Swedish quantum computer applied to chemistry for the first time

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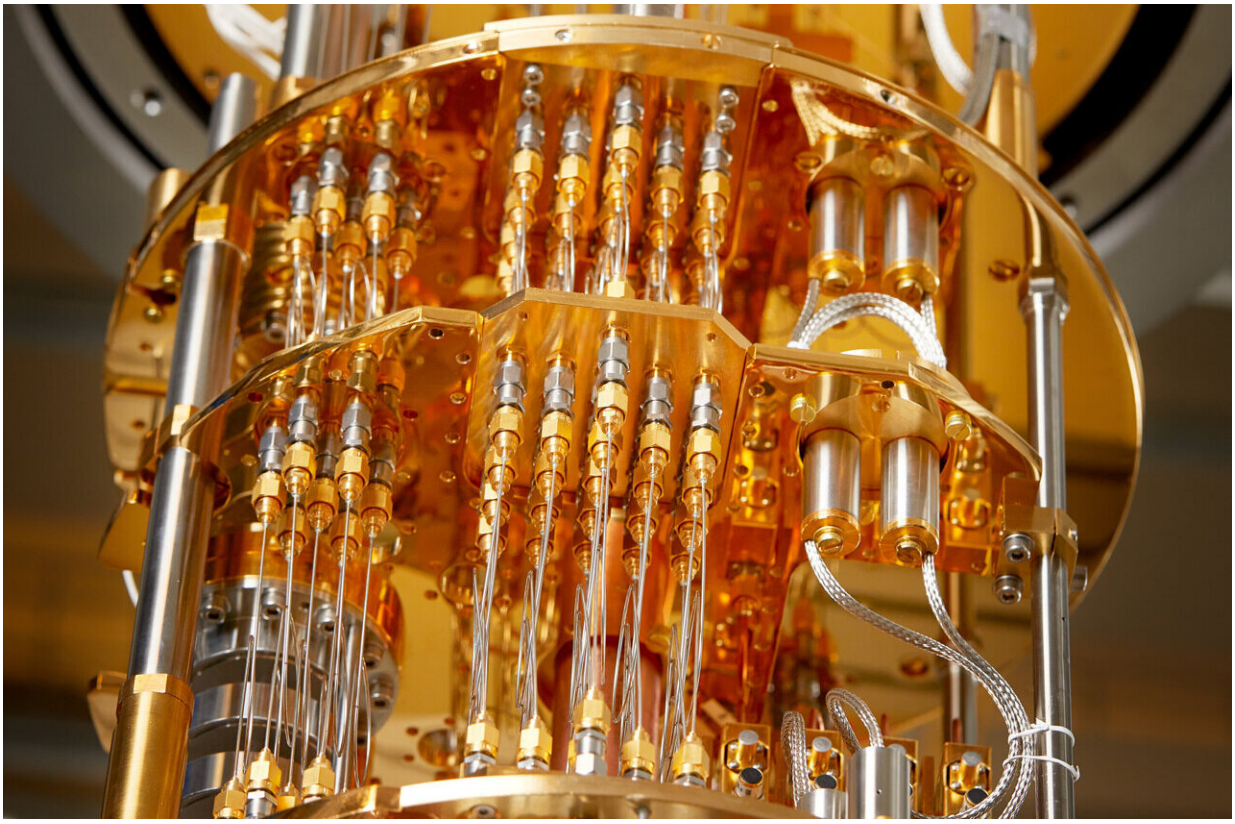

The quantum computer at Chalmers with the outer shielding of the dilution refrigerator removed. Credit: Chalmers/Anna-Lena Lundqvist

There are high expectations that quantum computers may deliver revolutionary new possibilities for simulating chemical processes. This

could have a major impact on everything from the development of new pharmaceuticals to new materials. Researchers at Chalmers University have now, for the first time in Sweden, used a quantum computer to undertake calculations within a real-life case in chemistry.

"Quantum computers could in theory be used to handle cases where electrons and atomic nuclei move in more complicated ways. If we can learn to utilize their full potential, we should be able to advance the boundaries of what is possible to calculate and understand," says Martin Rahm, Associate Professor in Theoretical Chemistry at the Department of Chemistry and Chemical Engineering, who has led the study.

Within the field of quantum chemistry, the laws of quantum mechanics are used to understand which chemical reactions are possible, which structures and materials can be developed, and what characteristics they have. Such studies are normally undertaken with the help of super computers, built with conventional logical circuits. There is however a limit for which calculations conventional computers can handle. Because the laws of quantum mechanics describe the behavior of nature on a subatomic level, many researchers believe that a quantum computer should be better equipped to perform molecular calculations than a conventional computer.

"Most things in this world are inherently chemical. For example, our energy carriers, within biology as well as in old or new cars, are made up of electrons and atomic nuclei arranged in different ways in molecules and materials. Some of the problems we solve in the field of quantum chemistry are to calculate which of these arrangements are more likely or advantageous, along with their characteristics," says Martin Rahm.

A new method minimizes errors in the quantum chemical calculations

There is still a way to go before quantum computers can achieve what the researchers are aiming for. This field of research is still young and the small model calculations that are run are complicated by noise from the quantum computer's surroundings. However, Martin Rahm and his colleagues have now found a method that they see as an important step forward. The method is called Reference-State Error Mitigation (REM) and works by correcting for the errors that occur due to noise by utilizing the calculations from both a quantum computer and a conventional computer.

"The study is a proof-of-concept that our method can improve the quality of quantum-chemical calculations. It is a useful tool that we will use to improve our calculations on quantum computers moving forward," says Martin Rahm. The article, "Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry," is published in the *Journal of Chemical Theory and Computation*.

The principle behind the method is to first consider a reference state by describing and solving the same problem on both a conventional and a quantum computer. This reference state represents a simpler description of a molecule than the original problem intended to be solved by the quantum computer. A conventional computer can solve this simpler version of the problem quickly. By comparing the results from both computers, an exact estimate can be made for the amount of error caused by noise. The difference between the two computers' solutions for the reference problem can then be used to correct the solution for the original, more complex, problem when it is run on the quantum processor.

By combining this new method with data from Chalmers' quantum computer Särimner the researchers have succeeded in calculating the intrinsic energy of small example molecules such as hydrogen and lithium hydride. Equivalent calculations can be carried out more quickly

on a conventional computer, but the new method represents an important development and is the first demonstration of a quantum chemical calculation on a quantum computer in Sweden.

"We see good possibilities for further development of the method to allow calculations of larger and more complex molecules, when the next generation of quantum computers are ready," says Martin Rahm.

Quantum computer built at Chalmers

The research has been conducted in close collaboration with colleagues at the Department of Microtechnology and Nanoscience. They have built the quantum computers that are used in the study, and helped perform the sensitive measurements that are needed for the chemical calculations.

"It is only by using real quantum algorithms that we can understand how our hardware really works and how we can improve it. Chemical calculations are one of the first areas where we believe that quantum computers will be useful, so our collaboration with Martin Rahm's group is especially valuable," says Jonas Bylander, Associate Professor in Quantum Technology at the Department of Microtechnology and Nanoscience.

More information: Phalgun Lolur et al, Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry, *Journal of Chemical Theory and Computation* (2023). DOI: 10.1021/acs.jctc.2c00807

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