Virtual Reality for Understanding Artificial-Intelligence-driven Scientific Discovery with an Application in Quantum Optics

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Abstract

Recent advances in Artificial Intelligence (AI) have led to new solutions for scientific problems. Yet, to fully exploit the potential of these tools, human researchers must understand the AI-generated proposals to extrapolate the findings, a task for which current algorithms are unsuited. To assist researchers in analyzing complex AI-generated solutions, we introduce `AriadneVR` , an immersive virtual reality (VR) environment for the visualization and manipulation of graphs. In particular, our tool works with an abstract representation of quantum optics experiments using colored weighted graphs. To showcase the benefits of our software, we present a new resource-efficient 3-dimensional entanglement swapping scheme and a 3-dimensional 4-particle GHZ state analyzer. Our results show the potential of VR to enhance researchers' ability to extract knowledge from graph-based generative AI, a widely used data representation in science.

1 Introduction

Virtual reality (VR) immerses the user in a 3D simulated environment, often interactive. Modern VR headsets feature stereoscopic rendering on top of the head and gaze tracking that, combined with gesture controllers, allow the user to move in all spatial degrees of freedom. This technology has found applications in many fields[1], such as entertainment, education [2, 3, 4], engineering [5, 6, 7], medicine [8, 9, 10, 11, 12, 13], or data science [14, 15]. In the natural sciences, VR helps to visualize and analyze complex data, often three-dimensional, such as molecules [16, 17, 18, 19, 20], astronomical data [21, 22, 23], or even neural network models [24, 25, 26], attempting to make

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Artificial Intelligence (AI) explainable [27]. Beyond improving our understanding of data, having effective visualization tools can help us develop more, better, and safer AI [28, 29]. Working directly with the data is also possible with some VR frameworks, like in interactive molecular simulations [30, 31].

Here, we introduce `AriadneVR` , a web VR tool to visualize and edit graphs. We focus on colored weighted graphs, an abstract representation of quantum optics experiments[32, 33, 34]. Within the virtual environment, the user can visualize the graphs as a whole or decompose them in perfect matchings, a set of subgraphs of high relevance in the colored graph framework (see Fig. 1). Moreover, when adding or removing elements of the graph, the program keeps track of how this affects the encoded experiment, updating it after every modification. Finally, in Section 4, we show two successful use cases of our technology, starting with AI-generated designs[35] and extrapolating the findings to larger new systems.

2 Background

2.1 Graph representation of quantum optics experiments

Previous work mapped a wide range of quantum optics experiments into multicolored weighted graphs[32, 33, 34]. In the simplest version of the framework, vertices indicate the optical path followed by the photons to reach a certain photodetector[36]. The edges connecting them show the creation of a photon pair, via spontaneous parametric down-conversion, and each photon reaches the detector/node at the end of the edge. The (complex) weight of the edge indicates the amplitude associated with the creation process of the photon pair. Finally, the colors indicate the different quantum modes accessible to the photons, such as polarization, orbital-angular momentum, or frequency, to name some. Photon pairs might not share the same mode and therefore the edges are often bicolored.

Experimentally, multiple probabilistic sources will emit photon pairs that reach the different photodetectors simultaneously. The detectors are unaware of which sources the photons came from. As shown in Fig. 1, this leads to a superposition of creation events with multiple photon pairs, represented by different edge combinations. In practice, we post-select only those creation events in which every detector is reached by a single photon simultaneously. Those are the edge combinations where every vertex has degree one, the so-called perfect matchings. The superposed states can come from a single perfect matching (like in Fig. 1) or from the addition of many of them.

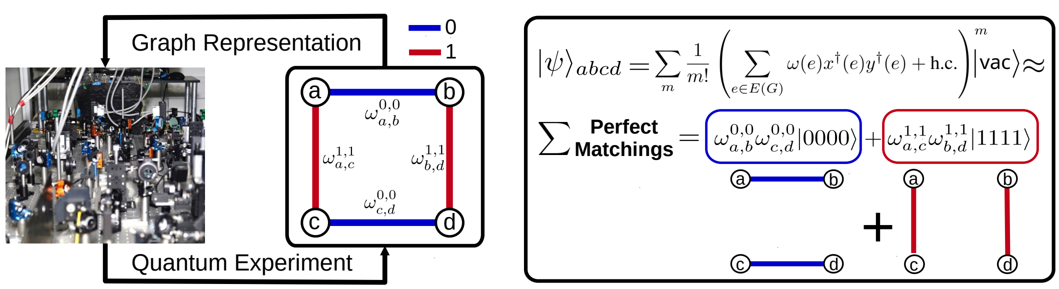

Figure 1: **Graph-based representation of quantum optics experiments.** The color edges, labeled in this case with real positive weights, map into a series of creation operators. The resulting state is, after post-selecting perfect matching contributions, a coherent superposition of two quantum states. The experiment to generate the (GHZ) state can be derived from the graph.

