Edge-coloured graphs with only monochromatic perfect matchings and their connection to quantum physics

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Abstract

Krenn, Gu, and Zeilinger initiated the study of PMValid edge-colourings because of their connection to a problem from quantum physics. A graph is defined to have a PMValid k-edge-colouring if it admits an edge colouring (not necessarily proper) with k colours, with the property that all perfect matchings are monochromatic and each of the k colour classes contains at least one perfect matching. The matching index of a graph G, $\mu(G)$, is defined as the maximum value of k for which G admits a PMValid k-edge-colouring. It is easy to see that $\mu(G) \geqslant 1$ if and only if G has a perfect matching (due to the trivial 1-edge-colouring, which is PMValid). Bogdanov observed that for all graphs non-isomorphic to K_4, $\mu(G) \leqslant 2$; $\mu(K_4) = 3$. However, the characterization of graphs for which $\mu(G) = 1$ and $\mu(G) = 2$ was not known. In this work, we answer this question. Using this characterization, we also give a fast algorithm to compute the value of $\mu(G)$ for a graph G. In view of our work, the structure of PMValid k-edge-colourable graphs is now fully understood for all k. Our characterization also has implications for the aforementioned quantum physics problem. In particular, it settles a conjecture of Krenn and Gu for a subclass of graphs.

Mathematics Subject Classifications: 05C70, 05C15, 05C75, 05C85, 81P40

1 Introduction

We will be considering only simple, finite, undirected, and loopless graphs. For a graph G, let $V(G)$ and $E(G)$ denote the set of vertices and edges, respectively. For $S \subseteq V(G)$, $G[S]$ denotes the induced subgraph of G on S. The cardinality of a set $\mathcal{S}$ is denoted by $|\mathcal{S}|$. For a positive integer r, $[r]$ denotes the set $\{1, 2, \ldots, r\}$. We refer to a cycle with n vertices as C_n and the complete graph with n vertices as K_n. The degree of a vertex v is denoted as $d(v)$. The minimum degree of G and the maximum degree of G are denoted as $\delta(G)$ and $\Delta(G)$, respectively.

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A graph is matching covered if every edge of it is part of at least one perfect matching. If an edge e is not part of any perfect matching M, then we call e to be *redundant*. By removing all redundant edges from the given graph G, we get its unique maximum matching covered subgraph $mcg(G)$. In an edge-colouring of G, each edge e is associated with a colour which is denoted using a natural number. We emphasise that this need not be a proper edge-colouring. If exactly k colours are used in an edge-colouring, we call it a k-edge-colouring. G_c represents an edge-coloured graph formed by a k-edge-colouring c over graph G.

Definition 1 (PMValid)**.** On a graph G, a k-edge-colouring c is said to be *PMValid* if:

- All perfect matchings are monochromatic
- Each of the k colour classes contains at least one perfect matching

In other words, the k-edge colouring c is PMValid if in its restriction to the edges of $mcg(G)$, all the k colours appear in some edge of $mcg(G)$ and for each edge e, all the perfect matchings containing e are monochromatic with colour $c(e)$.

The study of PMValid edge-colourings was initiated by Krenn, Gu, and Zeilinger because of its connection to a problem from quantum physics [14].

Definition 2 (Matching index)**.** Given a graph G, its *matching index* $\mu(G)$ is defined as the maximum value of k for which G admits a PMValid k-edge-colouring.

If c is a PMValid k-edge-colouring on G, we say that G_c is *perfectly monochromatic* and $\mu(G, c) = k$. More generally, when all perfect matchings of an edge-coloured graph G_c are monochromatic, let $\mu(G, c)$ denote the number of colours whose colour class contains a perfect matching; if G_c has no perfect matching, set $\mu(G, c) = 0$. If some perfect matching of G_c is not monochromatic, we leave $\mu(G, c)$ undefined. Then $\mu(G)$ is the maximum value of $\mu(G, c)$ over all edge-colourings c for which $\mu(G, c)$ is defined. It is easy to see that $\mu(G) = \mu(mcg(G))$.

Question 3. For each $i \in \mathbb{N}$, can one characterize all graphs for which $\mu(G) = i$?

Bogdanov observed the following [2, 14]:

Theorem 4. *For a graph G which is non-isomorphic to K_4, $\mu(G) \leqslant 2$; $\mu(K_4) = 3$.*

We note that a weaker statement, namely $\mu(G) \leqslant 3$ for all graphs, follows from a result of Thomason [22] on uniquely (proper) edge colourable graphs. A graph is said to be uniquely proper k-edge colourable if it has exactly one proper edge colouring using exactly k colours up to the permutation of the colours. For example, consider the star graph $K_{1,k}$. It is uniquely proper k-edge-colourable, since any proper k-edge-colouring of $K_{1,k}$ must assign different colours to different edges; hence there is only one such colouring up to permutation of colours. Thomason proved [22] that, for $k \geqslant 4$, $K_{1,k}$ is the only uniquely proper k-edge-colourable graph.

Now, to show that $\mu(G) \leqslant 3$, suppose that there is a graph with $\mu(G) = k > 3$. Then, for some $k \geqslant 4$, there exists a graph G with a PMValid k-edge-colouring c. Consider the k-regular subgraph G' of G_c formed by taking the union of one perfect matching from each of the k colour classes. It is easy to see that the colouring induced by c on G' is also PMValid; in other words, G'_c has exactly k perfect matchings, and all of them are monochromatic. Clearly, c is indeed a proper k-edge colouring of G'. It is not difficult to see that there cannot be any other proper k-edge colouring for G', other than the ones obtainable by permutation of colours from c. From the result of Thomason, [22], such a graph G' must be isomorphic to $K_{1,k}$. But $K_{1,k}$ does not even have a perfect matching, which is a contradiction.

It is easy to see that if G has at least one perfect matching, a trivial 1-edge-colouring on G is PMValid. Hence $\mu(G) = 0$ if and only if G does not have a perfect matching. This implies that for every graph G, which is non-isomorphic to K_4 and has a perfect matching, $\mu(G)$ is 1 or 2 (from Theorem 4). However, the characterization of the graphs based on whether their matching index is 1 or 2 remained unknown.

1.1 Our results

Our main result is such a characterization of graphs based on the value of their matching index being 1 or 2 in Theorem 6. This, in turn, gives a complete characterization of all graphs based on the value of their matching index. We now develop some notation which is useful for stating our result.

Let G be a Hamiltonian graph of even order. Consider any Hamiltonian cycle C and label its vertices $0, 1, 2, 3, \ldots 2n-1$ in a clockwise direction along C. We interchangeably refer to vertex $i \mod 2n$ as i. The vertices $\{1, 3, \ldots, 2n-1\}$ are referred to as *odd vertices* with respect to C and the vertices $\{0, 2, \ldots, 2n-2\}$ are referred to as *even vertices* with respect to C. The edges of the Hamiltonian cycle C are defined to be C-edges. The edges between two vertices of the same parity are defined to be *legal* edges with respect to C. Every edge $e = \{i, j\}$ partitions the remaining vertices of graph into two parts $\mathcal{P}(e) = \{i+1, i+2, \ldots j-1\}$ and $\mathcal{P}'(e) = \{j+1, j+2 \ldots, i-1\}$ with respect to C. If an edge e' has one endpoint in $\mathcal{P}(e)$ and the other endpoint in $\mathcal{P}'(e)$, then e' and e are said to be *crossing* each other with respect to C and the pair of edges e, e' is referred to as a *crossing* pair with respect to C.

Let the legal edges (with respect to C) $e = \{2i_1+1, 2i_2+1\}$ and $e' = \{2j_1, 2j_2\}$ cross each other (with respect to C) and, without loss of generality, assume that the vertices $2i_1+1, 2j_1, 2i_2+1, 2j_2$ appear clockwise on C. We say that e, e' form a *drum* with respect to C if $e' = \{2j_1, 2j_2\} = \{2i_2, 2i_1\}$ or $e' = \{2j_1, 2j_2\} = \{2i_1+2, 2i_2+2\}$. In other words, an end vertex of e and an end vertex of e' must be adjacent on the cycle (that is, there should be a C-edge between them) and the remaining end vertices of e, e' must also be adjacent on the cycle C.

Definition 5. $\mathcal{H}$ is defined to be the family of even-order matching-covered Hamiltonian graphs with at least 6 vertices such that all graphs $G \in \mathcal{H}$ satisfy the following: There *exists* a Hamiltonian cycle C of G such that Properties 1, 2 and 3 are satisfied with respect to the vertex labelling obtained from a clockwise cyclic ordering of C.

Property 1. *All edges of G are C-edges or legal edges with respect to C.*

Property 2. *Every crossing pair (with respect to C) of G forms a drum with respect to C.*

Property 3. *Each legal edge (with respect to C) of G is part of exactly one drum with respect to C.*

An example graph G is shown in Figure 1, which satisfies Properties 1, 2 and 3 with respect to the cyclic orderings along two different Hamiltonian cycles. As the properties are satisfied with respect to at least one cycle, $G \in \mathcal{H}$. This special class of graphs also happens to be equivalent to the set of matching covered graphs with a matching index of 2.

