Krenn-Gu Conjecture for Sparse Graphs

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Abstract

Greenberger–Horne–Zeilinger (GHZ) states are quantum states involving at least three entangled particles. They are of fundamental interest in quantum information theory, and the construction of such states of high dimension has various applications in quantum communication and cryptography. Krenn, Gu and Zeilinger discovered a correspondence between a large class of quantum optical experiments which produce GHZ states and edge-weighted edge-coloured multi-graphs with some special properties called the *GHZ graphs*. On such GHZ graphs, a graph parameter called *dimension* can be defined, which is the same as the dimension of the GHZ state produced by the corresponding experiment. Krenn and Gu conjectured that the dimension of any GHZ graph with more than 4 vertices is at most 2. An affirmative resolution of the Krenn-Gu conjecture has implications for quantum resource theory. Moreover, this would save huge computational resources used for finding experiments which lead to higher dimensional GHZ states. On the other hand, the construction of a GHZ graph on a large number of vertices with a high dimension would lead to breakthrough results.

In this paper, we study the existence of GHZ graphs from the perspective of the Krenn-Gu conjecture and show that the conjecture is true for graphs of vertex connectivity at most 2 and for cubic graphs. We also show that the minimal counterexample to the conjecture should be 4-connected. Such information could be of great help in the search for GHZ graphs using existing tools like PyTheus. While the impact of the work is in quantum physics, the techniques in this paper are purely combinatorial, and no background in quantum physics is required to understand them.

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1 Introduction

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, which is local (i.e. information can be transmitted maximally with the speed of light) and realistic (i.e. properties exist prior to and independent of their measurement) [2]. Later, in 1989, Greenberger, Horne, and Zeilinger (abbreviated as GHZ) studied what would happen if more than two particles are entangled [8]. 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 [4, 21]. While the study of such states started purely out of fundamental curiosity [24, 16, 17], they are now used in many applications in quantum information theory, such as quantum computing [11]. They are also essential for early tests of quantum computing tasks [28], and quantum cryptography in quantum networks[22].

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Zeilinger became a co-recipient of the Nobel Prize for Physics in 2022, for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science. We note that the work on experimentally constructing GHZ states is at the heart of Zeilinger's Nobel prize-winning work [1]. Increasing the number of particles involved and the dimension of the GHZ state is essential both for foundational studies and practical applications. Motivated by this, a huge effort is being made by several experimental groups around the world to push the size of GHZ states. Photonic technology is one of the key technologies used to achieve this goal [28, 27]. The Nobel Laureate himself, with some co-authors, proposed a scheme of optical experiments in order to achieve this, which gives an opportunity for graph theorists to get involved in this fundamental research: In 2017, Krenn, Gu and Zeilinger [14] discovered (and later extended [10, 9]) a bridge between experimental quantum optics and graph theory. 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 an edge-coloured edge-weighted graph, though the edge-colouring goes a little beyond what graph theorists are used to. Conversely, every edge-coloured edge-weighted graph (also referred to as an experiment graph) can be translated into a concrete experimental setup. This technique has led to the discovery of new quantum interference effects and connections to quantum computing [10]. Furthermore, it has been used as the representation of efficient AI-based design methods for new quantum experiments [15, 23].

However, despite several efforts, a way to generate a GHZ state of dimension $d > 2$ with more than $n = 4$ photons with perfect quality and finite count rates without additional resources [13] could not be found. This led Krenn and Gu to conjecture that it is not possible to achieve this physically (stated in graph theoretic terms in Conjecture 6). They have also formulated this question purely in graph theoretic terms and publicised it widely among graph theorists for a resolution [19]. We now formally state this problem in graph-theoretic terms and explain its equivalence in quantum photonic terms. For a high-level overview of how the experiments are converted to edge-coloured edge-weighted graphs, we refer the reader to the appendix of [6]. For the exact details, the reader can refer to [14, 10, 9, 13].

1.1 Graph theoretic preliminaries and notations

We first define some commonly used graph-theoretic terms. For a graph G, let $V(G), E(G)$ denote the set of vertices and edges, respectively. We use $\kappa(G)$ to denote the vertex connectivity of G. For $S \subseteq V(G)$, $G[S]$ denotes the induced subgraph of G on S. $\mathbb{N}, \mathbb{N}_0, \mathbb{C}$ denote the set of natural numbers, non-negative numbers and complex numbers, respectively. The cardinality of a set $\mathcal{S}$ is denoted by $|\mathcal{S}|$. For a positive integer r, $[r]$ denotes the set $\{1, 2 \ldots, r\}$. Given a multi-graph, its skeleton is its underlying simple graph. We do not consider self-loops in multi-graphs.

Usually, in an edge colouring, each edge is associated with a natural number. However, in such edge colourings, the edges are assumed to be monochromatic. But in the graphs corresponding to experiments, we are allowed to have bichromatic edges, i.e. one half coloured by a certain colour and the other half coloured by a different colour. For example, in the graph shown in Figure 1a, the simple edge between vertices 4 and 6 is a bichromatic edge. We develop some new notation to describe bichromatic edges.

Each edge of a multi-graph can be thought to be formed by two half-edges, i.e., an edge e between vertices u and v, consists of the half-edge starting from the vertex u to the middle of the edge e (hereafter referred to as the u-half-edge of e) and the half-edge starting from the vertex v to the middle of the edge e (hereafter referred to as the v-half-edge e). Thus, the edge set E of the multi-graph gives rise to the set of half-edges H, with $|H| = 2|E|$. For an edge e between vertices u and v, we may denote the v-half-edge of e by e_v and u-half edge of e by e_u. Consider the edge e between vertices 4 and 6 in Figure 1a. The 4-half edge of e (e_4) is of colour red, and the 6-half edge (e_6) is of colour green.

