

NPA Hierarchy for Quantum Isomorphism and Homomorphism Indistinguishability

based on a joint work with D.E. Roberson, T. Seppelt, and P. Zeman.

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July 9, 2026

Venue: Quantum Constraint Satisfaction Problems, A Satellite workshop of ICALP 2026.

Introduction

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- Homomorphism indistinguishability provides a unified framework for studying relaxations of graph isomorphism arising from a wide range of fields including model theory, optimization, algebraic graph theory, machine learning, and category theory.

Homomorphism Indistinguishability

The class \mathcal{F}	The relation $G \cong_{\mathcal{F}} H$
All graphs	Isomorphism [Lovász 1967]
Cycles	Cospectrality
Cycles & paths	Cospectral & cospectral complements
Trees	Fractional isomorphism [Dvořák 2010]
Treewidth $\leq k$	Indistinguishable by k -WL [Dvořák 2010]
Treedepth $\leq k$	Ind. by FOL w/ counting of quantifier rank $\leq k$ [Grohe 2020]

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\mathcal{L}_k	k^{th}-level of Lasserre hierarchy is feasible. [Seppelt & Roberson 2024]
\mathcal{P}_k	k^{th} level of NPA is feasible for (G, H)-isomorphism game

Theorem [KRSZ26]

Let G, H be two graphs on the same number of vertices. Then, for each $k \in \mathbb{N}$, there is a class of planar graphs \mathcal{P}_k , such that the following are equivalent:

- 1 The k^{th} -level of the NPA hierarchy for the (G, H) -graph isomorphism game is feasible
- 2 G and H are homomorphism indistinguishable over \mathcal{P}_k , i.e., $G \cong_{\mathcal{P}_k} H$.

Consequences

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- Another consequence of our main result is a randomized polynomial time algorithm deciding *exact feasibility* of each level of the NPA hierarchy for quantum isomorphism.
- We are currently working on extending this algorithm to a larger class of semidefinite programs, including the NPA hierarchy of relaxations for Linear Constraint System games.

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- In each round, the referee picks two vertices g and g' from the graph G (uniformly at random) and sends them to Alice and Bob respectively. Alice and Bob are required to respond with vertices h and h' from the graph H respectively.
- The referee then decides if they win or lose based on
 $V : V(G) \times V(G) \times V(H) \times V(H) \rightarrow \{0, 1\}$

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

The Graph Isomorphism Game

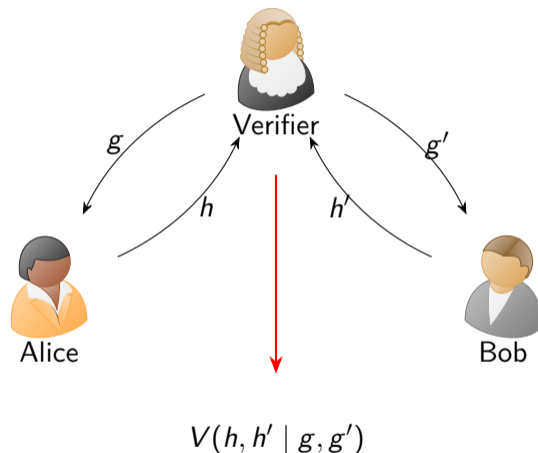


Figure: The Graph Isomorphism Game

- A *quantum strategy* for the graph isomorphism game involves mutually commuting POVMs $\{E_{gh}\}_{h \in V(H)} \subseteq \mathcal{B}(\mathcal{H})$ and $\{F_{g'h'}\}_{h' \in V(H)} \subseteq \mathcal{B}(\mathcal{H})$ for each $g, g' \in V(G)$ and an entangled state $|\psi\rangle \in \mathcal{B}(\mathcal{H})$ shared between Alice and Bob.

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- Upon receiving the questions g, g' measure their part of the shared entangled state $|\psi\rangle$ by using the POVMs $\{E_{g,h}\}_{h \in V(H)}$ and $\{F_{g',h'}\}_{h' \in V(H)}$ respectively. Hence, the probability that they output h, h' given the questions g, g' , is given by

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- Such a quantum strategy is *perfect* if $V(h, h' \mid g, g') = 0$ implies that $p(h, h' \mid g, g') = 0$. In this case, the graphs are said to be *quantum isomorphic*.

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Theorem [AMR⁺19]

Two graphs G, H are quantum isomorphic if and only if there is a unital C^* -algebra \mathcal{A} equipped with a tracial state ρ and projections $\{P_{gh}\}_{g \in V(G), h \in V(H)} \subseteq \mathcal{A}$ such that:

- 1 $\sum_{h' \in V(H)} P_{gh'} = \sum_{g' \in V(G)} P_{g'h} = 1$ for all $g \in V(G)$ and $h \in V(H)$.
- 2 The operator matrix $P = [P_{g,h}]_{g \in V(G), h \in V(H)}$ satisfies $A_G P = P A_H$.

