# Quantum Experiments and Graphs: Multiparty States as Coherent Superpositions of Perfect Matchings

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We show a surprising link between experimental setups to realize high-dimensional multipartite quantum states and graph theory. In these setups, the paths of photons are identified such that the photon-source information is never created. We find that each of these setups corresponds to an undirected graph, and every undirected graph corresponds to an experimental setup. Every term in the emerging quantum superposition corresponds to a perfect matching in the graph. Calculating the final quantum state is in the #P-complete complexity class, thus it cannot be done efficiently. To strengthen the link further, theorems from graph theory—such as Hall's marriage problem—are rephrased in the language of pair creation in quantum experiments. We show explicitly how this link allows one to answer questions about quantum experiments (such as which classes of entangled states can be created) with graph theoretical methods, and how to potentially simulate properties of graphs and networks with quantum experiments (such as critical exponents and phase transitions).

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When a pair of photons is created, and one cannot—even in principle—determine what its origin is, the resulting quantum state is a coherent superposition of all possibilities [1,2]. This phenomenon has found a manifold of applications such as in spectroscopy [3], in quantum imaging [4], for the investigation of a complementarity [5], in superconducting cavities [6], and for investigating quantum correlations [7]. By exploiting these ideas, the creation of a large number of high-dimensional multipartite entangled states has recently been proposed [8] (inspired by computer-designed quantum experiments [9]).

Here we show that graph theory is a very good abstract descriptive tool for such quantum experimental configuration: Every experiment corresponds to an undirected graph, and every undirected graph is associated with an experiment. On the one hand, we explicitly show how to translate questions from quantum experiments and answer them with graph theoretical methods. On the other hand, we rephrase theorems in graph theory and explain them in terms of quantum experiments.

An important example for this link is the number of terms in the resulting quantum state for a given quantum experiment. It is the number of perfect matchings that exists in the corresponding graph—a problem that lies in the #P-complete complexity class [10]. Furthermore, the link can be used as a natural implementation for the experimental investigation of quantum random networks [11].

*Experiments and graph.*—The optical setup for creating a 3-dimensional generalization of a 4-photon Greenberger-Horne-Zeilinger state [12,13] is shown in Fig. 1(A) [8]. The experiment consists of three layers of two down-conversion crystals each. Each crystal can create a pair of photons in the state $|0,0\rangle$, where the mode number could correspond to the orbital angular momentum (OAM) of photons [14–16], or some other (high-dimensional) degree-of-freedom. A laser pumps all of the six crystals coherently, such that two pairs of photons are created in parallel. Four-fold coincidence (i.e., four photons are detected simultaneously in detector $a$, $b$, $c$, and $d$) can only happen if the two photon pairs are created in crystals I and II, or in crystals III and IV, or in crystals V and VI. In every other case, there is at least one path without a photon, which is neglected by postselection. Between each layer, the modes are shifted by $+1$. This example leads to the final state $|\psi\rangle = (1/\sqrt{3})(|0,0,0,0\rangle + |1,1,1,1\rangle + |2,2,2,2\rangle)$.

The corresponding graph is shown in Fig. 1(B). Every optical path $a$, $b$, $c$, $d$ in the experiment corresponds to a vertex in the graph, and every crystal forms an edge between the vertices. A four-fold coincidence count happens if a subset of the edges contains each of the four vertices exactly once. Such a subset is called *perfect matching* of the graph. In the above example, there are three perfect matchings (two green edges, two blue edges, and two red edges), thus there are three terms in the quantum state. We can therefore think of our quantum state

 

