## Contributors

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# Project description and questions

In this activity, you will read three articles and then choose one on which to focus. For the one you choose to investigate further, identify outreach articles about it and submit a written response to the questions below. The objective is for you to bridge quantum simulations towards business and technology. Please read the directions below carefully and complete the assignment in full.

Begin by reading the **abstracts** of the following articles:

- 1. Observation of a Many-Body Dynamical Phase Transition with a 53-qubit Quantum Simulator. *Nature*, volume 551, pages 601–604 (30 November 2017) [PDF download]
- 2. Scalable Quantum Simulation of Molecular Energies. *Physical Review X*, vol. 6 (2016), pp. 031007 [PDF download]
- 3. Hardware-efficient Variational Quantum Eigensolver for Small Molecules and Quantum Magnets. *Nature*, volume 549, pages 242–246 (14 September 2017) [PDF download]

Do not worry if you don't understand all the technical details on these articles. It is enough to skim through the text omitting those details and focus on discussion, conclusion and context.

Prepare responses (300-500 words) for **each** of the following questions below.

- 1. These are three experimental demonstrations of quantum simulations. Noting 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?
- 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?
- 3. Imagine that you are responsible for investing the money of 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?

## Intro and list of articles

Before answering the questions, we will list the journal articles we found, by also providing some citations in the end. Citations explain our reasoning, but in the article we directly mentioned only a couple of them. Later, we will use the citations and the article summaries to support our arguments.

Out of three papers, we chose the first one - "Observation of a Many-Body

Dynamical Phase Transition with a 53-qubit Quantum Simulator" (I).

For this paper, we found 4 journal articles. For "Scalable Quantum Simulation of Molecular Energies" (II) we found 3, and for "Hardware-efficient Variational Quantum Eigensolver for Small Molecules and Quantum Magnets" - 2 articles.

## Links

#### Article I:

https://www.nature.com/articles/nature24654

https://arxiv.org/abs/1708.01044

- 1. Largest quantum simulations using 53 qubit trapped ions and another with 51 Ryberg atom

  (https://www.nextbigfuture.com/2017/11/largest-quantum-simulations-using-53-qubit-trapped-io
  ns-and-another-with-51-ryberg-atoms.html)
- 2. The Largest Quantum Simulator With 53 Qubits

  (https://www.rankred.com/the-largest-quantum-simulator-with-53-qubits/)
- 3. Best-yet quantum simulator with 53 qubits could really be useful <a href="https://www.newscientist.com/article/2155132-best-yet-quantum-simulator-with-53-qubits-could-really-be-useful/">https://www.newscientist.com/article/2155132-best-yet-quantum-simulator-with-53-qubits-could-really-be-useful/</a>)
- 4. Quantum simulators wield control over more than 50 qubits, setting new record: Atoms provide a robust platform for observing quantum magnets in action <a href="https://www.sciencedaily.com/releases/2017/11/171129131434.htm">https://www.sciencedaily.com/releases/2017/11/171129131434.htm</a>)
- 5. \*\*\*\*\*Quantum simulation with individual control of 53 qubits Trapped Ion Quantum Information

(http://iontrap.umd.edu/2017/12/01/quantum-simulation-with-individual-control-of-53-qubits/)

#### Article II:

https://ai.google/research/pubs/pub44815

https://arxiv.org/abs/1512.06860

1. Progress to an exact quantum description of chemistry with the first completely scalable quantum simulation of a molecule

(https://www.nextbigfuture.com/2016/07/progress-to-exact-quantum-description.html)

2. Quantum computers may revolutionize chemistry

(https://www.techspot.com/news/65639-quantum-computers-may-revolutionize-chemistry.html)

3. First completely scalable quantum simulation of a molecule

(https://phys.org/news/2016-07-scalable-quantum-simulation-molecule.html)

#### Article III

https://www.nature.com/articles/nature23879

https://arxiv.org/abs/1704.05018

1. New Approach to Simulate Chemistry with Quantum Computing;

IBM Pioneers New Approach to Simulate Chemistry with Quantum Computing (same article published by different journals)

