Quantum Computing and Energy Storage Research

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Introduction

Energy is the most important resource in the modern world. People in developed countries use large amounts of energy for many different purposes, including (but not limited to) lighting, cooking, climate control, transportation, and communication. This energy can be retrieved from various sources, such as nuclear reactions, fossil fuels, sunlight, and wind. In developing countries, access to electrical energy is capable of improving quality of life by allowing the use and development of many devices and advancements which otherwise might be out of reach.

Perhaps the most important consideration, then, is how to store all of this energy. This is very important for a variety of reasons. In energy production, good storage technologies can make up for the intermittency of certain sources, such as the sunlight or wind. In daily use, smart phones and laptop computers have become increasingly important to everyday life, for communication, recreation, and work; these devices rely on batteries for power. Additionally, transportation often uses fuels, such as gasoline or coal, to store the energy needed to drive a vehicle. However, these fuels exist in limited supply and have negative impacts on both the environment and public health.

As society tries to move away from these traditional fuels, it becomes necessary to replace the energy which they provide with different options. In the case of energy production, this often means replacing fossil fuels with renewable energy sources such as wind or solar. As noted above, however, these resources are often intermittent, and a solid foundation of energy storage is necessary for them to be able to provide consistent energy. The same can be said of electric vehicles, the rising alternative to traditional gasoline vehicles. In order to compete, and thus become more common, electric vehicles need batteries which are able to charge more quickly and to travel further using that charge, while also being affordable for an average person.

An important factor in all of the above improvements is chemistry. The chemical properties of a battery determine its charging speed, its energy density, and its cost. A promising direction for research into these improvements in battery technology is the use of quantum computers. Quantum computers could be able to accurately model molecules and chemical interactions, making it easier to research new materials for use in energy storage. The use of quantum computers could help push battery development forward and speed up the development of phones, cars, and renewable energy production.

Classical Chemical Modeling

The goal of any chemical modeling process is to solve the Schrödinger equation and find the ground state of the modeled molecule. In other words, modeling seeks to find the lowest energy state of the molecule's Hamiltonian. This ground state determines the structure and interactive properties of the molecule (Kandala, Mezzacapo, et al., 2017). Classical computers are capable of achieving this in a few different ways, including density functional theory (DFT), Monte Carlo methods, and tensor networks (Ho, McClean, Ong, 2018).

The most common of these methods in modern chemical modeling is density functional theory (Ho, McClean, Ong). To fully model a quantum chemical system, it is necessary to solve the many-body Schrödinger equation for all nuclei and electrons in the system. The mass of nuclei allows them to be approximated as point-particles using what is called the Born-Oppenheimer approximation (Hasnip, Refson, et al., 2014). Electrons, on the other hand, are not so simple. Because of its complexity, the many-body Schrödinger equation is too difficult for current classical technologies to solve outright. Density functional theory allows for the calculation of energy of a system based on the fact that "the energy of the system is a unique functional of the electron density" (Hasnip, Refson, et al.). Thus, by modeling the density of the electrons instead of the full many-body wave function used in the Schrödinger equation, DFT is able to massively simplify the modeling and calculation necessary to find the lowest energy state of the system.

Unfortunately, density functional theory is flawed as a method for computational modeling of quantum chemical systems. DFT modeling relies on several approximations, such as the aforementioned Born-Oppenheimer approximation. Approximations will always bring some form of error. The amount of error any given approximation causes can vary based on the chemical property being examined and based on the materials being examined (Ho, McClean, Ong). This also means that DFT requires an increasingly expert hand, as knowledge of the different methods, their limitations, and chemistry become more and more necessary (Ho, McClean, Ong).

Of course, density functional theory is not the only method which researchers can use to model chemical properties and processes. The other possibilities mentioned above, quantum Monte Carlo and tensor network methods, have certain advantages over DFT. One of these advantages is that they can be systematically refined for accuracy (Ho, McClean, Ong). The

major disadvantage of these methods is computational cost. Quantum Monte Carlo, for example, has what is called the "sign problem." The computational costs of avoiding this sign problem in a quantum Monte Carlo simulation or of storing the entire many-body wave function in other methods become large quickly, especially as the system of interest grows more complex with larger molecules and more particles and interactions to model (Ho, McClean, Ong). This means that modeling complex systems with these methods may take a very long time and a large amount of computational resources.