Theorem 6. *For any graph H with $|V(H)| > 4$, $\mu(H) = 2$ if and only if $mcg(H) \in \mathcal{H}$.*

We prove Theorem 6 in Section 3. We also give a fast algorithm that runs in time $O(|V(G)||E(G)|)$ to find the matching index of a graph in Section 4. The bottleneck of our runtime is the subroutine of finding the matching covered graph of G. Our characterization has some interesting applications to a conjecture from quantum physics. We present them in Subsection 2.3.

2 Quantum Physics Background

The graph-theoretic problem discussed in this paper is strongly motivated by an earlier work [14], the authors of which are prominent quantum physicists, one of whom is a Nobel laureate in Physics in 2022. In this section we present the connection between this problem and quantum physics in an over-simplified way so that even graph theorists who are not familiar with quantum physics may be able to understand the connection just enough to work on the problem.

2.1 Motivation

Quantum entanglement theory implies that two particles can influence each other even though they are separated over large distances. In 1964, Bell demonstrated that quantum mechanics conflicts with our classical understanding of the world [1]. Later, in 1989, Greenberger, Horne, and Zeilinger (abbreviated GHZ) studied what can happen if more than two particles are entangled [6]. Such states in which three particles are entangled ($|GHZ_{3,2}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$) were observed, rejecting local-realistic theories [3, 18].

Although the study of such states began purely out of fundamental curiosity [21, 15, 16], they are now used in many applications in quantum information theory, such as quantum computing [9]. They are also essential for early tests of quantum computing tasks

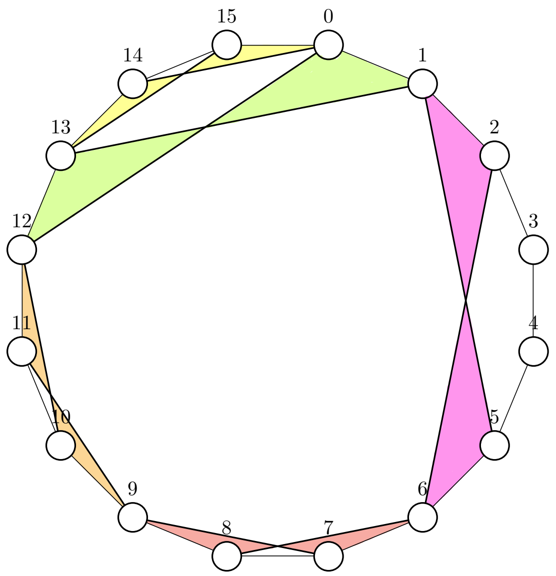


Figure 1: A graph G satisfying Properties 1, 2 and 3 with respect to the cyclic orderings of two different Hamiltonian cycles. Note that in the figure on left, the ordering is with respect to the Hamiltonian cycle C_1 and the edge $e = \{1, 5\}$ is a legal edge with respect to G, C_1. In the figure on right, the ordering is with respect to the Hamiltonian cycle C_2 and the same edge e is now labelled $\{1, 2\}$. Note that e is a C_2-edge and not a legal edge with respect to G, C_2. Each drum is shaded with a different colour.

[24] and for quantum cryptography in quantum networks [19]. Increasing the number of particles involved and the dimension of the GHZ state is essential both for foundational studies and for practical applications. Motivated by this, several experimental groups around the world are putting in a huge effort to push the size of GHZ states. Photonic technology is one of the key technologies used to achieve this goal [24, 23].

Recall that an edge colouring of a graph G is the assignment of some colour to each edge of G. It is possible to visualize G by drawing it in the 2-dimensional plane, such that each vertex u is represented by a point (also denoted by u for convenience) and each edge (u, v) is represented by a line segment between the points u and v. With this visualization in mind, each edge can be seen as composed of two half-edges, namely the half-edge starting from the point u to the centre of the line segment (hereafter referred to as the u-half-edge of (u, v)) and the half-edge starting from point v to the centre of the line segment (referred to as the v-half-edge). The notion of edge colouring can be extended to the notion of half-edge colouring: a half-edge colouring of G assigns some colour to each half-edge of G (as shown in Figure 3). Note that in a half-edge colouring, edge (u, v) may get bi-coloured, with the u-half-edge getting one colour and the v-half-edge getting another colour. If both the u-half-edge and the v-half-edge get the same colour, then we say that the edge (u, v) is monochromatic; otherwise it is bichromatic. If all edges of G are monochromatic with respect to a half-edge colouring c, then c can be considered as an edge colouring of G for the purpose of this paper.

In 2017, using the notion of half-edge colouring, Krenn, Gu, and Zeilinger [14] discovered a bridge between experimental quantum optics and graph theory, which they later extended [8, 7]. They observed that large classes of quantum optics experiments (including those containing probabilistic photon pair sources, deterministic photon sources, and linear optics elements) can be represented as half-edge coloured multi-graphs when there is *no destructive interference*. Conversely, every half-edge coloured multi-graph can be translated into a concrete experimental setup. When there is destructive interference, to capture the experiments, it is required to associate a complex-valued weight to each edge of the graph, in addition to the colours. We note that while there are some experiments for constructing GHZ states that do not fall into this category, these half-edge-coloured graphs capture many prominent ones.

Remark 7. Though we use the concept of half-edge colouring to present the connection between quantum optics experiments and graphs, by the end of the next subsection it will be clear to the reader why only PMValid edge colourings need to be studied in the case where there is no destructive interference.

2.2 Connection to Graph Theory

We will now present a very high-level overview of the relationship between half-edge coloured graphs and quantum photonic experiments. We warn the reader that the way we have written this description may deviate from the physicist's view of the experiment. To make it accessible to graph theorists with no background in quantum physics, we have abstracted out the main features that are required to understand and solve this problem. For accurate technical details of this framework, we refer the reader to [14].

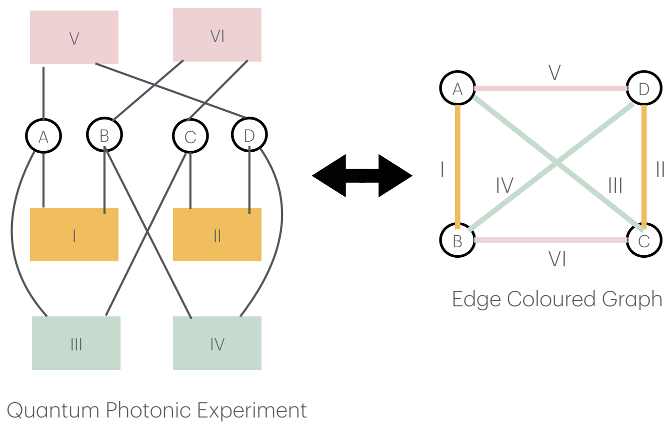


Figure 2: A quantum photonic experiment and the corresponding edge-coloured graph.

We will first see how an experiment $\mathcal{E}$ corresponds to the half-edge coloured graph G_c. Several crystals are positioned in the optical setup, and each of them is intersected by laser beams. Also, several photon detectors are positioned. Photon detectors will be interpreted as vertices and crystals will be interpreted as the edges of the corresponding

Quantum experiment	Graph theory
Optical setup with crystals $\mathcal{E}$	G_c
Crystals	Edges
Photon detectors	Vertices
Mode number	Colour
Multi-photonic configuration	Perfect matching
GHZ state	PMValid G_c
k-dimensional GHZ state	$\mu(G, c) = k$
n-particle GHZ state	$\lvert V(G)\rvert = n$

Table 1: Quantum photonic experiments and graph theory.

graphs, as we will explain shortly. When the laser passes through a crystal, it generates an entangled photon pair. Each photon in the pair is associated with a mode number which could represent different degrees of freedom. Graph theorists may imagine that the mode number of the photon is a colour associated with the photon. The experiment designer can lead each of these photons into a prearranged optical path. Note that which photon should take which path can be prearranged. These photons travel along their optical paths towards a photon detector. We emphasize that the two photons of the entangled pair created in the same crystal enter two different optical paths and reach two different photon detectors. Graph theorists may imagine that the crystal is positioned at the centre of the line segment that corresponds to an edge (with respect to a 2-dimensional drawing of the graph as described earlier) and the photons of the entangled pair generated in the crystal, travel along the two half-edges to two different vertices, which are the end points of that edge. The colour of the photon that travels along a half-edge is the same as the colour of the half-edge. In other words, an x-coloured half-edge of an edge corresponds to the optical path along which the x-coloured photon generated in the crystal that corresponds to this particular edge moves along. For example, in Figure 2, the photons generated in the crystal VI have optical paths leading to the photon detectors B, C. So, one can associate the edge, say VI, with the pair of vertices B and C, in the corresponding graph.

Note that many optical paths from different crystals may reach the same photon detector: In other words, in our graph multiple edges may be incident on the same vertex. However, each photon detector is only capable of detecting one photon at a time. Because the photons are generated as entangled pairs, they are always detected in pairs. In other words, if the photon that moved from crystal VI towards the photon detector B, got detected by the photon detector B, then the other photon of the pair which moved towards the photon detector C, would also get detected by C. This may sound weird to the uninitiated, but it is a consequence of the quantum phenomenon of entanglement. Thus, one can think of the detection event as capturing several entangled photon pairs rather than individual photons. A multiphotonic configuration is an event in which all photon detectors detect a photon. This can be seen as pairs of entangled photons (which in turn correspond to the crystals that created the pairs and thus to the corresponding set of edges) covering all photon detectors (vertices) exactly once. For graph theorists, what gets detected is precisely a perfect matching.

