NPA Hierarchy for Quantum Isomorphism and Homomorphism Indistinguishability*

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Abstract

Mančinska and Roberson [FOCS'20] showed that two graphs are quantum isomorphic if and only if they are homomorphism indistinguishable over the class of planar graphs. Atserias et al. [JCTB'19] proved that quantum isomorphism is undecidable in general. The NPA hierarchy gives a sequence of semidefinite programming relaxations of quantum isomorphism. Recently, Roberson and Seppelt [ICALP'23] obtained a homomorphism indistinguishability characterization of the feasibility of each level of the Lasserre hierarchy of semidefinite programming relaxations of graph isomorphism. We prove a quantum analogue of this result by showing that each level of the NPA hierarchy of SDP relaxations for quantum isomorphism of graphs is equivalent to homomorphism indistinguishability over an appropriate class of planar graphs. By combining the convergence of the NPA hierarchy with the fact that the union of these graph classes is the set of all planar graphs, we are able to give a new proof of the result of Mančinska and Roberson [FOCS'20] that avoids the use of the theory of quantum groups. This homomorphism indistinguishability characterization also allows us to give a randomized polynomial-time algorithm deciding exact feasibility of each fixed level of the NPA hierarchy of SDP relaxations for quantum isomorphism.

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1 Introduction

Two graphs G and H are said to be *homomorphism indistinguishable* over a class of graphs $\mathcal{F}$, written $G \cong_{\mathcal{F}} H$, if for every graph $F \in \mathcal{F}$, the number of homomorphisms from F to G is the same as the number of homomorphisms from F to H. A classic result from [Lov67] states that two graphs G and H are isomorphic if and only if they are homomorphism indistinguishable over all graphs. Since then, several relaxations of graph isomorphism from fields as diverse as finite model theory [Dvo10, Gro20, FSS24], algebraic graph theory [DGR18], optimisation [GRS25, RS24], machine learning [XHLJ18, MRF+19, ZGD+24], and category theory [DJR21, AJP22, MS22] were found to be homomorphism indistinguishability relations over suitable graph classes. Recently, a coherent theory which addresses the descriptive and computational complexity of homomorphism indistinguishability relations has begun to emerge [Rob22, Sep23, Neu24, Sep24a], cf. the monograph [Sep24b].

A ground-breaking connection between quantum information and homomorphism indistinguishability was found by Mančinska and Roberson [MR20]: They showed that two graphs are quantum isomorphic if and only if they are homomorphism indistinguishable over all planar graphs. Quantum isomorphism, as introduced by [AMR+19], is a natural relaxation of graph isomorphism in terms of the graph isomorphism game, where two cooperating players called Alice and Bob try to convince a referee that two graphs are isomorphic. A perfect deterministic strategy exists for the (G, H)-isomorphism game if and only if the graphs G and H are isomorphic. Two graphs G and H are said to be *quantum isomorphic*, written $G \cong_q H$, if there is a perfect quantum strategy (G, H)-isomorphism game, i.e., a perfect strategy making use of local quantum measurements on a shared entangled state.

The proof of Mančinska's and Roberson's result [MR20] heavily relies on certain esoteric mathematical objects called quantum groups. In more detail, the main idea of the proof is to interpret homomorphism tensors of bilabelled graphs as intertwiners of the quantum automorphism groups of the respective graphs.

Another recent result from [RS24] also obtained a homomorphism indistinguishability characterisation for each level of the Lasserre hierarchy of semidefinite programming (SDP) relaxations for the integer program for isomorphism between two graphs. More precisely, for each

$k \in \mathbb{N}$, the authors of [RS24] constructed a class of graphs $\mathcal{L}_k$ such that the k^{th}-level of the Lasserre hierarchy of SDP relaxations of the integer program for deciding whether G and H are isomorphic is feasible if and only if G and H are homomorphism indistinguishable over the graph class $\mathcal{L}_k$.

It was also shown in [AMR+19] that deciding quantum isomorphism of graphs is undecidable—contrary to deciding isomorphism of graphs, which is clearly decidable and currently known to be solvable in quasipolynomial time [Bab16]. This motivates the study of relaxations of quantum isomorphism. The NPA hierarchy [NPA08], which can be thought of as a noncommutative analogue of the Lasserre hierarchy, is a sequence of SDP relaxations of the problem of determining if a given joint conditional probability distribution arises from quantum mechanics. In particular, the NPA hierarchy can be used to formulate a hierarchy of SDP relaxations for the problem of deciding whether two graphs are quantum isomorphic.

In light of results from [MR20, RS24], it is natural to ask if the feasibility of each level of these SDP relaxations of quantum isomorphism can be characterised as a homomorphism indistinguishability relation over some family of graphs. Such a characterisation would make the NPA hierarchy subject to the emerging theory of homomorphism indistinguishability. For example, a recent result [Sep24a] asserts that, over every minor-closed graph class of bounded treewidth, homomorphism indistinguishability can be decided in randomized polynomial time. The NPA relaxation, being a semidefinite program, can be solved using standard techniques such as the ellipsoid method. However, such techniques can, in polynomial time, only decide the approximate feasibility of a system. A homomorphism indistinguishability characterisation of the NPA hierarchy would imply, for each of its levels, the existence of a randomized polynomial-time algorithm for deciding exact feasibility [Neu24, Sep23, Sep24a].

1.1 Main Results

Our main contribution is a homomorphism indistinguishability characterization for each level of the NPA hierarchy, as formalized by the following theorem.

Theorem 1.1 (Main Theorem). *For graphs G and H and $k \in \mathbb{N}$, the following are equivalent:*

(i) *there is a solution for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game;*
(ii) *there is a level-k quantum isomorphism map from G to H;*
(iii) *G and H are algebraically k-equivalent;*
(iv) *G and H are homomorphism indistinguishable over the family of graphs $\mathcal{P}_k$.*

In particular, the k^{th}-level of the NPA hierarchy is feasible for the (G, H)-isomorphism game if and only G and H are homomorphism indistinguishable over the graph class $\mathcal{P}_k$. Here, $\mathcal{P}_k$ is a bounded-treewidth minor-closed class of planar graphs, which we construct by interpreting the NPA systems of equations in light of a correspondence between combinatorics (bilabelled graphs) and algebra (homomorphism tensors) which underpins many recent results regarding homomorphism indistinguishability [MR20, GRS25, RS23, RS24].

As a corollary of Theorem 1.1, we devise a randomized polynomial-time algorithm for deciding the exact feasibility of each level of the NPA hierarchy. To that end, we first show that the graph classes $\mathcal{P}_k$ are minor-closed and of bounded treewidth, which is a graph parameter roughly measuring how far is a graph from a tree. Hence, a recent result from [Sep24a] implies that, for each $k \in \mathbb{N}$, there exists a randomized polynomial-time algorithm for deciding homomorphism indistinguishability over $\mathcal{P}_k$. We strengthen this result by making the dependence on the parameter k effective.

Theorem 1.2. *There exists a randomized algorithm which decides, given graphs G and H and an integer $k \geq 1$, whether the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game is feasible. The algorithm always runs in time $n^{O(k)}k^{O(1)}$ for $n := \max\{|V(G)|, |V(H)|\}$, accepts all YES-instances, and accepts NO-instances with probability less than one half.*

1.2 Proof Techniques

The main algebraic-combinatorial tools we use are bilabelled graphs and their homomorphism tensors. *Bilabelled graphs* are graphs with distinguished vertices which are said to carry labels. To a bilabelled graph $\boldsymbol{F} = (F, u, v)$ and an unlabelled graph G, one can associated the *homomorphism tensor* $\boldsymbol{F}_G \in \mathbb{N}^{V(G) \times V(G)}$ such that $\boldsymbol{F}_G(x, y)$ for $x, y \in V(G)$ is the number of homomorphisms $h \colon F \to G$ such that $h(u) = x$ and $h(v) = y$. For example, the bilabelled graph $\boldsymbol{A} = (A, u, v)$ with $V(A) = \{u, v\}$ and $E(A) = \{uv\}$ denotes the complete 2-vertex graph each of whose vertices u and v carry one label. In the case of $\boldsymbol{A}$, the matrix $\boldsymbol{A}_G$ is just the adjacency matrix of G. The fruitfulness of this construction stems from a correspondence between combinatorial operations on bilabelled graphs and algebraic operations on homomorphism tensors. For example, the *matrix product* $(\boldsymbol{F}_1)_G \cdot (\boldsymbol{F}_2)_G$ yields the homomorphism tensor of the bilabelled graph obtained by taking the *series composition* of $\boldsymbol{F}_1$ and $\boldsymbol{F}_2$.

We prove Theorem 1.1 by interpreting the NPA relaxation as a system of equations whose constraints involve homomorphism tensors and algebraic operations. Applying the aforementioned algebro-combinatorial correspondence, the graph class $\mathcal{P}_k$ is then obtained by reading the constraints as a description of a graph class via bilabelled graphs and combinatorial operations. To that end, we first give various reformulations of the NPA systems of equations as listed in Items (ii) and (iii) of Theorem 1.1. The proofs follow the outline below:

- In Theorem 3.6, we first show that a principal submatrix of a certificate for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game can be interpreted as a the Choi matrix of a completely positive map from $M_{V(G)^k}(\mathbb{C})$ to $M_{V(H)^k}(\mathbb{C})$ with certain properties. Such a completely positive map is known as a level-k quantum isomorphism map. We also show that the Choi matrix of such a level-k quantum isomorphism map (uniquely) extends to a certificate for the k^{th}-level of the NPA hierarchy for quantum isomorphism, thus showing that the existence of such a map is equivalent to the feasibility of the k^{th}-lvel of the NPA hierarchy.
- In Theorem 3.9, restrictions of the aforementioned completely positive maps are then shown to be algebra homomorphisms mapping homomorphism tensors of $\mathcal{Q}_k$ for G to homomorphism tensors of $\mathcal{Q}_k$ for H, where $\mathcal{Q}_k$ is the set of *atomic graphs* which form the building blocks for the graph class $\mathcal{P}_k$. Such an algebra homomorphism is called an *algebraic k-equivalence.*
- Lastly, in Theorem 4.4, we use the correspondence between combinatorial operations on graphs and algebraic operations on their homomorphism tensors to show that the existence of an algebraic k-equivalence is equivalent to homomorphism indistinguishability over $\mathcal{P}_k$.

The overall structure of the proof of Theorem 1.1 is inspired by the proof of the main result of [RS24], however, due to the "noncommutativity" of the NPA hierarchy, additional difficulties arise. For example, the proof of inner-product compatibility of the graph classes $\mathcal{L}_k$ from [RS24] is trivial, while proving the same for our graph classes $\mathcal{P}_k$ requires a creative construction in Lemma 4.2.

We take a more thorough look at the graph classes $\mathcal{P}_k$ in Section 4.2. We show that the set of underlying graphs of the union of the bilabelled graph classes $\mathcal{P}_k$ is the set of all planar graphs. By combining this result with the convergence of the NPA hierarchy, we derive a substantially simpler proof of the homomorphism indistinguishability characterization of quantum isomorphism given in [MR20]. In particular, we are able to avoid the use of heavy machinery for dealing with compact quantum groups, which formed one of the main ingredients of the proof in [MR20].