Thus, the primary methods for classical modeling of quantum chemical systems are flawed. While density functional theory is scalable, the approximations necessary to achieve this scalability can result in varying degrees of error; on the other hand, quantum Monte Carlo and tensor network methods are capable of accurately modeling chemical systems, but at a computational cost that is not scalable as complexity increases. Research into improving these methods is ongoing, and classical modeling of quantum systems is still a valuable tool for materials research. However, these still may not be the best methods for modeling chemical systems.

Quantum Chemical Modeling

As mentioned previously, the goal of chemical modeling "is to solve for the ground-state energy of many-body interacting fermionic Hamiltonians" (Kandala, Mezzacapo, et al.). In quantum computing, this is achieved by mapping the wave equations of electrons to the wave equations of qubits, resulting in a Hamiltonian problem on a set of qubits (Kandala, Mezzacapo, et al.). Given a k-local Hamiltonian, this means finding the ground-state eigenvalue E_G and the ground state $|\phi_G\rangle$ such that

$$H|\phi_G\rangle = E_G|\phi_G\rangle$$

(Kandala, Mezzacapo, et al.).

The rise of quantum computing seems promising for chemical modeling. Because particle wave equations are mapped directly to qubit wave equations on which operations can then be performed, quantum computers have the potential to provide near exact solutions to problems in an amount of time similar to that taken by approximations performed on classical computers (Ho, McClean, Ong). This also means that the in-depth knowledge needed to utilize certain classical computational methods is less necessary. For example,

while density functional theory requires knowledge of different functionals, as well as how and why they are used, in addition to the base knowledge of the system being modeled, quantum methods require less of the specific knowledge of the methods themselves (Ho, McClean, Ong). In other words, quantum computation may make computational models more accessible for a wide audience. Additionally, quantum computing offers the possibility to model specific complex situations which classical simulation is not able to match, which could help to further push research into improved electronic and battery technologies forward (Ho, McClean, Ong).

In fact, research and use of quantum computing methods for chemical modeling are already underway. In an article published in *Nature* in 2017, IBM researchers showed promising results in the use of quantum computing to model larger molecules than had previously been modeled by a quantum computer. The team used variational quantum eigensolvers (VQEs) to model the ground states of molecules, a method which combines the strengths of classical and quantum computing to find a result (Kandala, Mezzacapo, et al.). In this method, a quantum computer prepares a trial state based on a set of parameters. The expectation of the energy is then passed to a classical optimizer, which improves the parameters. These parameters are then used to generate a new trial state, and the process continues (Kandala, Mezzacapo, et al.).

The researchers used VQEs with a seven-qubit superconducting quantum processor to find the ground state energies of H_2, LiH, and BeH_2 (Kandala, Mezzacapo, et al.). Each of the eight electron orbitals necessary to model these compounds was mapped to a single qubit, with the $1s'$ up and down orbitals omitted because of symmetry; this ultimately resulted in six orbitals being mapped to six qubits (Kandala, Mezzacapo, et al.). To generate trial states, the team used natural entangling properties of their hardware, described by H_0, a drift Hamiltonian (Kandala, Mezzacapo, et al.). The entangling operators are represented by the unitary matrix $U_{\text{ENT}} = e^{-iH_0\tau}$, "where τ is the evolution time" (Kandala, Mezzacapo, et al.). Next, they used Z and X gates to create single-qubit Euler rotations $U^{q,i}(\boldsymbol{\theta}) = Z^q_{\theta_1^{q,i}} X^q_{\theta_2^{q,i}} Z^q_{\theta_3^{q,i}}$, "where $\boldsymbol{\theta}$ represents the Euler angles, q identifies the qubit, and $i = 0, 1, \ldots, d$ refers to the depth position" (Kandala, Mezzacapo, et al.). They began the process with every qubit in the $|0\rangle$ state, "applying d entanglers U_{ENT} that alternate with N Euler rotations" (Kandala, Mezzacapo, et al.). What this means is that the final trial state output by the quantum processor was given

by

$$|\phi(\boldsymbol{\theta})\rangle = \prod_{q=1}^{N}[U^{q,d}(\boldsymbol{\theta})]\times U_{\mathrm{ENT}}\times\prod_{q=1}^{N}[U^{q,d-1}(\boldsymbol{\theta})]\times\cdots\times U_{\mathrm{ENT}}\times\prod_{q=1}^{N}[U^{q,0}(\boldsymbol{\theta})]|00\ldots0\rangle$$

