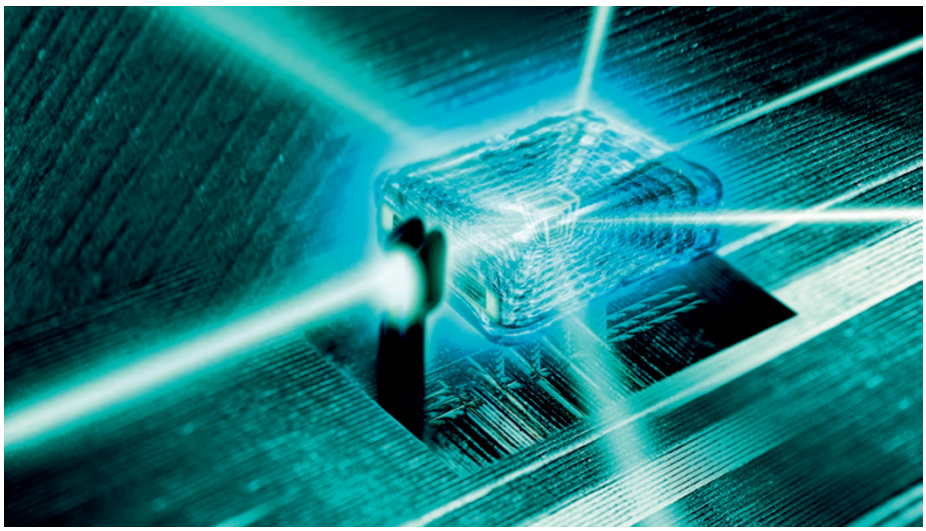
Quantum reform

Leonie Mueck

Quantum computers potentially offer a faster way to calculate chemical properties, but the exact implications of this speed-up have only become clear over the last year. The first quantum computers are likely to enable calculations that cannot be performed classically, which might reform quantum chemistry — but we should not expect a revolution.

It had been an exhausting day at the 2012 International Congress of Quantum Chemistry with countless presentations reporting faster and more accurate methods for calculating chemical information using computers. In the dry July heat of Boulder, Colorado, a bunch of young researchers decided to end the day with a cool beer, but the scientific discussion didn't fade away. Thoughts on the pros and cons of all the methods — the approximations they involved and the chemical problems that they could solve — bounced across the table, until somebody said "Anyway, in a few years we will have a quantum computer and our approximate methods will be obsolete".

An eerie silence followed. What a frustrating thought! They were devoting their careers to quantum chemistry — working tirelessly on applying the laws of quantum mechanics to treat complex chemical problems with a computer. And in one fell swoop, would all of those efforts be wasted as chemists turn to quantum computers and their enormous computing power?



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Quantum-chemical cravings

Ever since its beginnings, quantum chemistry has been on a starvation diet — adapting to limited computational resources like an organism adapts to a scarcity of nutrients. In the 1920s and 1930s, the great forefathers of the subject already knew the exact mathematical laws to describe the quantum mechanical behaviour of electrons in molecules. But, as Paul Dirac put it, "the exact application of these laws leads to equations much too complicated to be soluble". Dirac proved to be quite the prophet — even for today's supercomputers, using the Schrödinger equation to exactly calculate properties of even simple molecules is too complicated. But just like with a starvation diet, quantum chemists adapted to the restricted computational resources, building their vocation around the development of ever more sophisticated approximations to the exact solutions. This has resulted in a wealth of quantum chemical methods, each of them offering a different trade-off between accuracy and computational feasibility.

Enter the universal quantum computer. This dream machine would basically work like a normal digital computer; it would be programmable and could carry out any imaginable algorithm. But instead of electronic circuits representing bits, it would contain quantum circuits representing quantum bits — or qubits. These can be constructed using all sorts of quantum systems like nuclear spins or the electronic states of ions trapped in electromagnetic fields. "Right now we are in the very early stages of quantum computing in terms of actual implementation," explains Krysta Svore from Microsoft Research. But once this dream machine has become reality, the expected quantum leap in computing power promises an end to quantum chemistry's starvation diet, providing the resources to calculate exact solutions to the previously unsolvable equations and removing the need for approximate methods.

However, in the past year, researchers have started to clarify exactly what changes the first generation of quantum computers will bring. And although we will probably be able to perform computations that we cannot do on a 'classical' computer, it does not look like all the conventional quantum-chemical methods will become obsolete or that quantum chemists will be out of their jobs in the foreseeable future. Instead of a quantum revolution, it looks like we will be confronted with a quantum reform.