The type of edge colouring that we consider in this paper is more aptly called a *half-edge colouring*. It is a function from H to $\mathbb{N}_0$, say $c : H \to \mathbb{N}_0$. (Note that we use non-negative numbers to name the colours.) In other words, each half-edge gets a colour. An edge is called monochromatic if both its half-edges get the same colour (in which case we may use $c(e)$ to denote this colour); otherwise, it is called a bi-chromatic edge. In Figure 1a, the colour 0 is shown in red, and the colour 1 is shown in green. It is easy to see that $c(e_4) = 0$ and $c(e_6) = 1$ (recall that e is the simple edge between vertices 4 and 6). Consider the edge e' between vertices 1 and 6. As $c(e'_1) = c(e'_6) = 0$, e' is monochromatic and moreover, $c(e') = 0$. We then assign a weight $w(e) \in \mathbb{C}$ to each such coloured edge e. We denote the multi-graph G with the edge colouring c and edge weights $w(e)$ as G_c^w.

We call a subset P of edges in this edge-weighted edge-coloured graph a perfect matching if each vertex in the graph has exactly one edge in P incident on it.

▶ **Definition 1.** *The weight of a perfect matching P, $w(P)$ is the product of the weights of all its edges* $\prod_{e \in P} w(e)$

▶ **Definition 2.** *The weight of an edge-coloured edge-weighted multi-graph G_c^w is the sum of the weights of all perfect matchings in G_c^w.*

A vertex colouring vc associates a colour i to each vertex in the graph for some $i \in \mathbb{N}$. We use $vc(v)$ to denote the colour of vertex v in the vertex colouring vc. A vertex colouring vc *filters out* a sub-graph $\mathcal{F}(G_c, vc)$ of G_c on $V(G_c)$ where for an edge $e \in E(G_c)$ between vertices u and v, $e \in E(\mathcal{F}(G_c, vc))$ if and only if $c(e_u) = vc(u)$ and $c(e_v) = vc(v)$. Filtering also extends to weighted graphs where the weight of each edge in $\mathcal{F}(G_c^w, vc)$ is the same as its weight in G_c^w. Let vc be a vertex colouring in which $1, 2, 3, 6$ are associated with the colour green and $4, 5$ are associated with the colour red. The filtering operation of vc on the edge-coloured graph G_c^w shown in Figure 1a is given in Figure 1b. A vertex colouring vc is defined to be feasible in G_c^w if $\mathcal{F}(G_c^w, vc)$ has at least one perfect matching. It is easy to see that each perfect matching P is part of $\mathcal{F}(G_c^w, vc)$ for a unique vertex colouring vc. Such a P is said to induce vc. It is interesting to notice that there is a partition of perfect matchings (not edges) based on the vertex colourings.

▶ **Definition 3.** *The weight of a vertex colouring vc in the multi-graph G_c^w is denoted by $w(G_c^w, vc)$ and is equal to the weight of the graph $\mathcal{F}(G_c^w, vc)$.*

The weight of a vertex colouring, which is not feasible, is zero by default.

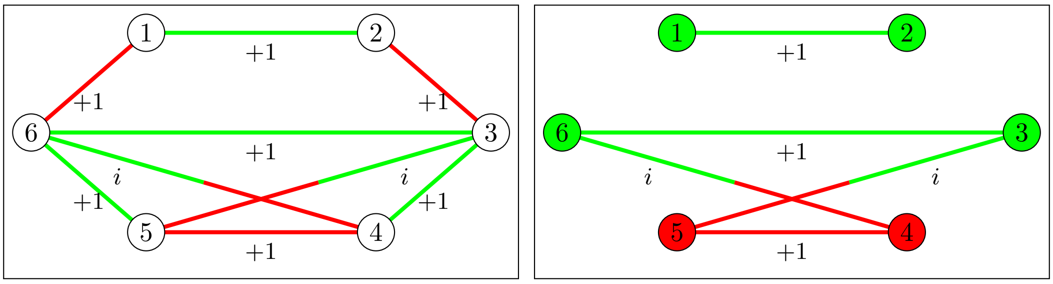
▶ **Definition 4.** *An edge-coloured edge-weighted graph is said to be GHZ, if:*

1. *All feasible monochromatic vertex colourings have a weight of* 1.
2. *All non-monochromatic vertex colourings have a weight of* 0.

An example of a GHZ graph is shown in Figure 1a.

▶ **Definition 5.** *The dimension of a GHZ graph G_c^w, $\mu(G, c, w)$ is the number of feasible monochromatic vertex colourings (having a weight of* 1*).*

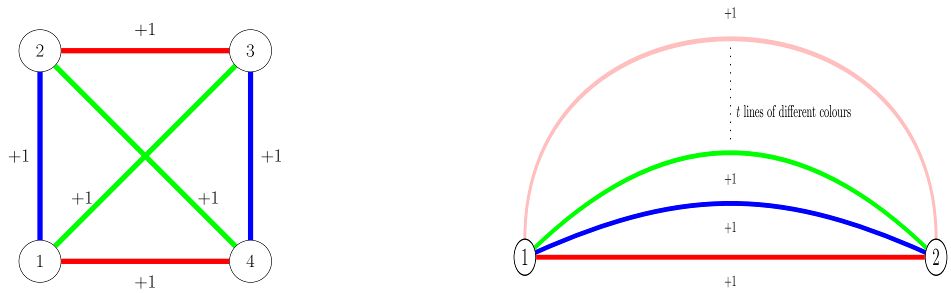
For a given multi-graph G (experimental set up), many possible edge-colourings (mode numbers of photons) and edge-weight (amplitude of photon pairs) assignments may lead it a GHZ graph (GHZ state). Finding a GHZ graph with n vertices and dimension d would



(a) An edge coloured edge-weighted graph G_c^w.

(b) $\mathcal{F}(G_c^w, vc)$, where $vc(i)$ is green for $i \in [1, 2, 3, 6]$ and red for $i \in [4, 5]$.

Figure 1 *vc*-Filtering of a graph.



(a) K_4 with 3 dimensions.

(b) K_2 with t dimensions.