In this case, one can construct a perfect strategy p such that

$$p(h, h' \mid g, g') = \rho(P_{gh} P_{g'h'}).$$

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- What makes it particularly interesting is that the hierarchy converges, i.e., the limit of the optimal value of the SDP relaxations is equal to the *quantum value* of the game.
- We present a synchronous version of the NPA hierarchy for the isomorphism game.

First Level of the NPA Hierarchy (Intuition)

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- By using the GNS construction, we may assume that \mathcal{A} is represented on a Hilbert space \mathcal{H} by a map $\pi : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H})$ and there is a unit vector $|\psi\rangle \in \mathcal{H}$ such that

$$\rho(a) = \langle \psi | \pi(a) | \psi \rangle .$$

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- Now, consider the set of vectors $|v_{gh}\rangle = \pi(P_{gh})|\psi\rangle$ for $g \in V(G)$ and $h \in V(H)$ and let \mathcal{R} denote their gram matrix. Note that all the information for judging whether this strategy is perfect is contained in \mathcal{R} . Indeed, we have

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- Also note that \mathcal{R} satisfies certain properties. For example, for any $g', g \in V(G)$ we have $\sum_{h, h' \in V(H)} \mathcal{R}_{gh, g'h'} = \sum_{h, h' \in V(H)} \langle \psi | \pi(P_{gh}P_{g'h'}) | \psi \rangle = \langle \psi | \psi \rangle = 1$.

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- These conditions are affine and can be used to give an SDP relaxation of quantum isomorphism, which is the first level of the NPA hierarchy. For higher levels, we consider matrices indexed by longer words in $\Sigma := V(G) \times V(H)$.

A Synchronous NPA Hierarchy for Quantum Isomorphism

For two graphs G, 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:

- $\mathcal{R}_{\epsilon, \epsilon} = 1$.
- $\mathcal{R}_{s, t} = \mathcal{R}_{s', t'}$ 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 $s, t \in \Sigma^*$.
- 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

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

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

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- a graph F ,
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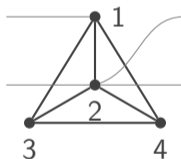


Figure: $\mathbf{F} = (K_4, (1, 2), (2, 2))$

Homomorphism Tensors


Let $\mathbf{F} = (F, \mathbf{u}, \mathbf{v})$ be a k, l -bilabelled graph and G be a graph. The *homomorphism tensor* of \mathbf{F} for G is $\mathbf{F}_G \in \mathbb{C}^{V(G)^k \times V(G)^l}$ whose (\mathbf{x}, \mathbf{y}) -entry is the number of homomorphisms $h: F \rightarrow G$ such that $h(\mathbf{u}_i) = \mathbf{x}_i$ and $h(\mathbf{v}_j) = \mathbf{y}_j$ for all $i \in [k]$ and $j \in [l]$.

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Operations on bilabelled graphs: Series composition

Theorem. For a graph G and bilabelled graphs F, F' ,

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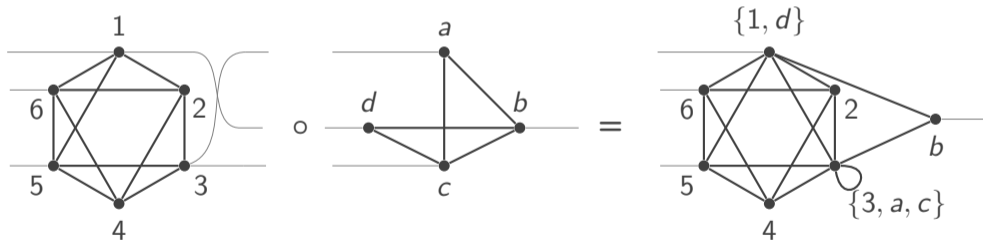
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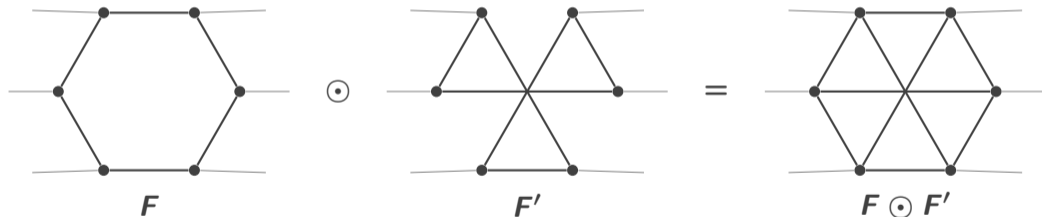
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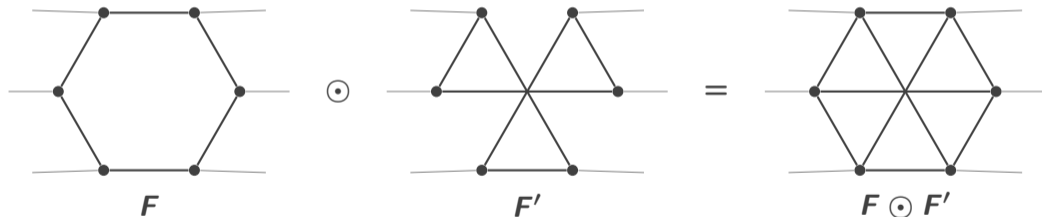