2.2 Patterns and symmetries of the experimental designs

Multiple experimental realizations, with different types of modes, can be derived from a single graph. This simple and abstract representation has enabled a successful top-down strategy for experimental design. The approach starts by setting a large fully connected graph with a certain number of modes (colors). Then, alternating weight optimization and edge pruning the algorithm reach the smallest graph that fulfills the experiment requirements. The *PyTheus* library[35] offers the fastest implementation of this approach, which we use in Section 4 to verify some of our proposed designs and explore reduced search spaces of graphs.

Small abstract graphs are much easier to understand and interpret that the different experimental setups that one can derive from them. Pattern recognition is straightforward in small graphs and has led to the discovery of several families of solutions, from entanglement generation to measurement schemes[32, 34, 35, 37]. However, as the number of nodes (particles) and colors (modes) increases, so does the difficulty of finding new patterns. Additionally, the increase of the search space's dimensions jeopardizes the computational feasibility of the top-down approach. With our new software, `AriadneVR`, we have simplified the search.

3 AriadneVR

`AriadneVR` is a web-based virtual reality application for better visualization, analysis, and manipulation of colored graphs. It is developed with the open-source framework *A-Frame* using HTML and JavaScript on a Meta Quest 2 (formerly Oculus). The software runs locally in the headset's browser, requiring neither installation nor an external computer for 3D rendering. The actual VR environment is shown in Fig. 2c, while the other 3D figures displayed were produced with *Blender*, including the ones from Fig. 3.

To enhance the search for new patterns, our tool enables direct visualization and manipulation of the graphs. Within the 3D environment, the user can edit the graph arrangements by grabbing and dragging its vertices, as well as add/remove edges. While doing the latter, the software keeps track of how these modifications affect the number of perfect matchings, and by extension the final states. The different perfect matchings can also be displayed as individual graphs.

The modified graphs can be saved to the headset and uploaded into the host platform. These stored graph files can be downloaded and edited in later sessions. The new constrained topologies can be used as a starting point in the PyTheus top-down search, drastically accelerated by the reduction of the exploration space (number of edges) and the decrease of perfect matchings. Moreover, to streamline the search for symmetries and patterns, the edges can be drawn without assigning them colors, representing a connection where all possible edges are in the initial graph.

Except for the colorless edges, our software follows the representation introduced with the PyTheus library. Spherical nodes are the standard way to represent the detectors. Cubical nodes show ancilla detectors, which assist in creating various states and performing certain operations. Pyramidal vertices indicate single incoming photons. The black shapes in the middle of the edges indicate negative real weights. For the solutions found in this work, all weights were real.

To facilitate the visualization of the graphs, we computed beforehand their initial 3D layout with the Kamada-Kawai-algorithm [38], implemented with the Python library `igraph`[39]. This initial arrangement and other features of the graphs are stored on the host platform. With this information and the library *THREE.js*, the A-Frame constructs a model from the graph.

While `AriadneVR` is built for analyzing quantum optics experiments, its core functionality is visualizing and editing small and medium-sized colored graphs. Therefore, if presented in the appropriate format, our tool can also work with other types of graphs. However, since `AriadneVR` is directly processed by the VR headset, the framerate decreases with larger graphs. That is not a serious limitation for us: graphs which are too large for the headset to process are too convoluted to grasp. In such scenario, the number of terms and interactions to consider is so large that we would rather work on simplifying the representation.

For projects which do require the rendering of huge networks, like those from social sciences, external computational power might be required. For such cases, software like *VRNetzer* [15] is better suited.

4 Applications

To illustrate the potential of immersive and interactive 3D environments in general and our software in particular, we want to highlight two successful use cases of our tool. Both examples involve entangled states of many photons and dimensions. The non-local properties of these states are the cornerstone of multiple quantum communication schemes [40, 41].

