

CHEMICAL PHYSICS

A quantum-computing advantage for chemistry

Error-mitigated Hartree-Fock computation is performed with up to 12 superconducting qubits

By **Xiao Yuan**

Quantum computers potentially have computational power greater than that of their classical counterparts. The recent demonstration of “quantum supremacy” on Google’s 53-qubit Sycamore quantum processor (1) has reinforced this idea, but it remains unknown whether the next generation of quantum computers will be able to solve classically intractable problems of practical interest. On page 1084 of this issue, Rubin *et al.* (2) take steps toward answering this question with an experimental implementation of Hartree-Fock calculations of molecular electronic energies on a superconducting processor. Although the calculations performed are also efficient to run on classical computers, the experiment demonstrates many of the key building blocks for quantum chemistry simulation and paves the way toward achieving quantum advantage for problems of chemical interest.

Using controllable quantum systems to simulate quantum mechanical problems in chemistry and physics was the brainchild of Richard Feynman, who remarked in the 1980s that “If you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful

problem, because it doesn’t look so easy” (3). Since then, there has been substantial theoretical and experimental progress toward this goal. In particular, the rapid recent development of superconducting qubits, such as Google’s Sycamore quantum processor, has enabled quantum supremacy, which samples from the outputs of random quantum circuits more efficiently than appears possible with even the largest classical supercomputers (1).

Rubin *et al.* investigate the performance of this same processor to determine the electronic structure of molecular systems. Such an accomplishment would have academic as well as commercial value, as it could enable the design of improved catalysts or new medicines. Since the first quantum algorithm for quantum computational chemistry was proposed in 2005 (4), there have been numerous developments to reduce its computational cost (5, 6). One of the most influential developments is that of the variational quantum eigensolver (VQE), which reduces the burden on the quantum processor by leveraging a classical coprocessor (7) (see the figure).

Prior proof-of-principle VQE experiments have realized electronic structure calculations with up to six qubits (8). It is still an open question as to whether the VQE can solve classically intractable instances of the electronic structure problem, which may require on the order of 100 qubits. As the prob-

lem size increases, so too does the quantum circuit depth (the number of layers of gates; five in the figure) required to realize the quantum algorithm. Even if the quality of the qubits is maintained while the processor is scaled up, larger processors with deeper circuits will lead to an increased error rate for the calculation. Assessing whether this build-up of errors is fatal for the VQE is one of the most pressing open questions in the field of quantum computing.

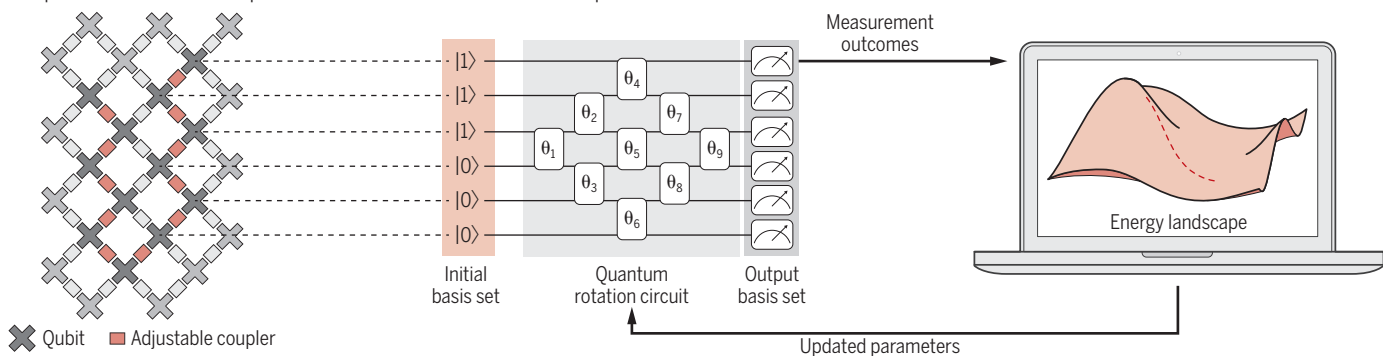
Rubin *et al.* take steps to address these open questions through an experimental VQE implementation using 6 to 12 qubits. The experiment implements the Hartree-Fock method for calculating the binding energy of hydrogen chains and the isomerization of diazene. The Hartree-Fock method provides approximate solutions to the electronic structure problem and is a classically tractable calculation. It is typically used as an initial step in quantum computational approaches to solving the electronic structure problem.

Nonetheless, this VQE experiment demonstrates many of the key components for large-scale VQE implementations, including electronic state preparation, Hamiltonian measurement for any one- and two-particle reduced-density matrix elements, two error mitigation techniques, and outer-loop classical optimization. Together, these features lead to the successful extension of prior investigations into quantum computational

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A variational quantum eigensolver

A parameterized quantum circuit, with properly prepared initial states and with the aid of a classical co-processor, approximates the wave function of a chemical compound. The circuit corresponds to the one Rubin *et al.* used for six-qubit Hartree-Fock calculation.