Corollary 1.3. *For graphs G and H, the following are equivalent:*

1. *for every k, there is a solution for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game,*
2. *G and H are homomorphism indistinguishable over $\bigcup_{k \in \mathbb{N}} \mathcal{P}_k$, the class of all planar graphs,*

3. *G and H are quantum isomorphic.*

The proof of Theorem 1.2 relies on the characterisation of the NPA hierarchy as homomorphism indistinguishability relations from Theorem 1.1. That is, instead of attempting to solve the NPA systems of equations, the algorithm decides whether the input graphs are homomorphism indistinguishable over the graph class $\mathcal{P}_k$. This is done by computing a basis for the finite-dimensional vector space spanned by the homomorphism tensors of the bilabelled graphs in $\mathcal{P}_k$. To that end, the algorithm utilises the inductive definition of the graph class $\mathcal{P}_k$ in terms of generators and combinatorial operations. Being linear or bilinear, their algebraic counterparts can be used to efficiently compute this basis via a fixed-point procedure, which terminates after polynomially many steps. Randomization is only necessary to deal with integers which would otherwise grow to exponential size in the course of the computation. To overcome this issue, the algorithm relies on linear algebra over finite fields of prime characteristics which are chosen at random.

1.3 Outline

The paper begins by covering some of the preliminaries in Section 2. We introduce bilabelled graphs and homomorphism tensors in Section 2.1, which are our main tools to relate the algebraic question of feasibility of the NPA hierarchy to a combinatorial problem of homomorphism indistinguishability. We then introduce the graph isomorphism game and a suitable version of the NPA hierarchy for the graph isomorphism game in Section 2.2. The proof of Theorem 1.1 will be broken down into a series of simpler theorems, namely Theorems 3.6, 3.9 and 4.4. This is done in Section 3 and the beginning of Section 4. In Section 4.2 we study the graph classes $\mathcal{P}_k$ in more detail and finish the proof of Corollary 1.3, thus providing the promised alternative proof of the main result of [MR20]. In Section 5, we show that there is a polynomial time randomized algorithm for each fixed level of the NPA hierarchy for quantum isomorphism.

2 Preliminaries

All graphs in this article are undirected, finite, and without multiple edges, unless stated otherwise. A graph is said to be *simple* if it does not contain any loops. A *homomorphism* $h\colon F \to G$ from a graph F to a graph G is a map $V(F) \to V(G)$ such that for all $uv \in E(F)$ it holds that $h(u)h(v) \in E(G)$. Note that this implies that any vertex in F carrying a loop must be mapped to a vertex carrying a loop in G.

Write $\hom(F, G)$ for the number of homomorphisms from F to G. For a family of graphs $\mathcal{F}$ and graphs G and H we write $G \cong_{\mathcal{F}} H$ if G and H are *homomorphism indistinguishable over* $\mathcal{F}$, i.e., if $\hom(F, G) = \hom(F, H)$ for all $F \in \mathcal{F}$. Since the graphs G and H into which homomorphisms are counted are throughout assumed to be simple, looped graphs in $\mathcal{F}$ can generally be disregarded as they do not admit any homomorphisms into simple graphs. For background on homomorphism indistinguishability, see [Sep24b].

Given a finite set Ω, we denote the symmetric group containing all permutations of Ω by $\mathfrak{S}_\Omega$. Given a natural number $k \in \mathbb{N}$, we will denote We use $\mathfrak{S}_k$ to denote $\mathfrak{S}_{[k]}$. We shall use $\mathscr{C}(1, \dots, k, 2k, \dots, k+1)$ to denote the group of cyclic permutations of the set $\Omega :=$ $\{1, \dots, k, 2k, \dots, k+1\}$, i.e., the cyclic subgroup of $\mathfrak{S}_\Omega$ generated by the transposition (12).

2.1 Bilabelled Graphs and Homomorphism Tensors

We recall the following definitions from [MR20, GRS25].

For $k, l \geq 1$, a (k,l)-*bilabelled graph* is a tuple $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ where F is a graph and $\boldsymbol{u} = (u_1, \dots, u_k) \in V(F)^k$, $\boldsymbol{v} = (v_1, \dots, v_l) \in V(F)^l$. The $\boldsymbol{u}$ are the *in-labelled vertices* of $\boldsymbol{F}$ while the $\boldsymbol{v}$ are the *out-labelled vertices* of $\boldsymbol{F}$. Given a graph G, the *homomorphism tensor* of

$\boldsymbol{F}$ for G is $\boldsymbol{F}_G \in \mathbb{C}^{V(G)^k \times V(G)^l}$ whose $(\boldsymbol{x}, \boldsymbol{y})$-entry is the number of homomorphisms $h \colon F \to G$ such that $h(\boldsymbol{u}_i) = \boldsymbol{x}_i$ and $h(\boldsymbol{v}_j) = \boldsymbol{y}_j$ for all $i \in [k]$ and $j \in [l]$.

For a (k,l)-bilabelled graph $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$, write $\operatorname{soe}(\boldsymbol{F}) \coloneqq F$ for the underlying unlabelled graph of $\boldsymbol{F}$. If $k = l$, write $\operatorname{Tr}(\boldsymbol{F})$ for the unlabelled graph underlying the graph obtained from $\boldsymbol{F}$ by identifying $\boldsymbol{u}_i$ with $\boldsymbol{v}_i$ for all $i \in [l]$. For $\sigma \in \mathfrak{S}_{k+l}$, write $\boldsymbol{F}^\sigma \coloneqq (F, \boldsymbol{x}, \boldsymbol{y})$ where $\boldsymbol{x}_i \coloneqq (\boldsymbol{uv})_{\sigma(i)}$ and $\boldsymbol{y}_{j-k} \coloneqq (\boldsymbol{uv})_{\sigma(j)}$ for all $1 \leq i \leq k < j \leq k+l$, i.e. $\boldsymbol{F}^\sigma$ is obtained from $\boldsymbol{F}$ by permuting the labels according to σ. We also define $\boldsymbol{F}^* \coloneqq (F, \boldsymbol{v}, \boldsymbol{u})$ the graph obtained by swapping in- and out-labels.

Let $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ and $\boldsymbol{F}' = (F', \boldsymbol{u}', \boldsymbol{v}')$ be (k,l)-bilabelled and (m,n)-bilabelled, respectively. If $l = m$, write $\boldsymbol{F} \cdot \boldsymbol{F}'$ for the (k,n)-bilabelled graph obtained from them by *series composition*, whose underlying unlabelled graph obtained from the disjoint union of F and F' by identifying $\boldsymbol{v}_i$ and $\boldsymbol{u}'_i$ for all $i \in [l]$. Multiple edges arising in this process are removed. The in-labels of $\boldsymbol{F} \cdot \boldsymbol{F}'$ lie on $\boldsymbol{u}$, the out-labels on $\boldsymbol{v}'$.

If $k = m$ and $l = n$ write $\boldsymbol{F} \odot \boldsymbol{F}'$ for the *parallel composition* of $\boldsymbol{F}$ and $\boldsymbol{F}'$. The underlying unlabelled graph of the (k,l)-bilabelled graph $\boldsymbol{F} \odot \boldsymbol{F}'$ is the graph obtained from the disjoint union of F and F' by identifying $\boldsymbol{u}_i$ with $\boldsymbol{u}'_i$ and $\boldsymbol{v}_j$ with $\boldsymbol{v}'_j$ for all $i \in [k]$ and $j \in [l]$. Again, multiple edges are dropped. The in-labels of $\boldsymbol{F} \odot \boldsymbol{F}'$ lie on $\boldsymbol{u}$, the out-labels on $\boldsymbol{v}$.

As observed in [MR20, GRS25], the benefit of these combinatorial operations is that they have an algebraic counterpart. Formally, for all graphs G and all (l,l)-bilabelled graphs $\boldsymbol{F}, \boldsymbol{F}'$, it holds that $\operatorname{soe}(\boldsymbol{F}_G) = \hom(\operatorname{soe} \boldsymbol{F}, G)$, $\operatorname{Tr}(\boldsymbol{F}_G) = \hom(\operatorname{Tr} \boldsymbol{F}, G)$, $(\boldsymbol{F}_G)^\sigma = (\boldsymbol{F}^\sigma)_G$, $(\boldsymbol{F} \cdot \boldsymbol{F}')_G = \boldsymbol{F}_G \cdot \boldsymbol{F}'_G$, and $(\boldsymbol{F} \odot \boldsymbol{F}')_G = \boldsymbol{F}_G \odot \boldsymbol{F}'_G$, where $\operatorname{soe}(X)$ denotes the sum of elements, Tr denotes the trace, $\cdot$ denotes matrix multiplication and $\odot$ denotes Schur product.

Slightly abusing notation, we say that two graphs G and H are homomorphism indistinguishable over a family of bilabelled graphs $\mathcal{S}$, in symbols $G \cong_{\mathcal{S}} H$ if G and H are homomorphism indistinguishable over the family $\{\operatorname{soe} \boldsymbol{S} \mid \boldsymbol{S} \in \mathcal{S}\}$ of the underlying unlabelled graphs of the $\boldsymbol{S} \in \mathcal{S}$.

We conclude this subsection by defining the notion of a minor of bilabelled graphs.

Definition 2.1 ([RS24])**.** Let $\boldsymbol{M}$ and $\boldsymbol{F}$ be (k,l)-bilabelled graph. Then, M is said to be a *bilabelled minor* of $\boldsymbol{F}$, written $\boldsymbol{M} \leq \boldsymbol{F}$, if it can be obtained from $\boldsymbol{F}$ by applying a sequence of the following bilabelled minor operations:

1. edge contraction
2. edge deletion
3. deletion of unlabelled vertices.

We note that the if a bilabelled graph $\boldsymbol{M}$ is a bilabelled minor of $\boldsymbol{F}$, then M is a minor of F [RS24, Lemma 4.12]. Similarly, if $\boldsymbol{F}$ is a bilabelled graph and M is a graph such that M is a minor of F, there exists a bilablled graph $\boldsymbol{M'}$ such that M' is the union of M with some unlabelled vertices [RS24, Lemma 4.13].

Remark 2.1.1 (drawing bilabelled graphs)*.* Throughout the paper we will depict bilabelled graphs as follows. To draw a bilabelled graph $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$, we draw the graph F and attach i^{th} input "wire", depicted in grey, to u_i and j^{th} output wire to v_i. Vertices can have multiple input/output wires attached to them. The input and output wires extend to the far right and far left of the picture respectively. Finally, in order to indicate which input/output wire is which, we draw them so that they occur in numerical order (first at the top) at the edges of the picture. See Fig. 1(a) for an example of a bilabelled graph and Fig. 1(b) for an illustration of series and parallel composition, defined above.

2.2 The Graph Isomorphism Game

We begin this section by defining the graph isomorphism game. We refer the reader to [AMR+19] for more details.