Figure 2 GHZ graphs.

immediately lead to an experiment which result in a d-dimensional GHZ state with n particles. For each such GHZ graph, a dimension is achieved. The maximum dimension achieved over all possible GHZ graphs with the unweighted uncoloured simple graph G as their skeleton is known as the *matching index* of G, denoted by $\mu(G)$. In Figure 2b, we have an edge-coloured edge-weighted GHZ K_2 of dimension t. Note that t can be arbitrarily large. Therefore, $\mu(K_2) = \infty$. However, only two particles are involved; for a GHZ state to form, we need more than two particles. Therefore, such a construction will not give a GHZ state. We note that the matching index is defined for a simple graph G by taking the maximum over all possible multi-graphs with a skeleton G. For instance, the simple graph K_2 has only one edge. However, we considered all possible multi-graphs having a skeleton K_2 to define $\mu(K_2)$.

It is easy to see that if a graph has a perfect matching, it must contain an even number of vertices. So, we consider matching indices of graphs with even and at least 4 vertices for the rest of the manuscript. From Figure 2a, we know that $\mu(K_4) \geq 3$ and, despite the use of huge computational resources [15, 23, 20], this is the only (up to an isomorphism) known graph of the matching index at least 3. Any graph with a matching index of at least 3 and $n > 4$ vertices would lead to a new GHZ state of dimension at least 3 with $n > 4$ entangled particles. Motivated by this, this problem has been extensively promoted[19, 12]. Krenn and Gu conjectured that

▶ **Conjecture 6.** *If* $|V(G)| > 4$, *then* $\mu(G) \leq 2$

Several cash rewards were also announced for a resolution of this conjecture [12]. We note the following implications of resolving this conjecture

1. Finding a counterexample for this conjecture would uncover new peculiar quantum interference effects of a multi-photonic quantum system using which we can create new GHZ states

2. a. Proving this conjecture would immediately lead to new insights into resource theory in quantum optics
   b. Proving this conjecture for different graph classes would help us understand the properties of a counterexample and guide experimentalists in finding it. This is particularly important since huge computational efforts are going into finding such graphs [15, 23, 20].

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 the edge e to be redundant. By removing all redundant edges from the given graph G, we get its unique maximum matching covered sub-graph $mcg(G)$. 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 and w make G a GHZ graph, they also make $mcg(G)$ a GHZ graph and $\mu(G, c, w) = \mu(mcg(G), c, w)$. Therefore, $\mu(G) = \mu(mcg(G))$.

One can also notice that, if there are two edges, say e, e' between vertices u and v such that $c(e_u) = c(e'_u)$ and $c(e_v) = c(e'_v)$, then they can be replaced with an edge e'' such that $w(e'') = w(e) + w(e')$,$c(e''_u) = c(e_u)$ and $c(e''_v) = c(e_v)$. Such a reduction will retain the GHZ property and dimension of the graph. Therefore, in the rest of the manuscript, we only deal with such reduced graphs, i.e, between two vertices between vertices u and v and given $i, j \in [\mu(G)]$ there exists at most one edge e such that $c(e_u) = i$ and $c(e_v) = j$. We also note that, if an edge e has weight 0, it can be treated as if the edge were absent.

1.2 Related work

No destructive interference. The special case of all edges having a real positive weight corresponds to the case when there is no destructive interference. With this restriction, Krenn-Gu conjecture was resolved due to the following observation by Bogdanov [3].

▶ **Theorem 7.** *In a coloured multi-graph G_c with $|V(G)| > 4$, if there exist three monochromatic perfect matchings of different colours, then there must be a non-monochromatic perfect matching.*

Due to this result, when there is no destructive interference, every matching covered graph non-isomorphic to K_4 can achieve a maximum dimension of 1 or 2 and thus can be classified into Type 1 and Type 2 graphs(See [6] for detailed discussion). Chandran and Gajjala [6] gave a structural classification for Type 2 graphs. They further proved that for any half-edge colouring and edge weight assignment on a simple Type 2 unweighted uncoloured graph, a dimension of 3 or more can not be achieved! The computational aspects of the vertex colourings arising from these experiments were studied by Vardi and Zhang [25, 26]

Absence of bi-coloured edges. The problems get easier in the absence of bi-coloured edges and have opened up work in several directions. We list some of the known results in this direction. Cervera-Lierta et al. [5] used SAT solvers to prove that if the number of vertices is 6 or 8, the maximum dimension achievable is 2 or, at most, 3, respectively. Chandran and Gajjala [7] proved that the maximum dimension achievable for an $n > 4$ vertex graph is less than $\frac{n}{\sqrt{2}}$.

Unrestricted results. For the general case, the only known result is due to Mantey [18]. He proved the following theorem using the Gröbner basis.

▶ **Theorem 8.** *If $|V(G)| = 4$, then $\mu(G) \leq 3$. Moreover, if $\mu(G, c, w) = 3$, then between any pair of vertices in G_c^w, there is exactly one non-zero edge (and isomorphic to the coloured graph shown in Figure 2a).*

Surprisingly, there is no known analytical proof even for such *small* graphs. We encourage the reader to attempt to prove Theorem 8 to understand the difficulty arising due to multi-edges. One has to tune 54 variables which can be complex numbers (the number of possible edges when 3 colours are allowed) such that 81 equations (the number of possible vertex colourings when 3 colours are allowed) are satisfied, even for graphs as small as 4 vertex graphs.

1.3 Our results

We give the first results, which resolve the Krenn-Gu conjecture for a large class of graphs in the completely general setting, that is, when both bi-coloured edges and multi-edges are allowed. We prove that the Krenn-Gu conjecture is true for all graphs with vertex connectivity at most 2 in the full version.

▶ **Theorem 9.** *For a graph G, if $\kappa(G) \leq 2$, then $\mu(G) \leq 2$.*

Our next main contribution is a reduction technique, which implies Theorem 10. We explain and prove our reduction in Section 2. We introduce a scaling lemma in Section 1.4, which gives us an equivalent version of Krenn-Gu conjecture and which may turn out to be more useful in some situations.

▶ **Theorem 10.** *Given a graph G with $\kappa(G) \leq 3$ and $V(G) > 4$, there exists a graph G' with $|V(G')| \leq |V(G)| - 2$ and $\mu(G') \geq \mu(G)$.*

Due to Theorem 10, a minimal counter-example (a counter-example with the minimum number of vertices) to Krenn-Gu conjecture must be 4-connected. Using Theorem 10, we can resolve Krenn-Gu conjecture for some interesting graph classes like cubic graphs (that is, 3 regular graphs). We prove Theorem 11 and Theorem 12 in Section 2.3.