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Other operations: transposition, trace, and cyclic permutations.

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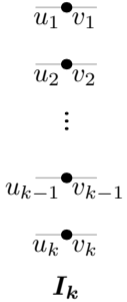
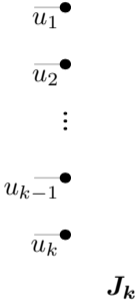
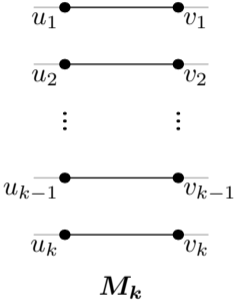
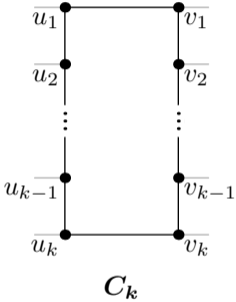


Figure: Atomic Graphs

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- 1 \mathcal{Q}_k^P to be the set of all minors of \mathbf{C}_k ;
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- 3 $\mathcal{Q}_k = \mathcal{Q}_k^P \cup \mathcal{Q}_k^S$.

Then \mathcal{P}_k is the class of (k, k) -bilabelled graphs generated by the elements of \mathcal{Q}_k under

- series composition,
- parallel composition with the elements of \mathcal{Q}_k^P ,
- transpose,
- and cyclic permutations.

Definition. $\mathcal{P}_k = \{F : \exists(F, \mathbf{u}, \mathbf{v}) \in \mathcal{P}_k\}$

The k^{th} level of the NPA hierarchy for the (G, H) -isomorphism game is feasible



There is a level- k quantum isomorphism map from G to H



G and H are homomorphism indistinguishable over \mathcal{P}_k

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- As a consequence of our main result, we may write the following:

Corollary [KRSZ26]

The following are equivalent:

- 1 $G \cong_q H$
- 2 $G \cong_{\mathcal{P}} H$, where $\mathcal{P} = \bigcup_{k=1}^{\infty} \mathcal{P}_k$.

Homomorphism Indistinguishability over Planar Graphs

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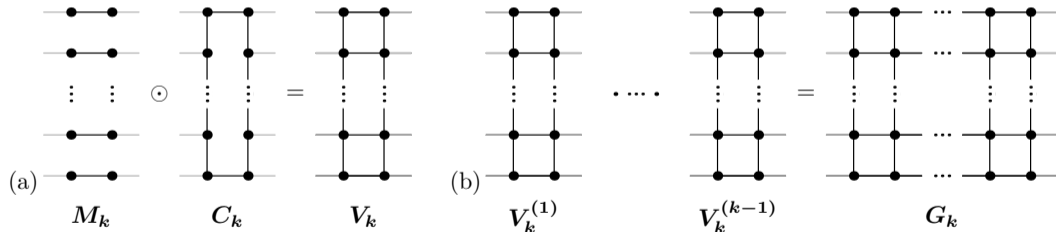
- One can easily show that each \mathcal{P}_k contains only of planar graphs. Hence, to establish Mančinska and Roberson's result, we need to show that \mathcal{P} contains all planar graphs.

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Homomorphism Indistinguishability over Graph Classes of Bounded Treewidth

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- *Treewidth* is a parameter that determines how close a graph is to being a tree. For example, forests have treewidth 1, series-parallel graphs have treewidth 2, and the $k \times k$ grid has treewidth k .
- In [Sep24], Seppelt showed that homomorphism indistinguishability over minor-closed graph classes of bounded treewidth can be decided in polynomial time by a randomized algorithm.

Randomized Polynomial Time Algorithm for the NPA hierarchy

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- The graph classes \mathcal{P}_k that we construct are minor-closed and have treewidth at most $3k - 1$. Hence, it follows that there is a randomized polynomial time algorithm deciding exact feasibility of each level of the NPA hierarchy for the graph isomorphism.
- We improve upon this result by making the dependence on k *explicit*:

Theorem [KRSZ26]

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.

Thank You!

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