Quantum Experiments and Graphs: Multiparty States as coherent superpositions of Perfect Matchings

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(Dated: May 19, 2017)

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 correspond 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 grpah. Calculating the final quantum state is in the complexity class #P-COMPLETE, thus 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. This link allows to answer questions about quantum experiments (such as which classes of entangled states can be created) with graph theoretical methods, and potentially simulate problems in Graph Theory with quantum experiments.

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. Twenty-five years ago, Wang, Zou and Mandel (originally suggested by Zhe-Yu Ou) have used that idea in a remarkable way [1, 2]: They coherently overlapped one of the output modes from each crystal ($|b\rangle = |d\rangle$ in Fig. 1A), such that the *which-crystal information* for the photon in d never exists in the first place. That leads to $|\psi\rangle = 1/\sqrt{2}\,(|a\rangle + |c\rangle)\,|d\rangle$, where one photon is in d and the second photon is in a coherent superposition of being in a and in c. This phenomenon has found a manifold of applications such as in spectroscopy [3], in quantum imaging [4], for the investigation of complementarity [5], in superconducting cavities [6] and for investigating quantum correlations [7].

In a variation of that idea, both output modes from the two crystals are overlapped such that the paths of the photons are identical (Fig. 1B). By adding phases between the two crystals, one obtains $|\psi\rangle = (|a, b\rangle + \exp(i\phi)|a, b\rangle) = (1 + \exp(i\phi))|a, b\rangle$, which means that by changing the phase ϕ, one can enhance or surpress the creation of photons – a phenomenon denoted as *frustrated* generation of photon pairs [8]. If instead of phase shifters one would add mode shifters between the crystals (for instance, the crystal produces two horizontal polarized photons, and the mode-shifter changes horizontal to vertical), one creates an entangled two-photon state $|\psi\rangle = 1/\sqrt{2}(|H_a, H_b\rangle + |V_a, V_b\rangle)$ [9]. By exploiting these ideas, the creation of a large number of high-dimensional multipartite entangled states has been proposed recently [10] (inspired by computer-designed quantum experiments [11]).

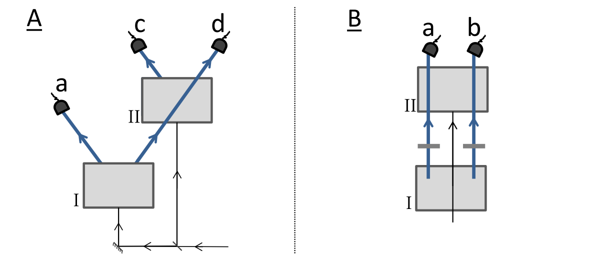

Figure 1. **A**: The experiment introduced in [1] consists of two crystals, pumped by a laser (depicted in black) which create one pair of photons (either in crystal I or in crystal II), and one of the paths is overlapped. If the two possibilities are prepared such that one cannot distinguish in which crystal the photons have been created, the final state consists of a photon in d and a coherent superposition of the second photon being in a or in c. **B**: In this experiment, both arms are overlapped. If the grey elements between the two crystals are phase-shifters, the two crystals can either constructivly or destructivly interfere, leadering to larger or smaller numbers of photons in the output a and b [8]. If the grey elements are mode-shifters, one creates an entangled state [9]. In can be chosen by the experimentalist whether the photons emerge colinear or at an angle from the crystal. For simplicity, the laser is not drawn anymore in the following examples.

Here we show that such experimental configurations can be systematically described with Graph Theory: Every experiment corresponds to an undirected Graph, and every undirected Graph is associated with an experiment. On the one hand, it allows to translate questions from quantum experiments and answer them with graph theoretical methods. On the other

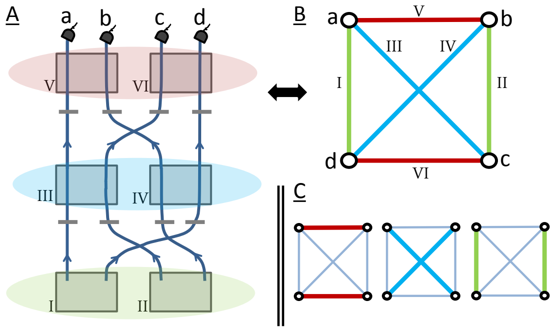

Figure 2. **A**: An optical setup which can create a 3-dimensional 4-photon GHZ-state with the method of Path Identity. It consists of three layers of crystals, in between there are variable mode- and phase-shifters (depicted in grey). **B**: The corresponding graph with four vertices (one for each path), six edges (one for each crystal). Every layer of crystals leads to a four-fold coincidence count. **C**: That corresponds to a *perfect matching* or *1-factor* in the graph.

hand, theorems in Graph Theory can be rephrased and understood with 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 complexity class #P-COMPLETE. Futhermore, the link between quantum experiments and graph theory helps to understand which high-dimensional multipartite quantum states is experimentally accessible.