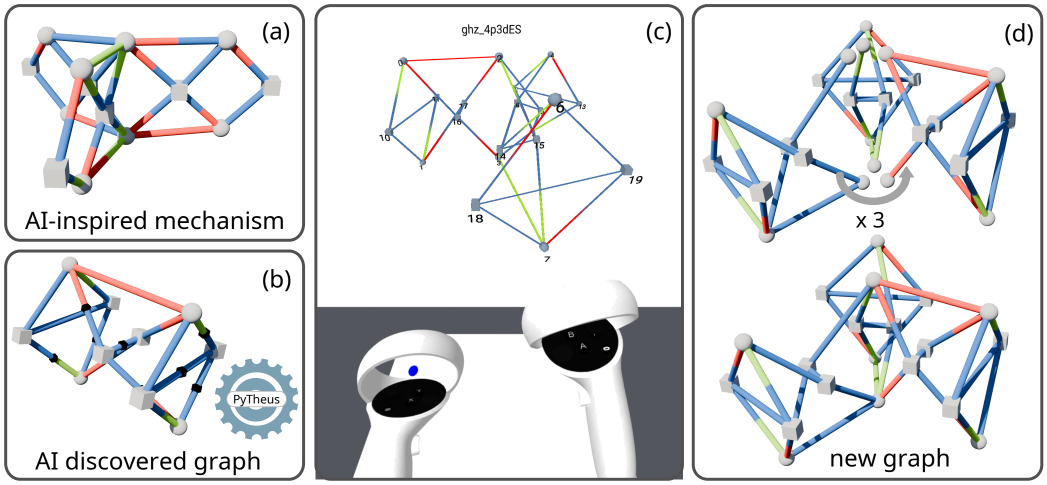

Figure 2: **VR assisted discovery of new designs for efficient high dimensional entanglement swapping.** Previous PyTheus designs performed efficient 2-dimensional entanglement between 3 pairs of particles. The designs were manually expanded to a 2-dimensional entanglement between 3 photon pairs, the 'arms' of the structure, and a 3-dimension photon pair in the center **(a)**. The manually found pattern and the PyTheus solution for 2-pair 3-dimensional swapping **(b)** were combined within the virtual environment **(c)** producing a larger entanglement swapping for 4 photon-pairs with 3-dimensions **(d)**. Notice that the final graph combines the 'arms' of our solution with a subgraph of the Pytheus solution. The spherical nodes are the optical paths (detectors) where the entangled pairs go, while the cubic ones are ancillas that enable the process.

The first example, shown in Fig. 2, is a 3-dimensional entanglement swapping scheme between (up to) 4 photon pairs. It is an extension of the original entanglement swapping protocol, in which two parties share two entangled particles that never interacted[42]. To find the solution we first saw that, with minor modifications, we could add a fourth pair of entangled photons to one of the graphs described in the PyTheus paper (solution 77), which produced a 2-dimensional entanglement between 3 pairs of particles. Remarkably, the 4th pair was different from the previous: it was a three-dimensional entangled pair. That drew our attention to another example of the PyTheus paper: the 2 entangled pairs of 3-dimensional photons (solution 78). Comparing and tinkering with both solutions we found out how to combine them into the final setup of 4 entangled pairs of 3-dimensions. The trick was to add the regular structures of our solution into a subgraph of the PyTheus solution.

The second example, shown in Fig. 3, required far less human input. We started analyzing the 3-dimensional 3-particle GHZ analyzer of the PyTheus paper (solution 80). Examining the structure of its perfect matchings, i.e. seeing how the different contributions interfered, we guessed the topology of a similar state with more particles. By constraining the geometry of our initial graph we reduced its original 124 edges to only 74 of them. This not only decreased the dimensionality of the search space but reduced the number of perfect matchings and, therefore, the contributions to the final state. With such simplification, we were able to find the solution in a domestic computer within minutes.

Later on, for comparison, we tried to obtain suitable solutions (high fidelity, low number of edges) starting from the complete graph with 124 edges. Due to the large number of perfect matchings, we had to run PyTheus on a high-performance computer with hundreds of gigabytes of RAM. Finding a solution took, starting from the full graph, around 3 hours on average. In the same machine, starting from the 74-edge subgraph, we needed less than 5 minutes to find an equally good solution. Moreover, the reduction of computed terms also allows for the smaller graph to be run in a domestic computer.

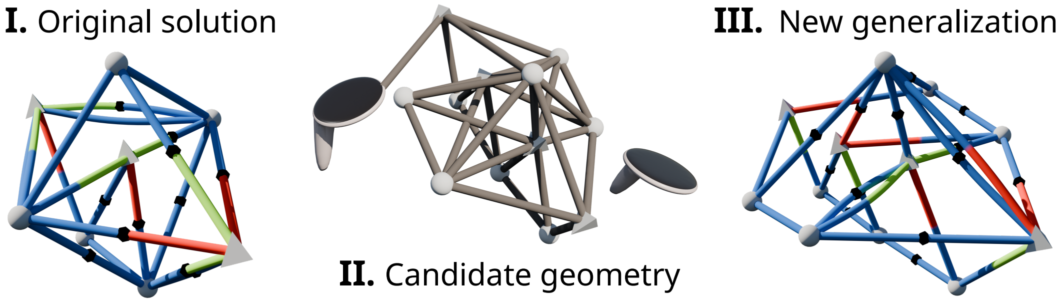

Figure 3: **Restricting the geometry of the initial graph reduces the search space and accelerates optimization.** Observing the structure of a PyTheus solution for 3-photon 3-dimensional GHZ-state analyzer **(I)** we made a guess of the geometry for larger graphs **(II)**. Our constraints reduced the search space of the larger graph (from the 124 of a complete graph to 74 edges) which led to a 4-particle generalization of the 3-dimensional GHZ-state analyzer **(III)**.

5 Conclusions

We have showcased the potential of VR environments for discovering and analyzing quantum optics experiments. The search and exploitation of patterns with the graph representation provided us experimental solutions that, by direct search, would have taken weeks for PyTheus to compute, and only if the memory permitted. Moreover, even when the patterns were vague we could test our intuitions and symmetry constraints and find solutions faster with fewer computational resources.

Adding new tools to our VR environment is a straightforward path for future updates. However, we are also interested in humbler setups, such as phone VR headsets. Having to reduce the available toolbox, these cheaper alternatives still offer excellent visualization capacities, avoiding software bloating. That would facilitate the adoption of our software and make it a handy tool to develop medium-sized graphs. That could go hand in hand with expanding our tool's applications in other fields. The design of quantum circuits [43] or the development of ZX-graphs [44] are interesting use cases of graph representations within neighbor domains.

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