Note that the output of the experiment is obtained by measuring the mode numbers of the photons detected in each photon detector. Graph theorists can imagine that when a photon is detected by a photon detector (vertex) that photon (or equivalently the corresponding half-edge) imparts its colour to the vertex. When a perfect matching gets detected, the output is a vertex colouring, where the colour of vertex u equals the colour of the u-half-edge of the edge in the perfect matching that covers u. (Note that the vertex colouring here need not be proper.)

A multiphotonic configuration is considered pure if all the detectors register photons with the same mode number (i.e., if the detected perfect matching is monochromatic). If different mode numbers are detected across the detectors, the configuration is impure (i.e., the perfect matching is non-monochromatic). For creating GHZ states, it is essential to ensure that only pure configurations are generated. What does a GHZ state mean to the graph theorist? Recall that a vertex colouring is monochromatic if all the vertices are assigned the same colour. It is non-monochromatic if there are at least two vertices, say u and v, such that colour$(u) \neq$ colour(v). For the experiment to produce a GHZ state, the vertex colourings that appear as output with non-zero "probability" should be always monochromatic. In other words, a non-monochromatic vertex colouring should never appear as output. When we consider the case where destructive interference is not playing any role, i.e., when we are restricting ourselves to unweighted half-edge coloured graphs as experiments as described earlier, to guarantee that no non-monochromatic vertex colouring can appear as output, we have to make sure that there are no non-monochromatic perfect matchings in the graph. Note that in a monochromatic perfect matching, all the edges have the same colour. In a non-monochromatic perfect matching either there are two edges e_1 and e_2 such that $colour(e_1) \neq colour(e_2)$ or it contains a bichromatic edge.

If k pure configurations are generated (that is, if there are k colours such that monochromatic vertex colourings of these colours can appear with non-zero "probability" in the output) then the GHZ state would have dimension k. Moreover, if n photon detectors are used, then we get an n-particle GHZ state. It follows that the number of particles involved equals the number of vertices of the graph. Clearly the dimension refers to the number of different monochromatic vertex colourings that can materialise as output, which in the 'no destructive interference' case translates to the number of colours such that there exists a monochromatic perfect matching for each of those colours.

It is easy to see that to define an experiment that produces a GHZ state, in the absence of destructive interference, we need only to consider graphs with monochromatic edges; any crystal that produces a "bi-chromatic" entangled pair can be removed, since they cannot be part of any perfect matching. This means that when studying this case, we can restrict our attention to edge colourings, rather than half-edge colourings. Some careful thought would convince the reader that we can even assume that there are no multi-edges when studying the "no destructive interference" case, since, if there exists a multi-graph without any non-monochromatic perfect matching and having at least one monochromatic perfect matching for exactly k colours, then there exists a simple graph also having the same properties. In brief, as promised in the earlier subsection, the "no destructive interference" case can be understood purely using the concept of PMValid k-edge-colourings in simple graphs, as we do it in this paper. More precisely, one can now see that Question 8 is equivalent to Question 3.

Question 8. Can one characterize experiments (under the conditions described in [14]) which would lead to $|GHZ_{n,k}\rangle$, a k-dimensional n-particle GHZ state?

On the other hand, half-edge colourings and multiple edges between two vertices can play a role if destructive interference is allowed, unless the experiment designer decides to remove the crystals leading to bichromatic edges or multiple edges between two vertices. To understand the case where destructive interference is allowed, we first need to understand the concept of weights. A complex number is associated with each edge; this is the weight $w(e)$ of that edge.

Now, the weight of a perfect matching M is defined to be $w(M) = \prod_{e \in M} w(e)$. The weight $w(M)$ is related to the "probability" of the event that the perfect matching M gets detected. For our purpose, we will describe this weight as the "probability" itself, though we should warn the reader that it is not probability in the usual sense; in particular, $w(M)$ is a complex number and not necessarily a real number in $[0, 1]$. If three different perfect matchings M_1, M_2 and M_3 induce a vertex colouring c (and there are no other perfect matchings that induce c), then the "probability" that the vertex colouring c appears in the output equals $w(M_1) + w(M_2) + w(M_3)$.

In view of the above discussion, note that when destructive interference is allowed, to guarantee that in the output no non-monochromatic vertex colouring appears, it is not necessary to make sure that there are no non-monochromatic perfect matchings in the graph that describes the experiment. It is sufficient to ensure that the weight of all non-monochromatic vertex colourings is 0. The dimension is the number of monochromatic vertex colourings whose weights are non-zero. The problem, as originally formulated, requires that the weight of each of these monochromatic vertex colourings be exactly 1, but it is shown in [4] that it is sufficient to assume that they are non-zero, since it is easy to normalize the edge weights so that each non-zero weight of a vertex colouring is translated to exactly 1. We explain the weighted version formally in Section 5.

2.3 Application

Though we are mainly studying the "no destructive interference case" in this paper, our characterization has some interesting implications for the more general edge-weighted version of this problem described in the previous subsection that we discuss in Section 5.

We show how to use our characterization to resolve the Krenn-Gu conjecture (Conjecture 33) for the class of graphs $\mathcal{H}$ (recall Definition 5). That is, if G is a graph such that in the unweighted case the matching index is 2, then even by allowing complex weights on the edges or by replacing the edge colouring by an arbitrary half-edge colouring (details in previous section and in Section 5), the dimension cannot become higher than 2. This fact is formally stated in Theorem 34 in Section 5. The consequence of our characterization towards the Krenn-Gu conjecture was recognized by quantum physicists by awarding the quantum-graph best paper award to a preliminary version of this work [12].

Remark 9. For readers who are more familiar with the language of quantum physics, we refer them to the earlier works [14, 8, 7, 13] for more details on the translation of quantum photonic experiments to the edge-weighted version. We deal with the graph-theoretic question posed by quantum physicists as it is.

3 Proof of Theorem 6

3.1 Preliminaries

Throughout this section, we assume that the graph G is not isomorphic to K_4. We first prove some simple structural properties of an edge-coloured graph G_c based on its $\mu(G, c)$ value.

If an even cycle contains disjoint monochromatic perfect matchings of different colours, we call it a cycle with alternating colours. We now present a simple theorem about edge-coloured graphs.

Theorem 10. *For an unweighted edge-coloured graph G_c, where G is the underlying graph that is not isomorphic to K_4 and c is the colouring, the statements* 1 *through* 4 *are true about the following conditions.*

Condition 1. *G_c is perfectly monochromatic.*

Condition 2. *G_c has a perfect matching.*

Condition 3. *G_c has a Hamiltonian cycle with alternating colours.*

1. *$\mu(G, c)$ is not defined if and only if Condition 1 is false.*

2. *$\mu(G, c) = 0$ if and only if Condition 1 is true and Condition 2 is false.*

3. *$\mu(G, c) = 1$ if and only if Conditions 1 and 2 are true and Condition 3 is false.*

4. *$\mu(G, c) = 2$ if and only if Conditions 1, 2 and 3 are true.*

Proof. Statement 1 is true by definition. It is also easy to see that Condition 3 implies Condition 2. Therefore, when Statement 2 is true, it follows that Condition 3 is also false, along with Condition 2.

If Condition 1 is true and Condition 2 is false, as there are no perfect matchings, $\mu(G, c) = 0$. If $\mu(G, c) = 0$, G_c must be perfectly monochromatic by Statement 1. Therefore, if there is a perfect matching it must be monochromatic. But that would imply $\mu(G, c) \geqslant 1$. Therefore, there is no perfect matching in G_c. Therefore, statement 2 is true.

We prove that if Conditions 1 and 2 are true and Condition 3 is false, then $\mu(G, c) = 1$. If Condition 1 and Condition 2 are true then $\mu(G, c) \geqslant 1$ by statement 1 and statement 2.

Towards a contradiction, let $\mu(G,c) \neq 1$. It follows that $\mu(G,c) \geqslant 2$. Therefore, there are at least two colours, say red and blue, with a monochromatic perfect matching. Consider the union of a red perfect matching and a blue perfect matching. It must be a disjoint union of even cycle(s) with alternating colours. Clearly, each cycle can be decomposed into two perfect matchings of different colours. If it is a disjoint union of at least two cycles, then by selecting the red perfect matching from one cycle and blue perfect matchings from the remaining cycles, we can construct a non-monochromatic perfect matching. This contradicts the assumption that Condition 1 is true. Therefore, the union of a red and a blue perfect matching is a Hamiltonian cycle with edges of alternating colours. But Condition 3 is false by assumption, a contradiction.

If Conditions 1, 2 and 3 are true, since there are two monochromatic perfect matchings of different colours which can be formed by selecting the edges of the same colour from the Hamiltonian cycle with alternating colours, $\mu(G,c) \geqslant 2$. As Condition 1 is true, we know that $\mu(G,c) \leqslant 2$ by Theorem 4. Therefore, $\mu(G,c) = 2$.