(Kandala, Mezzacapo, et al.). This setup was designed to be hardware efficient, not requiring complicated gates and intricate circuits which may not have worked fast enough for computations to be completed before the entangled particles lost coherence and error overtook the system. For the same reason, the researchers found that they received the best results from keeping the depth of their circuit small. This is despite the fact that, in an ideal system, more depth should provide a more accurate state (Kandala, Mezzacap, et al.).

This case highlights some of the flaws in quantum computational methods for chemical modeling. While quantum computing has much potential for providing exact solutions to quantum chemical problems in a reasonable amount of time, there are also many factors which currently limit how useful it can be. The IBM researchers describe at multiple points in the *Nature* article how concerns about decoherence affected their design process, as they sought to minimize the amount of time which their circuit would take in order to reduce the chances of errors. Yet this also shows hope for the use of quantum computing in this area of research. The IBM team was able to work around error-inducing factors and find the ground state energy of compounds ranging in size from H_2 to BeH_2. While the results were not perfect, there is hope that improvements in quantum computing technology will lead to improvements here, as well. This is a promising outcome for the future of quantum computing's usefulness.

As further proof of the implications of this research, another IBM team has used a similar methodology to model even larger compounds. In a 2020 paper published on arXiv, researchers from IBM and Daimler used the principles from the 2017 *Nature* article to model the dominant chemical products of lithium-sulphur batteries. This paper was published in *The Journal of Chemical Physics* in 2021. Lithium-sulfur batteries theoretically have both a high energy capacity and a high energy density, and the aim of this research was to better understand the chemical processes in the battery and more concretely describe their potential (Rice, Gujarati, et al., 2021). The researchers also modelled the compounds on classical computers using full configuration interaction (FCI), comparing the concrete results of the classi-

cal computations to the results of the quantum algorithm (Rice, Gujarati, et al.). FCI is a way to simulate chemical problems classically with exact diagonalization; according to IBM, the largest chemical problems solved this way "comprise around 22 electrons and 22 orbitals," and the full calculation would be expected to take over a week (Garcia, 2020). The particular molecules of interest in this article were lithium hydride (LiH), hydrogen sulfide (H_2S), lithium sulfide (Li_2S), and lithium hydrogen sulfide (LiSH). The researchers modeled these compounds using a five-qubit quantum processor, the IBM Q Valencia (Rice, Gujarati, et al.). Classical simulations of quantum computers were also considered. Overall, the team was able to model the ground state and dipole moment of the described compounds very accurately. The authors do note a potential difference in error between the modeling of ionic and covalent bonds, which could have interesting implications for the future of quantum modeling (Rice, Gujarati, et al.).

Again, this article highlights some flaws with quantum computation and its use in chemical modeling. The authors themselves acknowledge working around limitations including the limited number of available qubits and a lack of full availability of quantum error correction (Rice, Gujarati, et al.). Yet the paper also shows that research in the use of quantum computation in the simulation of chemical problems continues, with researchers using each other's work to push forward. Additionally, the paper shows that quantum modeling is already being applied toward real world problems. As more research is performed, the use of quantum computing in chemical modeling becomes closer to reality.

Conclusion

If quantum computers become more powerful, with more qubits and fault tolerance, then quantum computing methods will be better for modeling quantum chemical systems than classical systems. While good classical modeling methods exist and are improving, they are unable to match the combination of accuracy and speed which quantum computers have the potential to provide. The industry seems to understand this, too, with several major technology companies investing in quantum computing. For example, as mentioned, the IBM quantum computing team was working with Daimler, which is the parent company of Mercedes-Benz, on modeling battery chemistry. Quantum computing has the potential to revolutionize energy storage

technology, allowing for batteries which charge more quickly, provide power longer, and, hopefully, cost less.

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