New algorithms advance the computing power of early-stage quantum computers

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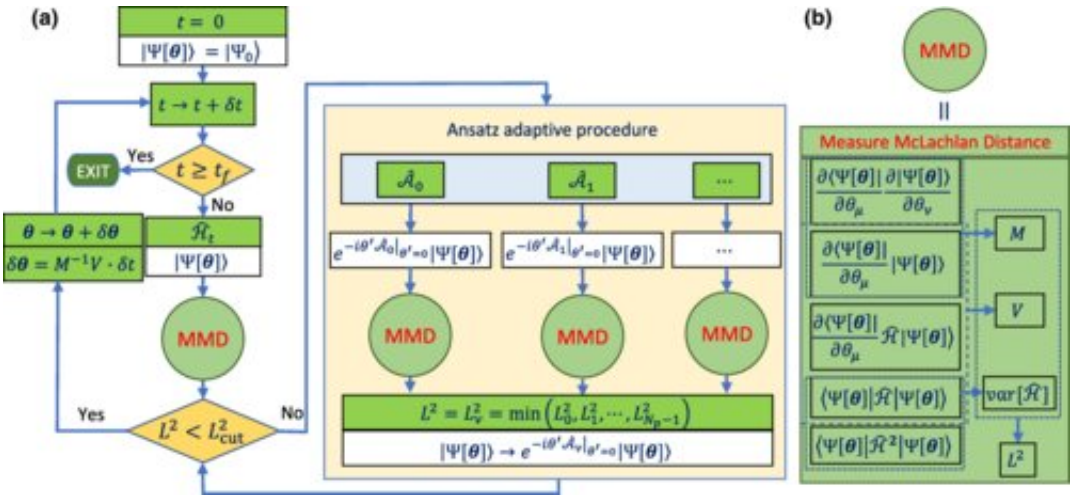

Schematic illustration of the AVQDS algorithm. The flow chart of AVQDS is plotted in (a). The details of the MMD module, which measures the McLachlan distance for a given variational wave function Ψ [θ] and time-dependent Hamiltonian ^H_t, are shown in (b). The circuits to measure matrix M and vector V can be found in Ref. [27]. Note that in the ansatz adaptive procedure, one only needs to measure the incremental elements in M and V, which are added in a given step. Credit: DOI: 10.1103/PRXQuantum.2.030307

A group of scientists at the U.S. Department of Energy's Ames Laboratory has developed computational quantum algorithms that are capable of efficient and highly accurate simulations of static and dynamic properties of quantum systems. The algorithms are valuable tools to gain greater insight into the physics and chemistry of complex

materials, and they are specifically designed to work on existing and near-future quantum computers.

Scientist Yong-Xin Yao and his research partners at Ames Lab use the power of advanced computers to speed discovery in condensed matter physics, modeling incredibly complex quantum mechanics and how they change over ultra-fast timescales. Current high performance computers can model the properties of very simple, small quantum systems, but larger or more complex systems rapidly expand the number of calculations a computer must perform to arrive at an accurate model, slowing the pace not only of computation, but also discovery.

"This is a real challenge given the current early-stage of existing quantum computing capabilities," said Yao, "but it is also a very promising opportunity, since these calculations overwhelm classical computer systems, or take far too long to provide timely answers."

The new algorithms tap into the capabilities of existing quantum computer capabilities by adaptively generating and then tailoring the number and variety of "educated guesses" the computer needs to make in order to accurately describe the lowest-energy state and evolving quantum mechanics of a system. The algorithms are scalable, making them able to model even larger systems accurately with existing current "noisy" (fragile and prone to error) quantum computers, and their near-future iterations.

"Accurately modeling spin and molecular systems is only the first part of the goal," said Yao, "In application, we see this being used to solve complex materials science problems. With the capabilities of these two algorithms, we can guide experimentalists in their efforts to control materials' properties like magnetism, superconductivity, chemical reactions, and photo-energy conversion."

"Our long-term goal is to reach 'quantum advantage' for materials— to utilize quantum computing to achieve capabilities that cannot be achieved on any supercomputer today," said Ames Laboratory Scientist Peter Orth.

More information: Yong-Xin Yao et al, Adaptive Variational Quantum Dynamics Simulations, *PRX Quantum* (2021). DOI: 10.1103/PRXQuantum.2.030307

Niladri Gomes et al, Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation, *Advanced Quantum Technologies* (2021). DOI: 10.1002/qute.202100114

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