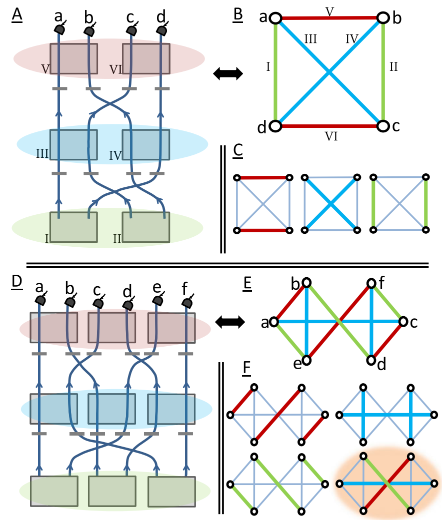


FIG. 1. (A) An optical setup which can create a 3-dimensional 4-photon GHZ-state with the method of *entanglement by path identity* [8]. It consists of three layers of crystals, and in between there are variable mode- and phase-shifters (depicted in grey). (B) The corresponding graph with four vertices (one for each path) and six edges (one for each crystal). Every layer of crystals leads to a four-fold coincidence count. (C) These correspond to three disjoint *perfect matchings,* or *1-factors,* in the graph. (D) An optical setup for creating 3-dimensional entanglement with six photons. (E) The corresponding graph. (F) It has four perfect matchings, thus the corresponding quantum state has four terms. One terms comes from each of the three layers (the GHZ terms), and one additional term comes from different layers (the *Maverick*-term, with orange background). For that reason, the resulting quantum state has not the form of a GHZ state. In the Supplemental Material [17], we show how to construct the experimental setup from a given graph.

as a coherent superposition of the perfect matchings in the corresponding graph. The correspondence between quantum optical setups and graph theoretical concepts are listed in Table I.

Now, what will happen when we add more crystals in each layer? As an example, in Fig. 1(D), three crystals in each layer produce six photons, there are three layers which make the photons 3-dimensionally entangled. Surprisingly

TABLE I. The analogies between quantum experiments involving multiple crystals and graph theory.

| Quantum experiment | Graph theory |
|---|---|
| Optical setup with crystals | Undirected graph $G(V, E)$ |
| Crystals | Edges $E$ |
| Optical paths | Vertices $V$ |
| $n$-fold coincidence | Perfect matching |
| #(terms in quantum state) | #(perfect matchings) |
| Maximal dimension of photon | Degree of vertex |
| $n$-photon $d$-dimensional GHZ state | $n$-vertex graph with $d$ disjoint perfect matchings |

however, in contrast to the natural generalization of the 4-photon case in Fig. 1(A)–(C) (and in contrast to what some of us wrote in [8]), the resulting state is not a high-dimensional GHZ state. In contrast to the previous case, there are four perfect matchings, thus the resulting quantum state has four terms [Fig. 1(F)]. One perfect matching comes from each of the layers (which are the terms expected for the GHZ state), and one additional perfect matching arises due to a combination of one crystal from each layer (which we call the *Maverick* term). If the mode shifter between the layers is $+1$ as before, the Maverick term has $|1_a, 1_c\rangle$ from the blue layer, $|2_b, 2_d\rangle$ from the green layer, and $|0_e, 0_f\rangle$ from the red layer. This leads to the final state

$$|\psi\rangle = \frac{1}{2}(|0,0,0,0,0,0\rangle + |1,1,1,1,1,1\rangle + |2,2,2,2,2,2\rangle + |1,2,1,2,0,0\rangle). \quad (1)$$

A GHZ state can only appear when all perfect matchings are *disjoint*, meaning that every edge appears only in one perfect matching. Otherwise, additional terms are present in the quantum state.

When the number of layers of crystals is increased to four (with three crystals per layer) and modes are shifted by $+1$ as before (and no phase shifters are used), there are eight terms in the resulting quantum state: Four GHZ-like terms and four additional Maverick terms. For five layers, the resulting 6-photon quantum state consists of 15 terms (5 GHZ-like terms and 10 additional Maverick terms), entangled in five dimensions (see Supplemental Material [17]). In general, $n$ crystals in one layer produce $2n$ photons. One can design setups with $d = (2n-1)$ layers, which correspond to a complete graph $K_{2n}$ (in a complete graph, every vertex is connected with every other one exactly once). It produces a state with $[(2n)!/n!2^n]$ terms, $(2n-1)$ of them are GHZ-like (see Supplemental Material [17]). By changing the mode shifters and phase shifters between the layers, a vast amount of different quantum states can be created.

