Conceptual understanding enabled by efficient automated design of quantum optical setups

M. Krenn[a,b,c], J.S. Kottmann[b], N. Tischler[d] and A. Aspuru-Guzik[b,c]

[a] *Max Planck Institute for the Science of Light, Erlangen, 91058, Germany.*

[b] *Departments of Chemistry and Computer Science, University of Toronto, Toronto, Ontario M5S 3H6, Canada.*

[c] *Vector Institute for Artificial Intelligence, Toronto, Ontario M5G 1M1, Canada.*

[d] *Centre for Quantum Computation and Communication Technology (Australian Research Council), Centre for Quantum Dynamics, Griffith University, Nathan, QLD 4111, Australia.*

Photons are a core ingredient for many quantum technologies that promise advances for communication, computation, and sensing beyond the capabilities of their classical counterparts. However, designing experimental photonic setups (such as setups to generate quantum states of interest) often eludes human intuition, while systematic schemes [1] so far only provide solutions for restrictive scenarios. For this reason, a range of computational methods for designing quantum optical experiments has been introduced, including genetic algorithms, optimization of parametrized setups, topological search augmented with machine learning, and active learning approaches [2]. Unfortunately, these algorithms entail significant drawbacks, such as inefficient discovery rates, requirements for large sets of training data, or the specialization on narrow problem sets. And critically, it has been unclear how new scientific ideas and understanding can be systematically extracted from the solutions provided by the computer algorithms.

In this work (published in Ref. [3]), we present THESEUS, an automated design algorithm for quantum photonics with a highly interpretable representation that allows physicists to understand the solutions obtained. THESEUS is applicable to discrete-variable quantum photonics problems (including heralded states, post-selected states, deterministic photon sources, and probabilistic photon sources); it requires no training data and is orders of magnitude faster than previous, comparable approaches. THESEUS makes use of a graph-based representation of quantum optical experiments that is interpretable and amenable to an automated design approach. As an important feature, it allows simplifying the solution to its conceptual core, from where physicists can interpret, understand, and generalize the underlying ideas and concepts. We apply THESEUS to solve several previously open questions about quantum experiments that involve complex multiphotonic entanglement.

[1] N. VanMeter, P. Lougovski, D. Uskov, K. Kieling, J. Eisert and J.P. Dowling, *Phys. Rev. A* **76**, 063808 (2007).

[2] M. Krenn, M. Erhard, and A. Zeilinger, *Nat. Rev. Phys. 2,* **649** (2020).

[3] M. Krenn, J.S. Kottmann, N. Tischler and A. Aspuru-Guzik, *Phys. Rev. X* **11**, 031044 (2021).