New algorithms to determine eigenstates and thermal states on quantum computers

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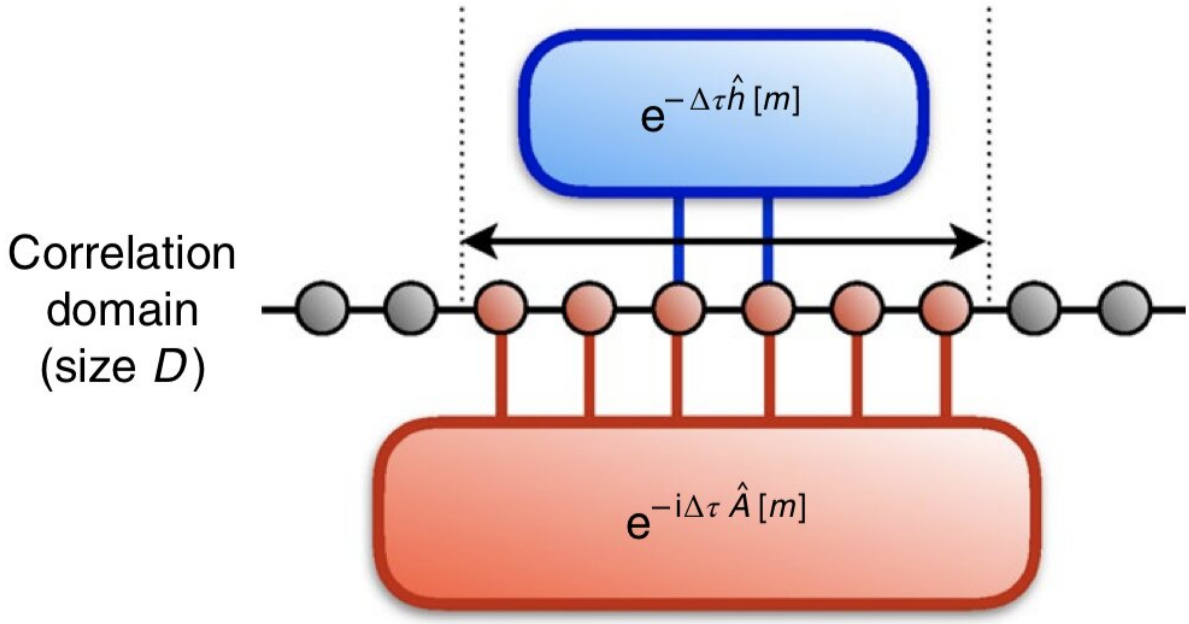

Image capturing the essence of how the researchers represented imaginary-time evolution by unitary transformations that one can turn into a quantum circuit. Credit: Motta et al.

Determining the quantum mechanical behavior of many interacting particles is essential to solving important problems in a variety of scientific fields, including physics, chemistry and mathematics. For instance, in order to describe the electronic structure of materials and

molecules, researchers first need to find the ground, excited and thermal states of the Born-Oppenheimer Hamiltonian approximation. In quantum chemistry, the Born-Oppenheimer approximation is the assumption that electronic and nuclear motions in molecules can be separated.

A variety of other scientific problems also require the accurate computation of Hamiltonian ground, excited and thermal states on a quantum computer. An important example are combinatorial optimization problems, which can be reduced to finding the ground state of suitable spin systems.

So far, techniques for computing Hamiltonian eigenstates on quantum computers have been primarily based on phase estimation or variational algorithms, which are designed to approximate the lowest energy eigenstate (i.e., ground state) and a number of excited states. Unfortunately, these techniques can have significant disadvantages, which make them impracticable for solving many scientific problems.

A research collaboration between the groups of Garnet Chan, Fernando Brandao, and Austin Minnich at the California Institute of Technology (Caltech) has recently led to the development of three new algorithms that could help to overcome the limitations of existing phase estimation and variational methods. These algorithms, dubbed quantum imaginary time evolution, quantum Lanczos and quantum METTS algorithms, were presented in a paper published in *Nature Physics*.

"Determining ground, excited and thermal states is of course an important problem in quantum computing, but the algorithms to tackle it on contemporary hardware typically require important quantum resources, such as deep quantum circuits (i.e. comprising many quantum gates, and thus prone to decoherence and imperfect implementation) and ancillary (i.e. additional) qubits—or non-linear noisy classical parameter optimizations," Mario Motta, one of the researchers who carried out the

study, told Phys.org.

The key aim of the recent study carried out by the researchers at Caltech was to develop new quantum algorithms for determining ground, excited and thermal states on quantum computers. The researchers tried to circumvent the practical limitations of existing techniques for computing Hamiltonian states by leveraging notions from classical computer physics, such as imaginary-time evolution, exact diagonalization and finite-temperature state sampling, ultimately extending these notions to quantum computing algorithms beyond what previously accomplished.

"Our algorithms are based on the notion of imaginary-time evolution, which is akin to a cooling process," Motta explained. "Suppose that we can prepare a quantum mechanical system in a simple but inaccurate approximation for the ground state, a trial wave function. By applying this cooling process to the system, we can systematically remove spurious excitations from the trial wave function, thereby gradually approaching the ground state. This is the content of the quantum imaginary-time evolution (QITE) algorithm."

The three algorithms developed by the Caltech researchers are somewhat similar to classical techniques for finding ground and excited states. By collecting information as imaginary-time evolution unfolds, however, these algorithms can formulate and solve an eigenvalue problem that provides access to specific excited states, employing a quantum variant of the Lanczos approach, a well-established mathematical technique to compute eigenvalues and eigenvectors.

"Of course, imaginary-time evolution can also be used to cool a system from infinite to finite (greater than zero) temperature, and thus to compute finite-temperature properties, as we do in our QMETTS algorithm," Motta said.

The quantum imaginary time evolution algorithm and Lanczos algorithm proposed by the researchers have several advantages over existing and classical techniques. For instance, as they are rooted in physical intuition, they can be implemented on contemporary quantum hardware and do not require deep circuits, ancillary qubits and complicated parameter optimizations, which are indispensable for other quantum algorithms.

"The most meaningful achievement of our study was the conception of a suite of new algorithms for the study of many-many-body systems on contemporary quantum computers," Motta said. "Our algorithms bring useful insights to the Physics field: in particular, they show how the combination of ideas and techniques from different fields of science can be synergistically combined to produce innovative techniques."

In their study, Motta and his colleagues demonstrated the effectiveness of the algorithms they developed by implementing them on the Rigetti quantum virtual machine and Aspen-1 quantum processing unit. In these demonstrations the algorithms performed remarkably well, comparing favorably to existing techniques for computing Hamiltonian ground, excited and thermal states.

The new algorithms developed by this team of researchers could be used in a variety of studies that involve quantum simulations and optimization. In addition, they could be refined and extended to meet the needs of individuals research projects.

"Our future research will be directed towards expanding the predictive power of the algorithms we developed," Motta said. "For example, by computing properties beyond the energy, such as density operators and correlation functions, and devising systematic and efficient strategies to study arbitrary many-body systems (comprising bosons and fermions, with particular emphasis on molecules)."

More information: Mario Motta et al. Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution, *Nature Physics* (2019). DOI: 10.1038/s41567-019-0704-4