Now one could ask what types of GHZ states are possible, in general, using the experimental scheme above. We show a proof based on graph theory which answers that question. For that, we first translate the quantum physics question "*Which d-dimensional GHZ states can be created?*" into the graph theory question "*Which undirected graphs exist with d perfect matchings which all are disjoint?*". The proof strategy is to construct a graph with a maximum number of disjoint perfect matchings, starting from $n$ vertices [24]. The concept and the proof are described in Fig. 2. We find that one can create arbitrarily large 2-dimensional GHZ states, and a 3-dimensional 4-photon GHZ state. In an analogous way, different questions in such quantum experiments can be translated and answered with graph theory.

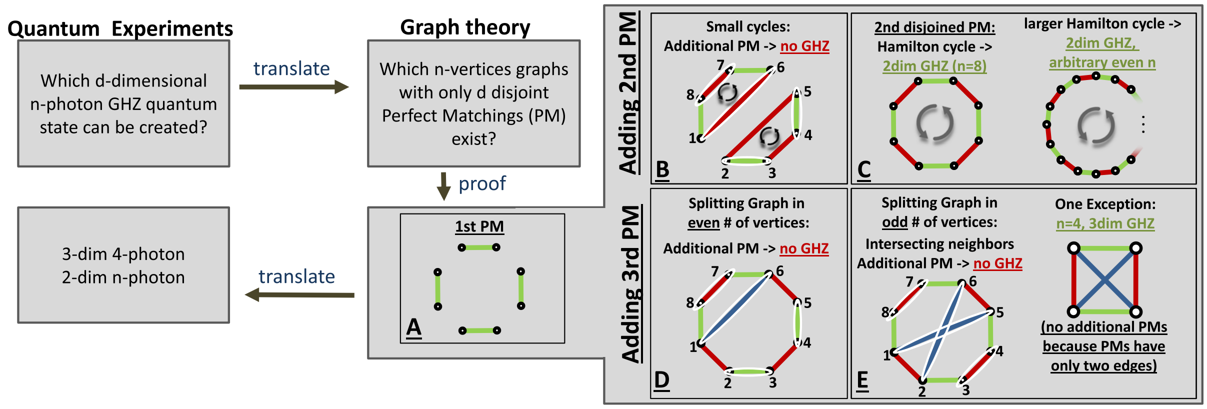


FIG. 2. Application of the bridge between quantum experiments and graph theory: As a concrete example, we ask which $d$-dimensional $n$-photon GHZ states can be created experimentally with this method. The idea of the proof is to construct a graph starting with $n$ vertices without edges. We try to maximize the number of *disjoint* perfect matchings (PMs) by adding appropriate edges to the graph [24]. In disjoint PMs, every edge appears in only one perfect matching. The example in the figure is for $n = 8$, but the proof works for any arbitrary even $n$. Step I: In **A**, we add the first PM to a set of eight vertices (green). Step II: In **B**, we add more edges to construct a second PM (red). Whenever the new PM, together with the first (green) PM, creates more than one cycle (here: edges 1-6,6-7,7-8,8-1; and 2-3,3-4,4-5,5-2), we immediately find an additional Maverick PM (indicated with white boundary, edges 1-6,2-3,4-5,7-8). Thus the graph cannot represent a GHZ state (as a GHZ state has only disjoint perfect matchings). The only choice for the second PM is to create together with the first PM *one* cycle that visits every vertex—a Hamilton cycle, shown in **C**. Hamilton cycles consist of 2 PMs, and therefore correspond to 2-dimensional GHZ states. It can be arbitrarily large, and thus there can be arbitrarily large $n$-photon 2-dimensional GHZ states. Step III: Starting with the Hamilton cycle, we try to add a third PM with blue edges. In **D**, we observe that if the new edge splits the graph into an even number of vertices (upper part: vertices 7,8; lower part: vertices 2,3,4,5), we always find a new Maverick PM. It consists of the new edge (here: 1–6) and edges from the Hamilton cycle (here edges 2-3,4-5,7-8). We learn—as we require only disjoint perfect matchings—no edge of a new PM should split the graph into even numbers of vertices (otherwise Maverick PMs appear). Finally, in **E** we try to add edges that split the graph into an odd number of vertices. We observe that in every additional PM there are at least two neighboring edges that intersect (neighboring edges start from consecutive vertices; here—shown in blue—they start at vertex 1 and vertex 2). This pair always forms a new Maverick PM with additional edges from the Hamilton cycle (here: 1-5,2-6,3-4,7-8). There is one exception for the case of $n = 4$: There can be a 3rd disjoint PM, because a Maverick PM needs at least 3 edges (2 blue ones and one from the Hamilton cycle). Therefore, a 4-photon 3-dimensional GHZ state can be created, while for $n > 4$, GHZ states can only be created with $d = 2$.

