Centre for Quantum Technologies

ANNUAL REPORT

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Visitor Notes: Jacob Biamonte

Categorical Models of Quantum Information in the Simulation of Many-Body Systems

CQT attracts both long and short term visitors from all over the world. Jacob Biamonte, a Research Fellow at the University of Oxford and Lecturer in Physics at St Peter's College, explains the results of his two collaborative visits with several members of CQT staff, including Stephen Clark. Their work involved using higher mathematics to create a new theory of tensor network states and has numerous practical applications in the simulation of physical systems.

It was quite the honour to be asked to contribute to CQT's annual report by outlining my experience as a visitor. I agreed instantly and after a bit of thought, I came to realise that my CQT visits and a lot of what's happened since are traced back to a single instant.

That instant: occurred when I was signing up for coffee in the common room of Wolfson College at the University of Oxford. A large part of the Oxford accounting system requires no electricity, and many of those spending time here sign for small expenditures often enough to see their signature evolve slowly into, say, a line with some bumps, or another slur of the pen. On this occasion, however, I noticed something elegant scribed on the page – the name of "V. Vedral". I still recall the flavescent paper, and the excitement when I realised that Vlatko Vedral, the long-awaited Wolfson Physics Fellow, had finally arrived. I recognized Vlatko's name as one of the founders of entanglement theory, and later that year ended up paying him with a Cuban cigar in exchange for a guest lecture in the course I organize. He spent several years in Oxford early in his research career and is now a Principal Investigator at CQT.

From Candle-Light Accounting to Collaboration

I've become accustomed to the shock people get when they realise that I, as a physicist, dabble in a strange branch of higher mathematics known as category theory. Vlatko, on the other hand, he seemed to like the idea of figuring out if category theory can tell us something we didn't already know about quantum information science (or at the very least, he was not openly opposed to it). It was around the time we met when I realised that category theory could precisely describe one of the deepest and most powerful theories being used in quantum physics: the theory of tensor network states. This was some time ago, and we have now been able to produce several notable results new to both tensor network theory and category theory, and in the process we've made pioneering steps towards connecting these two fields.

Computer simulations of physical processes form the backbone of many technological developments. For example, quantum chemistry simulations enable scientists to better understand large molecules used in pharmaceuticals. An aspect of the theory of tensor network states is an approach to efficiently describe complex states of physical systems by a connected network of components called tensors. This approach has proven useful in attempts to simulate quantum systems for many reasons: the most elementary perhaps being that many tensor networks require little memory storage. It struck me that the range of expressiveness of the existing mathematical theory of tensor network states and the associated graphical language would be broadened by elevating the theory to a rigorous tool. At the same time, this ended up allowing us to expose hosts of internal algebraic structure. Category theory with its long history in mathematics provided a way to achieve this.

Through Vlatko, I met Stephen Clark and Dieter Jaksch, both leading experts on the (then current) theory of tensor network states. Stephen is employed by CQT and Dieter is a Visiting Professor at the Centre. Although they both spend time in Oxford, we were all too busy locally, so we had to take a plane to Singapore, meet at CQT and then collaborate around the clock. I made two month-long visits in 2010. I won't have the space to give CQT's visitor program the respect it deserves for enabling us to work daily to develop our new framework. I also won't have room to go into details of how exciting it was for the three of us to meet the well known mathematician John Baez on his visit to Oxford – especially when we realised he was on his way to CQT for two years and that we all had many common interests. Instead, I'll skip to our results.

Out of the necessity for improvements to the current tensor network theory and the opportunity presented by noticing its similarity to category theory, we have developed a categorical approach to tensor network simulations that binds techniques across disciplines and creates a more expressive and powerful tensor network theory. The existing tensor network approach revolves around ways to approximate quantum states. What we have done boils down to creating a much better way to control the way states are expressed, making it possible to "zoom in" and expose new found internal structure.

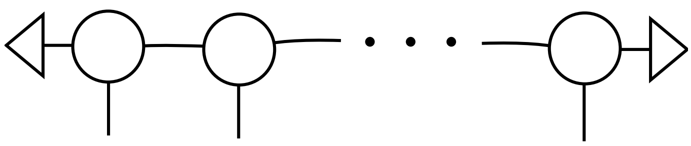


Figure 1: Tensor network states in the current formalism have this generic form. The legs on the bottom index spin degrees of freedom.