If $\mu(G,c) = 1$, then it is easy to see that Conditions 1 and 2 are true. Condition 3 must be false, because if it is true, that would imply $\mu(G,c) = 2$, as proved above. Similarly, if $\mu(G,c) = 2$, then it is easy to see that Conditions 1 and 2 are true. Condition 3 must be true, because if it is false, that would imply $\mu(G,c) = 1$, as proved above. $\square$

3.2 Definitions

For a graph G of even order and with a Hamiltonian cycle C, we define some more notation with respect to G and C. Let the vertices be $0, 1, 2, 3, \ldots, 2n-1$ in a clockwise direction along the cycle C. We interchangeably refer to vertex $i \mod 2n$ as i. An odd-even edge is called *illegal* if it is not a C-edge. Recall that odd-odd edges and even-even edges are called *legal* edges. It is easy to see that the edges of the graph can be classified into legal edges, illegal edges, and C-edges.

Recall that every edge $e = \{i,j\}$ partitions the remaining vertices of the cycle into two parts $\mathcal{P}(e) = \{i+1, i+2, \ldots j-1\}$ and $\mathcal{P}'(e) = \{j+1, j+2 \ldots, i-1\}$. The partition weight of e is defined as equal to $\min\{|\mathcal{P}(e)|, |\mathcal{P}'(e)|\}$. Note that both $|\mathcal{P}(e)|, |\mathcal{P}'(e)|$ are odd (even) for legal (illegal) edges. If $|i-j|$ is odd, we define $\mathbf{M}_{i,j} = \{\{i, i+1\}, \{i+2, i+3\} \ldots, \{j-1, j\}\}$, a perfect matching formed by the alternate C-edges clockwise from i to j.

Recall that if an edge e' has one endpoint in $\mathcal{P}(e)$ and the other endpoint in $\mathcal{P}'(e)$, then e' and e are said to be crossing each other. We say that a pair of crossing edges form a *legal crossing pair* if both edges are legal. We say that a legal crossing pair is a *nice* crossing pair if one of the edges is odd-odd and the other edge is even-even.

Recall that a drum D, say with vertices $2i_1+1, 2i_1+2, 2i_2+1, 2i_2+2$ partitions the remaining vertices of the cycle into two parts, $\mathcal{P}(D) = \{2i_2+3, 2i_2+4, \ldots 2i_1\}$ and $\mathcal{P}'(D) = \{2i_1+3, 2i_1+4 \ldots 2i_2\}$. It follows that $|\mathcal{P}(D)|, |\mathcal{P}'(D)|$ are even for a drum by the definition. We refer to the paths along C from $2i_2+2$ to $2i_1+1$ through $\mathcal{P}(D)$ and from $2i_1+2$ to $2i_2+1$ through $\mathcal{P}'(D)$ as straps of the drum. The length of a strap is the number of edges on the path. We refer to $\min\{|\mathcal{P}(D)|, |\mathcal{P}'(D)|\}$ as the partition weight of the drum D. Note that a drum is a 4-cycle with 2 C-edges forming a pair of opposite edges and a nice crossing pair forming the remaining two opposite edges.

It is important to note that even though there might be structures similar to drums formed by two illegal crossing edges, which partition the cycle into two odd parts, we *do not* refer to them as drums. Only nice crossing pairs can form drums. It follows that if we colour the edges of the Hamiltonian cycle with alternating colours, both the C-edges of a drum will get the same colour. We make a few observations regarding the Hamiltonian cycles of G in Subsection 3.3.

Remark 11. We emphasize that legal edges, illegal edges, C-edges, crossing pairs and drums are defined with respect to a graph and a vertex labelling along the clockwise direction of a Hamiltonian cycle C. For example, for a graph G, the legal edges with respect to C might not be legal edges with respect to a different Hamiltonian cycle C'. See Figure 1.

3.3 Observations

We refer to a Hamiltonian cycle with alternating red-blue edges as a red-blue alternating Hamiltonian cycle C. For graphs with such a Hamiltonian cycle C, whose vertices are labelled in clockwise cyclic order along C, we use the colouring convention that the edges of C of the form $\{2i-1, 2i\}$ are red and the edges of the form $\{2i, 2i+1\}$ are blue. We call a drum in G_c monochromatic if all 4 edges of the drum have the same colour.

Condition 4. *G is a matching covered graph with a colouring c for which $\mu(G,c) = 2$ and $|V(G)| = 2n \geqslant 6$. From Theorem 10, it has at least one red-blue alternating Hamiltonian cycle, say C. Label the vertices in clockwise cyclic order with respect to C so that colouring convention is satisfied.*

We now make some observations about unweighted edge-coloured graphs that satisfy Condition 4, which we will later use to prove the structural characterization of graphs where $\mu(G) = 2$.

Remark 12. Note that all the observations made below for G_c are with respect to a vertex labelling along the clockwise cyclic ordering of red-blue alternating Hamiltonian cycle C from Condition 4. For instance, in Observation 13, we only claim that there are no illegal edges with respect to a cyclic ordering along C.

Observation 13. *If Condition 4 is true, G_c has no illegal edges.*

Proof. Towards a contradiction, let there be an illegal edge. Let it be $\{1, 2j\}$ for some $j \in [2, n-1]$, without loss of generality. Consider the perfect matching

$$M = \{\{1, 2j\}\} \bigcup \mathbf{M}_{2,2j-1} \bigcup \mathbf{M}_{2j+1,0},$$

see Subsection 3.2 for the notation. As an illegal edge cannot be a C-edge, both $\mathbf{M}_{2,2j-1}$ and $\mathbf{M}_{2j+1,0}$ are non-empty. Observe that every edge of $\mathbf{M}_{2,2j-1}$ is blue and every edge of $\mathbf{M}_{2j+1,0}$ is red by the colouring convention of C. Thus M is a non-monochromatic perfect matching, contradicting that G_c is perfectly monochromatic. □

Observation 14. *If Condition 4 is true, all nice crossing pairs of G_c must form monochromatic drums.*

Proof. First, we prove that all nice crossing pairs form a drum. Towards a contradiction, let there be a nice crossing pair $\{2i_1+1, 2i_2+1\}$ and $\{2j_1, 2j_2\}$ that do not form a drum. Without loss of generality, we assume that $2i_1+1, 2j_1, 2i_2+1, 2j_2$ are in a clockwise direction on the cycle C. There is a perfect matching

$$\mathbf{M} = \{\{2i_1+1, 2i_2+1\}, \{2j_1, 2j_2\}\} \bigcup \mathbf{M}_{2i_1+2,2j_1-1} \bigcup \mathbf{M}_{2j_1+1,2i_2} \bigcup \mathbf{M}_{2i_2+2,2j_2-1} \bigcup \mathbf{M}_{2j_2+1,2i_1}$$

We see that $\mathbf{M}_{2j_2+1,2i_1} \bigcup \mathbf{M}_{2j_1+1,2i_2}$ is contained in the red colour class and $\mathbf{M}_{2i_1+2,2j_1-1} \bigcup \mathbf{M}_{2i_2+2,2j_2-1}$ is contained in the blue colour class by the colouring convention of C. If either of these two is empty, the crossing pair forms a drum. Therefore, both are non-empty and $\mathbf{M}$ is a non-monochromatic perfect matching.

Now we show that every drum is monochromatic. Towards a contradiction, let there be a non-monochromatic drum. Recall (see the definition of a drum) that non-adjacent C-edges e_1, e_2 of a drum are of the same colour, say red. Therefore, e_1, e_2 are part of the red perfect matching M formed by all red edges of C. Let the crossing pair of the drum be e_3, e_4. Consider the perfect matching $M' = M - \{e_1, e_2\} \bigcup \{e_3, e_4\}$. Since G has at least 6 vertices, $M - \{e_1, e_2\}$ has at least one edge of the red colour. As it is a non-monochromatic drum, at least one of e_3, e_4 must be blue. Therefore, M' is a non-monochromatic perfect matching. But all perfect matchings of G_c are monochromatic as G_c is perfectly monochromatic. This is a contradiction. Therefore, all nice crossing pairs must form monochromatic drums. ☐

Observation 15. *If Condition 4 is true, every legal edge of G_c is contained in exactly one drum.*

Proof. Let the legal edge be $e = \{1, 2j+1\}$ and of colour red, without loss of generality. Recall that e can only be part of the drums with non-adjacent cycle edges $\{1, 2\}, \{2j+1, 2j+2\}$ or $\{0, 1\}, \{2j, 2j+1\}$ by definition. We claim that the latter possibility can be ruled out. This is because e cannot form a drum with the legal edge $e' = \{0, 2j\}$, since $\{e, e'\}$ would form a nice crossing pair and the drum formed by $\{e, e'\}$ would have to be monochromatic by Observation 14. However, $\{0, 1\}$ and $\{2j, 2j+1\}$, which would form the C-edges of that drum, are blue by the colouring convention of C. Therefore, e can be part of at most one drum. A similar argument holds even if e was of the colour blue or e was an even-even edge.

We define a legal edge e_1 to be saturated if, for every perfect matching M containing e_1, there exists another legal edge $e_2 \in M$ forming a drum with e_1. We now claim that all legal edges are saturated. Suppose not. Without loss of generality, let $e = (1, 2j+1)$ have the minimum partition weight among all the legal edges that are not saturated. Let $[2, 2j]$ be the smaller among $\mathcal{P}(e)$ and $\mathcal{P}'(e)$, without loss of generality. Let M be the perfect matching which makes e not saturated, i.e. there is no edge e' in M, which forms a drum with e. By assumption on minimality of e, all the edges part of M with both its vertices in $[2, 2j]$ would be C-edges and the pairs of non-C-edges of drums. It is easy to see that a pair of non-C-edges of drums match the same number of odd vertices and even vertices, and a C-edge also matches the same number of odd vertices and even vertices. Therefore, all the edges part of M with both its vertices in $[2, 2j]$ match the same number of odd vertices and even vertices in $[2, 2j]$. However, since there are j even vertices and $j-1$ odd vertices in $[2, 2j]$, an even vertex in $[2, 2j]$ must match with a vertex in $[2j+2, 0]$. Such a vertex in $[2j+2, 0]$ must also be even since illegal edges are absent by Observation 13. It follows that this even-even edge crosses e, and since e is an odd-odd edge, they form a nice crossing pair. Therefore, they must form a drum from Observation 14 and hence e is saturated. Contradiction.

