Conceptual understanding through efficient inverse-design of quantum optical experiments

Mario Krenn,[1, 2] Jakob S. Kottmann,[1] Nora Tischler,[3] and Alán Aspuru-Guzik[1, 2, 4]
[1] *Department of Chemistry & Computer Science, University of Toronto, Canada.*
[2] *Vector Institute for Artificial Intelligence, Toronto, Canada.*
[3] *Centre for Quantum Dynamics, Griffith University, Brisbane, Australia.*
[4] *Canadian Institute for Advanced Research (CIFAR) Lebovic Fellow, Toronto, Canada*

The design of quantum experiments can be challenging for humans. In experimental quantum optics, A.I. methods have therefore been introduced to solve the inverse-design problem [1]. While some computer-designed experiments have been successfully demonstrated in laboratories, these algorithms generally are slow, require a large amount of data or work for specific platforms that are difficult to generalize.

Here we present THESEUS [2], an efficient algorithm for the design of quantum experiments, which we use to solve several open questions in experimental quantum optics. The algorithm's core is a physics-inspired, graph-theoretical representation of quantum states, which makes it significantly faster than previous comparable approaches. The improvement in speed shows that THESEUS is ready to go beyond benchmarks, and be applied to the **discovery of new scientific targets** and – more importantly – to the development of new scientific insights and understanding.

Scientific understanding is essential to the epistemic aims of science [3], but rarely addressed in applications of artificial intelligence to the natural sciences. In the philosophy of science, pragmatic criteria have been found for *scientific understanding*, in particular by de Regt's award-winning work [3, 4]. He describes that scientists can understand a phenomenon *if they can recognise qualitatively characteristic consequences without performing exact calculations.* We connect this criterion to our discoveries: We discover the first implementation of high-dimensional GHZ states, important classes of heralded photonic states and new experimental configurations of previously unknown transformations. In all of these cases, we identify the underlying conceptual cores of the solution. We use them to generalize the solutions to many other, large classes of states and transformations – without additional calculations.

Connecting to de Regt's criterion that argue that scientific understanding is connected with the skill to use concepts fruitfully, *without exact calculations*, our algorithm has been the source of scientific understanding for multiple instances. This is in stark contrast to typical A.I. applications in the natural sciences, where the solution of a parameter optimisation is the final product, without the intention of discovering new scientific ideas. Hence, in a broader sense, the ability of our algorithm goes beyond simple optimisation, and enters the realm of providing scientific insights and allowing for scientific understanding. Finally, we believe that insights from the philosophy of science can be productive guiding principles in the development of new A.I. algorithms for physics.

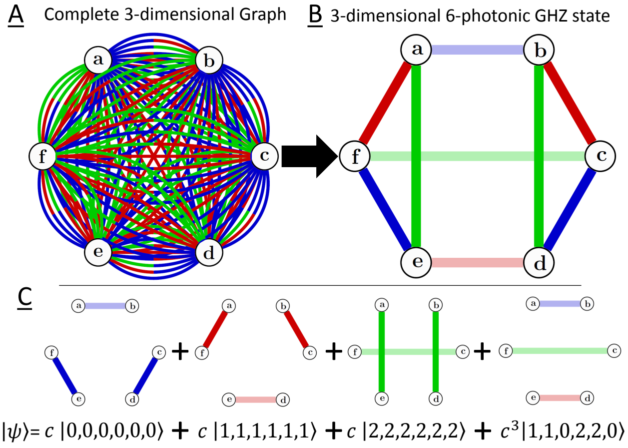

Figure 1. **Finding a 3-dimensional 6-photonic GHZ state. A:** The complete graph of six vertices (six paths) and three colours (three dimensions) is the initial state. **B:** The solution for a 6-photonic 3-dimensional GHZ state. **C:** The scientific interpretation and understanding comes from perfect matchings of weighted graphs, and can be immediatly generalized by human scientists.

[1] M. Krenn, M. Erhard and A. Zeilinger, Computer-inspired Quantum Experiments. *Nature Reviews Physics, in press, arXiv:2002.09970* (2020).
[2] M. Krenn, J. Kottmann, N. Tischler and A. Aspuru-Guzik, Conceptual understanding through efficient inverse-design of quantum optical experiments. *arXiv:2005.06443* (2020).
[3] H.W. De Regt and D. Dieks, A contextual approach to scientific understanding. *Synthese* **144**, 137 (2005).
[4] H.W. De Regt, Understanding scientific understanding. *Oxford University Press* (2017).