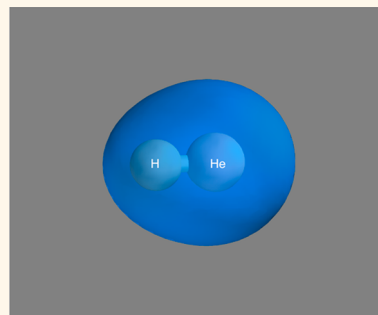


The Promise of Quantum Simulation

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ABSTRACT Quantum simulations promise to be one of the primary applications of quantum computers, should one be constructed. This article briefly summarizes the history of quantum simulation in light of the recent result of Wang and co-workers, demonstrating calculation of the ground and excited states for a HeH^+ molecule, and concludes with a discussion of why this and other recent progress in the field suggest that quantum simulations of quantum chemistry have a bright future.



In 1982, the physicist Richard Feynman noted that it is hard for classical computers to simulate some quantum mechanical systems. But, he observed, “Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws,”¹ then this simulation would become far easier. With this suggestion, Feynman inaugurated the field of quantum computing and introduced the idea that quantum computers change the boundaries of computational complexity.

Simulation of quantum physical systems is thus the first “killer app” of quantum computing. Since then, several other fast quantum algorithms have emerged, notably Peter Shor’s algorithm for integer factorization and discrete logarithms² and Lov Grover’s algorithm for unstructured search.³ Quantum simulation remains one of the primary applications of quantum computers, should one be constructed. It is arguably the most intriguing and potentially valuable of all the known quantum algorithms, with potential impact in chemistry,⁴ materials science,⁴ and elementary particle physics.⁵

The canonical quantum simulation algorithm uses the same subroutine as Shor’s integer factorization algorithm—the quantum Fourier transform—but instead of using it to reveal the period of a modular function, simulation uses it to estimate the energies of a Hamiltonian. It does this using Kitaev’s algorithm for quantum phase estimation,⁶ which efficiently reveals the phase (and thus the eigenvalue) of an eigenvector of a unitary

operation. Abrams and Lloyd^{7,8} showed that a broad class of Hamiltonians could be efficiently simulated (and thus probed using phase estimation) using a Suzuki–Trotter expansion. They applied their results to the Hubbard model and suggested that these techniques would lead to an exponential speed-up over classical computing resources. Somma and co-workers⁹ extended quantum simulation to many more systems by showing that the Jordan–Wigner transformation¹⁰ could be used to map the creation/annihilation operators that often define quantum mechanical Hamiltonians into N -qubit operators. This paved the way for quantum simulation of quantum chemistry.

Quantum simulation is arguably the most intriguing and potentially valuable of all the known quantum algorithms, with potential impact in chemistry, materials science, and elementary particle physics.

Quantum chemistry addresses the problem of describing the electronic structure of molecules and materials, which provides information about how they dissociate, react, absorb light, and interact with other molecules

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and materials. Typically, quantum chemical methods describe molecular electronic states as products of single-electron states generated from a variety of effective Hamiltonians, including Hartree–Fock¹¹ and density functional theory (DFT).^{12,13} A huge variety of interesting chemical systems are well described either by these product states or by simple perturbations of them. However, these methods break down in systems involving strongly correlated electrons. For these molecules, quantum chemists fall back on brute force methods, the most accurate (and arduous) of which is full configuration interaction (CI).¹⁴

Full CI considers the many-body Hamiltonian formed by all the possible ways of distributing N electrons into M one-electron states. Because the number of such configurations grows combinatorially with N and M , full CI computations require [classical] computational resources that scale exponentially with the molecule's size. This kind of scaling rapidly surpasses the capacity of any existing computer, so quantum chemists have developed a variety of "truncated" approximations to full CI. Typically, these involve configurations that can be generated using just a few excitations from the ground-state electronic configuration. Unfortunately, although truncated CI wave functions can be evaluated with only polynomial resources, they are known to lack properties that are required for quantitative chemical predictions, such as size consistency.¹⁵ Related perturbational approaches, such as coupled-cluster approaches,¹⁶ include size consistency but often lack strict variational bounds on the energy. So, although both truncated CI and coupled-cluster methods often give excellent energies in practice, they are incomplete solutions to chemical simulation because they lack certain properties of the full CI method. For the chemical problems where these methods fail, fully quantum simulation à la Feynman might be the only viable approach.