The scale of the problem

Although there are confusingly many approximations that are used in quantum chemistry, it has been very successful. "Quantum chemistry has become a very mature field," explains Gus Scuseria, a quantum chemist from Rice University in Houston, Texas. Today, all chemists can get their hands on user-friendly programs to calculate ground-state energies, molecular geometries or spectral parameters, using clever approximations to the exact solution. This exact solution is called full configuration interaction (FCI) — and it takes full account of electron–electron interactions, unlike the more simplistic methods that just approximate those interactions by crude averaging. To carry out FCI calculations the necessary computational resources are enormous and they grow — or scale — exponentially with the system size,

which is measured by the number of spin orbitals in the molecule. That means you can realistically perform such calculations only on atoms and tiny molecules with a handful of electrons in a few spin orbitals.

The methods that quantum chemists have developed to sensibly approximate the FCI solution bring down the computational resources to something bearable — that is you can comfortably calculate chemical properties of molecules with a few hundred atoms within hours or days on a supercomputer. The approximations have an effect on how the required computational resources scale with system size: rather than scaling exponentially, they scale polynomially, that is if N is the number of spin orbitals, the scaling is N^x. The value of x depends on, the exact approximations that you make: the smaller x, the cruder the approximation and the larger the errors. But a smaller x also means that you need less computational resources and can treat larger molecules in less time. In other words, the methods form a hierarchy in terms of computational resources and accuracy. As a rule of thumb, you can comfortably use N^7 methods to treat a few tens of atoms and get a result that is accurate enough for most chemical purposes. For very large molecules, there are even tricks to bring N^6 methods down to linear scaling while keeping errors to a minimum.

But there is a caveat. "85 years after Schrödinger's equation we have solved half of the problems," Scuseria demurs. For quite some time, he has been unsuccessfully racking his brain about the notorious 'multireference' or 'strong correlation' cases that make up the unsolved half. If two or more electronic states of a molecule are very close in energy, all the elegant approximations used to bring the scaling down no longer hold. Unfortunately, this happens for some of the most interesting chemical problems, such as understanding transition-metal compounds, bond-breaking and single-molecule magnets to name just a few. And some of the most enigmatic problems in physics belong to the class of strong-correlation problems, too, for example high-temperature superconductivity. Scuseria sighs. He would love to perform quantum-chemical calculations on big metal clusters — like tetramers of the well-known single-molecular magnet fragment $[Mn_{12}]$ — but it's a strong correlation problem. There are methods giving you "some results", Scuseria explains, but at present there are none that give you the right answer for every case of strong correlation.

A quantum computer would solve this problem using a completely different strategy, one that greatly reduces the scaling of FCI calculations and makes them far quicker to compute. "If we have exact solutions to the Schrödinger equations at hand, which is what a quantum computer promises, then we will be able to predict — always." says Alan Aspuru-Guzik from Harvard University. In other words, quantum chemists could stop worrying about approximations and just solve problems exactly. The main reason for the speed-up is simple: on a classical computer, the electronic wave function — which contains all the information about how the electrons behave in a molecule — needs a huge amount of memory to be stored. The number of required bits scales exponentially with the number of spin orbitals, hence the exponential scaling of FCI calculations. But, being quantum systems themselves, quantum computers represent electrons in molecules much more effortlessly — the number of necessary qubits only grows linearly with the number of spin orbitals. Consequently, you also need fewer operations to manipulate the qubits, explains Aspuru-Guzik. Back in 2005 he showed, theoretically, that an FCI calculation indeed scales polynomially on a quantum computer[1].

And since then he has been developing algorithms for quantum chemistry on quantum computers — although there is no quantum computer yet to implement anything of interest. Apart from a few proof-of-principle calculations of the hydrogen molecule and $He–H^+$ the field has little experimental work to show for itself[2,3]. For a calculation of one of Scuseria's $[Mn_{12}]$ fragments you'd need at least 500 qubits — and we are far from having a quantum computer of that size. But Aspuru-Guzik is optimistic: "We will see this in our lifetime," he says. Matthias Troyer, from ETH Zürich, is bold enough to be more specific. "First we need one qubit that's really stable long-term, for a few hours or a few days, and that can be manipulated," Troyer says. It needs to be stable enough to perform in the order of a trillion operations on it without making too many errors. Troyer thinks this could be achieved within 5–10 years. "And then another 10 years and we have a small quantum computer — but that's optimistic," he says.