▶ **Theorem 11.** *If the maximum degree of a graph G is 3, Conjecture 6 is true.*

▶ **Theorem 12.** *If the minimum degree of a graph G is 3, then $\mu(G) \leq 3$*

1.4 Reformulation of Krenn-Gu conjecture

Recall that we denote the weight of the vertex colouring vc over a set of vertices $U \subseteq V(G)$ as $w(U, vc)$, which is the sum of weights of all perfect matching on $G[U]$ which induce the vertex colouring vc on U and we denote the monochromatic vertex colouring $vc : V \to \{i\}$ by $\mathbf{i}_V$.

For a graph G, let $U, U' \subseteq V(G)$. Let $vc : U \to \mathbf{N}$ and $vc' : U' \to \mathbf{N}$. If $vc(v) = vc'(v)$ for all $v \in U \cap U'$, we call vc, vc' to be compatible with each other. When vc, vc' are compatible, we define their union $[vc \cup vc'] : U \cup U' \to \mathbf{N}$ as follows: $[vc \cup vc'](v) = vc(v)$ for $v \in U$ and $[vc \cup vc'](v) = vc'(v)$ for $v \in U'$.

We broaden the definition of GHZ graphs to *g-GHZ* graphs. An edge-coloured edge-weighted graph G_c^w satisfying the following properties is defined to be g-GHZ

1. All feasible monochromatic vertex colourings have a non-zero weight (instead of necessarily being 1).
2. All non-monochromatic vertex colourings have a weight of 0.

Note that this generalization allows each of the monochromatic vertex colourings to have different weights. The dimension of a g-GHZ graph is the number of feasible monochromatic vertex colourings. For a graph G, the maximum dimension achievable over all possible g-GHZ colouring and weight assignments is its *generalized matching index* $\mu_g(G)$.

▶ **Conjecture 13.** *$\mu_g(K_4) = 3$ and for a graph G which is non-isomorphic to K_4, $\mu_g(G) \leq 2$.*

We prove that Conjecture 6 and Conjecture 13 are equivalent. Trivially, a counter-example to Conjecture 6 would immediately give a counter-example to Conjecture 13. We prove that any counter-example to Conjecture 13 would also yield a counter-example to Conjecture 6 in Lemma 14. This reformulation is more suitable for our proofs in the following sections.

▶ **Lemma 14** (Scaling lemma). *If there is a graph G_c^w, which is g-GHZ, then there is a graph $G_c^{w'}$, which is a GHZ graph with the same dimension.*

Proof. We denote the weight of the vertex colouring $w(\mathbf{i}_V, G)$ using $W(i)$. Note that by definition of g-GHZ graphs, the weight of a monochromatic colouring $W(i)$ is always non-zero. So, for each edge $e \in G_c$ whose half-edges are of colour i, j, we assign the weight

$$w'(e) = w(e)(W(i)W(j))^{-1/n}$$

Let M be a matching in G_c, which induces the vertex colouring vc_M. The weight of an edge $e \in M$ between vertices u, v will be,

$$w'(e) = w(e)(W(vc_M(u))W(vc_M(v)))^{-1/n}$$

As each vertex is incident by exactly one edge of the perfect matching M, the weight of M will be

$$w'(M) = w(M) \prod_{v \in V} W(vc_M(v))^{-1/n}$$

Since the weights of all perfect matchings which induce a vertex colouring, vc will increase by a factor of $\prod_{v \in V} W(vc(v))^{-1/n}$, the weight of the vertex colouring vc will be

$$w'(vc) = w(vc) \prod_{v \in V} W(vc(v))^{-1/n}$$

As $w(vc)$ is zero for all non-monochromatic vertex colourings, $w'(vc)$ will remain to be zero.

For a monochromatic vertex colouring $vc = \mathbf{i}_V$, we know that $vc(v) = i$ for all $v \in V$. Therefore, $w'(\mathbf{i}_V) = w(\mathbf{i}_V)((w(\mathbf{i}_V))^{-1/n})^n = 1$

Therefore, $G_c^{w'}$ is a GHZ graph. ◀

2 Reduction

We prove a stronger theorem than Theorem 10 as stated below.

▶ **Theorem 15.** *Let G be a multi-graph with a vertex cut S of size 3. Let V_1 and V_2 be a partition of $V(G) \setminus S$ such that V_1 and V_2 are non-empty and there are no edges between V_1 and V_2 in G. Moreover, let $|V_1|$ be odd and $|V_2|$ be even. There exists a graph G' such that $|V(G')| \leq |V_1| + 3 \leq |V(G)| - 2$ and $\mu(G') \geq \mu(G)$.*

Let w, c be a colouring and weight assignment of G for which $\mu(G, c, w) = \mu(G)$. Then G' would be a graph on the vertex set $V_1 \bigsqcup S$. The edge set, the edge weight function and the edge colouring of G' would be the same as in $G[V_1 \bigsqcup S]$ except for the edges with both endpoints inside S; We redefine the set of edges, edge-weight function, edge-colouring within S. Let c' and w' represent the edge-colouring and the edge-weight function of G'. We will show that $\mu(G') \geq \mu(G', c', w') = \mu(G, c, w) = \mu(G)$.

Let $V = V(G)$ and $S = \{u_1, u_2, u_3\}$. Note that any perfect matching of G, should match an odd number of vertices of S to V_1 (since $|S|$ is odd). Therefore the perfect matchings of G can be grouped into 4 types:

Type 0: Let $\mathcal{P}_0$ denote the set of all perfect matchings on $G[V_1 \cup S]$ in which all the three vertices of S are matched with vertices in V_1. Let $W_0(vc)$ denote the sum of weights of the perfect matchings from $\mathcal{P}_0$ that induce the vertex colouring vc on $V_1 \bigsqcup S$. Let $\mathcal{P}'_0$ denote the set of all perfect matchings on $G[V_2]$. Let $W'_0(vc)$ denote the sum of weights of the perfect matchings from $\mathcal{P}'_0$ that induce the vertex colouring vc on V_2. Type 0 perfect matchings of G are the perfect matchings that belong to $\mathcal{P}_0 \times \mathcal{P}'_0$. Clearly, the sum of the weights of Type 0 perfect matchings that induce the colouring vc equals $W_0(vc)W'_0(vc)$.