Since the graph is matching covered, we know that every legal edge is part of at least one perfect matching. As every legal edge is saturated, it follows that every legal edge is also part of a drum. □

Observation 16. *If Condition 4 is true, each C-edge of G_c can be part of at most one drum.*

Proof. Let a C-edge e be part of two drums, say D_1, D_2 towards a contradiction. From Observation 15, the legal edges in both drums must be disjoint. Let them be e_1, e_1' in drum D_1 and e_2, e_2' in drum D_2. Let e_1, e_2 be the edges incident on even end point of e and e_1', e_2' be the edges incident on the odd end point of e. Observe that one of $\{e_1, e_2'\}$ and $\{e_1', e_2\}$ cross each other. It follows that they form a nice crossing pair and hence form a drum $D_3 \notin \{D_1, D_2\}$ by Observation 14. However, a legal edge can be part of only one drum by Observation 15. Contradiction. □

Observation 17. *If Condition 4 is true, all legal crossing pairs of G_c are nice.*

Proof. Towards a contradiction, let there be a legal crossing pair e, e', which is not nice. Without loss of generality, let both of them be odd-odd edges. From Observation 15, e must form a drum D with an even-even edge, say e''. As e, e' cross, they cannot be incident on the same vertex. As e' is odd-odd and e'' is even-even, they cannot be incident on the same vertex. Therefore, e' should be incident on a vertex from $\mathcal{P}(D)$ and a vertex from $\mathcal{P}'(D)$. Therefore, e', e'' cross each other. As they are a nice crossing pair, from Observation 14, they must form a drum. Therefore, e'' is part of two drums. But from Observation 15, e'' is part of exactly one drum. Contradiction. □

Observation 18. *If Condition 4 is true, all crossing pairs of G_c form monochromatic drums.*

Proof. All crossing pairs are legal since there are no illegal edges by Observation 13. All legal crossing pairs are nice from Observation 17. All nice crossing pairs form monochromatic drums from Observation 14. Therefore, all crossing pairs form monochromatic drums. □

Observation 19. *If Condition 4 is true, every vertex v of G_c can have at most two red edges and at most two blue edges incident on it. Moreover, if the vertex has two red(blue) edges incident on it, both of those red(blue) edges must be part of a red(blue) drum.*

Proof. Let the two cycle edges incident on v be e_1, e_2. Without loss of generality, let e_1 be red and e_2 be blue. Every C-edge can be part of at most one drum from Observation 16. In addition, all drums are monochromatic from Observation 18. Therefore, e_1 can be part of at most one red drum and e_2 can be part of at most one blue drum.

Recall that other than C-edges, only legal edges are incident on v from Observation 13. Every legal edge incident on vertex v must be part of a unique drum from Observation 15. But each of these drums must contain a cycle edge incident on v. It follows that v can be part of at most one red drum and at most one blue drum, and therefore, v can have at most two red edges and two blue edges incident on it. □

Observation 20. *If G is a matching covered graph and $\mu(G) = 2$, then $\Delta(G) \leqslant 4$.*

Proof. If $|V(G)| < 6$, it is easy to see that $\Delta(G) \leqslant 4$. We now assume that $|V(G)| \geqslant 6$. As $\mu(G) = 2$, there is a colouring c such that $\mu(G, c) = 2$. It follows from Theorem 10 that Condition 4 holds. Therefore, from Observation 19, on each vertex of G_c, at most two red edges and at most two blue edges are incident. Therefore, the degree is at most 4 for any vertex on G and hence $\Delta(G) \leqslant 4$. □

Observation 21. *If Condition 4 is true, all Hamiltonian cycles of G_c are red-blue alternating cycles.*

Proof. Any Hamiltonian cycle can be partitioned into two perfect matchings. Since G_c is perfectly monochromatic, both these perfect matchings must be monochromatic. Therefore, the Hamiltonian cycle is either a red-blue alternating cycle or a monochromatic cycle.

There is a red-blue alternating Hamiltonian cycle, say C_2, from Theorem 10. Towards a contradiction, let there be a monochromatic Hamiltonian cycle C_1. Without loss of generality, let all the edges of C_1 be of colour red. Therefore, every vertex must have at least two red edges incident on it. From Observation 19, every vertex can have at most two red edges incident on it. It follows that all red edges of the graph form a Hamiltonian cycle C_1. From Observation 19, since all vertices have 2 red edges incident on them, each vertex must be part of a drum with respect to C_2. Therefore, the monochromatic red Hamiltonian cycle C_1 must contain a red monochromatic drum, which is a 4-cycle. This is possible only when C_1 is a 4-cycle. But $|V(G)| \geqslant 6$ from Condition 4. Contradiction. It follows that there are no monochromatic red Hamiltonian cycles. Using a similar argument, it can be proved that there are no monochromatic blue Hamiltonian cycles. Therefore, all Hamiltonian cycles of G_c are red-blue alternating cycles. □

Observation 22. *If Condition 4 is true and G is not a cycle, a drum D exists such that all vertices in $\mathcal{P}(D)$ have degree 2.*

Proof. Among all drums, let D be a drum that has the smallest partition weight equal to $|\mathcal{P}(D)|$. Let D be formed by the crossing edges e_1, e_2. If $\mathcal{P}(D) = \emptyset$, the observation trivially holds. Therefore, we assume that $\mathcal{P}(D)$ has at least 1 vertex. Towards a contradiction, assume that there is a vertex v in $\mathcal{P}(D)$ with degree greater than 2. Therefore, there exists some legal edge e_3, incident on $v \in \mathcal{P}(D)$.

From Observation 15, e_3 must be part of some drum D' along with a crossing edge e'_3. As e_1, e_2 are part of exactly one drum D, e'_3 or e_3 cannot be in $\{e_1, e_2\}$, as in that case there would be another drum involving e_1 or e_2 other than D. From Observation 18, as all crossing pairs are drums, neither e_3 nor e'_3 can cross e_1 or e_2. Therefore, both C-edges of D' must be on the strap of D along $\mathcal{P}(D)$. Therefore, $|\mathcal{P}(D)| > |\mathcal{P}(D')|$. But this contradicts the assumption that D has the smallest partition weight. $\square$

3.4 Structural characterization of graphs for which $\mu(G) = 2$

Recall the definition of $\mathcal{H}$ (from Definition 5). Let $\mathcal{H}'$ be the family of even-order matching-covered Hamiltonian graphs with at least 6 vertices such that all graphs $G \in \mathcal{H}'$ satisfy the following: For *all* Hamiltonian cycles C of G, Properties 1, 2 and 3 are satisfied with respect to the vertex labelling obtained from a clockwise cyclic ordering of C.

Observe that Properties 1, 2 and 3 are satisfied for all cycles for $\mathcal{H}'$ and for some cycle for $\mathcal{H}$. It is easy to see that $\mathcal{H}' \subseteq \mathcal{H}$. Surprisingly, we show that the two classes $\mathcal{H}'$ and $\mathcal{H}$ are, in fact, the same!

Lemma 23. *For any graph H with $|V(H)| > 4$, if $\mu(H) = 2$, then $mcg(H) \in \mathcal{H}'$*

Proof. Let $G = mcg(H)$. If $\mu(H) = 2$, then $\mu(G) = 2$. It follows that there exists a perfectly monochromatic colouring c such that $\mu(G, c) = 2$. From Theorem 10, G has a perfect matching implying that the order of G is even; Moreover, G_c has at least one alternating red-blue Hamiltonian cycle. Therefore, Condition 4 holds for G_c. From Observation 21, all Hamiltonian cycles of G_c are alternating red-blue cycles. Therefore, with respect to any Hamiltonian cycle of G Condition 4 holds. It follows that Properties 1, 2 and 3 hold due to Observations 13, 18 and 15 respectively. Therefore, $mcg(H) \in \mathcal{H}'$. $\square$

Lemma 24. *If $mcg(H) \in \mathcal{H}$, then $\mu(H) = 2$.*

Proof. Let $G = mcg(H)$. We first show that for any graph $G \in \mathcal{H}$, there is an edge colouring c such that $\mu(G, c)$ is 2.

By definition of $\mathcal{H}$, there exists an even order Hamiltonian cycle, C with respect to which Properties 1, 2 and 3 are satisfied. Colour C with alternating red and blue colours. Notice that all uncoloured edges are legal due to Property 1. Consider a legal edge e, due to Property 3, it is part of a unique drum D having another legal edge e', where e, e' form a crossing pair. By the definition of a drum, both the non-adjacent C-edges of D must be of the same colour with respect to the colouring c. Colour e, e' with the same colour as the non-adjacent C-edges of D. Do this for all legal edges. Due to Property 3, as each legal edge is part of exactly one drum, each legal edge gets coloured exactly once. Thus, we now have a colouring c for the entire graph. We now prove that this colouring c is perfectly monochromatic.