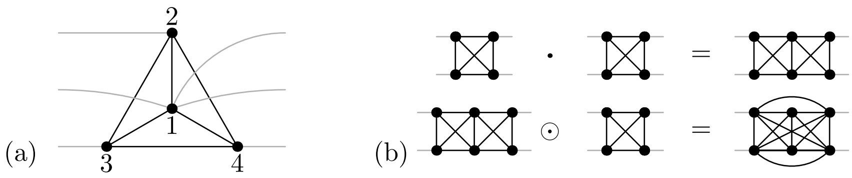

Figure 1: (a) $\boldsymbol{F} = (K_4, (2,1,3), (1,1,4))$. (b) And example of series and parallel composition.

Definition 2.2. Let G, H be two graphs with $|V(G)| = |V(H)|$. The (G,H)-isomorphism game is cooperative game involving two players Alice and Bob, and the verifier. It is played as follows:

- In each round of the game, the verifier chooses two vertices $g, g' \in V(G)$ (sampled uniformly and independently) and sends them to Alice and Bob respectively.
- Alice and Bob are not allowed to communicate during a round of the game, i.e. after receiving their question from the verifier. However, they are free to strategize before the game starts.
- Alice and Bob respond with vertices $h, h' \in V(H)$, respectively.
- The verifier decides whether Alice and Bob win or lose this round of the game based on the rule function or predicate $V(h, h' \mid g, g')$ which is given by

$$V(h, h' \mid g, g') = \begin{cases} 1 & \text{if } \mathrm{rel}_G(g, g') = \mathrm{rel}_H(h, h') \\ 0 & \text{otherwise} \end{cases}$$

Here $\mathrm{rel}_G(g, g') = \mathrm{rel}_H(h, h')$ if and only if both pairs of vertices are adjacent, non-adjacent, or identical.

Alice and Bob can employ a wide array of strategies to play this game. A *deterministic strategy* is one that involves two functions $f_A, f_B \colon V(G) \to V(H)$, where Alice and Bob respond with $f_A(g), f_B(g')$ when presented with the questions g, g' respectively. A *perfect strategy* is one that always wins the game for Alice and Bob.

The predicate necessitates that $f_A = f_B$ for any perfect deterministic strategy (f_A, f_B). Indeed, if $g = g'$, one sees that $f_A(g) = f_B(g)$ for all $g \in V(G)$. Similarly, it is not too difficult to show that $f_A = f_B = f$ is a graph isomorphism, if it is a perfect deterministic strategy. It is also clear that if Alice and Bob answer according to some isomorphism $f \colon V(G) \to V(H)$, then this is a perfect strategy. Hence, the perfect deterministic strategies of the (G,H)-isomorphism game are in bijective correspondence with the isomorphisms of G and H.

Alice and Bob can also make use of *probabilistic strategies*. A probabilistic strategy is given by joint conditional probability distributions $(p(h, h' \mid g, g'))_{g,g' \in V(G), h,h' \in V(H)}$. Probabilistic strategies are often called *correlations* in the literature. We shall denote the set of correlations indexed by the input sets X, Y and the output sets A, B by $P(X, Y, A, B)$. In the case where $X = Y$ and $A = B$, we shall use the notation $P(X, A)$ instead.

It is easy to see that a probabilistic strategy is a perfect strategy for the (G,H)-isomorphism game if and only if $V(h, h' \mid g, g') = 0$ implies that $p(h, h' \mid g, g') = 0$ for all $g, g' \in V(G)$ and $h, h' \in V(H)$. We also note that any perfect probabilistic strategy for the (G,H)-isomorphism game satisfies that $p(h, h' \mid g, g) = 0$ for all $h \neq h' \in V(H)$ and $g \in V(H)$. Such correlations are known as *synchronous correlations*.

2.2.1 Quantum Isomorphism of Graphs

Throughout this paper, we shall be working with what is known as the commuting operator model of quantum mechanics. As discussed earlier, Strategies making use of a shared state are known as *quantum strategies*. We refer the reader to [NC10] for a more thorough overview of fundamentals of quantum information.

Definition 2.3. A *quantum strategy* for the (G, H)-isomorphism game consists of a shared *state*, i.e. a unit vector $\psi \in \mathcal{H}$ in some Hilbert space $\mathcal{H}$ and self-adjoint projections $\{E_{g,h}\}_{g\in V(G),h\in V(H)} \subseteq \mathcal{B}(\mathcal{H})$ and $\{F_{g',h'}\}_{g'\in V(G),h'\in V(H)} \subseteq \mathcal{B}(\mathcal{H})$ such that:

- $\sum_h E_{gh} = I_{\mathcal{H}}$ and $\sum_h F_{g,h} = I_{\mathcal{H}}$
- $E_{g,h}F_{g',h'} = F_{g',h'}E_{g,h}$ for all $g, g' \in V(G)$ and $h, h' \in V(H)$.

When Alice and Bob receive the questions g, g' from the verifier, they use the PVMs $\{E_{g,h}\}_{h\in V(H)}$ and $\{F_{g',h'}\}_{h'\in V(H)}$ to perform a measurement on their part of the shared state ψ. In this case, the conditional probability of outputting h, h' when Alice and Bob receive the questions g, g' is given by $p(h, h' \mid g, g') = \langle\psi, E_{g,h}F_{g',h'}\psi\rangle$.

Two graphs G, H are said to be *quantum isomorphic*, written $G \cong_q H$ if there is a perfect quantum strategy for the (G, H)-isomorphism game. Two graphs that are isomorphic are also quantum isomorphic as all deterministic can be realised as quantum strategies. However, the converse is not true, i.e. there exist non-isomorphic graphs that are quantum isomorphic. Once again, we refer the reader to [AMR+19] for further details.

The existence of a perfect quantum strategy for the (G, H)-isomorphism game is characterized by the following proposition:

Proposition 2.4 ([AMR+19])**.** *Let G, H be two graphs with $|V(G)| = |V(H)|$. Then, the $G \cong_q H$ if and only if there exist a Hilbert space $\mathcal{H}$ and self-adjoint projections $\{E_{g,h}\}_{g\in V(G),h\in V(H)}$ such that:*

i. $\sum_{h\in V(H)} E_{g,h} = I_{\mathcal{H}}$ *for all* $g \in V(G)$,
ii. $\sum_{g\in V(G)} E_{g,h} = I_{\mathcal{H}}$ *for all* $h \in V(H)$,
iii. $E_{g,h}E_{g',h'} = 0$ *if* $V_{G,H}(h, h' \mid g, g') = 0$.

Given the first two conditions, the last condition is equivalent to:

$$(A(G) \otimes I_{\mathcal{H}})[E_{g,h}]_{g\in V(G),h\in V(H)} = [E_{g,h}]_{g\in V(G),h\in V(H)}(A(H) \otimes I_{\mathcal{H}}).$$

Furthermore, G and H are isomorphic if and only if there exist mutually commuting self-adjoint projections $\{E_{g,h}\}_{g\in V(G),h\in V(H)}$ satisfying the above conditions.

2.2.2 A Synchronous NPA Hierarchy for Quantum Isomorphism of Graphs

We shall focus on the NPA hierarchy for the graph isomorphism game in this subsection. We give a more detailed exposition of the NPA hierarchy in Appendix B. First, we introduce some notation that will be used throughout the paper and in Appendix B.

Let $\Sigma = V(G) \times V(H)$. The set of all finite strings in the alphabet Σ will be denoted by Σ^*. Similarly if $k \in \mathbb{N}$, Σ^k and $\Sigma^{\leq k}$ denote the set of all strings of length k and the set of all strings of length at most k respectively. ε is used to denote the empty string in Σ^*, and we use the following operations on strings:

- Let $s \in \Sigma^*$ be a string given by $s_1 \cdots s_k$, we denote the *reversed string* $s_k \dots s_1$ by s^R.
- Let $s, t \in \Sigma^*$ be strings given by $s_1 \cdots s_k$ and $t_1 \cdots t_l$ respectively. We denote their *concatenation* $s_1 \cdots s_k t_1 \cdots t_l$ by st.

With this notation in our hand, we now give the definition of a certificate for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game.

Definition 2.5. For two graphs G, H with $|V(G)| = |V(H)|$, a *certificate* for the k^{th} level of the NPA hierarchy of the (G, H)-isomorphism game is a positive semidefinite matrix $\mathcal{R} \in M_{\Sigma^{\leq k}}(\mathbb{C})$ such that:

(i) $\mathcal{R}_{\varepsilon,\varepsilon} = 1$
(ii) $\mathcal{R}_{s,t} = \mathcal{R}_{s',t'}$ for all $r, s, r', s' \in \Sigma^{\leq k}$, such that $s^R t \sim (s')^R(t')$, where we define $\sim$ to be the coarsest equivalence relation satisfying the following two properties:
  - For each $x, a \in X \times A$, $s(x, a)(x, a)t \sim s(x, a)t$ for all $s, t \in \Sigma^*$.

- $st \sim ts$ for all words $s, t \in \Sigma^*$.

(iii) For all words $s, s' \in \Sigma^{\leq k}$, $g \in V(G)$, $h \in V(H)$ such that $s(g,h)s' \in \Sigma^{\leq k}$, one has

$$\sum_{h' \in V(H)} \mathcal{R}_{s(g,h')s',t} = \mathcal{R}_{ss',t} \text{ for all } t \in \Sigma^{\leq k} \tag{1}$$

$$\sum_{g' \in V(G)} \mathcal{R}_{s(g',h)s',t} = \mathcal{R}_{ss',t} \text{ for all } t \in \Sigma^{\leq k} \tag{2}$$

$$\sum_{h' \in V(H)} \mathcal{R}_{t,s(g,h')s'} = \mathcal{R}_{t,ss'} \text{ for all } t \in \Sigma^{\leq k} \tag{3}$$

$$\sum_{g' \in V(G)} \mathcal{R}_{t,s(g',h)s'} = \mathcal{R}_{t,ss'} \text{ for all } t \in \Sigma^{\leq k} \tag{4}$$

(iv) For all $s, t \in \Sigma^{\leq k}$, if there exist consecutive $gh, g'h' \in \Sigma$ in $s^R t$ such that $\mathrm{rel}(g, g') \neq \mathrm{rel}(h, h')$ then $\mathcal{R}_{s,t} = 0$.

We shall say that the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game is *feasible* if there exists a certificate for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game.

Given a perfect strategy for the (G, H)-isomorphism game, where $\{E_{g,h}\}_{g \in V(G), h \in V(H)}$ are Alice's measurement operators and the shared state is ψ, we can construct a certificate for any level of the NPA hierarchy in the following way: for level-k, we consider the Gram matrix of the vectors $\{E_{g_1,h_1} \cdots E_{g_l,h_l} \psi\}_{g_1 h_1 \cdots g_l h_l \in \Sigma^{\leq k}}$.

The following proposition shows that the NPA hierarchy for the graph isomorphism game converges, i.e there is a solution for each level of the NPA hierarchy for the (G, H)-isomorphism if an only if $G \cong_q H$. A proof of the statement can be found in Appendix B. Proposition 2.6 gives two of the implications in Corollary 1.3, specifically it shows that items (1) and (3) are equivalent.