A link between quantum physics and graph theory has been drawn before, but for different reasons. For example, in *Graph states* [12, 13], which are related to the resources for measurement-based quantum computation [14], the vertices of the Graph correspond to qubits in a quantum state, and the edges correspond to correlations between two qubits. In different works, the *Laplacian* of a graph has been interpreted as the density matrix of a quantum state, which allowed to investigate new entanglement criteria [15].

Experiments and Graph – The optical setup for creating a 3-dimensional generalization of a 4-photon Greenberger-Horne-Zeilinger state [16, 17] is shown in Fig. 2A. 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 [18–20] 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. One photon in each of the four paths, i.e. a four-fold coincidence, 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 in post-selection. For example, if a photon pair is created in crystal I and one in III, there will be two photons in path a, but no photon in path b. Between each layer, the photons can be manipulated. For example if the modes are shifted by +1 between every layer (in the case of OAM, this can be done with holograms), photons from the green layer are shifted twice, photons from the blue layer are shifted once and photons in the red layer stay in their initial state. This example leads to the final state $|\psi\rangle = 1/\sqrt{3}\left(|0_a,0_b,0_c,0_d\rangle + |1_a,1_b,1_c,1_d\rangle + |2_a,2_b,2_c,2_d\rangle\right)$ (where the subscript correspond to the path of the photon).

The corresponding graph is shown in Fig. 2B. Every optical path a, b, c, d in the experiment corresponds to a vertex in the graph, every crystal forms an edge between the vertices. A four-fold coincidence count happens when a subset of the edges are incident to

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
layers of crystals	disjoint perfect matchings
#(terms in quantum state)	#(perfect matchings)
maximal dimension of photon	degree of vertex

Table I. The analogies between Quantum Experiments involving multiple crystals and Graph Theory.

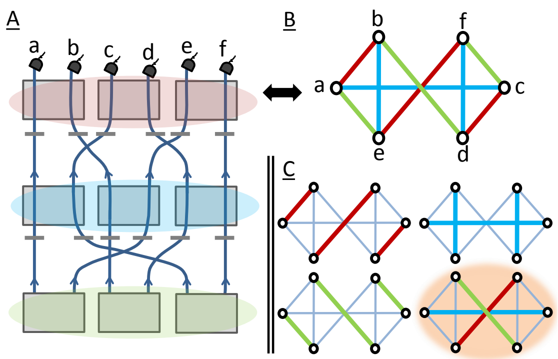

Figure 3. **A**: An optical setup for creating 3-dimensional entanglement with 6 photons. **B**: The corresponding graph consists of 6 vertices and 9 edges, and each layer of crystals corresponds to a 1-factor (depicted in green, blue and red). **C**: This graph has four perfect matchings, thus the corresponding 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 red background). For that reason, the resulting quantum state has not the form of a GHZ state.

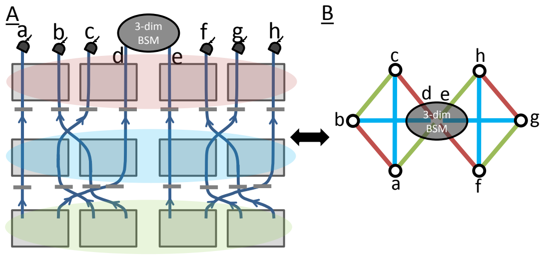

Figure 4. **A**: Two experiments which each create a 3-dimensional 4-photon entangled GHZ state can be combined with a 3-dimensional Bell-State measurement. **B**: In the corresponding graph, the vertices d and e are merged. Merging the two graphs can be understood as a generalized multi-photon high-dimensional entanglement swapping.