In order to build 3-dimensional GHZ-type experiments with six photons (without extra terms), one can use two copies of the 3-dimensional 4-photon GHZ state [presented in Fig. 1(A)], and combine them with a 3-dimensional Bell-state measurement [25,26]. In the graph this is represented by two graphs that are merged (see Supplemental Material [17]). Many other classes of entangled states, such as a two-dimensional W-state [27,28] or asymmetrically entangled Schmidt-Rank Vector (SRV) [29,30], can be created by exploiting multigraphs (graphs with more then one edge between two vertices), as shown in the Supplemental Material [17].

An important result is that calculating the final quantum state cannot be done efficiently: Counting the number of perfect matchings in a graph (i.e., calculating the number of terms in the resulting quantum state) is in the #P-complete complexity class. In a bipartite graph, it is equivalent to computing the permanent of the graph's biadjacency matrix [10] (see Supplemental Material for such an experimental setup [17]). Furthermore, for general graphs, counting the number of perfect matchings corresponds to calculating the *Hafnian* (a generalization of the permanent) of the graph's adjacency matrix. Even for approximating the Hafnian, there is no known deterministic algorithm that runs in polynomial time [31,32]. An example is given in Fig. 3(A) for a random graph, its corresponding perfect matching and Hafnian in Fig. 3(B)–(C), and the corresponding quantum setup in Fig. 3(D).

While the information about the number of terms is encoded in every $n$-photon quantum state emerging from the setup, the question is how one can obtain this information (or approximate it) efficiently. Measurements in the computation basis are not sufficient, otherwise it could be calculated classically as well. One direction would be to investigate the *frustrated generation* of multiple qubits [33] (for instance, by using phase shifters instead of mode shifters between each crystal), or by analyzing multiphoton, high-dimensional entanglement detections [34]. A detailed investigation of the link between the outcome of such experiments and complexity classes would be valuable, but it is outside the scope of this Letter.

As it is possible to generate experimental setups for arbitrary undirected graphs, the presented scheme is also a natural and inexpensive implementation of quantum

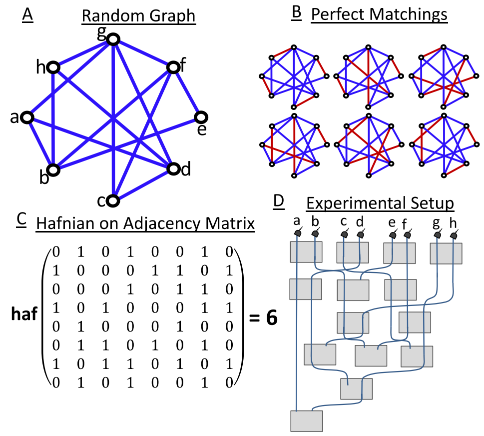


FIG. 3. Random graph or quantum random network—and its connection to quantum experiments. (A) A random graph with 8 vertices and 14 edges. (B) The perfect matchings corresponding to the random graph. (C) They can be calculated with the matrix function *Hafnian*, which is a generalization of the *permanent*. Both are very expensive to calculate. (D) The corresponding quantum experiment. Each of the terms in its quantum state corresponds to a perfect matching in the graph. It can also be seen as a quantum random network, to study network properties in the quantum regime.