Type *i*: For $i \in \{1, 2, 3\}$, Let $\mathcal{P}_i$ denote the set of perfect matchings of $V_1 \bigsqcup \{u_i\}$, and let $\mathcal{P}'_i$ denote the set of perfect matchings of $V_2 \bigsqcup (S \setminus \{u_i\})$. Let $W_i(vc)$ denote the sum of weights of all perfect matchings from $\mathcal{P}_i$ that induce the vertex colouring vc on $V_1 \bigsqcup \{u_i\}$ and $W'_i(vc)$ denote the sum of weights of all perfect matchings from $\mathcal{P}'_i$ that induce the colouring vc on $V_2 \bigsqcup (S \setminus \{u_i\})$. Type i matchings of G are the perfect matchings that belong to $\mathcal{P}_i \times \mathcal{P}'_i$. Clearly, the sum of weights of Type i perfect matchings that induce the colouring vc equals $W_i(vc)W'_i(vc)$. From the above discussion, it is easy to see that

$$w(vc) = \sum_{i \in \{0,1,2,3\}} W_i(vc)W'_i(vc) \tag{1}$$

Recall that c_{V_2} denotes the monochromatic vertex colouring with the colour c on V_2. Let us partition $[\mu(G)]$ into $\mathcal{C}_1 \sqcup \mathcal{C}_2$ such that $c \in \mathcal{C}_1$, if and only if there exists some colouring c' on $V_1 \sqcup S$ such that $W'_0(c_{V_2})W_0(c') \neq 0$. The remaining colors from $[\mu(G)]$ belong to $\mathcal{C}_2$ (Note that this happens if $W'_0(c_{V_2}) = 0$ or if for all colourings c' on $V_1 \sqcup S$, $W_0(c') = 0$.). We will now prove Theorem 15 in two cases. When $\mathcal{C}_1 = \emptyset$ (Theorem 1) and $\mathcal{C}_1 \neq \emptyset$ (Theorem 2)

▶ **Theorem 1.** *Let G be a multi-graph with a vertex cut of size 3. If $\mathcal{C}_1 = \emptyset$ (as defined earlier), then $\mu(G) \leq \mu(K_4)$*

▶ **Theorem 2.** *Let G be a multi-graph with a vertex cut of size 3. If $\mathcal{C}_1 \neq \emptyset$ (as defined earlier), then there exists a graph G' such that $|V(G')| \leq |V_1| + 3 \leq |V(G)| - 2$ and $\mu(G') \geq \mu(G)$. Recall that V_1 and V_2 is a partition of $V(G) \setminus S$ such that V_1 and V_2 are non-empty and there are no edges between them. Moreover $|V_1|$ is odd and $|V_2|$ is even.*

2.1 Construction for Theorem 1

Let $V(G') = \{v_0, v_1, v_2, v_3\}$. The reader may mentally map the vertices v_1, v_2, v_3 to the vertices u_1, u_2, u_3 of the vertex cut S and v_0 to the set of vertices V_1. Note that G' is a multi-graph (without self loops) and each pair of vertices from $V(G')$ may have many edges between them. In fact, we would define $\mu(G)^2$ number of edges between each pair of vertices in $\{v_0, v_1, v_2, v_2\}$, one edge for each ordered pair in $[\mu(G)] \times [\mu(G)]$.

Let $i, j \in \{1, 2, 3\}$ with $i \neq j$. Let $(p, q) \in [\mu(G)] \times [\mu(G)]$. We will define an edge e for each such (p, q) between v_i and v_j. This edge e would be coloured such that the v_i-half edge of e (i.e., e_{v_i}) has colour p and the v_j-half edge of e (i.e., e_{v_j}) has colour q. The weight of the edge would be $w(e) = \sum_{c \in \mathcal{C}_2} w(c_{V_2} p_{u_i} q_{u_j})$ The reader may recall that $c_{V_2} p_{u_i} q_{u_j}$ represents the colouring in which V_2, u_i, u_j are coloured with c, p, q respectively. Its weight is the weight of the induced subgraph of G on $V_2 \cup \{u_i, u_j\}$ filtered out by the colouring $c_{V_2} p_{u_i} q_{u_j}$. In this case, $\mathcal{C}_1 = \emptyset$; so $\mathcal{C}_2 = [\mu(G)]$; and therefore there are $\mu(G)$ terms in the summation.

We will now consider the edges between v_0 and v_i, when $i \in \{1, 2, 3\}$. Let $(p, q) \in [\mu(G)] \times [\mu(G)]$. We will define an edge e for each such (p, q) between v_0 and v_i. This edge e would be coloured such that the v_0-half edge of e (i.e., e_{v_0}) has colour p and the v_i-half edge of e (i.e., e_{v_i}) has colour q. The weight of such an edge e is defined as $w(e) = w(p_{V_1} q_{u_i})$

2.2 Proof of construction for Theorem 1

Consider any vertex colouring $vc : V' \to \mathbf{N}$ on G'. We will prove that $w(V(G'), vc) = 0$, if vc is non-monochromatic and $w(V(G'), vc) = 1$, if vc is monochromatic.

Let the vertex colouring vc be $i_{v_0} j_{v_1} k_{v_2} l_{v_3}$. To find the weight of vc, we consider the subgraph of G' filtered out by vc. For instance, between the vertices v_2 and v_3, the colouring vc would filter exactly one edge, and such an edge would have the v_2-half edge of colour k and v_3-half edge of colour l. Clearly, this gives a graph which is isomorphic to K_4 (with some edges possibly getting a weight of zero). Observe that there are only three perfect matchings in K_4. So, it is now easy to find the weight of vc by enumeration.