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 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. 3A, three crystals in each layer produce 6 photons, there are three layers which make the photons 3-dimensionally entangled. Surprisingly however, in contrast to the natural generalisation of the 4-photon case in Fig. 2 (and in contrast to what some of us wrote in [10]), 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. 3C). One perfect matching comes from each of the layers (which are the terms expected for the GHZ state), and one additional arises due to a combination of one crystal from each layer (which we call *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

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

When the number of layers of crystals is increased to four, there are eight terms in the resulting quantum state. For five crystals, the resulting 6-photon quantum state consists of 15 terms, entangled in 5 dimensions (see Appendix). In general, n crystals in one layer produce $2n$ photons. One can design setups with $d = (2n-1)$ independent layers of crystals which can be arbitrarily controlled by the experimentalist.

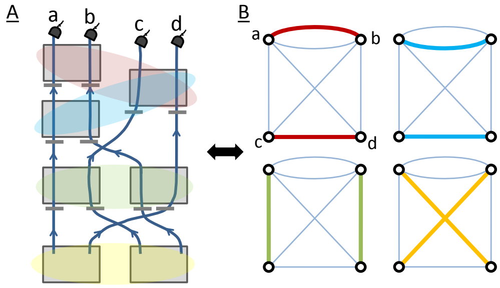

Figure 5. **A**: An optical setup, where two crystals emit into the same path, can be used to realize many entangled states, such as the W-state $|\psi\rangle = 1/2\left(|0,0,0,1\rangle + |0,0,1,0\rangle + |0,1,0,0\rangle + |1,0,0,0\rangle\right)$ or a high-dimensional asymmetrically entangled state $|\psi\rangle = 1/2|0\rangle\left(|0,0,0\rangle + |1,0,1\rangle + |2,1,0\rangle + |3,1,1\rangle\right)$, where one photon acts as trigger. By changing the mode- and phase-shifters between the crystals, one arrives at different states. **B**: Such experiments can be consistently described with multiple edges that are incident to the same two verices. By looking at the perfect matchings, it is easy to understand what modes the individual crystals have to produce to obtain the desired state (for example, shown in [10]).

Such a complete set of layers correspond to complete graphs K_{2n} (in a complete graph, every vertex is connected with every other one exactly once), and the structure of the layers is called 1-Factorization. A 1-Factorization of the graph G(V,E) is a partitioning of the graph's edges into disjoined subgraphs (called 1-factors), where each 1-factor has the same number of vertices as G(V,E) – and in contrast to the factorization of natural numbers, it doesn't need to be unique [21]. Every 1-Factor of the 1-Factorization can be controlled independently in the quantum experiment (such as the GHZ terms in Fig. 3C), while additional perfect matchings lead to additional terms (such as the Maverick term in Fig. 3C).

In order to build 3-dimensional GHZ-type experiments with 6 photons (without extra terms), one can use two copies of the 3-dimensional 4-photon GHZ state (presented in Fig. 2A), and combined them with a 3-dimensional Bell-state measurement [22, 23] as shown in Fig. 4A and B. Triggering on one of the 9 Bell states leads to

$$|\psi\rangle = \frac{1}{\sqrt{3}}\big(|0,0,0,0,0,0\rangle + |1,1,1,1,1,1\rangle + |2,2,2,2,2,2\rangle\big), \quad (2)$$

which is a 6-photon, 3-dimensional GHZ state. This can be generalized to multi-photon 3-dimensional GHZ states with more copies chained together. The operation is a generalisation of entanglement swapping [24, 25] to multi-photonic systems [26] with more than two dimensions. In the graph it can be represented by two graphs that are merged.

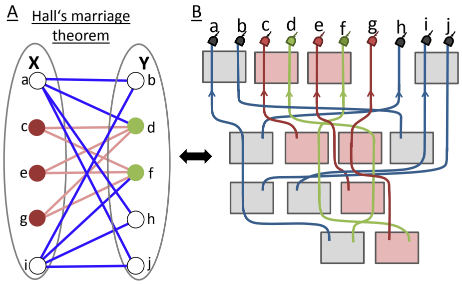

Figure 6. A theorem from Graph theory: Hall's marriage theorem **A**: For a bipartite graph with equal number of elements in X and Y, Hall's theorem gives a necessary and sufficient condition for the existence of a perfect matching. That happens when for every subset in $W \in X$, the number of neighbors 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) have only two neighbors in Y (d, f – indicated in green), thus there can not 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 can not be a 10-fold coincidence count.

Many other classes of entangled states, such as two-dimensional W-state [27, 28] or asymmetrically entangled Schmidt-Rank Vector (SRV) [29, 30] can be created by exploiting asymmetry in the experimental setups, as shown in Fig. 5A. Here, two crystals connect the photons in the same path. The corresponding graph has more then one edge between two vertices – a so-called multigraph (Fig. 5B).