We first prove that, for a drum D with a crossing pair e, e' and a perfect matching M, either $\{e, e'\} \subseteq M$ or $\{e, e'\} \bigcap M = \emptyset$. Towards a contradiction, let there be a perfect matching M, which contains e but not e'. As e is legal, $|\mathcal{P}(e)|$ and $|\mathcal{P}'(e)|$ are odd. Since M cannot match the vertices of $\mathcal{P}(e)$ within itself and every vertex must be covered by

M, there must be an edge $e'' \in M$ crossing e. But every crossing pair forms a drum due to Property 2 and e is part of only one drum due to Property 3. Therefore, e'' must be e'. Thus, $e' \in M$. Contradiction.

We now prove that the colouring c is perfectly monochromatic. Towards a contradiction, let there be a non-monochromatic perfect matching M. If M contains legal edges, they come in pairs such that each pair belongs to a drum. Clearly, all these pairs of legal edges that belong to M are disjoint from Property 3. Replace each such crossing pair in M with the associated pair of C-edges of the corresponding drum to form a new perfect matching M'. Observe that since all drums are monochromatic, we are replacing a pair of crossing edges with C-edges of the same colour. It follows that since M is a non-monochromatic perfect matching, M' must also be a non-monochromatic perfect matching. However, M' is a perfect matching from the Hamiltonian cycle C, which is alternately coloured. Thus, M' must be monochromatic. This is a contradiction.

Therefore, G_c has no non-monochromatic perfect matchings. Therefore, G_c is perfectly monochromatic. Since there are two perfect matchings of different colours in C, $\mu(G, c) = 2$. Therefore, $\mu(G) \geqslant 2$. From Theorem 4, $\mu(G) \leqslant 2$. It follows that $\mu(G) = 2$ and hence $\mu(H) = 2$. □

Lemma 25. $\mathcal{H} = \mathcal{H}'$

Proof. It is easy to see that $\mathcal{H}' \subseteq \mathcal{H}$ by definition. Consider any matching covered graph $G \in \mathcal{H}$. From Lemma 24, $\mu(G) = 2$. As $\mu(G) = 2$, from Lemma 23, $G \in \mathcal{H}'$. It follows that $\mathcal{H} \subseteq \mathcal{H}'$ and hence $\mathcal{H} = \mathcal{H}'$. □

By Lemma 23, if $\mu(H) = 2$, then $mcg(H) \in \mathcal{H}'$. But from Lemma 25, $\mathcal{H}' = \mathcal{H}$. Finally, from Lemma 24, if $mcg(H) \in \mathcal{H}$ then $\mu(H) = 2$. Therefore, Theorem 6 follows.

4 Algorithm to find the matching index

We first prove Lemma 26, which is useful to prove the correctness of our algorithm.

Lemma 26. *Let G be a matching-covered graph with $\mu(G) = 2$. Let $v \in V(G)$ and let $\mathcal{M}(e)$ denote the set of all perfect matchings of G containing the edge $e \in E(G)$. There exist two edges e_1, e_2 incident on v such that $M_1 \bigsqcup M_2$ is a Hamiltonian cycle of G, for any $M_1 \in \mathcal{M}(e_1)$ and any $M_2 \in \mathcal{M}(e_2)$.*

Proof. Let c be a perfectly monochromatic colouring of G such that $\mu(G, c) = 2$. From Theorem 10, G_c is perfectly monochromatic and has a red-blue alternating Hamiltonian cycle C. For a vertex v, let two of its incident edges from C be e_1, e_2. Without loss of generality, let e_1 be red and e_2 be blue. For those e_1, e_2, we prove that $M_1 \bigsqcup M_2$ is a Hamiltonian cycle of G_c, for any $M_1 \in \mathcal{M}(e_1)$ and $M_2 \in \mathcal{M}(e_2)$.

Since e_1 is red, and G_c is perfectly monochromatic, all perfect matchings in $\mathcal{M}(e_1)$ must be monochromatic red perfect matchings by definition. Similarly, all perfect matchings in $\mathcal{M}(e_2)$ must be monochromatic blue perfect matchings. Therefore, $M_1 \bigcap M_2 = \emptyset$ and $M_1 \bigsqcup M_2$ must be a disjoint union of even cycle(s) of alternating colours. If it is a disjoint union of at least two even cycles, then by selecting the red perfect matching from one cycle and blue perfect matchings from the remaining cycles, we can construct a non-monochromatic perfect matching. However, this is not possible as G_c is perfectly monochromatic. Therefore, $M_1 \bigsqcup M_2$ is a Hamiltonian cycle. $\square$

Algorithm 1: To decide whether a non-trivial matching covered graph non-isomorphic to K_4 has matching index 1 or 2

Pick any $v \in V(G)$, arbitrarily.
$\mathcal{C} \leftarrow \emptyset$
if $d(v) \geqslant 5$ **then**
  $\mu(G) \leftarrow 1$ `// See Observation 20`
else
  for *all pairs of edges* $\{e_1, e_2\}$ *incident on* v **do**
    Pick arbitrary perfect matchings M_1, M_2 such that $e_1 \in M_1$ and $e_2 \in M_2$
    if $M_1 \bigcup M_2$ *is a Hamiltonian cycle* **then**
      $\mathcal{C} \leftarrow \mathcal{C} \bigcup \{M_1 \bigcup M_2\}$
    end
  end
end
if $\mathcal{C} = \emptyset$ **then**
  $\mu(G) \leftarrow 1$ `// See Lemma 26`
else
  Pick any $C \in \mathcal{C}$ arbitrarily ;
  if *Properties 1, 2, 3 are satisfied in* G *with respect to* C **then**
    $\mu(G) \leftarrow 2$ `//` $G \in \mathcal{H}'$`, See Lemma 25`
  else
    $\mu(G) \leftarrow 1$ `//` $G \notin \mathcal{H}$`, See Theorem 6`
  end
end

4.1 Proof of correctness

Proof. From Theorem 4, if H is isomorphic to K_4, $\mu(H) = 3$. From Theorem 10, $\mu(H) = 0$ if and only if there is no perfect matching in H. The absence of a perfect matching can be checked using an algorithm of Micali and Vazirani [17] in $O(\sqrt{|V|}|E|)$ time.

We now know that $\mu(H) = 1$ or 2. We first find the maximum matching covered subgraph $G = mcg(H)$ in $O(|V||E|)$ time using a deterministic algorithm due to Carvalho and Cheriyan [5]. It can also be computed in $O(|V|^{2.376})$ time using a randomized algorithm due to Rabin and Vazirani [20]. As $\mu(G) = \mu(H)$, it is now sufficient to find $\mu(G)$ as described in Algorithm 1. The overview of Algorithm 1 is described below, along with its correctness.

If G is not Hamiltonian, $\mu(G) = 1$ from Theorem 10. If G is Hamiltonian and we know a Hamiltonian cycle C of G, it is easy to check if G satisfies Properties 1, 2 and 3 with respect to C in $O(|E|)$ time. Due to Theorem 6, if all three properties are satisfied with respect to C, then $G \in \mathcal{H}$ and hence $\mu(G) = 2$. If any of the properties is not satisfied with respect to C, $G \notin \mathcal{H}' = \mathcal{H}$ (from Lemma 25) and hence $\mu(G) = 1$. However, finding Hamiltonian cycles in general graphs is an NP-hard problem. Fortunately, since we are only interested in graphs where $\mu(G) = 2$, we can give a simple efficient algorithm that returns a Hamiltonian cycle of G, using Lemma 26.

We pick any vertex $v \in V(G)$, arbitrarily. Note that the maximum degree is at most 4 when $\mu(G) = 2$ from Observation 20. Therefore, we try to find a Hamiltonian cycle only when $d(v) \leqslant 4$. There are at most $\binom{4}{2} = 6$ pairs of edges incident on v. Since G is a matching covered graph, for each pair $\{e_1, e_2\}$, we can find arbitrary perfect matchings M_1, M_2 containing e_1, e_2 respectively, using any maximum matching algorithm [17]. If their union is not a Hamiltonian cycle for all $\binom{4}{2}$ pairs, then $\mu(G) = 1$ from Lemma 26. If their union is a Hamiltonian cycle C for at least one pair, then we check if $G \in \mathcal{H}$ or $G \notin \mathcal{H}'$ with respect to C. Recall that since G is a matching covered graph, by Theorem 6, $\mu(G) = 2$ if and only if $G \in \mathcal{H}' = \mathcal{H}$. $\square$

We note that one can also rephrase our result, i.e. Theorem 6 in terms of SPQR trees. SPQR trees are a decomposition of a biconnected graph with respect to its triconnected components. There is a known linear-time implementation for finding such decompositions [11, 10]. One can use such a linear time algorithm to find the SPQR tree of the matching covered graph G as a black box to detect graphs with matching index 2. However, the bottleneck is finding the matching covered graph $G = mcg(H)$ in both approaches, which takes $O(|V||E|)$ time. We present the current algorithm as it naturally follows from the structural classification.

