

Question1: These are three experimental demonstrations of quantum simulations. Nothing its relative date of publication, describe your chosen paper's impact in the business trade press. Do you feel it had the largest influence of the three? Why or why not?

1. Observation of a many-body¹ dynamical phase transition² with a 53-qubit quantum simulator.

1.1 Objectives of this quantum simulator

Here a quantum simulator is used composed of up to 53 qubits to:

1. study non-equilibrium dynamics³ in the transvers-field Ising model^{4,5} with long-range interactions.
2. Observe a dynamical phase transition after a sudden change of the Hamiltonian, in a regime in which conventional statistical mechanics does not apply.

1.2 Implementation of this quantum simulator

The qubits are represented by the spins of trapped ions, which can be prepared in various initial pure states. We apply a global long-range Ising interaction with controllable strength and range, and measure each individual qubit with an efficiency of nearly 99 per cent. Such high efficiency means that arbitrary many-body correlations between qubits can be measured in a single shot, enabling the dynamical phase transition to be probed directly and revealing computationally intractable features that rely on the long-range interactions and high connectivity between qubits.

1.3 Magnitude of business opportunities

The field has advanced tremendously since the 1960s. Subsequent decades saw great progress in addressing new many-body systems - such as those exhibiting the Kondo effect, disordered systems, superfluid helium-3, and unconventional superconductors - and the development of new tools, such as functional integrals and the renormalization group.

1.4 Some of the impacted audience

The understanding of such nonequilibrium behavior is of great interest to a wide range of subjects, from social science and cellular biology to astrophysics and quantum condensed matter physics.

1.5 Outreach articles

1. <http://www.arxiv-vanity.com/papers/1708.01044/>
2. <https://www.cambridge.org/am/academic/subjects/physics/condensed-matter-physics-nanoscience-and-mesoscopic-physics/introduction-many-body-physics?format=HB>

2. Scalable quantum simulation of molecular energies.

1.1 Objectives of this quantum simulator

A programmable array of superconducting qubits^{6,7} is used to compute the energy surface of molecular hydrogen using two distinct quantum algorithms.

1.2 Implementation of this quantum simulator

1. The unitary coupled cluster method using the variational quantum eigen solver is experimentally executed. Efficient implementation of predicts the correct dissociation energy⁸ to within chemical accuracy of the numerically exact result.
2. The canonical quantum algorithm for chemistry is experimentally demonstrated, which consists of Trotterization and quantum phase estimation.

We compare the experimental performance of these approaches to show clear evidence that the variational quantum eigensolver is robust to certain errors. This error tolerance inspires hope that variational quantum simulations of classically intractable molecules may be viable in the near future.

Our findings suggest that the quantum simulation of classically intractable molecules may be possible without the overhead of quantum error correction.

My chosen paper is “Scalable quantum simulation of molecular energies” and I do believe it can have the largest influence of the three for its great magnitude of business opportunities and the vast impacted audience which I will mention below.

1.3 Magnitude of business opportunities

“...nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical...” - Richard Feynman, Simulating Physics with Computers

1. The researchers are aiming to create a quantum computer that is capable not only of computing single molecule energies, but entire

chemical systems. As one example, they would like to be able to simulate what happens as bacteria do their work in producing fertilizer—a process they note that currently consumes approximately 2 percent of global energy produced. That would mean developing a universal quantum computer, which, not coincidentally, is a goal Google has set for itself.

2. It is thought that quantum computers will be most useful in replicating and simulating reality, particularly modelling chemical reactions. Numerous computer science researchers around the world and billions of dollars has been invested to create them, and it is believed that these new super-powerful computers will be available within the next 50 years.

"Though many theoretical and experimental challenges lay ahead, a quantum enabled paradigm shift from qualitative / descriptive chemistry simulations to quantitative / predictive chemistry simulations could modernize the field so dramatically that the examples imaginable today are just the tip of the iceberg," Google's quantum software engineer Ryan Babbush, one of the lead authors on the study, wrote on the [Google Research blog](#).

1.4 Some of the impacted audience

1. The design of solar cells
2. Industrial catalysts
3. Batteries
4. Flexible electronic
5. Medicines
6. Materials
7. Understanding of high temperature superconductivity

1.5 Outreach articles

1. <https://phys.org/news/2016-07-scalable-quantum-simulation-molecule.html>
2. <https://www.ibtimes.co.uk/google-boasts-quantum-computing-breakthrough-first-display-real-world-use-1571823>
3. <https://journals.aps.org/prx/abstract/10.1103/PhysRevX.6.031007>

4. <https://ai.googleblog.com/2016/07/towards-exact-quantum-description-of.html>
5. <https://journals.aps.org/prx/pdf/10.1103/PhysRevX.6.031007>

3. Hardware-efficient variational quantum eigen solver for small molecules and quantum magnets.

1.1 Objectives of this quantum simulation

Determining the ground-state⁹ for molecules of increasing size, up to BeH_2 .

1.2 Requirements

- a. Up to six qubits
- b. More than hundred Pauli terms.
- c. Variational quantum eigensolver
- d. Prepared trial states
- e. Compact encoding of fermionic Hamiltonians
- f. Robust stochastic optimization routine

1.3 Some of the impacted audience

1. The results help to elucidate the requirements for scaling the method to larger systems and for bridging the gap between key problems in high-performance computing and their implementation on quantum hardware.