At least this is close enough for giant companies like Microsoft to get involved. Krysta Svore manages the Quantum Architecture and Computation group at Microsoft Research. "We want to be ready with killer applications should a quantum computer one day be built." she says to explain the rationale behind their efforts to design quantum computing algorithms for quantum chemistry. The essential requirement for a killer application is that the quantum computer must be better at solving the problem than a classical computer. "So far, the only thing that is feasible, that has the application potential, is quantum chemistry" concurs Troyer — at least for the first generation of small quantum computers with a few hundred qubits. And so Svore's group joined forces with Troyer and started to look at the prospects of quantum chemistry on quantum computers.

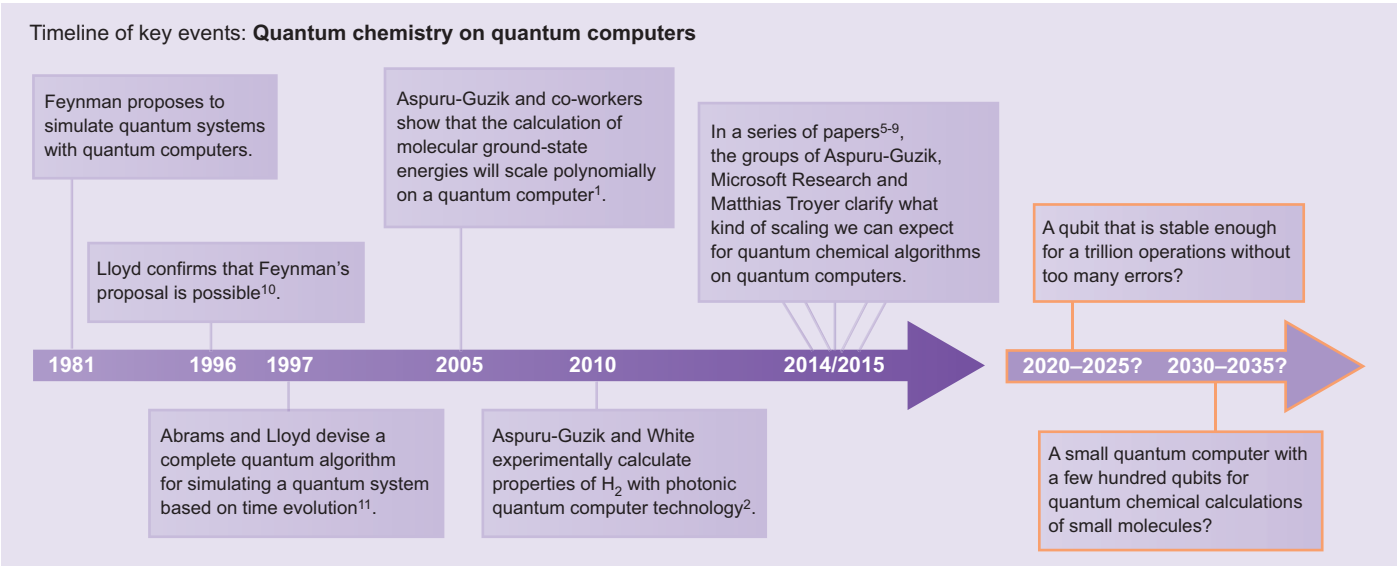
Their studies are carried out with a healthy dose of pragmatism; having proof that FCI calculations scale polynomially is a good start, but there are still some very practical questions that need answering. It is crucial to know what exactly the x in an N^x scaling would be to get an idea about how long calculations would actually take on quantum computers. The question is whether they will finish in an amount of time that a quantum chemist is willing to wait — say a few months. "If the scaling is N^{10}, it's faster than a classical computer but it might just take forever." Troyer says. And if that "forever" is too long for even the most patient quantum chemists, quantum chemistry will never be the killer application for quantum computers.

A quantum of solace

In 2014, advances in determining the exact scaling and designing algorithms to get it down to a practically manageable level have come so thick and fast that they even overwhelmed quantum-computing veteran Aspuru-Guzik. "It's been an interesting year," he says in reference to the progress that has been made in designing specific algorithms that use as few operations on the qubits as possible.