Proposition 2.6. *Let G, H be two graphs with $|V(G)| = |V(H)|$, and $\Sigma = V(G) \times V(H)$. Then, the (G, H)-isomorphism game has a perfect quantum strategy if and only if for each $k \in \mathbb{N}$, there exists a certificate for the k^{th}-level of the NPA hierarchy.*

3 NPA Hierarchy and Homomorphism Tensors

In this section, we shall give several algebro-combinatorial reformulations of the existence of a certificate for the k^{th} level of the NPA hierarchy of the graph isomorphism game. These reformulations allow us to interpret the existence of a certificate for the k^{th} level of the NPA hierarchy as a homomorphism indistinguishability characterization. Most of the proofs here are linear-algebraic in nature. We shall discuss the graph-theoretic implications of our results in the next section.

3.1 Quantum Isomorphism Relaxation via Completely Positive Maps

In this subsection, we show that a principal submatrix of a certificate for the k^{th}-level of the NPA hierarchy for quantum isomorphism can be interpreted as the Choi matrix (see Appendix A) of a completely positive map from $M_{V(G)^k}(\mathbb{C})$ to $M_{V(G)^k}(\mathbb{C})$ satisfying certain properties. We then show that the Choi matrix of such a completely positive map uniquely extends to a certificate for the k^{th}-level of the NPA hierarchy for quantum isomorphism. Thus feasibility of the k^{th}-level of the NPA hierarchy for the graph isomorphism game is equivalent to the existence of a completely positive map satisfying certain properties. In order to make these notions precise, we now introduce the atomic bilabelled graphs, which will be the building blocks of the graph classes that we shall construct in the next section.

Definition 3.1. Let $k \geq 1$. A (k,k)-bilabelled graph $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ is atomic if all its vertices are labelled. We define two classes of atomic graphs (see Figure 3.1):

- The class $\mathcal{Q}_k^P$ is the class of (k,k)-bilabelled minors of the graph $\boldsymbol{C}_k := (C_k, (1, \dots, k), (k+1, \dots, 2k))$ with $V(C_k) = [2k]$ and $E(C_k) = \{\{i, i+1\} : i \in [2k], i \neq k, 2k\} \cup \{\{1, k+1\}, \{k, 2k\}\}$.
- The class $\mathcal{Q}_k^S$ is the class of (k,k)-bilabelled graphs obtained by taking minors of the graph $\boldsymbol{M}_k := (M_k, (1, \dots, k), (k+1, \dots, 2k))$ with $V(M_k) = [2k]$ and $E(M_k) = \{\{i, i+k\} : i \in [k]\}$

Finally, we define $\mathcal{Q}_k := \mathcal{Q}_k^P \cup \mathcal{Q}_k^S$.

We also define two specific atomic graphs $\boldsymbol{J}_k, \boldsymbol{I}_k \in \mathcal{Q}_k$ for each $k \in \mathbb{N}$.

- $\boldsymbol{J}_k := (J_k, (1, \dots, k), (k+1, \dots 2k))$ with $V(J_k) = [2k]$ and $E(J_k) = \emptyset$
- $\boldsymbol{I}_k := (I_k, (1, \dots k), (1, \dots k))$ with $V(I_k) = [k]$ and $E(I_k) = \emptyset$

In other words, $\boldsymbol{J}_k$ and $\boldsymbol{I}_k$ are obtained from $\boldsymbol{M}_k$ by deleting and contracting all the edges respectively. These atomic graphs are special in the sense that one has $(\boldsymbol{J}_k)_G = J$ and $(\boldsymbol{I}_k)_G = I$ for all graphs G, where I and J are the identity and all ones matrix respectively. We also note that $\boldsymbol{J}_k \in \mathcal{Q}_k^S, \mathcal{Q}_k^P$ and $\boldsymbol{I}_k \in \mathcal{Q}_k^S$, but $\boldsymbol{I}_k \notin \mathcal{Q}_k^P$.

We can now define quantum isomorphism maps using the homomorphism tensors of the graphs in $\mathcal{Q}_k$:

Definition 3.2. Let G and H be graphs and $k \in \mathbb{N}$. A linear map $\Phi : \mathbb{C}^{V(G)^k \times V(G)^k} \to \mathbb{C}^{V(H)^k \times V(H)^k}$ is a *level k quantum isomorphism map* from G to H if the following holds:

$$\Phi \text{ is completely positive,} \tag{5}$$

$$\Phi(\boldsymbol{F}_G \odot X) = \boldsymbol{F}_H \odot \Phi(X) \text{ for all } \boldsymbol{F} \in \mathcal{Q}_k^P \text{ and } X \in \mathbb{C}^{V(G)^k \times V(G)^k}, \tag{6}$$

$$\Phi(I) = I = \Phi^*(I), \tag{7}$$

$$\Phi(J) = J = \Phi^*(J), \tag{8}$$

$$\Phi(\boldsymbol{F}_G) = \boldsymbol{F}_H \text{ for all } F \in \mathcal{Q}_k, \tag{9}$$

$$\Phi(\boldsymbol{X}^\sigma) = \Phi(\boldsymbol{X})^\sigma \text{ for all } \sigma \in \mathscr{C}(1, \dots, k, 2k, \dots, k+1). \tag{10}$$

Remark 3.2.1. Note that conditions (5) and (7) state that any level k quantum isomorphism map is a completely positive, trace-preserving, unital map. Also note that condition (9) implies the part of conditions (7) and (8) on the map Φ, and thus we are being a bit redundant. However, we do need to explicitly include the conditions on the adjoint Φ^*. Lastly, we are being a bit imprecise since we should really write $\boldsymbol{I}_G, \boldsymbol{I}_H, \boldsymbol{J}_G$, and $\boldsymbol{J}_H$.

We now prove some lemmas that will be useful for our proof that existence of a level k quantum isomorphism map is equivalent to the existence of a certificate for the k^{th} level of the NPA hierarchy.

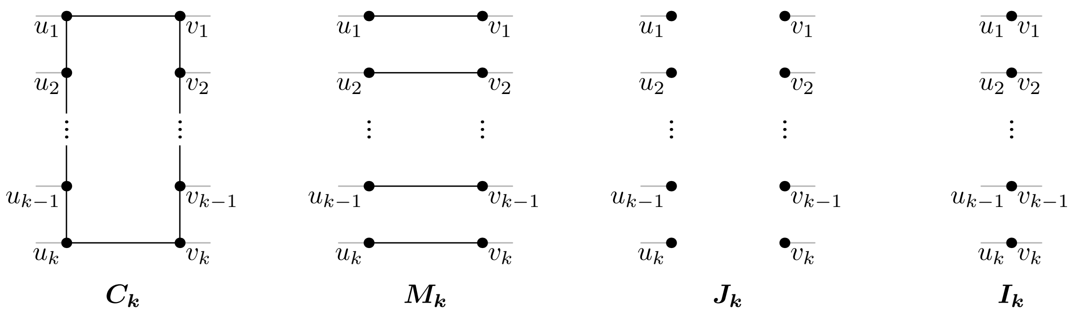

Figure 2: Atomic graphs.

Lemma 3.3. *Let G and H be graphs, $k \in \mathbb{N}$, and suppose that Φ is a level k quantum isomorphism map from G to H. If M is the Choi matrix of Φ, then $M_{s,t} = 0$ if any cyclic permutation of $s^R t$ contains consecutive terms gh and $g'h'$ such that $\mathrm{rel}(g, g') \neq \mathrm{rel}(h, h')$.*

Proof. TOPROVE 0 □

Lemma 3.4. *Let G and H be graphs and $k \in \mathbb{N}$. If Φ is a level k quantum isomorphism map from G to H, then $\Phi(\boldsymbol{F}_G X) = \boldsymbol{F}_H \Phi(X)$ and $\Phi(X \boldsymbol{F}_G) = \Phi(X)\boldsymbol{F}_H$ for all $\boldsymbol{F} \in \mathcal{Q}_k$ and $X \in \mathbb{C}^{V(G)^k \times V(G)^k}$.*

Proof. TOPROVE 1 □

For our last lemma we need to introduce some notation. For disjoint subsets $R_G, R_H \subseteq [k]$, and $s = g_1h_1 \dots g_kh_k \in (V(G) \times V(H))^k$, we denote by $s(R_G, R_H)$ the set of all strings $s' = g_1'h_1' \dots g_k'h_k'$ such that $g_i' = g_i$ for $i \notin R_G$ and $h_i' = h_i$ for $i \notin R_H$. For example, if $k = 3$ and $s = g_1h_1g_2h_2g_3h_3$, then

$$s(\{1\}, \{3\}) = \left\{g_1'h_1g_2h_2g_3h_3' \in (V(G) \times V(H))^3 : g_1' \in V(G),\ h_3' \in V(H).\right\}$$

Additionally, for any subset $R \in [k]$ we denote by $s \setminus R$ the substring of s obtained by removing its i^{th} entry for each $i \in R$.

Lemma 3.5. *Let G and H be graphs and suppose that Φ is a level k quantum isomorphism map from G to H. If M is the Choi matrix of Φ, then for any $s, t \in (V(G) \times V(H))^k$, disjoint subsets $S_G, S_H \subseteq [k]$, and disjoint subsets $T_G, T_H \subseteq [k]$, we have that*

$$\sum_{s' \in s(S_G, S_H),\ t' \in t(T_G, T_H)} M_{s',t'} \tag{11}$$

depends only on the equivalence class of the relation $\sim$ that $(s \setminus (S_G \cup S_H))^R (t \setminus (T_G \cup T_H))$ lies in.

Proof. TOPROVE 2 □

Theorem 3.6. *Let G and H be graphs and $k \in \mathbb{N}$. Then the following are equivalent:*

1. *The k^{th} level of the NPA hierarchy is feasible for the (G, H)-isomorphism game.*
2. *There exists a level k quantum isomorphism map from G to H.*
3. *There exists a level k quantum isomorphism map from H to G.*

Proof. TOPROVE 3 □

We remark that it follows from Definition 2.5 (ii) that the extension of the Choi matrix M to the certificate $\mathcal{R}$ is in fact unique.

The observant reader may have noticed that not all elements of $\mathcal{Q}_k^S$ were needed to prove that item (2) implies item (1) above. This is related to the fact that it is in fact possible to generate this unused bilabelled graphs from those that were used in the proof. However, redefining the set $\mathcal{Q}_k^S$ to only contain those that were used does not make it any easier to prove that (1) implies (2), and we will need these extra graphs later.

3.2 Isomorphisms Between Matrix Algebras

In this subsection, we shall see how a quantum isomorphism map restricts to a homomorphism between algebras containing homomorphism tensors for G to homomorphism tensors for H of graphs in $\mathcal{Q}_k$. This brings us a step closer to interpreting a solution for the K^{th}-level of the NPA hierarchy as a homomorphism indistinguishability result.

A matrix algebra $\mathcal{A} \subseteq M_{n^k}(\mathbb{C})$ is *S-partially coherent* if it is unital, self-adjoint, contains J, and is closed under Schur product with any matrix in S. Further, $\mathcal{A}$ is *cyclically-symmetric* if $A^\sigma \in \mathcal{A}$, for every $A \in \mathcal{A}$ and $\sigma \in \mathscr{C}(1, \dots, k, 2k, \dots, k+1)$.

