Spin clean-up method brings practical quantum computers closer to reality

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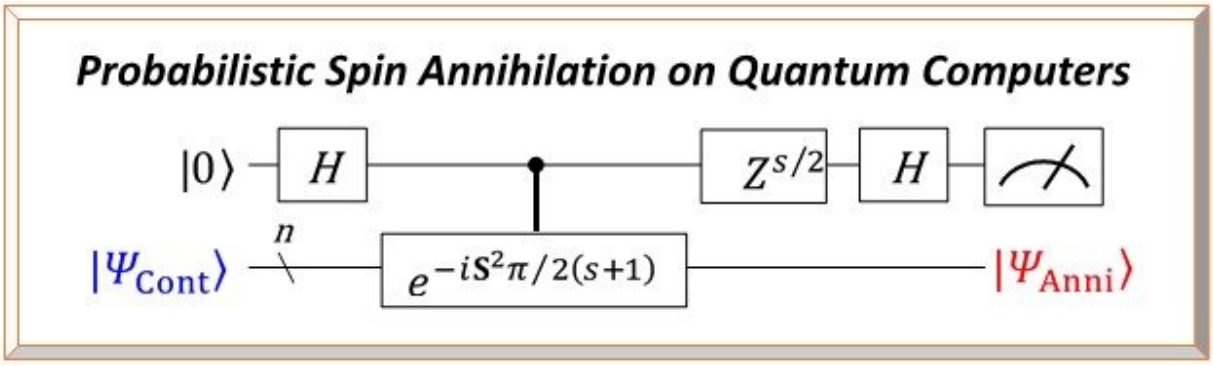

If the measurement outcome in the quantum circuit is the |0? state, the spin contaminated wave function |?Cont? is projected out onto the spin annihilated one |?Anni?. The rightmost part of the top line denotes the measurement. Credit: Kenji Sugisaki, Kazunobu Sato and Takeji Takui, Osaka City University

Quantum computers are the new frontier in advanced research technology, with potential applications such as performing critical calculations, protecting financial assets, or predicting molecular behavior in pharmaceuticals. Researchers from Osaka City University have now solved a major problem hindering large-scale quantum computers from practical use: precise and accurate predictions of atomic and molecular behavior.

They published their method to remove extraneous information from

quantum chemical calculations on Sept. 17 as an advanced online article in *Physical Chemistry Chemical Physics*, a journal of the Royal Society of Chemistry.

"One of the most anticipated applications of quantum computers is electronic structure simulations of atoms and molecules," said paper authors Kenji Sugisaki, Lecturer and Takeji Takui, Professor Emeritus in the Department of Chemistry and Molecular Materials Science in Osaka City University's Graduate School of Science.

Quantum chemical calculations are ubiquitous across scientific disciplines, including pharmaceutical therapy development and materials research. All of the calculations are based on solving physicist Erwin Schrödinger's equation, which uses electronic and molecular interactions that result in a particular property to describe the state of a quantum-mechanical system.

"Schrödinger equations govern any behavior of electrons in molecules, including all chemical properties of molecules and materials, including chemical reactions," Sugisaki and Takui said.

On classical computers, such precise equations would take exponential time. On quantum computers, this precision is possible in realistic time, but it requires "cleaning" during the calculations to obtain the true nature of the system, according to them.

A quantum system at a specific moment in time, known as a wave function, has a property described as spin, which is the total of the spin of each electron in the system. Due to hardware faults or mathematical errors, there may be incorrect spins informing the system's spin calculation. To remove these 'spin contaminants,' the researchers implemented an algorithm that allows them to select the desired spin quantum number. This purifies the spin, removing contaminants during

each calculation—a first on quantum computers, according to them.

"Quantum chemical calculations based on exactly solving Schrödinger equations for any behavior of atoms and molecules can afford predictions of their physical-chemical properties and complete interpretations on chemical reactions and processes," they said, noting that this is not possible with currently available classical computers and algorithms. "The present paper has given a solution by implementing a quantum algorithm on quantum computers."

The researchers next plan to develop and implement algorithms designed to determine the state of electrons in molecules with the same accuracy for both excited- or ground-state electrons.

More information: Kenji Sugisaki et al, A probabilistic spin annihilation method for quantum chemical calculations on quantum computers, *Physical Chemistry Chemical Physics* (2020). DOI: 10.1039/d0cp03745a

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