As an example, consider the vertex colouring in which v_0, v_1 are coloured red and v_2, v_3 are coloured green and blue, respectively. Its filtering is shown in Figure 3. Its weight would be $w_1 w'_1 + w_2 w'_2 + w_3 w'_3$.

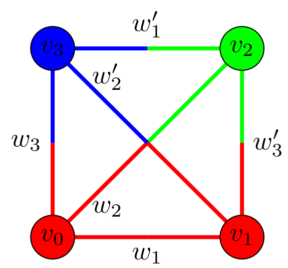


Figure 3 K_4 obtained by a filtering operation.

We will first compute the weight of perfect matching $\{\{v_0, v_1\}, \{v_2, v_3\}\}$ in vc. By substituting the edge weights from the construction, we get the weight of the perfect matching to be

$$= w(i_{V_1} j_{u_1}) \sum_{c \in [\mu(G)]} w(c_{V_2} k_{u_2} l_{u_3}) = \sum_{c \in [\mu(G)]} w(i_{V_1} j_{u_1}) w(c_{V_2} k_{u_2} l_{u_3})$$

As $w(i_{V_1} j_{u_1}) w(c_{V_2} k_{u_2} l_{u_3})$ is exactly the sum of weights of Type 1 perfect matchings for the vertex colouring $i_{V_1} j_{u_1} k_{u_2} l_{u_3} c_{V_2}$

$$= \sum_{c \in [\mu(G)]} W_1(i_{V_1} j_{u_1} k_{u_2} l_{u_3} c_{V_2}) W'_1(i_{V_1} j_{u_1} k_{u_2} l_{u_3} c_{V_2}) \tag{2}$$

Similarly, the weight of the weight of perfect matching $\{\{v_0, v_2\}, \{v_1, v_3\}\}$ in vc is

$$= \sum_{c\in[\mu(G)]} W_2(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})W'_2(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}) \tag{3}$$

and the weight of the weight of perfect matching $\{\{v_0, v_3\}, \{v_1, v_2\}\}$ in vc is

$$= \sum_{c\in[\mu(G)]} W_3(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})W'_3(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}) \tag{4}$$

As the weight of the vertex colouring vc' is the sum of these three perfect matchings, by adding the equations Equations (2)–(4), we get

$$w(vc') = \sum_{r\in\{1,2,3\}} \sum_{c\in[\mu(G)]} W_r(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})W'_r(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})$$

By rearranging the summation and using Equation (1),

$$= \sum_{c\in[\mu(G)]} \sum_{r\in\{1,2,3\}} W_r(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})W'_r(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}) = \sum_{c\in[\mu(G)]} w(i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2})$$

First suppose that $vc = i_{v_0}j_{v_1}k_{v_2}l_{v_3}$ is non-monochromatic. Clearly, $i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}$ is also non-monochromatic for all $c \in [\mu(G)]$. Since the weight of all such colourings is zero, their sum is also zero. It now follows that $w(vc) = 0$

On the other hand, suppose $vc = i_{v_0}j_{v_1}k_{v_2}l_{v_3}$ is monochromatic, i.e., $i = j = k = l$. Clearly, if $c = i$, $i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}$ is also monochromatic and has weight 1. If $c \neq i$, $i_{V_1}j_{u_1}k_{u_2}l_{u_3}c_{V_2}$ is non-monochromatic and has weight 0. Since we take the sum over all c, it now follows that $w(vc) = 1$.

2.3 Applications of construction for Theorem 1

▶ **Corollary 16.** *If the minimum degree of a graph G is 3, then $\mu(G) \leq 3$*

Proof. Let u be a three-degree vertex, and x, y, z be its neighbours. Let $V_1 = \{u\}$, $S = \{x, y, z\}$ and $V_2 = V \setminus \{u, x, y, z\}$. Note that there are no Type 0 matchings as u can match with at most one vertex in S in any perfect matching. Therefore, $W_0(c)$ is zero for all $c \in [\mu(G)]$. It is now easy to see that $\mathcal{C}_1 = \emptyset$. Therefore, from Theorem 1, $\mu(G) \leq \mu(K_4)$. From Theorem 8, it is known that the matching index of graphs with 4 vertices is at most 3. Therefore, $\mu(G) \leq \mu(K_4) = 3$. ◀

▶ **Corollary 17.** *Conjecture 6 is true for all graphs whose maximum degree is at most* 3.

Proof. From Corollary 16, we know that $\mu(G) \leq 3$. Towards a contradiction, let $\mu(G) = 3$ for graph with $|V(G)|$ >4 and maximum degree 3. Therefore, there exists a colouring c and weight assignment w such that $\mu(G, c, w) = 3$. Let the three colours be $1, 2, 3$.

We first claim that between any pair of vertices, there is at most one non-zero edge incident on it. Suppose not. Then, there exist vertices u and x_1 with multiple non-zero edge between them. Since the maximum degree of the skeleton G is at most 3, there exists a vertex set (for instance, all neighbours of u if the degree is 3) $\{x_1, x_2, x_3\}$ which separates u from the $V - \{u, x_1, x_2, x_3\}$. Let $V_1 = \{u\}$, $S = \{x_1, x_2, x_3\}$ and $V_2 = V \setminus \{u, x_1, x_2, x_3\}$. Recall that $\mathcal{C}_1 = \emptyset$. By the construction from Section 2.1, the weights of edges between u and the vertices $\{x_1, x_2, x_3\}$ remain unchanged. Therefore, we obtain a graph with 4 vertices of dimension 3 such that a pair of vertices have multiple non-zero edges between them. But this is not possible from Theorem 8. Therefore, there are no multi-edges in G_c^w.

Since the matching index is 3, there are perfect matchings (of non-zero edges) of colours $1, 2, 3$. Therefore, from Theorem 7, there must be at least one non-monochromatic perfect matching M (of non-zero edges), say inducing the non-monochromatic vertex colouring vc. But there is exactly one non-zero edge of colours $1, 2, 3$ incident on u. Therefore, for any vertex colouring vc, there can be at most one perfect matching M' inducing vc. It now follows that $w'(M) = w'(vc) = 0$. Therefore, there must be an edge, say of colour 1, whose weight is zero; hence, the monochromatic vertex colouring of 1 must be zero. Contradiction.

