Q&A
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The Variational Quantum Eigensolver – progress and near term applications for quantum chemistry
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Q1: I was struck by the slide you had for making the things that make the computation doable in a sense about the coherence and the overlaps and so on. I had this other naive view that the problems that arise that make it difficult for us to solve quantum chemistry problems on the classical computers, are indeed when we have a lot of delocalisation and a lot of issues around that. When we can find an effective way of localising things, we've found very clever algorithms for doing that and keeping things apart, and then, putting them together and clever DfT overlaps and so on, and so I'd rather hope that the quantum ones were at the opposite end, but you seem to be suggesting that's actually not entirely true here?

So you're right it's a very good point. First of all, it's unfortunately not entirely the case for contributors, but it's worth pointing out sort of two different aspects of this. The first one is we care about the problem being local, so we care about the cost function being local, but the wave functions of the wave function that we're modelling, doesn't have that much of a requirement, so the operations that we're doing on the qubits don't need to be local operations. So that means that we can create a model of the electronic wavefunction that is very, very highly entangled. And still, measure it against an operator or series of operator which isn't so Hamilton, which is a design so that each operator is very local. The advantage of this is obviously that you can model is very complex wave functions on the quantum computer, which is something that you shouldn't be able to do with sort of common conventional methods. But as you pointed out, actually this remains an open question. We're not sure yet whether we can actually produce this sort of wavefunctions intractable manner so with number of parameters that is small enough for it to be optimisable and with a depth that is shallow enough so that it can be implemented on the near-term quantum devices. So yes, it's a very narrow margin.

The other intriguing part that is where the mental exercise seems to be going, is that creating of those suitable Hamiltonians from the beginning. How hard is it to learn how to do this, starting from a sort of classical outlook of saying, "well, I can write down the treasure equation, and I can think of the normal sub orbitals that we use, or I can conceive of a basis set, or somehow…", translating that into this kind of SPIN type Hamiltonian which is, I guess, what we're going to do, it seems my colleagues who do NMR and so on are frequently, it's a language they work on and when think about, but not maybe a language that makes most of us chemists who came not doing quantum chemistry, but thinking that you can go and get a quantum answer. There are people in between who very happy with density matrices and whatever. I mean, what if your record if somebody's listening hear anything, right? I know a little bit about what quantum chemistry is. I need to go away and learn. Obviously, we're going to do a review, this is clearly the place to start… but what does one need to learn about to be able to think in that way? To go from a classically driven quantum Hamiltonian to something that is more amenable to a quantum computer?

It's a very deep question, so there's a lot to possibly to answer here, so I'll just try to summarise quickly. So the first thing is make sure you understand you know second quantisation. The reason why second quantisation exists for the representation of a molecule in terms of Firmenich operators, and I guess this is you know, core to quantum chemistry. So, any quantum chemistry textbooks will cover this. The next step is to understand why we why we needed to have this spin operators and why we cannot have the fermionic operators directly. And the main reason is because fermionic operators are very very abstract concepts which they defined for the need of sedimentation. They were defined by King in the 1920s for the need of verifying this, the antisymmetry of the of the electronic wavefunction. So, therefore now that we are with machines which are basically effectively spin states, qubits are spin state and that can only be measured on spin operators. We need to find a

translation of these somewhat archaic operators of the Firmenich into spin operators, which I'm glad we've been defining a very long time ago as well. But, we still need to find translation between another. And the issue is that you know spin operators themselves don't obey these anti-commuting relationship by default, and so therefore we need to construct the specific operators and and in a manner that they obey this, relationship. The very first paper about this actually predates you know any thoughts of quantum computing which is a paper by Jordan Wigner back in 1928, which basically shows that you can explicitly express the Firmenich operators into spin operators, and that's the very first attempt at doing so and obviously over the last couple of years many people have tried to make this more efficient. But, if you're interested in sort of understanding how this translation works, so the translation from the molecular structure to the Firmenich Hamilton into the quantum modelling, the first step is to look at the second quantisation and to understand how it works from a sort of quantum chemistry perspective and the second is probably to look at the Jordan Wigner encoding. Jordan are big on mapping and there is many resources on the Internet about this and that would be the basic point to understand this language that people in the quantum computing community talk about.

I'll just say the reason why I was asking that is that, we're holding these particular this group of seminars now because we think that it's really important for this network there to have resource available, to have a greater understanding of where quantum computing is going, and that we actually are looking to put on a set of workshops to actually provide some hands-on help and some guidance through this, at least in simple way. But when I'm looking at the various courses around, there doesn't seem to be a course that takes a sort of normal sort of chemist who knows a bit about quantum computing and quantum chemistry, and so knows something about some basic quantum mechanics, but doesn't know about quantum gates, but equally doesn't know the right bits and pieces. But they just didn't seem to be a course that starts from the right point, and so we're looking at doing that. This has been very helpful in trying to understand what algorithms one should concentrate on and where some background should come from. We'll have to have a chat with you as well.

I think bridging between the two communities is very challenging and it's very important, so I think you're on the right path.