Google Sycamore

The schematic shows the superconducting qubits and the adjustable couplers that connect them.

Quantum circuit

The input states of the wave function are initialized as $|0\rangle$ or $|1\rangle$. Each box with a parameter θ is a rotation gate that is compiled into two two-qubit gates and three single-qubit gates.

Classical calculation

The outcomes are fed into a classical computer that trains the parameters to learn the ground state of the system. The classical parameters that determine the wave function are fed back to the quantum computer, and the calculation is rerun.

chemistry. The techniques demonstrated in this work will likely form the foundation of future VQE experiments targeting classically intractable systems.

Perhaps the most important conclusions from the work of Rubin *et al.* are the necessity of tailoring algorithms to the quantum processor and the importance of error mitigation techniques. Because near-term quantum devices typically have restricted realizable gates, the ability to compile the circuit for a given architecture is crucial for simulation efficiency and accuracy. The methods showcased by Rubin *et al.* for realizing electronic states with nearest-neighbor gates shed light on how to implement more complicated calculations with restricted hardware topologies.

Even with the compilation methods discussed above, the presence of noise in these calculations is still a pressing issue. Rubin *et al.* show how to obtain accurate results despite this noise through the use of error mitigation strategies. The techniques used in this work are specialized for quantum simulations, exploiting particle conservation through local density matrix information and the N -representability conditions of fermionic systems. For the 12-qubit calculation with 72 two-qubit gates, the combined error mitigation techniques effectively improve the raw-state fidelity to >99%, which represents an increase of about two orders of magnitude.

Whether noisy intermediate-scale quantum computers will be able to surpass classical supercomputers in solving chemistry problems has become one of the most exciting questions in quantum computing. Preliminary calculations on small- and intermediate-sized systems have verified the feasibility of the most promising quantum algorithms. However, further work is needed to enable similar calculations to be performed for system sizes that are greater by one to two orders of magnitude. Experimentally, quantum devices need to be scaled up to hundreds or even thousands of qubits. The characterization of errors should be improved alongside a reduction in error rates. Theoretically, we seek more efficient algorithms and more effective error mitigation techniques, especially ones tailored for specific problems and quantum devices. ■

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A health worker fumigates homes in Managua, Nicaragua, to reduce the risk of mosquito-borne dengue and Zika viruses.

INFECTIOUS DISEASE

Zika virus increases risk of dengue disease

Interactions between Zika virus immunity and dengue disease have implications for vaccination

By Hannah Clapham

The dengue flavivirus (DENV) is a mosquito-borne virus that occurs in more than 100 countries and is known for inducing complex immunity in human infections. The first infection with one of the four DENV serotypes generally has a low risk of severe outcome. Subsequently, it is thought that there is a period of cross-protection in which infection with any serotype results in even lower risk of severe disease. After this period, an infection with a different serotype has a higher risk of severe disease (1). In 2015 to 2016, Zika virus (ZIKV, also mosquito-borne) spread rapidly across Central and South America and the Caribbean, where DENV is also endemic (2). Because ZIKV is also a flavivirus, whether prior infection with DENV alters Zika disease risk and vice versa became an important question as ZIKV spread. On page 1123 of this issue, Katzelnick *et al.* (3) studied the long-running dengue cohort in Nicaragua and found evidence that prior ZIKV infection increases dengue disease risk.

DENV infection can result in a range of outcomes, including asymptomatic, mild

flu-like illness and severe dengue, which is characterized by complications of bleeding and organ damage. ZIKV infections are mostly mild, except for a small proportion that result in Guillain-Barre syndrome (autoimmunity to peripheral nerves) or birth defects in infants born to mothers infected during pregnancy.

An initial DENV infection generates high levels of serotype cross-reactive neutralizing antibodies. However, these antibodies wane over time and are thought to reach “subneutralizing” levels. The more severe disease in subsequent infections is thought to arise in part from antibody-dependent enhancement, whereby these antibodies are able to bind to, but not neutralize, the virus, which can promote virus cell entry. To study the relationship between prior DENV infections and subsequent dengue outcome, a long-running cohort study is ideal. The cohort study in Managua, Nicaragua, running since 2004, has led to numerous insights into dengue immunity and disease. With the arrival of ZIKV, this study effectively expanded to include ZIKV infections, leading to the findings of Katzelnick *et al.*

For ZIKV infection after a DENV infection, in vitro testing of sera showed that previous DENV infection led to both neutralizing and enhancing responses to ZIKV (4).

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