5 Edge-weighted version

So far, we answered a natural graph-theoretic question arising from quantum photonic experiments: What is the structure of the graphs that admit a PMValid 2-edge colouring? In this section, we formalize the graphs that arise from the quantum optical experiments in the general case; namely when we allow destructive interference that was briefly discussed in Subsection 2.2. The interested reader can refer to [13] to know how these graphs correspond to the experiments.

We first develop some new notation to describe bichromatic edges. We denote the colours as natural numbers. One can imagine an edge $e = \{u, v\}$ to be of two halves, where the half containing u is represented by $u_h(e)$ and the half containing v is represented by $v_h(e)$. An edge colouring c associates a colour i to $u_h(e)$ and a colour j to $v_h(e)$ for some colours $i, j \in \mathbb{N}$ (as shown in Figure 3). For such an edge e, if $i \neq j$ we call e a bichromatic edge and if $i = j$, we call e a monochromatic edge. A weight assignment w assigns every edge e a weight $w(e) \in \mathbb{C} \setminus \{0\}$. (As a zero weight edge e is the same as the edge e being absent, we do not need to consider zero-weight edges.)

Definition 27. The weight of a perfect matching P, $w(P)$ is the product of the weights of all its edges $\prod\limits_{e \in P} w(e)$

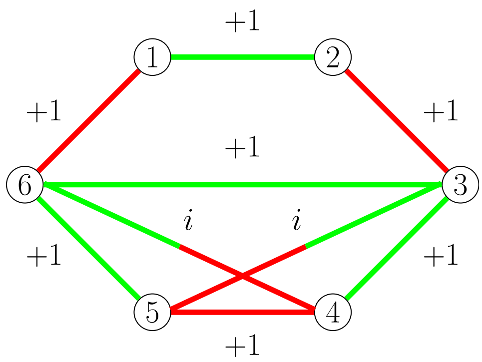


Figure 3: A 2-valid edge-coloured edge-weighted graph G_c^w (red corresponds to 0 and green corresponds to 1)

Definition 28. The weight of a graph G, $w(G) = \sum_{P \in \mathcal{P}} w(P)$ where $\mathcal{P}$ is the set of all perfect matchings of G.

A vertex colouring vc associates a colour i to each vertex in the graph where $i \in \mathbb{N}$. We use $vc(v)$ to denote the colour of vertex v in the vertex colouring vc.

Definition 29. For an edge-weighted edge-coloured graph G_c^w, each vertex colouring vc naturally defines an *edge-filtering* operation $\Theta_{vc}(G_c^w) = H_c^w$ as follows: $V(H_c^w) = V(G_c^w)$ and $e = \{u, v\} \in E(H_c^w)$ if and only if $e \in E(G_c^w)$ and $u_h(e), v_h(e)$ are coloured with $vc(u), vc(v)$ respectively.

We say that $\Theta_{vc}(G_c^w)$ is the vc-filtered subgraph of G_c^w. One may view $\Theta_{vc}(G_c^w)$ as the subgraph of G_c^w consisting of all the coloured edges e for which the colour on each half-edge agrees with the label of the corresponding vertex in vc.

Definition 30. The weight of a vertex colouring vc with respect to G_c^w is defined to be the weight of the subgraph of G_c^w filtered by vc, $w(vc, G_c^w) = w(\Theta_{vc}(G_c^w))$

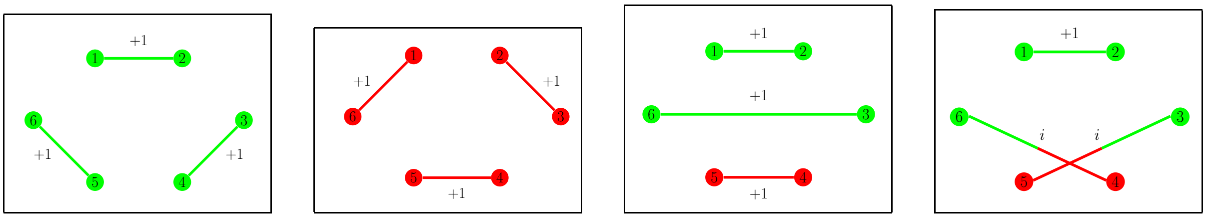
Note that if $\Theta_{vc}(G_c^w)$ does not have a perfect matching, then $w(vc) = 0$ by definition. When the graph G_c^w is understood from the context, we will use $w(vc)$ to denote $w(vc, G_c^w)$.

Definition 31. An edge-weighted edge-coloured graph G_c^w is said to be *valid* with dimension $\bar{\mu}(G, c, w)$ (or $\bar{\mu}(G, c, w)$-valid), if the following two conditions are satisfied:

1. There exists $\bar{\mu}(G, c, w)$ monochromatic vertex colourings with a weight of 1.
2. All vertex colourings other than the $\bar{\mu}(G, c, w)$ monochromatic vertex colourings of weight 1 have a weight of 0.

An example of a 2-valid edge-coloured edge-weighted graph is shown in Figure 3.

Definition 32. For a graph G, the maximum k such that there exists an edge colouring c and edge-weight assignment w for which G_c^w is k-valid (valid with dimension k) is defined to be $\bar{\mu}(G)$.



(a) $\Theta_{|111111\rangle}(G_c^w)$ (b) $\Theta_{|000000\rangle}(G_c^w)$ (c) $\Theta_{|111001\rangle}(G_c^w)$ (i) (d) $\Theta_{|111001\rangle}(G_c^w)$ (ii)

Figure 4: The vertex colourings induced by the perfect matchings of Figure 3.

In a graph G_c^w, for the weight of the non-monochromatic vertex colouring vc to be zero, it is not necessary that $\Theta_{vc}(G_c^w)$ does not have a perfect matching; the weights of perfect matchings can cancel each other. For instance, perfect matchings in Figures 4c and 4d add up to zero. However, when all edge weights are positive real numbers, such cancellations are not possible and hence there cannot be any non-monochromatic perfect matchings in G_c^w. Therefore, when all the weights are restricted to positive real values, the weighted problem would reduce to the unweighted problem of PMValid edge colourings which was discussed in the earlier sections. It is easy to see that $\bar{\mu}(G) \geqslant \mu(G)$ (Observation 38).

As we have observed already in terms of weights, the difference between the unweighted and weighted case is that essentially we are not restricted to only real positive weights but are allowed to take any complex weights. In quantum physics terms this is expressed by saying that destructive interference is allowed. Krenn and Gu made a conjecture that allowing destructive interference does not help to get a higher dimension (and hence a statement analogous to Theorem 4 for edge-weighted edge-coloured graphs will hold). The reader not familiar with quantum physics can safely discard these comments on destructive interference as the problem and its solution can be understood from a graph-theoretic point of view.

Conjecture 33 (Krenn-Gu Conjecture)**.** For a multigraph G that is not isomorphic to K_4, $\bar{\mu}(G) \leqslant 2$; $\bar{\mu}(K_4) = 3$.

Surprisingly, we prove that once the structure corresponds to $\mu(G) = 2$, then the freedom to choose any colouring (with possibly bichromatic edges) and to choose complex weight functions does not help to achieve a higher value of $\bar{\mu}(G)$ for simple graphs (i.e. destructive interference indeed does not help in this case as Krenn and Gu predicted for all cases).

Theorem 34. *For a simple graph G, if $\mu(G) \neq 1$, then $\bar{\mu}(G) = \mu(G)$.*

The above theorem is an application of our main result, which is the structural classification of graphs with $\mu(G) = 2$. We first observe that a certain gadget is present in the graphs with $\mu(G) = 2$, from Theorem 6. We then prove that this gadget would prevent from achieving a higher value of $\bar{\mu}(G)$ in Section 6. A natural question one can ask is if $\mu(G)$ and $\bar{\mu}(G)$ should always be the same. We prove that this is not the case in Subsection 6.3.

Observation 35. *There exists a graph G, with $\mu(G) = 1$ and $\bar{\mu}(G) = 2$.*

6 Proof of Theorem 34: Weighted case

6.1 Preliminaries for weighted edge-coloured graphs

We first make some simple observations for the weighted version. Let G_c^w be a valid edge-coloured edge-weighted graph. Note that a colouring c and a weight assignment w of G induces a colouring and a weight assignment for every subgraph of G, respectively. When there is no scope for confusion, we use c, w itself to denote this induced colouring and weight assignment, respectively. It is easy to see that if c, w makes G a k-valid edge-coloured edge-weighted graph, they also make $mcg(G)$ a k-valid edge-coloured edge-weighted graph and $\bar{\mu}(G, c, w) = \bar{\mu}(mcg(G), c, w)$. Therefore, $\bar{\mu}(G) = \bar{\mu}(mcg(G))$.

For $S \subseteq V(G)$, we define $\mathbf{i}_S$ to be the monochromatic vertex colouring using colour i over the induced subgraph $G_c^w[S]$. The weight of $\mathbf{i}_S$ is denoted by $w(\mathbf{i}_S) = w(\Theta_{\mathbf{i}_S}(G_c^w[S]))$. We emphasize that this weight is with respect to the induced subgraph $G_c^w[S]$. Let $G_c^w[\mathbf{i}, S]$ denote the subgraph of $G_c^w[S]$ formed by all monochromatic edges of $G_c^w[S]$ of colour i.