Therefore, $\mu(G) \leq 2$ when $|V(G)| > 4$. ◀

2.4 Construction for Theorem 2

Recall that $S = \{u_1, u_2, u_3\}$ is a vertex cut separating V_1 from V_2 in the graph G, where $|V_1|$ is odd, $|V_2|$ is even. Assume that $\mathcal{C}_1 \neq \emptyset$. For this case, we will construct an edge-weighted, edge coloured multi-graph G' with $V(G') = V_1 \cup S$ and $\mu(G') \geq \mu(G)$. Since $|V_2| \geq 2$, $|V(G')| \leq |V(G)| - 2$.

If a pair of vertices is such that at least one of them lies in V_1, then the set of edges in G' between this pair of vertices is the same as those in G with the same weights and colours. Between the pairs of vertices with both vertices from S, we define one edge for each pair of colours in $[\mu(G)] \times [\mu(G)]$. Thus there would be $(\mu(G))^2$ edges between each pair, $\{u_i, u_j\}, i \neq j$.

We now describe how to assign weight to a coloured edge e between the vertices u_i and u_j, where $i < j$ and $i, j \in \{1, 2, 3\}$ such that the u_i-half of e is coloured p and the u_j-half of e is coloured q.

$$w'(e) = \sum_{c \in \mathcal{C}_2} W(c_{V_2} p_{u_i} q_{u_j}) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W(c_{V_2} p_{u_i} q_{u_j})}{W(c_{V_2})} \tag{5}$$

▶ Remark 18. Recall that our plan is to remove V_2 and the edges incident on V_2 completely in order to get the reduced graph G'. This should be done without losing the information about the weights of monochromatic vertex colourings of V_2 to make sure that $\mu(G')$ does not become smaller than $\mu(G)$. The weight assignment is similar in spirit to the weight assignment done for the construction of Theorem 1. The expression here is more complicated in this case, because of the adjustments required to make it work: This will be clear when the reader goes through the proof carefully.

2.5 Proof of the construction for Theorem 2

Consider any vertex colouring $vc' : V_1 \cup S \to \mathbf{N}$ of G'. Let us denote vc' more explicitly, using the notation describe in Section 2.1, as $(\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}$. Note that α here is the vertex colouring induced on V_1 by the vertex colouring vc', i, j, k are the colours of u_1, u_2, u_3 respectively under the vertex colouring vc'. (Note that we use the notation $(\alpha)_{V_1}$ to emphasize that this is not necessarily a monochromatic colouring of V_1, using a single colour named α; rather it can be any vertex colouring, monochromatic or non-monochromatic.) We will use the notation of w' to denote the weights of vertex colourings of G' and its subgraphs and w to denote the weights of vertex colourings of G and its subgraphs. For example, $w(i_{V_1} j_S)$ is the weight of the vertex colouring $i_{V_1} j_S$ with respect to the edge-set of G, whereas $w'(i_{V_1} j_S)$ denotes the weight of the same vertex colouring with respect to the edge-set of G'. Our intention is to prove that $w'((\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}) = 0$, whenever $(\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}$ is non-monochromatic and $w'((\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}) \neq 0$, whenever $(\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}$ is monochromatic, i.e. $i = j = k$ and α is a monochromatic vertex colouring of V_1 using colour i, i.e. $(\alpha)_{V_1} = i_{V_1}$. The reader may note that we are not insisting the weight to be equal to 1 in the monochromatic case; non-zero is sufficient since we can then use the Scaling Lemma (Lemma 14) to scale the weights of the monochromatic vertex colourings to 1, thus constructing an edge-weight function w' and edge-colouring c' of G' such that $\mu(G', c', w') = \mu(G)$ implying $\mu(G') \geq \mu(G)$.

Recall that $vc' = (\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3}$ filters out a simple graph from G' and the weight of vc' is the sum of weights of all the perfect matchings (PMs) in this filtered out simple graph. Perfect matchings (PMs) of this graph can be grouped into 4 categories: (1) Type $0'$: PMs containing none of the edges with both endpoints in S. (2) Type $1'$: PMs containing the edge (u_2, u_3) (3) Type $2'$: PMs containing the edge (u_1, u_3) (4) Type $3'$: PMs containing the edge (u_1, u_2) For $t = 0, 1, 2, 3$, we denote the total weight of Type t' PMs by W'_t. Clearly $w'(vc') = \sum_{0 \leq t \leq 3} W'_t$.

Now let us consider a corresponding vertex colouring of G, $vc = (\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3} c_{V_2}$, which is obtained by taking the same vertex colouring vc' for $V_1 \cup S$, and then extending it by the monochromatic vertex colouring c_{V_2} of V_2, using the colour c. Since we may use any colour $c \in [\mu(G)]$ to extend the vertex colouring vc' of $V_1 \cup S$ to a vertex colouring of $V_1 \cup S \cup V_2$, it is more appropriate to call the extended colouring $(\alpha)_{V_1} i_{u_1} j_{u_2} k_{u_3} c_{V_2}$, it is better to denote $vc(c)$, rather than just vc.

The weight of vc on G can also be decomposed into 4 terms corresponding to 4 different groups of perfect matchings of the subgraph filtered out by vc from G.

(1) Type 0: The PMs in which all the three vertices of S are matched to vertices in V_1.

(2) Type t for $t = 1, 2, 3$: The PMs in which only u_t is matched to some vertex of V_1, and the remaining two vertices of S are either matched to each other or to vertices of V_2.

The total weight of the perfect matchings (in the the subgraph of G filtered out by the vertex colouring $vc(c)$) of Type$t, 0 \leq t \leq 3$ will be denoted by $W_t(c)$ where $c \in [u(G)]$. Clearly $w(vc(c)) = \sum_{0 \leq t \leq 3} W_t(c)$. Now we show that W'_t can be expressed as a (weighted) sum of $W_t(c)$ over the colours $c \in [\mu(G)]$.