(https://www.nextbigfuture.com/2017/09/new-approach-to-simulate-chemistry-with-quantum-computing.html)

(https://www.prnewswire.com/news-releases/ibm-pioneers-new-approach-to-simulate-chemistry-with-quantum-computing-300518270.html)

2. IBM Breaks Ground for Complex Quantum Chemistry

(https://www.hpcwire.com/2017/09/14/ibm-breaks-ground-complex-quantum-chemistry/)

### Question 1

All the articles came out the same year papers were published.

The chosen paper, judging by the content and number of articles, was very well received. According to I.1., 53-qubit simulator can be a key in building a universal computer. The same possibility is mentioned in I.2., according to which the simulator can result in actual quantum circuits and computers, with this time a wider range of applications. The idea of wider applications is mentioned in I.3. too. It states that while there are different, separate simulators built for different problems, this simulator has a chance to be improved and handle more than one program with one simulator only. The I.4. mentions the possible applications of the simulator and its possible improved version. If the current 53-qubit simulator explores magnetism, adding more qubits and making the number close to 100 can broaden the application range up to chemistry, material design, etc. Although I.5. is not a business trade press publication, but rather apiece from the webpage of the project, we included it to go through the funders and make conclusions. The list shows that they are research programs and special funds, no corporations. We wanted to note that.

Now a couple of words for the other two papers.

According to II.1., the project and its continuation can revolutionize the study of chemistry so much that the current results will be no big deal compared to the breakthroughs. The possible usage of the project in the future can be in "..design of solar cells, industrial catalysts, flexible electronics, batteries, medicines and more.", and solving the fertilizer problem as stated in II.2. Lastly, II.3. mentioned the possibility of building a universal computer in the future based on the project, by that, repeating the same prediction as for the article I.

III.1. provides a somewhat clear business strategy and vision on the usage of the project and future products (please see the citation). III.2. Lists possible discoveries linked to the project such as new small-molecule drugs or organic material.

## Question 2

For all three papers, we found almost the same amount of articles. We expected to find more for the large corporation research projects, but surprisingly, the university research project is also well discussed and popular. However, the visions mentioned in the articles differ. For the I paper the future applications are the possibility of a universal computer, usage not only in magnetism, but also in chemistry and medicine, and running multiple programs on the same simulator, instead of just one. In the case of the other two papers, the articles brought more specific examples of future usages, such as the design of solar cells, industrial catalysts, flexible electronics, batteries, and medicines for II, and drugs and organic material for III. This, of course, can simply be a result of the nature of the projects. We decided to note it anyway and consider the possibility that articles about corporation papers were more specific in terms of future usage. In the case of III.1., even reproduction steps are given for achieving goals. Our explanation for this "inequality" is the following: corporations have better business strategies and better opportunities to implement their projects or continue improving them. Universities can have ideas for projects, whether short-term or long term, but in terms of future implementations, they may face the problem of direct access to production or funding. Their products are more

general in the concept of usage. The corporations, on the other hand, develop their projects for achieving their goals and using them in their production. Additionally, one more, a bit sentimental reason. Researchers at universities are people genuinely interested in science. Their goals are more inclined to the idea of serving the science itself, rather than immediate profit. They are driven by curiosity. The research of the corporations is more production and profit-oriented. For corporation projects, the need to create a useful product that will give a good result. University projects can be a matter of interest and less of a profit, which is not true for corporations.

# Question 3

We would invest in the chosen project and here is why.