Definition 3.7. Let S_k be the set of homomorphism tensors of (k,k)-bilabelled atomic graphs for G in $\mathcal{Q}_k^P$. For a graph G, we define the algebra $\widehat{\mathcal{Q}}_G^k$ as the minimal cyclically-symmetrical S_k-partially coherent algebra containing homomorphism tensors of all (k,k)-bilabelled graphs in $\mathcal{Q}_k$ for G.

Definition 3.8. Two n-vertex graphs G and H are *algebraically k-equivalent* if there is *algebraic k-equivalence*, i.e., a vector space isomorphism $\varphi\colon \widehat{\mathcal{Q}}_G^k \to \widehat{\mathcal{Q}}_H^k$ such that

1. $\varphi(M^*) = \varphi(M)^*$ for all $M \in \widehat{\mathcal{Q}}_G^k$,
2. $\varphi(MN) = \varphi(M)\varphi(N)$ for all $M, N \in \widehat{\mathcal{Q}}_G^k$, n
3. $\varphi(\boldsymbol{F}_G \odot M) = \boldsymbol{F}_H \odot \varphi(M)$ for all $\boldsymbol{F} \in \mathcal{Q}_k^P$ and any $M \in \widehat{\mathcal{Q}}_G^k$,
4. $\varphi(I) = I$, $\varphi(J) = J$ and $\varphi(\boldsymbol{F}_G) = \boldsymbol{F}_H$ for all $\boldsymbol{F} \in \mathcal{Q}_k$,
5. $\varphi(M^\sigma) = \varphi(M)^\sigma$ for all $M \in \widehat{\mathcal{Q}}_G^k$ and $\sigma \in \mathscr{C}(1,\dots,k,2k,\dots,k+1)$.
6. φ is trace preserving.

Note that every algebraic k-equivalence is sum-preserving, i.e., $\operatorname{soe}(\varphi(X)) = \operatorname{soe}(X)$ for all $X \in \hat{\mathcal{Q}}_k$. Indeed, $\operatorname{soe}(\varphi(X)) = \operatorname{Tr}(J\varphi(X)) = \operatorname{Tr}(\varphi(JX)) = \operatorname{Tr}(JX) = \operatorname{soe}(X)$.

Theorem 3.9. *Let $k \geq 1$. Two graphs G and H are algebraically k-equivalent if and only if there is a level-k quantum isomorphism map from G to H.*

Proof. TOPROVE 4 □

4 Homomorphism Indistinguishability

In this section, we shall finish the proof of the main theorem by constructing the graph classes $\mathcal{P}_k$ such that homomorphism indistinguishability over $\mathcal{P}_k$ is equivalent to the feasibility of the k^{th}-level of the NPA hierarchy. As stated earlier, we shall start with the atomic graphs $\mathcal{Q}_k$ as our building blocks and construct the graph class $\mathcal{P}_k$ by series composition, cyclic permutation of labels, and parallel composition with appropriate graphs.

Definition 4.1. Let $\mathcal{P}_k$ be the class of (k,k)-bilabelled graphs generated by the set of atomic graphs $\mathcal{Q}_k$ under parallel composition with graphs from $\mathcal{Q}_k^P$, series composition, and the action of the group $\mathscr{C}(1,\dots,k,2k,\dots,k+1)$ on the labels.

We remark that the action of $\mathscr{C}(1,\dots,k,2k,\dots,k+1)$ on a bilabelled graph $\boldsymbol{F} \in \mathcal{P}_k$ corresponds to "rotating" the drawing of $\mathcal{F}$ (see e.g. Figure 3).

4.1 Inner-product Compatibility of $\mathcal{P}_k$

A class of (k,k)-bilabelled graphs $\mathcal{T}$ is said to be *inner-product compatible* if for all $\boldsymbol{R}, \boldsymbol{S} \in \mathcal{T}$, there is a $\boldsymbol{Q} \in \mathcal{T}$ such that $\operatorname{Tr}(\boldsymbol{R}^* \cdot \boldsymbol{S}) = \operatorname{soe}(\boldsymbol{Q})$.

Lemma 4.2. *The graph classes $\mathcal{P}_k$ are inner-product compatible for each $k \in \mathbb{N}$.*

Proof. TOPROVE 5 □

Theorem 4.3 ([RS24, Theorem 4.6])**.** *Let $\mathcal{S}$ be an inner-product compatible class of (k,k)-bilabelled graphs containing J. Write $\mathcal{S}_G$ for the homomorphism tensors $\{\boldsymbol{F}_G \mid \boldsymbol{F} \in \mathcal{S}\}$, and let $\mathbb{C}\mathcal{S}_G \subseteq M_{V(G)^k}(\mathbb{C})$ denote the vector space spanned by $\mathcal{S}_G$. Then, the following are equivalent:*

(i) *G and H are homomorphism indistinguishable over $\mathcal{S}$.*
(ii) *there exists a sum-preserving vector space isomorphism $\varphi : \mathbb{C}\mathcal{S}_G \to \mathbb{C}\mathcal{S}_H$ such that $\varphi(\boldsymbol{F}_G) = \boldsymbol{F}_H$ for all $\boldsymbol{F} \in S$.*

The next theorem completes the proof of Theorem 1.1.

Theorem 4.4. *Let $k \geq 1$. Two graphs G and H are homomorphism indistinguishable over $\mathcal{P}_k$ if and only if they are partially k-equivalent.*

Proof. TOPROVE 6 □

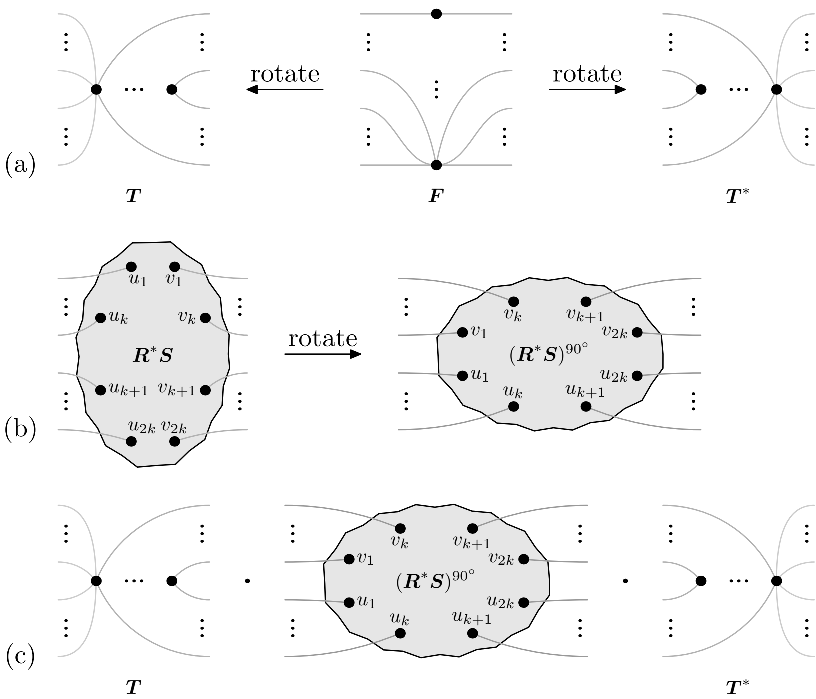

Figure 3: Inner-product compatibility in the even case.

4.2 Planarity and Minor-closedness of $\mathcal{P}_k$

In this subsection, we shall look at the graph classes $\mathcal{P}_k$ in more detail. The first thing we note is that for each $k \in \mathbb{N}$, one has that $\mathcal{P}_k \subseteq \mathcal{L}_k$, which were the classes of graphs constructed in [RS24] to obtain a homomorphism indistinguishability charatcterization for the Lasserre hierarchy of SDP relaxations of graph isomorphism. We include a brief overview of this in Appendix C and we refer the reader to [RS24] for more details. Indeed, for each $k \in \mathbb{N}$ it is not too difficult to see that $\mathcal{Q}_k \subseteq \mathcal{A}_k$ (where $\mathcal{A}_k$ are the atomic graphs used to construct $\mathcal{L}_k$ in [RS24]). Moreover, the set of allowed operations while constructing $\mathcal{P}_k$ from $\mathcal{Q}_k$ is also a subset of the set of operations allowed while constructing $\mathcal{L}_k$ from $\mathcal{A}_k$. In fact, for $k = 1$, it is not too difficult to show that $\mathcal{P}_k = \mathcal{L}_k$ is the set of all outerplanar graphs. We note here that the class $\mathcal{P}_k$ is not the set of k-outerplanar graphs for $k \neq 1$. For any $k \in \mathbb{N}$, one can construct a k-outerplanar graph in $\mathcal{P}_2$. The following lemma is immediate from [RS24, Lemma 4.7]:

Lemma 4.5. *Let $F \in \mathcal{P}_k$ be a (k,k)-bilabelled graph. Then, the treewidth of the underlying graph* soe F *is at most* $3k - 1$.

We now work towards giving an alternate proof of the main result of [MR20] that shows that two graphs are quantum isomorphic if and only if they are homomorphism indistinguishable over all planar graphs. Let $\mathcal{P} := \bigcup_{k=1}^{k} \mathcal{P}_k$. Then, it follows from the main theorem (Theorem 1.1) and convergence of NPA hierarchy (Proposition 2.6) that $G \cong_q H$ is equivalent to $G \cong_{\mathcal{P}} H$. This proves Corollary 1.3 with the exception of the claim in item (2) that $\mathcal{P}$ is the set of all planar graphs. We now work towards proving this final claim, thus completing the proof of Corollary 1.3.

First, we show that for each $k \in \mathbb{N}$, the graph class $\mathcal{P}_k$ only contains planar graphs. We begin by precisely defining what it means for a bilabelled graph to be planar. We use the definition given in [MR20].