▶ **Observation 19.** *For* $t = 1, 2, 3 : W'_t = \sum_{c \in \mathcal{C}_2} W_t(c) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_t(c)}{w(c_{V_2})}$

Proof. Let us calculate the total weight W'_1 of Type 1 perfect matchings of the vertex colouring $\alpha_{V_1} i_{u_1} j_{v_2} k_{v_3}$. (The case when $t = 2, 3$ is similar.) Clearly these PMs are obtained by adding the edge (u_2, u_3) of colour (j, k) to each perfect matching of the induced subgraph on $V_1 \cup \{u_1\}$ (after filtering out by the vertex colouring $\alpha_{V_1} i_{u_1}$). Therefore the total weight of these PMs can be written as $W'_1 = w'(\alpha_{V_1} i_{u_1}) w'(e)$ where e is the edge between u_2 and u_3 of colour (i, j), that is, the edge e with u_2-half of e coloured j and u_3-half of e coloured k. Now substituting for $w'(e)$, the right hand side of equation 5, we get

$$W'_1 = w'(\alpha_{V_1} i_{u_1}) \left(\sum_{c \in \mathcal{C}_2} w(c_{V_2} j_{u_2} k_{u_3}) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{w(c_{V_2} j_{u_2} k_{u_3})}{w(c_{V_2})} \right) \tag{6}$$

Note that $w'((\alpha)_{V_1} i_{u_1}) = w((\alpha)_{V_1} i_{u_1})$ since in the induced subgraph on $V_1 \cup \{u_1\}$ the edge set, weights and colour are same for both G and G'. It follows that,

$$W'_1 = \sum_{c \in \mathcal{C}_2} w((\alpha)_{V_1} i_{u_1})) w(c_{V_2} j_{u_2} k_{u_3}) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{w((\alpha)_{V_1} i_{u_1})) w(c_{V_2} j_{u_2} k_{u_3})}{w(c_{V_2})} \tag{7}$$

Noting that $w(\alpha_{V_1} i_{u_1}) w(c_{V_2} j_{u_2} k_{u_3}) = w(\alpha_{V_1} i_{u_1} j_{u_2} k_{u_3} c_{V_2}) = W_1(c)$ we get,

$$W'_1 = \sum_{c \in \mathcal{C}_2} w(\alpha_{V_1} i_{u_1} c_{V_2} j_{u_2} k_{u_3}) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{w(\alpha_{V_1} i_{u_1} c_{V_2} j_{u_2} k_{u_3})}{w(c_{V_2})} = \sum_{c \in \mathcal{C}_2} W_1(c) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_1(c)}{w(c_{V_2})}$$

Similar arguments allow us establish the required result for $t = 2, 3$ also. ◀

▶ **Observation 20.** $w(vc') = \sum_{c \in \mathcal{C}_2} w(vc(c)) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{w(vc(c))}{w(c_{V_2})}$

Proof. Now $w'(vc') = W_0' + W_1' + W_2' + W_3'$
$= W_0' + \sum_{c \in \mathcal{C}_2} (W_1(c) + W_2(c) + W_3(c)) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_1(c) + W_2(c) + W_3(c)}{w(c_{V_2})}$

Recall that for any colour $c \in [\mu(G)]$, $w(vc(c)) = W_0(c) + W_1(c) + W_2(c) + W_3(c)$. Note that for colours $c \in \mathcal{C}_2$, $W_0(c) = W_0'.w(c_{V_2})$; and therefore $W_1(c)+W_2(c)+W_3(c) = w(vc(c))$, the weight of the vertex colouring $\alpha_{V_1} i_{u_1} j_{u_2} k_{u_3} c_{V_2}$. Now W_0' can be trivially rewritten as $\frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_0'.w(c_{V_2})}{w(c_{V_2})}$. Since $W_0'.w(c_{V_2}) = W_0(c)$, this expression can be rewritten as $\frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_0(c)}{w(c_{V_2})}$.

So we can combine the terms of this expression, term by term with the terms inside the sum over $c \in \mathcal{C}_1$ and rewrite the expression as follows:

$$= \sum_{c \in \mathcal{C}_2} w(vc(c)) + \frac{1}{|\mathcal{C}_1|} \sum_{c \in \mathcal{C}_1} \frac{W_0(c) + W_1(c) + W_2(c) + W_3(c)}{w(c_{V_2})} \tag{8}$$

Since for colours $c \in \mathcal{C}_1$, $W_0(c) + W_1(c) + W_2(c) + W_3(c) = w(vc(c))$ we get the required result. ◀

If vc' is non-monochromatic, then $vc(c)$ is also non-monochromatic for any $c \in [\mu(G)]$. Therefore, $w(vc(c)) = 0$ for all c and hence $w'(vc') = 0$ from Observation 20.

If vc' is monochromatic, say of colour i, $vc(c)$ will be monochromatic if and only if $c = i$. Therefore, if $i \in \mathcal{C}_2$, then $w(vc') = w(vc(i)) = 1$. Similarly, if $i \in \mathcal{C}_1$, then $w'(vc') = \frac{1}{|\mathcal{C}_1| w(\mathbf{i}_{V_2})}$ from Observation 20. In both the cases this will be non-zero as required.

The weights can now be readjusted by the Scaling Lemma (Lemma 14) to get a GHZ graph.

2.6 Limitations of our reduction

A careful reader might observe that the difficulty in extending our reduction technique to cuts of larger size comes from the case when two newly introduced edges are part of the same perfect matching. For instance, for the case when there is a 4 vertex cut $\{u_1, u_2, u_3, u_4\}$ separating V_1, V_2 (both of even size) in G, one could try to extend our ideas and capture the weights from $V_2 \cup \{u_3, u_4\}$ and $V_2 \cup \{u_1, u_2\}$ on the edges $(v_3, v_4), (v_1, v_2)$ of G', respectively. However, this would create some extra terms in G' due to the perfect matchings in which (v_1, v_2) and (v_3, v_4) are contained. Such terms could destroy the GHZ property of G'. We believe that finding a way to bypass this difficulty and finding a more general reduction will resolve Krenn and Gu's conjecture for all graphs.

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