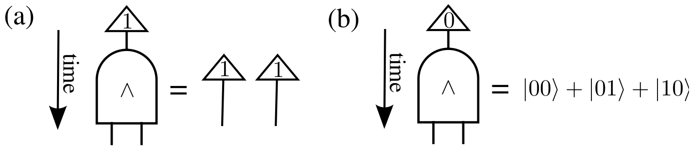


Figure 2: The quantum AND-state. This corresponds to a valid quantum operation, realisable in a quantum optics experiment.

Our results have opened a new door, leading to several novel results in both category theory and tensor networks. In particular, we have used the new framework to give a new solution to the quantum decomposition problem. Specifically, given a quantum state S, we are now able to directly construct a tensor network that describes the state S in terms of clearly defined building blocks. This solution became possible by synthesizing and tailoring several powerful modern techniques from higher mathematics: category theory, algebra and coalgebra and applicable results from classical network theory and graphical calculus.

Tensor Network States

A key idea behind using a tensor network based computer algorithm to describe a large class of quantum states efficiently is finding a way to approximate the state. Typically, this is done by a form of matrix factorisation known to experts as Vidal's iterative use of the SVD (skipping details, you simply throw away small singular values and truncate the Hilbert space). In many cases this provides highly accurate approximations of quantum states. The resulting matrix product states take essentially the form shown in Fig. 1.

Readers familiar with category theory might say, “this looks a lot like a string diagram, right?!” After digging through the details in a few collaborative meetings, John pinpointed the relation between these diagrams and his theory of spin networks (which he developed for use in quantum gravity).

Snap Shot: Categorical Tensor Network States

Our recent work concerns the development of a new tool set and corresponding framework to address problems in network descriptions of many-body physics and related disciplines. These tools and this framework is significantly different to and outside the range of methods used to date.

In the categorical network model of quantum states we present, each of the internal components that form our network building blocks are completely defined in terms of their mathematical properties, and these properties are given in terms of equations which have a purely graphical interpretation: category theory replaces ad hoc graphical methods in network descriptions of many-body physics and enables rigorous proofs to now be done graphically.

Say you have a quantum state, the quantum AND-state: |000>+|010>+|100>+|111>. If we draw this as a network (AND-tensor with two-inputs and one-output), and place a |1> on the output and run the network backwards, this leads to the product state |1>|1> (Fig. 2a). Now if we instead place a |0> on the output and run the network backwards, this leads to the entangled state |00>+|01>+|10> (Fig. 2b). The idea is we can now “wire” these quantum logic tensors together in a controllable way to create larger and larger tensor network states.

It turns out that our quantum logic-tensors enable us to translate a quantum state into a tensor network directly. For instance, the internal structure of a so-called W-state (|00…1>+|01…0>+|10…0>) as in Fig. 3.

Connecting the Dots

Categorical models of tensor network states enable us not only to “zoom out” and expose high-level structure, but also to “zoom in” and expose hidden algebraic structures that are not currently being considered in the tensor network simulation community. Enhancing the graphical language and mathematical component of these numerical methods should lead to the discovery of new theoretical models and numerical algorithms which challenge and shape our understanding of many-body physics.

Getting to the very bottom of why quantum systems are so difficult to simulate is one of those seemingly impossible research problems. It's bewildering but fascinating to explore. With each step towards better ways to handle complex quantum states, technological advancement follows. Adding quantum capability to simulations in physics and chemistry is of great commercial interest, meaning this research has the potential to attract R&D investment from Singapore and abroad.

Further reading

Citations and background information on tensor network states can be found at http://www.comlab.ox.ac.uk/activities/quantum/course/. This webpage is for a graduate course given at the University of Oxford in 2010, “The Quantum Theory of Information and Computation”, which I developed with Stephen Clark, Mark Williamson and Vlatko Vedral to foster the cross-communication needed to explore these multidisciplinary topics. This course will be given again at Oxford this year (with Dieter Jaksch) and we plan to give versions of this course at several leading research institutions and top universities, including Imperial College London, University College London and CQT (with several lectures by John Baez). For his trips to London, Vlatko doubled his fee: two Cuban cigars per lecture. What can we do?