1.4 Outreach articles

1. <https://scinapse.io/papers/2755255888>
2. <https://arstechnica.com/science/2017/09/quantum-computers-reach-deeper-find-ground-state-of-simple-hydrides/>

Some more relevant interesting articles:

1. <https://phys.org/news/2018-07-world-first-quantum-simulation-chemical-bonds.html>
 2. https://www.huffpost.com/entry/quantum-magnetism-first-time-physicists_n_3339243
 3. <https://phys.org/news/2020-04-topological-insulator-hybrid-approach-magnetic.html>
 4. <https://www.ibtimes.co.uk/storage-wars-atom-sized-magnets-are-future-when-world-runs-out-space-data-1636575>
-

1. **Many-body:** Many-body theory is an area of physics which provides the framework for understanding the collective behavior of large numbers of interacting particles, often on the order of Avogadro's number.
2. **Phase transition:** Phase transition is when a substance changes from a solid, liquid, or gas state to a different state. Every element and substance can transition from one phase to another at a specific combination of temperature and pressure.
3. **Non-equilibrium:** Non-equilibrium thermodynamics is a branch of thermodynamics that deals with physical systems that are not in thermodynamic equilibrium but can be described in terms of variables that represent an extrapolation of the variables used to specify the system in thermodynamic equilibrium.
4. **Ising model:** The Ising model is a mathematical model of ferromagnetism in statistical mechanics. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins" that can be in one of two states.
5. **Transvers-field Ising model:** A quantum version of the classical Ising model.
6. **Superconductivity:** is the set of physical properties observed in certain materials, wherein electrical resistance vanishes and from which magnetic flux fields are expelled.
7. **Superconducting quantum computing:** is an implementation of quantum computer in superconducting electronic circuits.
8. **Dissociation energy:** The energy needed to break every chemical bond in a molecule and completely separate all its atoms.
9. **Ground state energy:** The ground state is the lowest-energy state a quantum system can occupy. The ground state energy is the energy of that state.

Question 2: Two of the papers employ superconducting qubits, and were from research at large corporations, while one paper describes research using atomic qubits, performed at a research university. Based on how these results were received in the news press, can you see how the technology, and the research institution, made a difference in expectations for future developments?

Google, Microsoft, IBM and Intel are the four leading companies in quantum computing. The institute for quantum computing – university of Waterloo, university of Oxford, and Harvard Quantum initiative are among the top leading quantum computing research universities. In my opinion, corporations are leading in quantum computing compared to universities. I think finance is one of the main reasons since first these companies are rich themselves and also governments are willing to invest a lot of money on them. The second reason that comes to my mind is the influence of marketing and advertising. It goes without saying that people follow these well-known companies' news much more than universities' updates. In other words, the more you are followed and seen by people the more influence in business trade you can have. However, university research is undeniably important and their cooperation's with companies cannot be neglected. For instance, Google operates D-Wave quantum computer from their Quantum Artificial Intelligence Lab, which is hosted by the university's space research association and NASA. Additionally, IBM also announced a Partnership with a range of

universities to encourage greater study into quantum computing. It also recently invested in Cambridge Quantum Computing, which was one of the first startups to become a part of IBM's Q Network in 2018. One of the best-known companies in the technology world, Intel invested \$50 million in founding to QuTech(a research institute in the Delft University of Technology) in 2015. We all know that quantum computing is hard and I think it is a must that corporations and universities work jointly to speed up the development of these awesome and powerful computers and meet the quantum supremacy as soon as possible in order to have a chance to use the opportunities that quantum computers bring about to our lives.

Outreach articles:

1. <https://zen.yandex.ru/media/id/5e00b58843fdc000adb4baac/the-worlds-top-12-quantum-computing-research-universities-5e0643f016ef9000ac18eea4>
2. https://www.em360tech.com/business_agility/tech-features-featuredtech-news/top-10-quantum-computing-companies/

Question 3: Imagine you are responsible for investing the money for a company or a funding agency interested in the further development of quantum computation. Would you invest your money in your chosen paper's project? Why or why not?

* The article I have chosen to focus on is Scalable Quantum Simulation of Molecular Energies.

I would definitely invest money on this project as I truly believe that **quantum is the future** since it enables the industries to tackle problems they never would have attempted to solve before, and Scalable Quantum Simulation of Molecular Energies is just one more step in the right direction towards making a quantum computing a reality as **it can be useful to simulate nature**. Nature in its most basic building blocks is quantum, so if you want to exactly simulate any process in nature, you need a quantum simulator. Moreover, researchers have already successfully managed to use a quantum computer to simulate a hydrogen molecule, which would be the first step towards simulating the entire chemical systems and most experts agree that **quantum chemistry is going to be of the first killer apps of this emergent technology**. Scalable Quantum Simulation of Molecular Energies will have **huge impact on quantum chemistry** and it is one of the factors which makes this project worth investing both time and money.

In particular, quantum simulation of molecular energies promises significant advances in our understanding of chemistry, including precise predictions of chemical

reactions rates. These advances, which may require relatively few qubits to achieve, may have board industrial impact given the wide importance of chemistry.

Scalable Quantum Simulation of Molecular Energies can be useful for modelling chemical reactions in order to predict reaction rates, which will greatly speed up how medicines, solar cells, batteries, industrial catalysts and flexible electronics are designed. In other words, it can revolutionize our world.

Another reason which makes me interested in this project is that superconducting qubits are being used, which I believe is the most leading qubit modality in quantum computing today. I think superconducting qubits will be the first qubit modalities which will be highly scalable and for this reason, I think it positively effects the project growth speed.