In 2005, Aspuru-Guzik and co-workers¹⁷ applied iterative phase estimation and other techniques from quantum information theory to the full CI problem. Although their approach scales polynomially for the full CI problem, the exact scaling of their algorithm was unclear in 2005. However, their approach suggested that even modest quantum resources could potentially enable full CI simulations that outperform the largest, fastest supercomputers.

The first experimental demonstration of quantum full CI algorithm came 5 years later, when a photonic quantum information processor¹⁸ calculated the ground and electronically excited states for a minimal basis set description of H_2 using a 20-bit iterative phase estimation. Although this proof-of-principle computation did not provide any added insight into the nature of the H_2 bond, it demonstrated conclusively that the quantum phase estimation algorithm could produce accurate bonding and excitation energies, even in the face of the noise and decoherence inherent to imperfect physical qubits.

In this issue of *ACS Nano*, Wang and co-workers¹⁹ demonstrate a quantum calculation of the ground and excited states for a HeH^+ molecule, which is isoelectronic with H_2 but has differently charged nuclei. Wang *et al.* report the highest precision achieved to date in the quantum simulation of molecular energies; they surpass chemical precision by 10 orders of magnitude. Their quantum simulation was performed using 2 qubits from a diamond nitrogen vacancy (NV) center and represents the first implementation of the full CI algorithm on a solid-state qubit. As with the earlier demonstration,¹⁸ this result is most notable for verifying that these algorithms can be successfully implemented on actual qubits rather than just in theoretical idealizations.

The principle of quantum chemistry simulation has been proved. The next urgent question is how it will scale—how many qubits and

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how much time will be required to apply quantum simulation algorithms to larger, more general molecules. The time required scales with N , the number of basis functions used to describe the atomic orbitals that compose the molecule (adequate basis sets require 5–20 basis functions per atom), and/or Z , the maximum nuclear charge in the molecule. The initial analysis last year²⁰ suggested that quantum simulation algorithms might require $O(N^6)$ clock cycles. Although this is a huge advance, in principle, over the $O(e^N)$ scaling of exact classical simulation, it remains prohibitively intractable in practice. However, more careful analyses of the Suzuki–Trotter expansion have produced steady and rapid improvements in this scaling, first to $O(N^7)$,²¹ then to $O(N^{5.5})$,²² and, most recently, to $O(N^3Z^{2.5})$.²³

The best scaling known today suggests that, given a handful of good qubits, quantum simulation could produce practical, useful results. A closer look, however, suggests a less optimistic picture in the near future. Molecules with $N = 1000$ are routinely analyzed on laptop computers using DFT, the workhorse method of chemistry and materials science. The most optimistic scaling given above suggests that a quantum computer would need at least 10^9 operations to match what DFT can do on a laptop. Because qubits have far higher error rates than classical computers, such a large computation would absolutely demand quantum error correction.²⁴ Error correction imposes massive overhead in time, number

of qubits, and complexity because small quantum rotations have to be compiled into H, S, and T gates,²⁵ some of which must be exhaustively distilled from noisy resources.²⁶ These considerations suggest that practical quantum simulation of meaningful molecules is substantially more challenging than it appears at first—and perhaps infeasible in the near term.

Perhaps surprisingly, we remain optimistic. Although the demonstrations by Wang *et al.*¹⁹ and others are a long way from practical utility, they demonstrate that the principle is sound. It is widely believed that further algorithmic improvements are possible; after all, just in the past 2 years, we have seen the time scaling drop from $O(N^9)$ to $O(N^3Z^{2.5})$. Moderate improvements in scaling could dramatically change feasibility, and algorithms that avoid the Suzuki–Trotter expansion^{27–30} appear promising. Finally, we observe that some of the most promising candidates for near-term “quantum supremacy” (practical speed-ups over existing classical computers) are robust quantum simulation algorithms that may not require error correction, either by using device noise to mimic real-world noise in the simulated system or by leveraging shallow quantum circuits that run so quickly that errors do not accumulate. Analog quantum simulation⁴ is one such candidate and has been used to mimic Hubbard³¹ and spin³² Hamiltonians. Analog methods are not currently known for chemical or molecular systems, but these systems can be addressed within the variational eigensolver approach,³³ which leverages a small quantum computer to evaluate the energy terms of a parametric wave function that is varied by an associated classical computer-driven optimization. We believe that between the near-term promise of these nontraditional algorithms and steady progress toward the long-term goal of digital quantum simulation, quantum simulation of quantum chemistry has a bright future.

Conflict of Interest: The authors declare no competing financial interest.

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