Researchers optimize simulations of molecules on quantum computers

The net result is a much faster operation involving far fewer gates. That’s important because errors in quantum hardware increase as a function of both time and the number of operations.

The researchers then used this approach to explore a chemical, Mn_4O_5Ca, that plays a key role in photosynthesis. Using this approach, they showed it’s possible to calculate what’s called the “spin ladder,” or the list of the lowest-energy states the electrons can occupy. The energy differences between these states correspond to the wavelengths of light they can absorb or emit, so this also defines the spectrum of the molecule.

Faster, but not quite fast enough

We’re not quite ready to run this system on today’s quantum computers, as the error rates are still a bit too high. But because the operations needed to run this sort of algorithm can be done so efficiently, the error rates don’t have to come down very much before the system will become viable. The primary determinant of whether it will run into an error is how far down the time dimension you run the simulation, plus the number of measurements of the system you take over that time.

“The algorithm is especially promising for near-term devices having favorable resource requirements quantified by the number of snapshots (sample complexity) and maximum evolution

time (coherence) required for accurate spectral computation," the researchers wrote.

But the work also makes a couple of larger points. The first is that quantum computers are fundamentally unlike other forms of computation we've developed. They're capable of running things that look like traditional algorithms, where operations are performed and a result is determined. But they're also quantum systems that are growing in complexity with each new generation of hardware, which makes them great at simulating other quantum systems. And there are a number of hard problems involving quantum systems we'd like to solve.

In some ways, we may only be starting to scratch the surface of quantum computers' potential. Up until quite recently, there were a lot of hypotheticals; it now appears we're on the cusp of using one for some potentially useful computations. And that means more people will start thinking about clever ways we can solve problems with them—including cases like this, where the hardware would be used in ways its designers might not have even considered.

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