Observation 36. *For $S \subseteq V(G)$, let the connected components of $G_c^w[\mathbf{i}, S]$ be $\bigsqcup_{j=1}^{r} S_j = S$. Then the weight of its monochromatic vertex colouring $\mathbf{i}_S$ is*

$$w(\mathbf{i}_S) = \prod_{j=1}^{r} w(\mathbf{i}_{S_j})$$

Observation 37. $\bar{\mu}(G) \leqslant \delta(G)$

Proof. Let c, w be such that $\bar{\mu}(G, c, w) = \bar{\mu}(G)$. Note that in G_c^w, there are $\bar{\mu}(G)$ colour classes containing a monochromatic perfect matching. Therefore, any vertex v of G has at least one monochromatic edge incident on it from each of the $\bar{\mu}(G)$ colours. Therefore, v has degree at least $\bar{\mu}(G)$. Therefore, the minimum degree of G is at least $\bar{\mu}(G)$. □

Observation 38. $\bar{\mu}(G) \geqslant \mu(G)$

Proof. It is sufficient to prove that given an unweighted edge-coloured graph G_c which is PMValid, it is possible to assign weights w to the edges so that the graph G_c^w is $\mu(G)$-valid. We first note that any edge which is part of a perfect matching in G_c cannot be bichromatic, since c is PMValid. Let the colour of an edge e be represented by $c(e)$. Let $pm_{c(e)} > 0$ denote the number of monochromatic perfect matchings of colour $c(e)$ in G_c. Consider the weight function $w(e) = (pm_{c(e)})^{-2/n}$ on G_c. It is easy to see that the weight of each monochromatic perfect matching of colour $c(e)$ is ${pm_{c(e)}}^{-1}$ as each perfect matching has $n/2$ edges. Since there are $pm_{c(e)}$ many monochromatic perfect matchings of colour $c(e)$, the weight of all $\mu(G)$ monochromatic vertex colourings is 1. As all perfect matchings are monochromatic, all non-monochromatic vertex colourings have weight 0. Therefore, G_c^w is $\mu(G)$-valid. □

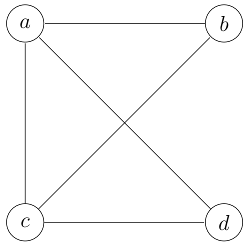


Figure 5: Gadget for Lemma 39

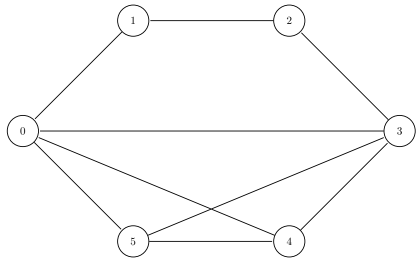


Figure 6: Example for Observation 35: Graph G with $\mu(G) = 1$ and $\bar{\mu}(G) = 2$

6.2 Proof of Theorem 34

Proof. If $\mu(G) = 0$, from Theorem 10, G has no perfect matching. Therefore, $\bar{\mu}(G) = 0 = \mu(G)$. If $\mu(G) = 3$, we know that G is K_4. As K_4 has 6 edges, it has at most 3 disjoint perfect matchings. Hence $\bar{\mu}(G) \leqslant 3$. We also know that $\bar{\mu}(G) \geqslant \mu(G) = 3$. Therefore $\bar{\mu}(K_4) = 3 = \mu(K_4)$.

We now prove that if $\mu(G) = 2$, then $\bar{\mu}(G) = 2$. Let $G' = mcg(G)$. If G' is a cycle, then $\delta(G') = 2$, and hence $\bar{\mu}(G) = \bar{\mu}(G') \leqslant 2$ by Observation 37. Together with Observation 38, this gives $\bar{\mu}(G) = 2$. We may therefore assume that G' is not a cycle.

From Observation 22, there exists a drum D in G' (with respect to some Hamiltonian cycle) such that all vertices of the smaller part, $\mathcal{P}(D)$, have degree 2. If $\mathcal{P}(D)$ is non-empty, then $\delta(G') \leqslant 2$ and from Observation 37, $\bar{\mu}(G) = \bar{\mu}(G') \leqslant 2$.

If $\mathcal{P}(D)$ is empty, then the strap between two vertices, say a, c of the drum D is just the cycle edge ac. Now, it is easy to see that a, c have degree 3. Let the other two vertices from the drum D be b, d such that $abcd$ is a 4-cycle as shown in Figure 5. We now prove that the existence of a slightly more general structure (of which Figure 5 is a special case) would imply that $\bar{\mu}(G) \leqslant 2$ in Lemma 39.

Lemma 39. *If G is not isomorphic to K_4 and there exist $a, b, c, d \in V(G)$ such that $d(a) = d(c) = 3$ and $abcd$ forms a 4-cycle, then $\bar{\mu}(G) \leqslant 2$.*

Proof. Let $S = V(G) - \{a, b, c, d\}$. If $S = \emptyset$, then, since G is not isomorphic to K_4, at least one of b and d has degree at most 2. Hence $\bar{\mu}(G) \leqslant 2$ by Observation 37. Thus, assume that $S \neq \emptyset$.

Towards a contradiction, let $\bar{\mu}(G) \geqslant 3$. As there is a degree-3 vertex, $\delta(G) \leqslant 3$. From Observation 37, $\bar{\mu}(G) \leqslant \delta(G) \leqslant 3$. Therefore, $\bar{\mu}(G) = 3$ and hence there exists a colouring c and weight w, such that G_c^w is 3-valid. Let the three colour classes be $1, 2, 3$. Note that as a, c have degree 3, they should have at least one monochromatic edge incident on them from each of the colour classes $1, 2, 3$. Therefore, they can neither have two edges from the same colour class incident on them or a bi-chromatic coloured edge incident on them. It is easy to see that all the edges of the cycle $abcd$ are monochromatic.

Also note that both the edges incident on b from the cycle $abcd$ cannot belong to the same colour class. This is because if ab, bc (which are monochromatic) have the same colour, say 1, a monochromatic perfect matching associated with the colour 1 must contain both ab and bc (as the only one 1-coloured monochromatic edge incident on a is ab and the only one 1-coloured monochromatic edge incident on c is bc). But there cannot be two edges from a perfect matching incident on b. The same observation holds for the vertex d, that is da and dc must have different colours.

Since 3 colour classes contain the 4 edges of the cycle $abcd$, a colour class must contain at least two of these edges. As these edges cannot be adjacent, without loss of generality, let ab and cd be of colour 1. Therefore, neither bc nor ad is coloured 1. Since ab and cd are the only colour-1 edges incident on a and c, respectively, every perfect matching contributing to $w(\mathbf{1}_{V(G)})$ contains ab and cd. Hence

$$w(\mathbf{1}_{V(G)}) = w(\mathbf{1}_S)w(ab)w(cd) = 1,$$

and therefore $w(\mathbf{1}_S) \neq 0$.

Consider the vertex colouring vc, where S is coloured 1, $\{b, c\}$ are coloured c_{bc}, and $\{a, d\}$ are coloured c_{ad}. Recall that c_{bc}, c_{ad} cannot be equal to 1. Since $S \neq \emptyset$, the vertex colouring vc is non-monochromatic, and hence validity gives $w(vc) = 0$. As a, c have three monochromatic edges of different colours incident on each of them, the only edge of colour c_{ad} incident on a is ad. Similarly, the only edge of colour c_{bc} incident on c is bc. Therefore, every perfect matching of $\Theta_{vc}(G_c^w)$ must contain the edges bc and ad. Hence

$$w(vc) = w(\mathbf{1}_S)w(bc)w(ad) = 0.$$

Since the edge weights are non-zero, we get $w(\mathbf{1}_S) = 0$, contradicting $w(\mathbf{1}_S) \neq 0$.

□

We know that $\bar{\mu}(G) \geqslant \mu(G) = 2$. Therefore, $\bar{\mu}(G) = 2$. □

6.3 Proof of Observation 35

Proof. We show that the graph G shown in Figure 6 satisfies $\mu(G) = 1$ and $\bar{\mu}(G) = 2$. The graph is matching covered: the cycle edges lie in alternating perfect matchings, the edge $\{0, 3\}$ lies in the perfect matching $\{\{0, 3\}, \{1, 2\}, \{4, 5\}\}$, and the edges $\{0, 4\}$ and $\{3, 5\}$ lie in the perfect matching $\{\{0, 4\}, \{1, 2\}, \{3, 5\}\}$. Hence $mcg(G) = G$.

Consider the cyclic ordering along the Hamiltonian cycle $C = (0, 1, 2, 3, 4, 5, 0)$ shown in Figure 6. The edge $\{0, 3\}$ is an illegal edge with respect to C, so Property 1 fails for this Hamiltonian cycle. By Lemma 25, $\mathcal{H} = \mathcal{H}'$; hence $G \notin \mathcal{H}$. Therefore, by Theorem 6, $\mu(G) \neq 2$. Since G is Hamiltonian and is not isomorphic to K_4, Theorem 4 implies $\mu(G) = 1$.

It remains to show that $\bar{\mu}(G) = 2$. The underlying graph in Figure 3 is isomorphic to the graph in Figure 6, by relabelling vertex 6 as 0. Since Figure 3 gives a 2-valid edge-coloured edge-weighted realization, we have $\bar{\mu}(G) \geqslant 2$. On the other hand, $\delta(G) = 2$, and hence $\bar{\mu}(G) \leqslant 2$ by Observation 37. Therefore $\bar{\mu}(G) = 2$. □

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