Definition 4.6. Given a (k,l)-bilabelled graph $\boldsymbol{G} = (G, \boldsymbol{a}, \boldsymbol{b})$ we define the graph G^0 as the graph obtained from G by adding a cycle $C = \alpha_1, \ldots, \alpha_k, \beta_l, \ldots, \beta_1$ and the edges $a_i\alpha_i$ and $b_j\beta_j$ for each $i \in [k]$ and $j \in [l]$, and say that $\boldsymbol{G}$ is planar if G^0 has a planar embedding where the

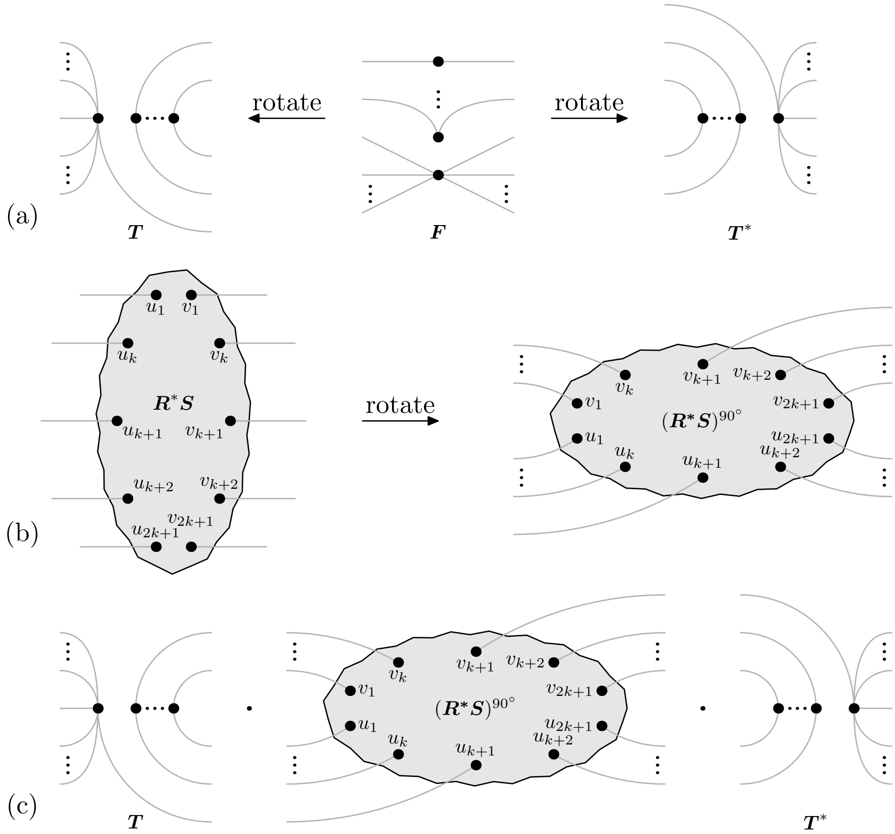

Figure 4: Inner-product compatibility in the odd case.

cycle C is the boundary of a face. We shall refer to C as the *enveloping cycle* of G^0, and usually consider planar embeddings where C is the boundary of the outer face.

Lemma 4.7. *For each $k \in \mathbb{N}$, the class of graphs $\mathcal{P}_k$ is contained in the set of all planar bilabelled graphs.*

Proof. TOPROVE 7 □

We will also need that the class $\mathcal{P}_k$ is closed under taking minors (recall the notion of minors of bilabelled graphs from Section 2.1) and that $\mathrm{soe}(\mathcal{P}_k)$ is closed under minors and disjoint unions. The proofs of these facts are almost identical to the analogous proofs for the class $\mathcal{L}_k$ used in [RS24]. Therefore, we will just state the results and comment on the very minor differences in the proofs.

Lemma 4.8. *For each $k \in \mathbb{N}$, the class of bilabelled graphs $\mathcal{P}_k$ is minor-closed.*

The proof of this follows the proof of Lemma 4.16 of [RS24] almost exactly. The only difference is as follows. In the proof, at one point some care must be taken to remove some unwanted isolated labelled vertices that become isolated and unlabeled after a series composition. To do this, prior to the series composition, a parallel composition is used which has the effect of merging the i^{th} labelled output vertex with the first input vertex. Such a parallel composition is not available in $\mathcal{P}_k$, rather only cyclically consecutive labelled vertices can be merged. However, the choice of merging with the first input was arbitrary, and the only thing truly necessary for the proof is that the unwanted isolated labelled vertex is merged with some labelled vertex which does not become an unwanted isolated unlabelled vertex after the series composition. This is easily accomplished in $\mathcal{P}_k$, since one can merge the unwanted isolated labeled vertex with one that is next to it in cyclic order (if this is also an unwanted isolated labelled vertex, then merge both with the next, etc.).

With the above lemma in hand, the proof of the following is identical to Lemma 4.9 in [RS24].

Lemma 4.9. *For each $k \in \mathbb{N}$, the class of graphs $\operatorname{soe}(\mathcal{P}_k)$ is minor-closed and union-closed.*

We now work towards showing that although each $\mathcal{P}_k$ has bounded treewidth, their union contains arbitrarily large grids

Lemma 4.10. *For each $k \in \mathbb{N}$, the class of graphs $\mathcal{P}_k$ contains the $k \times k$ grid.*

Proof. TOPROVE 8 □

We now need a standard result from graph minor theory that follows from [RS84]:

Theorem 4.11. *For every planar graph G, there is a natural number n_G such that G is a minor of the $n_G \times n_G$ grid.*

The following corollary is now immediate from Lemma 4.7, Lemma 4.9, Lemma 4.10 and Theorem 4.11:

Corollary 4.12. *The set $\mathcal{P} = \bigcup_{k\in\mathbb{N}} \operatorname{soe}(\mathcal{P}_k)$ is the set of all planar graphs.*

Recalling the discussion preceding Lemma 4.7, this completes the proof of Corollary 1.3, and thus gives us the promised alternative proof of the result of [MR20].

5 Exact Feasibility of NPA in Randomized Polynomial Time

Being a semidefinite program, the NPA relaxation can be solved using standard techniques such as the ellipsoid method. However, such techniques can, in polynomial time, only decide the approximate feasibility of a system. In this section, we use homomorphism indistinguishability to give a randomized algorithm for deciding whether any level of the NPA hierarchy is feasible exactly.

Theorem 1.2. *There exists a randomized algorithm which decides, given graphs G and H and an integer $k \geq 1$, whether the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game is feasible. The algorithm always runs in time $n^{O(k)}k^{O(1)}$ for $n := \max\{|V(G)|, |V(H)|\}$, accepts all YES-instances, and accepts NO-instances with probability less than one half.*

By a recent result [Sep24a, Theorem 1.1], homomorphism indistinguishability over every minor-closed graph class of bounded treewidth can be decided in randomized polynomial time. In Theorem 1.1, we have established that the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game is feasible for two graphs G and H if and only if they are homomorphism indistinguishable over $\mathcal{P}_k$. By Lemmas 4.5 and 4.9, the graph class $\mathcal{P}_k$ is minor-closed and of bounded treewidth. Hence, by [Sep24a, Theorem 1.1], the feasibility of the k^{th}-level of the NPA hierarchy can be decided in randomized polynomial time for every fixed k. However, this result assumes k to be fixed and not part of the input. Theorem 1.2 makes the dependence on k effective.

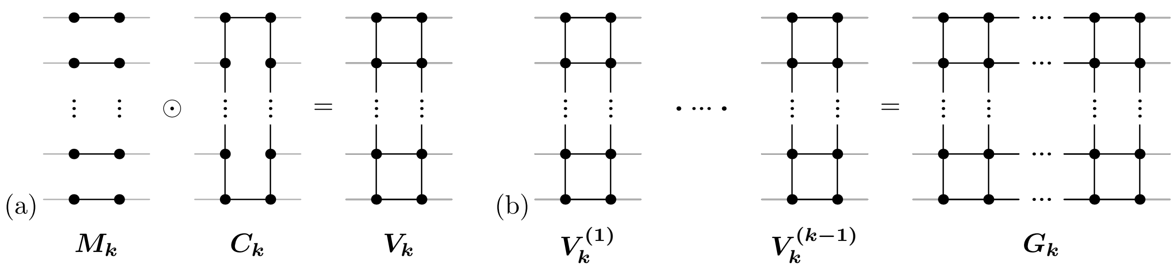

Figure 5: (a) Construction of the graphs $\boldsymbol{V}_k$. (b) Construction of the graph $\boldsymbol{G}_k$.

5.1 Modular Homomorphism Indistinguishability

As a first step towards Theorem 1.2, we show that it can be decided in deterministic polynomial time whether G and H are *homomorphism indistinguishable over $\mathcal{P}_k$ modulo a prime p*, i.e. $\hom(F, G) \equiv \hom(F, H) \mod p$ for all $F \in \mathcal{P}_k$. We choose to work over a finite field in order to avoid memory issues with too large integers.

Theorem 5.1. *There exists a deterministic algorithm which decides, given graphs G and H, an integer $k \geq 1$, and a prime p, whether G and H are homomorphism indistinguishable over $\mathcal{P}_k$ modulo p. The algorithm runs in time $n^{O(k)}(k \log p)^{O(1)}$ for $n := \max\{|V(G)|, |V(H)|\}$.*

The algorithm in Theorem 5.1 decides whether G and H are homomorphism indistinguishable over $\mathcal{P}_k$ by computing a basis B for the $\mathbb{F}_p$-vector space S spanned by homomorphism matrices of bilabelled graphs in $\mathcal{P}_k$. More precisely,

$$S := \operatorname{span}\{\boldsymbol{P}_G \oplus \boldsymbol{P}_H \mid \boldsymbol{P} \in \mathcal{P}_k\} \subseteq \mathbb{F}_p^{(V(G)^k \cup V(H)^k) \times (V(G)^k \times V(H)^k)}$$

where $\boldsymbol{P}_G \oplus \boldsymbol{P}_H := \begin{pmatrix} \boldsymbol{P}_G & 0 \\ 0 & \boldsymbol{P}_H \end{pmatrix}$. A basis $B \subseteq S$ can be computed iteratively as follows. We initialise B with the singleton set containing $\boldsymbol{J}_G \oplus \boldsymbol{J}_H$. Subsequently, we repeatedly apply the operation from Definition 4.1 to compute new vectors. Whenever a new vector is linearly independent from the vectors already in B, we add it to B. Since the dimension of S is at most $2n^{2k}$, this process terminates after a polynomial number of steps. This procedure is formally described in Algorithm 1.

In order to achieve a better runtime in Theorem 5.1, we give size-$O(k)$ sets $\mathcal{B}_k^P$ and $\mathcal{B}_k^S$ of bilabelled graphs generating $\mathcal{Q}_k^P$ and $\mathcal{Q}_k^S$. Let $\mathcal{B}_k := \mathcal{B}_k^P \cup \mathcal{B}_k^S$.

Lemma 5.2. *Let $k \geq 1$ and consider the following (k, k)-bilabelled graphs.*

- $\boldsymbol{J} := (J, (1, \dots, k), (k+1, \dots, 2k))$ *with* $V(J) = [2k]$ *and* $E(J) = \emptyset$,
- *for* $i \in [2k]$ *and* $j := i + 1$ *if* $i < 2k$ *and* $j := 1$ *otherwise, the graphs* $\boldsymbol{C}^{=i}$ *and* $\boldsymbol{C}^{\sim i}$ *which are obtained from* $\boldsymbol{J}$ *by, respectively, identifying or connecting the vertices* i *and* j,
- $\boldsymbol{I} := (I, (1, \dots, k), (1, \dots, k))$ *with* $V(I) = [k]$ *and* $E(I) = \emptyset$,
- *for* $i \in [k]$, *the graphs* $\boldsymbol{M}^{\neq i} = (M^{\neq i}, (1, \dots, k), (1, \dots, i-1, i', i+1, \dots, k))$ *with* $V(M^{\neq i}) = [k] \cup \{i'\}$, $E(M^{\neq i}) = \emptyset$ *and* $\boldsymbol{M}^{\sim i} = (M^{\sim i}, (1, \dots, k), (1, \dots, i-1, i', i+1, \dots, k))$ *with* $V(M^{\sim i}) = [k] \cup \{i'\}$, $E(M^{\sim i}) = \{ii'\}$.