- 1. They have a vision of the future of their product and we like it. According to I.4., researchers think that achieving the 100-qubit goal can broaden their field of study for magnetism to chemistry. Researchers are interested to continue their research of the project, which was revolutionary according to the articles. More time and funding will give even better results and we would like to see them. Also, their goal is to make a simulator running several programs instead of one. This sounds like another revolutionary and big step towards building universal quantum products.
- 1. We are intrigued by the fact they are using atomic qubits, instead of superconducting ones like corporations. The other two articles were about superconducting qubits, so we decided to do some research and see if they are more popular than atomic qubits in

general. It turned out, they are. Research and production are mainly focused on, while atomic qubits are less popular. However, as our article and separate research suggest, atomic qubits have an interesting potential that has chances to be uncovered. We find it very promising. Therefore, we would love to see if the research team's expectation of building universal quantum computers based on their simulations on atomic, not superconducting qubits will come true or not. The best way to do so is to try.

2. Our final reason is that we would love to support a university research project. Being students ourselves at a university, we see the importance of research projects in the lives of students, researchers, universities, and science in general. They are required to motivate students to pursue the career of research, which is the base of scientific breakthroughs. The more students get an opportunity to try research and dedicate time to it, the more scientific breakthroughs will become possible. Also, motivating current researchers with opportunities will help them maintain their favorite job and develop science. Leaving research only to the corporations is not a good approach. Wide research projects are left mainly to big companies, and by that scientists and researchers often have no choice but to work in a place that they do not want. Universities should have enough financing to encourage scientists and researchers to stay and work on their projects, and not migrate to big corporations for research fundings.

## Citations

I.1. "Given an even higher level of control over the interactions between spins, as already

demonstrated for smaller numbers of trapped-ion qubits, this same system can be upgraded to a universal quantum computer."

- I.2. "These types of quantum simulators would help scientists to implement quantum circuits, and ultimately quantum connect multiple ion chain together to develop a complete quantum computer with a wide range of applications."
- I.3. "The design for this simulator could lead to a true quantum computer one day.

Most quantum simulators are built to run one specific program, but the team thinks it should be possible to tweak their device to run multiple programs, rather than having to build a separate simulator for each program."

- I.4. "As they look to add even more qubits, the team believes that its simulator will embark on more computationally challenging terrain, beyond magnetism. "We are continuing to refine our system, and we think that soon, we will be able to control 100 ion qubits, or more," says Jiehang Zhang, the study's lead author and UMD postdoctoral researcher. "At that point, we can potentially explore difficult problems in quantum chemistry or materials design.""
- I.5. Funding information.

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- The Joint Quantum Institute at the University of Maryland Department of Physics and NIST
- · IARPA LogiQ Program, through ARO contract
- · ARO Atomic & Molecular Physics Program
- AFOSR Multidisciplinary University Research Initiative (MURI) on Optimal Measurements for Scalable Quantum Technologies
- AFOSR Multidisciplinary University Research Initiative (MURI) on Wiring Quantum Networks with Mechanical Transducers
- ARO Multidisciplinary University Research Initiative (MURI) on Modular Quantum Circuits
- · ARL Center for Distributed Quantum Networks
- NSF Physics Frontier Center at JQI (PFC@JQI)
- Intelligence Community Postdoctoral Fellowship Program.
- II.1. "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."
- II.2. "..the ability to do so could revolutionize the design of solar cells, industrial catalysts, flexible electronics, batteries, medicines and more. As you can see, it was incredibly accurate and inspires hope that the VQE technique may be able to solve classically intractable problems like the production of fertilizer mentioned earlier."
- II.3. "That would mean developing a universal quantum computer, which, not coincidently, is a goal Google has set for itself."

III.1. "For future quantum applications, IBM anticipates certain parts of a problem to be run on a classical machine while the most computationally difficult tasks might be off-loaded to the quantum computer. This is how businesses and industries will be able to adopt quantum computing into their technology infrastructure and solutions. To get started today, developers, programmers and researchers can run quantum algorithms, work with individual quantum bits, and explore tutorials and simulations on the IBM Q experience. As well, IBM has commercial partners exploring practical quantum applications through the IBM Research Frontiers Institute." III.2. "Exact predictions will result in molecular design that does not need calibration with experiment. This may lead to the discovery of new small-molecule drugs or organic material."