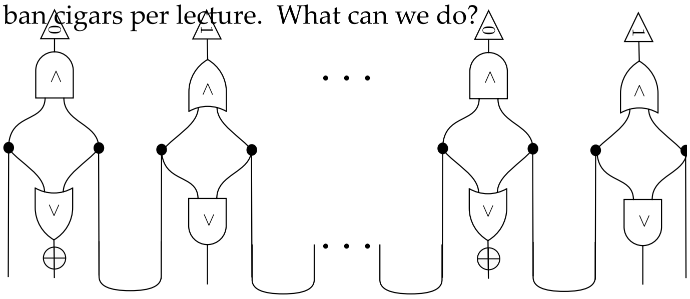
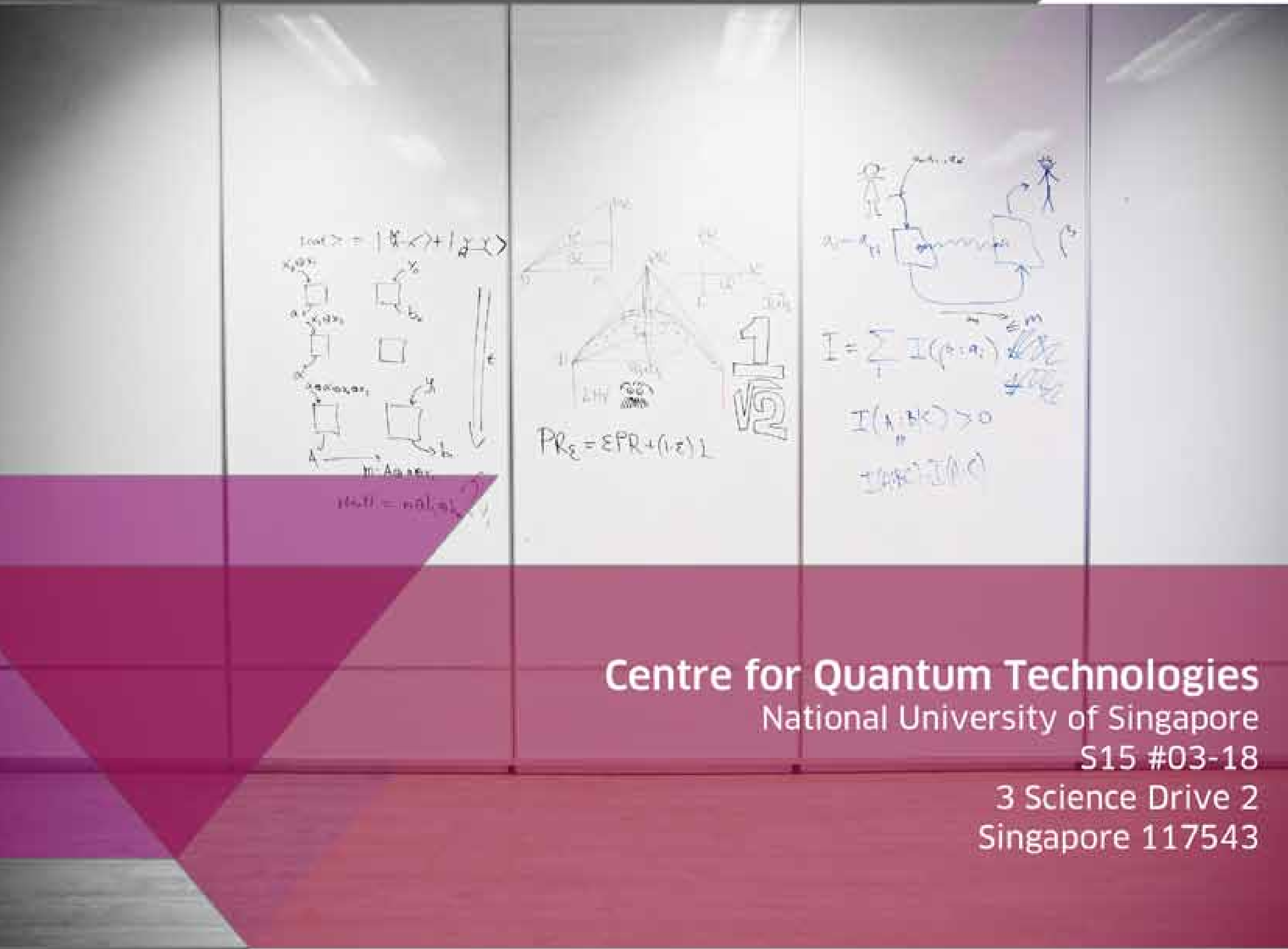


Figure 3: A tensor network state in our framework. Hosts of internal structure is exposed and the components that form the network are completely defined in terms of their mathematical properties by diagrammatic laws.



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