Then $\mathcal{Q}_k^P$ is generated by $\mathcal{B}_k^P := \{\boldsymbol{J}\} \cup \{\boldsymbol{C}^{=i}, \boldsymbol{C}^{\sim i} \mid i \in [2k]\}$ under parallel composition and $\mathcal{Q}_k^S$ is contained by the graph class generated by $\mathcal{B}_k^S := \{\boldsymbol{I}\} \cup \{\boldsymbol{M}^{\neq i}, \boldsymbol{M}^{\sim i} \mid i \in [k]\}$ under series composition.

Proof. TOPROVE 9 □

Lemma 5.3. *Algorithm 1 is correct.*

Proof. TOPROVE 10 □

Lemma 5.4. *Algorithm 1 terminates in time $n^{O(k)}(k \log p)^{O(1)}$ for $n := \max\{|V(G)|, |V(H)|\}$.*

Proof. TOPROVE 11 □

5.2 Reducing NPA to Modular NPA

If $G \not\equiv_{\mathcal{P}_k} H$, then there exists a graph $F \in \mathcal{P}_k$ such that $\hom(F, G) \neq \hom(F, H)$. Since $\hom(F, G), \hom(F, H) \leq n^{|V(F)|}$ for $n := \max\{|V(G)|, |V(H)|\}$, it follows that G and H are also not homomorphism indistinguishable over $\mathcal{P}_k$ modulo every prime p greater than $n^{|V(F)|}$. Unfortunately, there is a priori no bound on the size of F in terms of n. In this section, we give such a bound and thereby derive Theorem 1.2 from Theorem 5.1. For $l \in \mathbb{N}$, write $(\mathcal{P}_k)_{\leq l} := \{F \in \mathcal{P}_k \mid |V(F)| \leq l\}$.

Algorithm 1: Modular NPA.

Input: Graphs G and H, an integer $k \geq 1$, a prime p in binary.

Output: Whether G and H are homomorphism indistinguishable over $\mathcal{P}_k$ modulo p.

for every $\boldsymbol{A} \in \mathcal{B}_k$, compute the homomorphism matrices $\boldsymbol{A}_G \in \mathbb{F}_p^{V(G)^k \times V(G)^k}$ and $\boldsymbol{A}_H \in \mathbb{F}_p^{V(H)^k \times V(H)^k}$;
initialise $B \leftarrow \{\boldsymbol{J}_G \oplus \boldsymbol{J}_H\} \subseteq \mathbb{F}_p^{(V(G)^k \cup V(H)^k) \times (V(G)^k \cup V(H)^k)}$;
foreach $\boldsymbol{A} \in \mathcal{B}_k$ **do**
 if $\boldsymbol{A}_G \oplus \boldsymbol{A}_H \notin \operatorname{span}(B)$ **then**
  add $\boldsymbol{A}_G \oplus \boldsymbol{A}_H$ to B;
repeat
 foreach $\boldsymbol{A} \in \mathcal{B}_k^P$, $v \in B$ **do**
  $w \leftarrow (\boldsymbol{A}_G \oplus \boldsymbol{A}_H) \odot v$;
  if $w \notin \operatorname{span}(B)$ **then**
   add w to B;
 foreach $v_1, v_2 \in B$ **do**
  $w \leftarrow v_1 \cdot v_2$;
  if $w \notin \operatorname{span}(B)$ **then**
   add w to B;
 foreach $\sigma \in \mathscr{C}(1, \dots, k, 2k, \dots, k+1)$, $v \in B$ **do**
  $w \leftarrow v^\sigma$;
  if $w \notin \operatorname{span}(B)$ **then**
   add w to B;
until B *is not updated*;
if $\mathbf{1}_G^T v \mathbf{1}_G = \mathbf{1}_H^T v \mathbf{1}_H$ *for all* $v \in B$ **then**
 accept;
else
 reject;

Theorem 5.5. *Let $k \geq 1$. Let G and H be a graphs on at most n vertices. Let $f_k(n) := 2k \cdot 4^{n^{2k}}$. Then*

$$G \cong_{\mathcal{P}_k} H \iff G \cong_{(\mathcal{P}_k)_{\leq f_k(n)}} H.$$

Towards Theorem 5.5, we define the following complexity measure $\nu \colon \mathcal{P}_k \to \mathbb{N}$ inductively. If $\boldsymbol{Q} \in \mathcal{Q}_k$, then $\nu(\boldsymbol{Q}) := 1$. For $\boldsymbol{F} \in \mathcal{P}_k$, define $\nu(\boldsymbol{F})$ inductively as the least number $n \in \mathbb{N}$ such that there exist

1. $\boldsymbol{F}' \in \mathcal{P}_k$ and $\boldsymbol{Q} \in \mathcal{Q}_k^P$ such that $\boldsymbol{F} = \boldsymbol{Q} \odot \boldsymbol{F}'$ and $n = \nu(\boldsymbol{F}')$, or
2. $\boldsymbol{F}', \boldsymbol{F}'' \in \mathcal{P}_k$ such that $\boldsymbol{F} = \boldsymbol{F}' \cdot \boldsymbol{F}''$ and $n = \max\{\nu(\boldsymbol{F}'), \nu(\boldsymbol{F}'')\} + 1$, or
3. $\boldsymbol{F}' \in \mathcal{P}_k$ and $\sigma \in \mathscr{C}(1, \dots, k, 2k, \dots, k+1)$ such that $\boldsymbol{F} = (\boldsymbol{F}')^\sigma$ and $n = \nu(\boldsymbol{F}')$.

By Definition 4.1, $\nu \colon \mathcal{P}_k \to \mathbb{N}$ is well-defined.

Lemma 5.6. *Let $k \geq 1$. For every $\boldsymbol{F} \in \mathcal{P}_k$, it holds that $\boldsymbol{F}$ has at most $2k \cdot 2^{\nu(\boldsymbol{F})}$ vertices.*

Proof. TOPROVE 12 □

As in Section 5.1, we consider a sequence of nested spaces of homomorphism matrices. For $l \geq 1$, write

$$S_l := \operatorname{span}\{\boldsymbol{F}_G \oplus \boldsymbol{F}_H \mid \boldsymbol{F} \in \mathcal{P}_k, \nu(\boldsymbol{F}) \leq l\} \subseteq \mathbb{R}^{(V(G)^k \cup V(H)^k) \times (V(G)^k \cup V(H)^k)}.$$

Clearly, $S_1 \subseteq S_2 \subseteq \cdots \subseteq S := \bigcup_{l \geq 1} S_l$. The space S is of dimension at most $2n^{2k}$. The following lemma shows that $S_{2n^{2k}} = S$.

Lemma 5.7. *If $l \geq 1$ is such that $S_l = S_{l+1}$, then $S_l = S$.*

Proof. TOPROVE 13 $\square$

This concludes the preparations for the proof of Theorem 5.5.

Proof. TOPROVE 14 $\square$

It remains to derive Theorem 1.2 from Theorems 5.1 and 5.5.

Proof. TOPROVE 15 $\square$

6 Discussion

We have established a characterization of the feasibility of the k^{th}-level of the NPA hierarchy of relaxations for the (G, H)-isomorphism game in terms of homomorphism indsitingushability over the graph class $\mathcal{P}_k$. We know that $\mathcal{P}_k$ is a subclass of planar graphs, has bounded-treewidth, and is closed under taking minors. We only have an inductive description of the class $\mathcal{P}_k$ as being generated from $\mathcal{Q}_k$ using series composition, cyclic permutations, and parallel composition with atomic graphs from $\mathcal{Q}_k^P$. Thus, a natural question is to understand better the properties of the graphs in $\mathcal{P}_k$. Recall that $\mathcal{L}_k$ is the analogous class of graphs for the k^{th}-level of the Lasserre hierarchy of relaxations of the integer program for graph isomorphism.

Problem 6.1. *Is $\mathcal{P}_k$ equal to the intersection of $\mathcal{L}_k$ with the class of all planar bilabelled graphs?*

In the field of graph isomorphism testing, the k-dimensional Weisfeiler-Leman (k-WL) algorithm is an essential subroutine. It iteratively constructs an automorphism-invariant partition of the k-tuples of vertices of a graph. For some classes of graphs, the k-WL algorithm is sufficient to test isomorphism. This is closely related to the feasibility of the k^{th}-level of the Lassere hierarchy of SDP relaxations of the graph isomorphism integer program [RS24]. This motivates the following problem.

Problem 6.2. *Is there a class of graphs $\mathcal{C}$ for which the k^{th}-level of the NPA hierarchy determines quantum isomorphism and isomorphism does not coincide with quantum isomorphism on $\mathcal{C}$?*

Note that, for example, it is known that two trees are isomorphic if and only if they are quantum isomorphic, and that 1-WL determines if two trees are isomorphic. However, it would be interesting to find a class of graphs that can be quantum isomorphic without being isomorphic, and where we can decide quantum isomorphism by some fixed level of the NPA hierarchy.

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A Linear algebra

Recall that a linear map $\Phi : M_n(\mathbb{C}) \to M_k(\mathbb{C})$ is said to be *positive* if it maps all positive semidefinite matrices in $M_n(\mathbb{C})$ to positive semidefinite matrices in $M_k(\mathbb{C})$. Φ is said to be *completely positive* if for all $l \in \mathbb{N}$ the map $\mathbb{I}_l \otimes \Phi : M_n(\mathbb{C}) \otimes M_l(\mathbb{C}) \to M_k(\mathbb{C}) \otimes M_l(\mathbb{C})$ is positive, where $\mathbb{I}_l : M_l(\mathbb{C}) \to M_l(\mathbb{C})$ is the identity map.

The *Choi matrix* of a map $\Phi : M_n(\mathbb{C}) \to M_k(\mathbb{C})$ is the $nk \times nk$ matrix $\sum_{i,j=1}^{k} E_{ij} \otimes \Phi(E_{ij})$, where E_{ij} are the matrix units. It follows from a well known result of Choi [Cho75] that a linear map $\Phi : M_n(\mathbb{C}) \to M_k(\mathbb{C})$ is completely positive if and only if its Choi matrix is positive semidefinite.

