hamiltonian. The control variables $\vec{\theta}_k$ are then changed, for instance, with a gradient descent feedback mechanism on the estimated energies, until the lowest value for E_q is found. This corresponds to the set of controls θ_k^* that create the state with lowest energy—the groundstate E_g .

Simulations of this method for generating an ansatz show that a fixed, partial entanglement U_{ENT} (not a full CNOT) and a depth of approximately six entanglers is necessary to represent the groundstate of LiH with chemical accuracy (1 mHartree or better). Because Ansatz generation starts with all qubits in the groundstate, the first set of Z rotations of the operator $U^{q,0}(\vec{\theta})$ are not implemented. Therefore, for d entanglers the total number of independent parameters to generate the Ansatz is $p = N(3d + 2)$.

3. VQE Results for Three Molecules

The results of the VQE algorithm for the simulation of the Hamiltonians for H_2 using four qubits, LiH using four, and BeH_2 using six qubits are shown in Figure 2 a, b, and c. The figure includes exact groundstate energy (solid line), the VQE algorithm result averaged over repeated experiments, or shots, (solid circles) and a classical simulation of the VQE algorithm that accounts for decoherence and the effect of finite sampling (fuzzy regions). Here the molecular

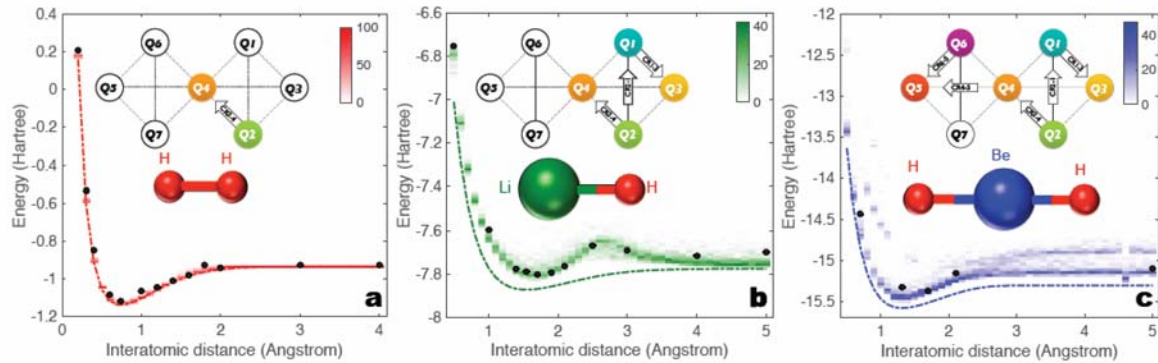


Figure 2. Experimental results (black circles), exact energy surfaces (dotted lines) and density plots (fuzzy) of outcomes from numerical simulations of three molecules. These results are for one entangler circuits ($d=1$). Error bars on the experimental data are much smaller than the circles. Figure reproduced from [7]

energies in units of Hartree as a function of interatomic distance; in the case of BeH_2 it is assumed that both bonds have the same length. For all three molecules, only one entangler was

used; otherwise the effect of decoherence overpowers the benefit of using larger depths. The energy discrepancies between the exact and quantum VQE algorithm agree qualitatively with a classical simulation including amplitude damping and dephasing noise, showing how decoherence affects the quantum computation.

4. Error Mitigation

Quantum information is fragile in all known qubit technologies; this is a consequence of the small energy difference between the ground and first excited states of the qubit, which are the two states comprising the computational basis for any qubit. Topological parity codes have been invented to protect quantum information by spreading a single qubit state across $\mathcal{O}(d^2)$ qubits, where d is the code distance [14]. However, the overhead of any known code which protects against all errors is very large— to implement many-body physics algorithms would require hundreds to thousands of physical qubits per protected logical qubit, and hundreds to thousands of these logical qubits to perform computations that are out of reach for conventional computers [6]. We are a long way away from the hundreds of thousands to millions of physical qubits necessary to perform fault-tolerant (error free) computations.

However, we have been exploring error mitigation techniques to reduce error without the large overhead required to correct all errors [15] which can be applied to NISQ hardware. We have implemented one of the ideas, Richardson extrapolation, to reduce the error of the VQE algorithm. The idea is elegant: if we could have an experimental parameter that we could vary to increase noise in the calculation, then we could measure energy as a function of that noise parameter and extrapolate to the noiseless value (theoretically). This approach would be valid as long as the source(s) of decoherence are time invariant over the period of the extrapolation experiments and as long as the noise itself is small compared to the average energy of the Hamiltonian being computed.

We have found a way to implement this error mitigation technique, given that the above assumptions hold. If we take a longer time to generate $|\psi(\vec{\theta}_k)\rangle$, the noise will be roughly proportional to the time taken. This is an easy "knob" for experimentalists since the time it takes to perform a rotation or entanglement operation on qubits is roughly proportional to the amplitude of the RF pulses applied. By stretching out the time of a pulse and reducing amplitude we can perform the same operation slower and slower.

In [16], error mitigation was applied to a variational quantum eigensolver, addressing the electronic structure problem for H_2 and LiH . The ability to mitigate for the effect of decoherence enabled access to longer circuit depths and achieved significant improvements in the estimates of the ground state energy for both molecules.

5. Conclusions

We have attempted to summarize progress simulating many-body systems with NISQ quantum computers. These algorithms are limited by errors in quantum gates and coherence; the PEA algorithm is more sensitive to hardware quality as it requires a polynomial circuit depth, while the VQE algorithm, which is linear in depth, is more robust. Newly-proposed error mitigation techniques have proven able to reduce VQE algorithm error, and this progress is likely to inspire more work on mitigation approaches with less overhead than required for full error correction. It is difficult to predict with certainty when or if NISQ hardware and these heuristic algorithms will improve to the point that we can solve problems intractable for conventional computers. Nevertheless, progress has been rapid and shows promise for these near-term algorithms solving many-body problems we can't now even attempt. This promise is being realized primarily because qubits can represent the highly-entangled states of many-body systems much more efficiently and natively than any conventional hardware.

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