A quantum algorithm for quantum chemistry looks fundamentally different from its classical counterpart. For example, when searching for the ground-state energy of a molecule with a classical algorithm, you first encode a rough guess of a molecule's wave function in a huge array of numbers. Then you search for the optimal solution iteratively. The corresponding quantum algorithm, on the other hand, proceeds in three steps. First, the wave function is encoded into qubits that are prepared in a quantum superposition state. This superposition is the pinch of magic in quantum computers, the resource making them more powerful simulators for quantum systems than classical computers. While classical bits can only assume the states 0 or 1, the laws of quantum mechanics allow qubits to be in a superposition between all the classical states and thus hold more information. The second step is for these qubits to search for the right answer while undergoing an evolution in time, and the third step involves a measurement being made to extract the desired information from the superposition state[4].

The heart of last year's progress lies in digging deeper into the second step — the evolution of the quantum system in time.



In order for the equations that underlie this time evolution to be encoded into logical operations that can be carried out by the qubits, they need to be broken down into discrete time steps. The bigger the steps, the fewer operations you need and that makes for better scaling. But if you make the steps too large, you introduce errors. "The question people have been trying to get their heads around recently is 'What is the largest time step that you can take without having large errors in your answer?'" Aspuru-Guzik says. In early 2014, Matthias Troyer and the Microsoft team were looking to answer this question and initial analysis revealed[5] that, to give accurate answers, the time steps required lead to a terrible scaling of N^9. But subsequent analysis and optimization by both teams has brought it down significantly[6–9]. The latest results show that the scaling might be as good as N^4 or N^3 in some cases, Svore says.

What exactly this progress means in practice depends on how fast the computer could perform individual operations; computer scientists call this the gate time. If trapped ions are used as qubits, the current gate time amounts to about 10 microseconds; the big rival technology — superconducting qubits — needs about 100 nanoseconds. "If we can get a machine with about 200 qubits and the gate time is not more than a microsecond then we have some really interesting applications." says Troyer. In other words, we could perform an FCI calculation that is intractable on a classical computer in minutes or maybe hours.

This is wonderful news for computer scientists. But what does it mean for chemists? Would this progress allow for treating problems of real chemical interest? In general, it seems that a quantum computer would have the biggest impact for small multireference problems. They are a nuisance in conventional quantum chemistry but are not too demanding for a small quantum machine with a few hundred to a thousand qubits. In this realm, studying Fe_2S_2 — the reactive centre in the electron transfer enzyme ferrodoxin — has established itself as both Troyer's and Aspuru-Guzik's favourite showcase problem. With the newly optimized algorithms, an FCI calculation on Fe_2Se_2 would indeed finish within minutes or hours on a 150-qubit quantum computer; no quantum chemist would even dare to dream that this calculation could be performed on a classical computer. But, for the first generation of quantum computers, fulfilling Scuseria's wish to treat $[Mn_{12}]$ tetramers will be a stretch. This is not only because it would need 2,000 qubits but depending on the gate time and exact scaling, Scuseria would also probably have to wait years for the calculation to finish. And that's nothing compared with studying high-temperature superconductors with quantum computers: optimistically assuming a gate time of about ten nanoseconds, Troyer estimates that this computation would last for as long as the age of the universe.

It does not look like the early generations of quantum computers will revolutionize the way we do quantum chemistry. Instead of transforming the maze of current quantum chemical methods into a highway, they will most likely add just another quick side road that one would use to solve a specific range of chemical problems. "It will be like now, the only difference is that we could do FCI on slightly bigger systems," Troyer comments. To get the best of both worlds, Troyer envisions quantum–classical hybrid methods: in metalloenzymes, like ferrodoxins, haemoglobins or cytochromes, small but multireference-ridden reactive metal centres could be calculated using a quantum computer while advanced linear-scaling methods from conventional quantum chemistry would be well-suited to treat the surrounding organic portion of the protein.

But much must happen before every chemist has a quantum computer handy so today's quantum chemists should not throw in the towel. Scuseria, at least, has by no means given up on conventional methods: "I believe that there is a polynomial-cost answer to the strong correlation problem. We just haven't found it yet." he says. And Troyer hopes that the developments in quantum computing will give rise to "quantum-competition inspired" leaps in solving the big problems in quantum chemistry with conventional methods. Instead of worrying over their beers that quantum computers could put them out of work, quantum chemists should channel their efforts and design better algorithms to treat small multireference cases. With the prospect of beating a quantum computer to keep you motivated, now seems to be the best time ever to devote a career to approximate methods in conventional quantum chemistry. ❐

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