An important result is that calculating the final quantum state can not be done efficiently: Counting the number of perfect matchings in a bipartite graph (i.e. calculating the number of terms in the resulting quantum state) is in the complexity class #P-complete, as it is equivalent to computing the permanent of the graph's biadjacency matrix [31] (see Appendix for such an experimental setup). Furthermore, for general graphs, counting the number of perfect matchings corresponds to calculating the *Hafnian* (a generalisation of the permanent) of the graph's adjacency matrix. Even for approximating the Hafnian there is no known deterministic algorithm which runs in polynomial time [32, 33].

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 *frustrated generation* of multiple qubits [8] (for instance, by using phase shifters instead of mode shifters between each crystal), or by analysing multi-photon high-dimensional entanglement detections [34]. A detailed investigation of the link between the outcome of such experiments and complexity classes would be valueable, but is outside the scope of this article.

Finally, to strenghen 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. 6A 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 [35]. A generalisation to general graphs, *Tutte's theorem* [36, 37], is shown in the Appendix. 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 analyse the emerging quantum states with methods from graph theory. The new link immediatly opens up many new directions for future research. For example, the analysation of the number of *maximal matchings* and *matchings* in a graph (called *Hosoya index* and often used in chemistry [38, 39]).

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 [40–42].

Furthermore it would be interesting how the merging of graphs (as done with a Bell-state measurement in Fig. 4A) can be generalized, and whether a combination with non-destructive measurements [43], can lead to larger classes of accessible states and how that can be described in the Graph theoretical framework. It would be interesting whether related techniques could be investigated in terms of Graph Theory as well, such as generating entanglement by propagation, detection and post selection [44], by using the indistinguishability [45–47] or by using linear optics [48].

The generation 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 [49, 50]) or 2-Factoriations (or general n-Factorizations, which would lead to n photons in one single arm).

We suggest that recent developments of integrated optics implementations of quantum experiments, where the photons are generated on a photonic chip [51–53], could be particularly useful to realize setups of the type proposed here.

ACKNOWLEGDEMENTS

The authors thank Manuel Erhard for useful discussions. X.G. thanks Lijun Chen for support. This work was supported by the Austrian Academy of Sciences (ÖAW), by the European Research Council (SIQS Grant No. 600645 EU-FP7-ICT) and the Austrian Science Fund (FWF) with SFB F40 (FOQUS). XG acknowlegdes support from the Major Program of National Natural Science Foundation of China (No. 11690030, 11690032), the National Natural Science Foundation of China (No.61272418).

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Supplemental Materials

APPENDIX I. ENTANGLEMENT OF 6 PHOTONS IN 5 DIMENSIONS - COMPLETE GRAPH K_6

An experiment with five layers and three crystals in each layer is shown in Fig. 7A. It corresponds to the complete graph K_6, which has one edge between each of its six vertices Fig. 7B. It has 15 perfect matchings, which are shown in Fig. 7C. For complete graphs K_{2n} with $2n$ vertices, the number of perfect matchings is $\#(PM) = \frac{(2n)!}{n!2^n}$.