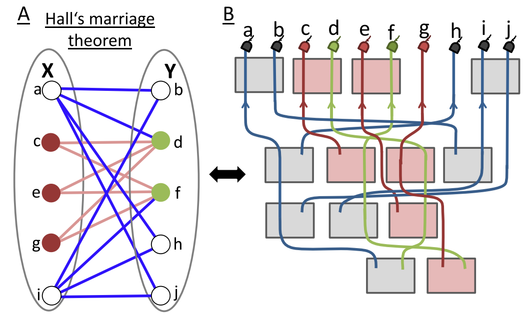


FIG. 4. A theorem from graph theory: Hall's marriage theorem (A) For a bipartite graph with equal number of elements in $X$ and $Y$, Hall's theorem gives a necessary and sufficient condition for the existence of a perfect matching. That happens when for every subset in $W \in X$, the number of neighbors in $Y$ is larger or equal than $|W|$. In the example graph, the subset of $X$ consisting of the vertices c, e, g (indicated in red) has only two neighbors in $Y$ (d, f—indicated in green), thus there cannot be a perfect matching. (B) For quantum experiments, the analog question is whether there can be $2n$-fold coincidences, given that $n$ crystals emit photon pairs. When the two photons are distinguishable (which corresponds to a bipartite graph), $2n$ folds can only happen when for every subset $W$ of signal photon paths the number of connected idler paths is larger or equal than $|W|$. In the example, the subset of signal photon paths (c, e, g—depicted in red) has only two corresponding idler paths (d, f—depicted in green), thus there cannot be a 10-fold coincidence count.

(random) networks (see Fig. 3). This could be used to experimentally investigate entanglement percolation [35–37] and critical exponents that lead to phase transitions in quantum random networks [11]. As an example, it has been shown that for large quantum networks with $N$ nodes, every quantum subgraph can be extracted with local operations and classical communication (LOCC) if the edges are connected with a probability $p \geq N^{-2}$ [11]. In close analogy to the experimental schemes here, $N$ is the number of output paths of photons, and $p$ corresponds to the probability for a down-conversion event in a single crystal. The quantum state for the edge between vertices $a$ and $b$, with mode number $\ell$ can be written as

$$|\psi_{a,b}\rangle = \Big[1 + p(\hat{a}^{\dagger}_{a,\ell}\hat{a}^{\dagger}_{b,\ell} - \hat{a}_{a,\ell}\hat{a}_{b,\ell}) + \frac{p^2}{2}(\hat{a}^{\dagger}_{a,\ell}\hat{a}^{\dagger}_{b,\ell} - \hat{a}_{a,\ell}\hat{a}_{b,\ell})^2 + \cdots\Big]|0\rangle, \quad (2)$$

where $p$ is the spontaneous parametric down-conversion probability. The complete quantum (random) network is a combination of all crystals being pumped coherently, which is a tensor product over all existing edges in the form of

$$|\psi_{\text{network}}\rangle = \bigotimes_{e(i,j)\in E} |\psi_{i,j}\rangle, \quad (3)$$

where $i$ and $j$ are the vertices that are connected by the edge $e \in E$.

Finally, to strengthen the link between quantum experiments and graph theory, we show that theorems from graph theory can be translated and reinterpreted in the realm of quantum experiments. In Fig. 4(A) and (B), we show *Hall's marriage theorem*, which gives a necessary and sufficient condition in a bipartite graph for the existence of at least one perfect matching [38]. A generalization to general graphs, *Tutte's theorem* [39,40], is shown in the Supplemental Material [17]. Both graph theory theorems can be understood in the language of quantum experiments.

To conclude, we have shown a strong link between quantum experiments and graph theory. It allows to systematically analyze the emerging quantum states with methods from graph theory. The new link immediately opens up many new directions for future research. For example, the analysis of the number of *maximal matchings* and *matchings* in a graph (called a *Hosoya index* and often used in chemistry [41,42]) in the context of quantum experiments.

A detailed investigation of links between these experiments and computation complexity classes, in particular the relation to computation complexity with linear optics would be interesting [43–45].

Furthermore, it would be interesting how the merging of graphs can be generalized with nondestructive measurements [46], whether it leads to larger classes of accessible states and how that can be described in the graph theoretical framework.

The generalization to other graph theoretical methods would be interesting, such as weighted graphs (which could correspond to variable down-conversion rates via modulating the laser power), hypergraphs (which would correspond to creation of tuples of photons, for instance via cascaded down-conversion [47,48]), or 2-factorizations (or general $n$-factorizations, which would lead to $n$ photons in one single arm).

Experimental implementations could not only create a vast array of well-defined quantum states, but could also investigate striking properties of quantum random networks in the laboratory.

Finally, we suggest that recent developments of integrated optics implementations of quantum experiments, where the photons are generated on a photonic chip [49–51], could be particularly useful to realize setups of the type proposed here.

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