Lemma A.1 ([MRV24, Lemma A.1]). *Let $\mathcal{A}$ and $\mathcal{B}$ be self-adjoint unital subalgebras of $\mathbb{C}^{n\times n}$ and $\varphi\colon \mathcal{A} \to \mathcal{B}$ be a trace-preserving isomorphism such that $\varphi(X^*) = \varphi(X)^*$ for all $X \in \mathcal{A}$. Then there exists a unitary $U \in \mathbb{C}^{n\times n}$ such that $\varphi(X) = UXU^*$ for all $X \in \mathcal{A}$.*

Lemma A.2 (Generalisation of [MRV24, Lemma 4.9]). *Let $\Phi_1, \Phi_2\colon M_n(\mathbb{C}) \to M_n(\mathbb{C})$ be two linear maps which are completely positive, trace-preserving, and unital. Then for any matrices X and Y such that $\Phi_1(X) = Y$ and $\Phi_2(Y) = X$ it holds that $\Phi_1(XW) = Y\Phi_1(W)$ and $\Phi_1(WX) = \Phi_1(W)Y$ for all $W \in M_n(\mathbb{C})$. Furthermore,*

i. *X and Y are cospectral in this case,*
ii. *and $\Phi_1^*(Y) = X$.*

Proof. TOPROVE 16 □

Lemma A.3 ([MRV24, Lemma 4.5]). *Let $D \in \mathbb{C}^{m\times n}$ be a matrix and $u \in \mathbb{C}^n$ and $v \in \mathbb{C}^m$. Then the following are equivalent:*

1. *$D(u \odot w) = v \odot (Dw)$ for all $w \in \mathbb{C}^n$,*
2. *$D_{ij} = 0$ whenever $v_i \neq u_j$,*
3. *$D^*(v \odot z) = u \odot (D^*z)$ for all $z \in \mathbb{C}^m$.*

B The NPA Hierarchy

Our treatment of the NPA hierarchy is based on [Wat20, Chapter 8]. Let $(p(a,b|x,y))_{x\in X, y\in Y, a\in A, b\in B}$ be a correlation in $P(X,Y,A,B)$. We now address the issue of determining if p is a quantum correlation, i.e. we ask if there are commuting PVMs $\{E_{xa}\}_{a\in A}$ and $\{F_{y,b}\}_{b\in B}$ for each $x \in X$ and $y \in Y$, and a state ψ such that $p(a,b|x,y) = \langle \psi, E_{xa}F_{yb}\psi\rangle$ for all $x \in X$, $y \in Y$, $a \in A$ and $b \in B$.

Note that in order to determine the correlation p, one only needs the vectors $\{E_{xa}\psi\}_{x\in X, y\in A}$ and $\{F_{yb}\psi\}_{y\in Y, b\in B}$. In particular, we note that all of this information is contained in the Gram Matrix of these vectors.

Let us define $\Sigma = (X \times A) \sqcup (Y \times B)$. We can now define an SDP relaxation of the problem of determining whether p is a quantum correlation, by searching for positive matrices R indexed by $\Sigma^{\leq 1}$ such that $R_{xa,yb} = p(a,b|x,y)$ for all $x \in X, y \in Y, a \in A, b \in B$. A Gram Matrix arising from an actual quantum strategy as described earlier also satisfies several other equations. For example, one always has that $\sum_a E_{x,a}\psi = \psi$ for all $x \in X$. Hence, we may restrict our search space to positive matrices indexed by $\Sigma^{\leq 1}$ that satisfy these additional constraints. Each of these additional constraints actually turns out to be affine. Hence, we get an SDP relaxation of the problem of determining if p is a quantum correlation as discussed earlier.

One can construct increasingly complicated SDP relaxations of this problem in a similar manner by searching over positive matrices indexed by longer words formed from the alphabet Σ. For each $k \in \mathbb{N}$, one searches over positive semidefinite matrices indexed by words from $\Sigma^{\leq}$.

This hierarchy of SDP relaxations is known as the *NPA hierarchy*, named after the authors of [NPA08] who introduced it, where the choice of k corresponds to different levels of the hierarchy.

We give more details in the next section. However, we shall restrict ourselves to the case of synchronous correlations and games. We refer the reader to [NPA08] for more details regarding the general case.

B.1 A Synchronous NPA Hierarchy

We choose our alphabet to be $\Sigma = X \times A$ instead of $(X \times A) \sqcup (X \times A)$, since we are restricting ourselves to synchronous correlations. We define $\sim$ to be the coarsest equivalence relation satisfying the following two properties:

1. For each $x, a \in X \times A$, $s(x,a)(x,a)t \sim s(x,a)t$ for all $s, t \in \Sigma^*$.
2. $st \sim ts$ for all words $s, t \in \Sigma^*$.

Definition B.1. A function $\phi : \Sigma^* \to \mathbb{C}$ is said to be *admissible* if:

1. $\phi(\varepsilon) = 1$
2. For all words $s, t \in \Sigma^*$, we have
$$\sum_{a \in A} \phi(s(x,a)t) = \phi(st)$$
for each $x \in X$.
3. For all words $s, t \in \Sigma^*$, we have
$$\phi(s(x,a)(y,b)t) = 0$$
for each $x, y \in X$ and $a, b \in A$ such that $V(a, b \mid x, y) = 0$.
4. For all words $s, t \in \Sigma^*$ satisfying $s \sim t$, we have $\phi(s) = \phi(t)$.

Similarly, an *admissible function of order k* is a function $\phi : \Sigma^{\leq 2k} \to \mathbb{C}$ satisfying above conditions. An *admissible operator of order k* is a positive semidefinite matrix $\mathcal{R} \in M_{\Sigma^{\leq k}}(\mathbb{C})$ such that there exists an admissible function $\phi : \Sigma^{\leq 2k}$ of order k satisfying $\mathcal{R}_{s,t} = \phi(s^R t)$.

We now state the result about the convergence of the NPA hierarchy for synchronous correlations from [Rus23] without a proof:

Lemma B.2 ([Rus23, Corollary 2]). *Let $p \in P(X, A)$ be a synchronous correlation. Then, $p \in C_q(X, A)$ if and only if for each $k \in \mathbb{N}$ there exists an admissible operator $\mathcal{R}^k$ of order k such that $\mathcal{R}^k_{(x,a),(y,b)} = p(a, b \mid x, y)$ for all $x, y \in X,\ a, b \in A$.*

B.2 Proof of Convergence of NPA Hierarchy for Quantum Isomorphism

We finish the proof of 2.6 as promised in Section 2.

Proof. TOPROVE 17 $\square$

C Lasserre Hierarchy for Graph Isomorphism

Recall that two graphs are isomorphic if and only if there exists a permutation matrix P such that $A_G P = P A_H$, where A_G and A_H denote the adjacency matrices of G and H respectively. The problem of checking whether or not two graphs G and H are isomorphic can be formulated as the integer program $\mathrm{ISO}(G, H)$ defined as follows:

$$
\begin{aligned}
\sum_{h \in H} X_{g,h} - 1 &= 1 \quad \text{for all } g \in V(G), \\
\sum_{g \in G} X_{g,h} - 1 &= 1 \quad \text{for all } h \in V(H), \\
X_{g,h} X_{g',h'} &= 0 \quad \text{for all } g, g' \in V(G),\ h, h' \in V(H) \\
&\qquad \text{such that } \mathrm{rel}_G(g, g') \neq \mathrm{rel}_H(h, h').
\end{aligned} \tag{12}
$$

where the variables $\{X_{g,h}\}$ are allowed take the values $0, 1$. An element $\{g_1h_1, \ldots, g_lh_l\}$ is said to be a *partial isomorphism* if $\mathrm{rel}(g_i, g_j) = \mathrm{rel}(h_i, h_j)$ for all $i, j \in [l]$. We can now consider the Lasserre hierarchy of SDP relaxations for $\mathrm{ISO}(G, H)$. We present the version used in [RS24].

Definition C.1. Let $k \geq 1$. The level-k Lasserre relaxation for graph isomorphism has variables y_I ranging over $\mathbb{R}$ for $I \in \binom{V(G) \times V(H)}{\leq 2k}$. The constraints are as follows:

$$
\begin{aligned}
M_t(y) \coloneqq (y_{I \cup J})_{I, J \in \binom{V(G) \times V(H)}{\leq t}} &\succeq 0, \\
\sum_{h \in V(H)} y_{I \cup \{gh\}} &= y_I \quad \text{for all } I \text{ s.t. } |I| \leq 2t - 2 \text{ and all } g \in V(G), \\
\sum_{g \in V(G)} y_{I \cup \{gh\}} &= y_I \quad \text{for all } I \text{ s.t. } |I| \leq 2t - 2 \text{ and all } h \in V(H), \\
y_I &= 0 \quad \text{if } I \text{ s.t. } |I| \leq 2t \text{ is not a partial isomorphism}, \\
y_\emptyset &= 1.
\end{aligned} \tag{13}
$$

In [RS24], for each $k \in \mathbb{N}$, a class of (k, k)-bilabelled graphs $\mathcal{L}_k$ was constructed such that for each the k^{th}-level of the Lasserre hierarchy $\mathrm{ISO}(G, H)$ is feasible if and only if G, H are homomorphism indistinguishable over $\mathcal{L}_k$. The construction of these graph classes $\mathcal{L}_k$ begins from *atomic graphs* $\mathcal{A}_k$ which are defined (k, k)-bilabelled graphs $\boldsymbol{F} = (F, \boldsymbol{u}, \boldsymbol{v})$ with all of its vertices labelled. Note that the the set of atomic graphs $\mathcal{A}_k$ is generated under parallel composition by the graphs

- $\boldsymbol{J} \coloneqq (J, (1, \ldots, k), (k+1, \ldots, 2k))$ with $V(J) = [2k]$, $E(J) = \emptyset$,
- $\boldsymbol{A}^{ij} \coloneqq (A^{ij}, (1, \ldots, k), (k+1, \ldots, 2k))$ with $V(A^{ij}) = [2k]$, $E(A^{ij}) = \{ij\}$ for $1 \leq i < j \leq 2k$,
- $\boldsymbol{I}^{ij}$ for $1 \leq i < j \leq 2k$ which is obtained from $\boldsymbol{A}^{ij}$ by contracting and removing the edge ij.

We dedicate this part of the paper to motivate the viewpoint that the NPA hierarchy is a noncommutative generalisation of the Lasserre hierarchy. This is indeed well known in the literature (see [NPA12, KSS23] for example), but we include this for the sake of completion.

One can construct an NPA like hierarchy of SDP relaxations of the problem of deciding if two graphs are isomorphic. If we make use of the characterization given in Proposition 2.4, a certificate $\mathcal{R}$ for the k^{th}-level of the NPA hierarchy constructed from a set of commuting projections also satisfies the following condition:

$$
\mathcal{R}_{g_1h_1 \ldots g_kh_k, g_{k+1}h_{k+1} \ldots g_{2k}h_{2k}} = \mathcal{R}_{g_{\sigma(1)}h_{\sigma(1)} \ldots g_{\sigma(k)}h_{\sigma(k)}, g_{\sigma(k+1)}h_{\sigma(k+1)} \ldots g_{\sigma(2k)}h_{\sigma(2k)}} \quad \text{for all } \sigma \in \mathbb{S}_{2k}. \tag{14}
$$

Now, it is not too difficult to see that the certificates for the k^{th}-level of the NPA hierarchy for the (G, H)-isomorphism game satisfying (14) are in bijective correspondence with certificates for the k^{th}-level of the Lasserre hierarchy. In particular, this implies that the feasibility of the k^{th}-level of the Lasserre hierarchy also implies the feasibility of the k^{th}-level of the NPA hierarchy. Hence, we should expect that $\mathcal{P}_k \subseteq \mathcal{L}_k$ for all $k \in \mathbb{N}$ which is indeed the case as we have seen.