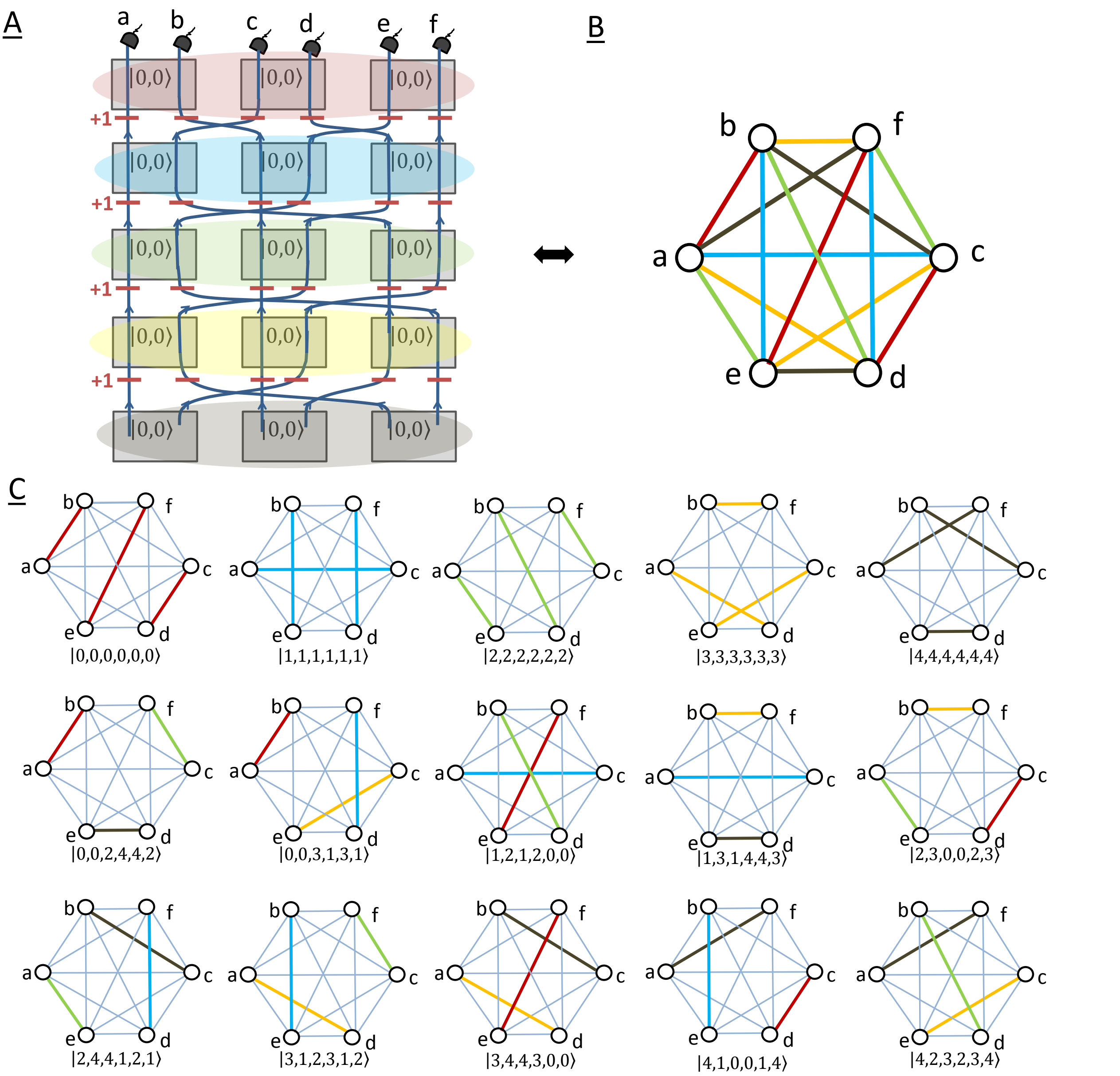

Figure 7. **A**: An experimental setup with five layers with three crystals each, which creates a 6-photon entangled state in five dimensions. **B**: It is represented by the complete graph K_6, and each of the five layers corresponds to one perfect matching (indicated by the edges with the same colors). **C**: A complete graph with six vertices has 15 perfect matchings. Five of them (first line) correspond to the five different layers which can be arbitrarily controlled in the experiment. The remaining ten perfect matchings (second and third line) correspond to combinations from different layers of crystals.

APPENDIX II. BIPARTITE GRAPHS

Counting the number of perfect matchings in a bipartite graph is in the complexity class #P-COMPLETE. In Fig. 8A, an experimental setup is shown which corresponds to the bipartite graph in Fig. 8B. The perfect matchings for this case can be found in Fig. 8C. They correspond to the number of terms in the resulting quantum state. The mode number of the different terms can be set for each crystal individually, thus one can simply see which states are possible.

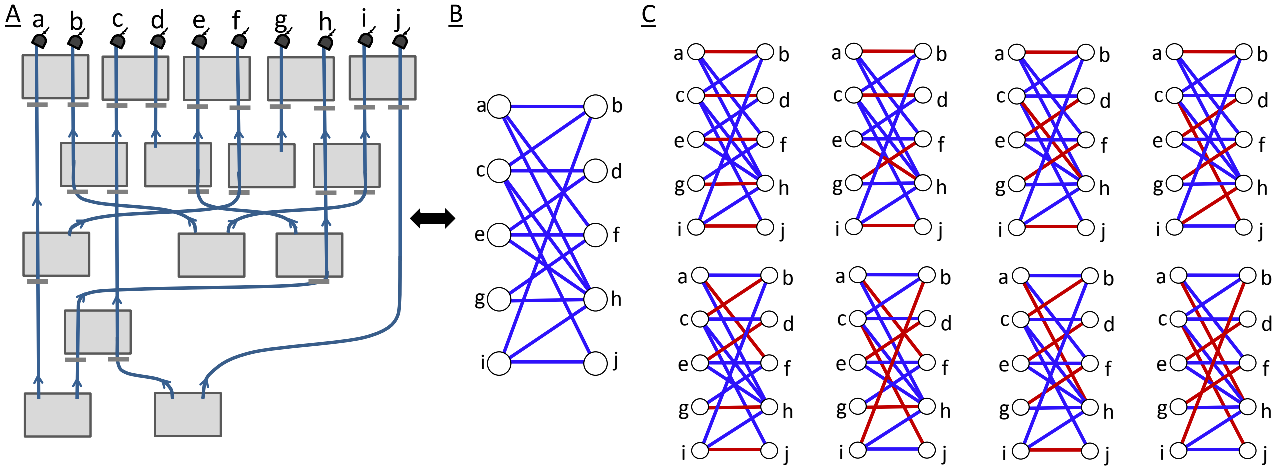

Figure 8. **A**: An optical setup which corresponds to a bipartite graph. It has ten paths and 15 crystals. **B**: The corresponding bipartite graph. The question how many terms the resulting quantum state will have is asking how many perfect matchings there are in the bipartite graph. **C**: In this example, there are eight perfect matchings, which are represented with red coloured edges.

APPENDIX III. PERFECT MATCHINGS IN GENERAL GRAPHS: TUTTE'S THEOREM

A different important result in Graph theory about perfect matchings is *Tutte's theorem*. It gives a necessary and sufficient condition for general graphs, when one can find perfect matchings (but not talking about how many). It is a generalisation of Hall's marriage theorem, which answers the same question for bipartite graphs. In Fig. 9A, the theorem is explained based on an example. That theorem can be understood with quantum experiments, as shown in Fig. 9B.

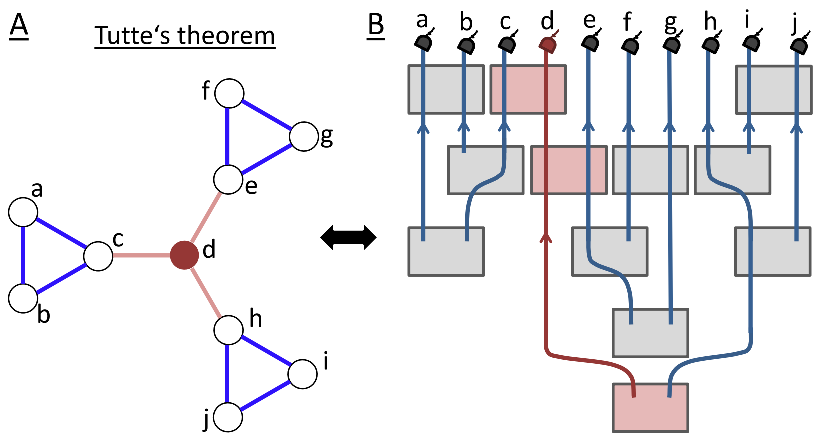

Figure 9. **A**: Tutte's theorem is a generalisation for arbitrary graphs. It says that in a graph $G(V, E)$ a perfect matching exists if and only if for every subset $U \in V$, the remaining subgraph $V - U$ has at most U connected components with an odd number of vertices. In the above example, if we chose $U = d$, the remaining subgraph has three connected components (abc, efg, hij), and each of them has an odd number of vertices. U has only one vertex, thus there is no perfect matching in this graph. **B**: The analog criterion for a general setup where each crystal produces indistinguishable photon pairs can be states as follows: For every combination of paths U, removing the paths and all connected crystals leads to several independent remaining setups S_r. Coincident counts can only occure if the number of S_r with odd numbers of paths is smaller than the number of paths in U. In the example, the subset $U = d$ does not fulfill the condition: By removing the path d and every connected crystal (depicted in red), S_r contains three independent subsetups (with paths abc, efg, hij), each of them have an odd number (three) of paths. It can be easily understood that subsetups with an odd number of crystals require one photon from the removed subset. If the number of subsetups, which require one photon, is larger than the number of paths removed, not every subsetup will receive a photon, thus there can not be an 2n-fold coincidence count.