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Terrington House
13-15 Hills Road
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Published by Cambridge Quantum

07 July 2017

Relaxations of Graph Isomorphism*†

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Abstract

We introduce a nonlocal game that captures and extends the notion of graph isomorphism. This game can be won in the classical case if and only if the two input graphs are isomorphic. Thus, by considering quantum strategies we are able to define the notion of quantum isomorphism. We also consider the case of more general non-signalling strategies, and show that such a strategy exists if and only if the graphs are fractionally isomorphic. We prove several necessary conditions for quantum isomorphism, including cospectrality, and provide a construction for producing pairs of non-isomorphic graphs that are quantum isomorphic.

We then show that both classical and quantum isomorphism can be reformulated as feasibility programs over the completely positive and completely positive semidefinite cones respectively. This leads us to considering relaxations of (quantum) isomorphism arrived at by relaxing the cone to either the doubly nonnegative (DNN) or positive semidefinite (PSD) cones. We show that DNN-isomorphism is equivalent to the previous defined notion of graph equivalence, a polynomial-time decidable relation that is related to coherent algebras. We also show that PSD-isomorphism implies several types of cospectrality, and that it is equivalent to cospectrality for connected 1-walk-regular graphs. Finally, we show that all of the above mentioned relations form a strict hierarchy of weaker and weaker relations, with non-singalling/fractional isomorphism being the weakest. The techniques used are an interesting mix of algebra, combinatorics, and quantum information.

1998 ACM Subject Classification G.2.2 Graph Theory

Keywords and phrases graph isomorphism, quantum information, semidefinite programming

Digital Object Identifier 10.4230/LIPIcs.ICALP.2017.76

* The full version of this work, including all of the proofs, is given in [3] (https://arxiv.org/abs/1611.09837) and [16].

† LM is supported by UK EPSRC under grant EP/L021005/1. DR is supported by Cambridge Quantum Computing Ltd. and the Engineering and Physical Sciences Research Council of the United Kingdom (EPSRC), as well as Simone Severini and Fernando Brandao. RS is partially supported by grant GA ČR P202-12-G061 and by grant LL1201 ERC CZ of the Czech Ministry of Education, Youth and Sports. SS is supported by the Royal Society, the EPSRC, and the National Natural Science Foundation of China (NSFC). AV is supported in part by the Singapore National Research Foundation under NRF RF Award No. NRF-NRFF2013-13. Part of this work was done while DR, and SS were visiting the Simons Institute for the Theory of Computing.

44th International Colloquium on Automata, Languages, and Programming (ICALP 2017).
Editors: Ioannis Chatzigiannakis, Piotr Indyk, Fabian Kuhn, and Anca Muscholl; Article No. 76; pp. 76:1–76:14
Leibniz International Proceedings in Informatics
Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

1 Introduction

Given graphs G and H, an *isomorphism* from G to H is a bijection $\varphi : V(G) \to V(H)$ such that $\varphi(g)$ is adjacent to $\varphi(g')$ if and only if g is adjacent to g'. When such an isomorphism exists, we say that G and H are *isomorphic* and write $G \cong H$. The notion of isomorphism is central to a broad area of mathematical research encompassing algebraic and structural graph theory, but also combinatorial optimization, parameterized complexity, and logic. The *graph isomorphism (GI) problem* consists of deciding whether two graphs are isomorphic. It is a question with fundamental practical interest due to the number of problems that can be reduced to it. Additionally, the GI problem has a central role in theoretical computer science as it is one of the few naturally defined problems in NP which is not known to be polynomial-time solvable or NP-complete. While there is a deterministic quasipolynomial algorithm for the GI problem [5], regardless of its worst case behavior, the problem can be solved with reasonable efficiency in practice (*e.g.* see [17]). In relation to the context of this paper, it is valuable to notice that the discussion around graph isomorphism has branched into the analysis of many equivalence relations that form hierarchical structures. Prominent instances are, for example, cospectrality, fractional isomorphism, *etc.* [4, 12, 26].

In this work we introduce the graph isomorphism game, which is played by non-communicating players and allows us to capture and extend the notion of graph isomorphism. We investigate three classes of strategies for this game: classical, quantum, and non-signalling. In the classical case, players can win the (G, H)-isomorphism game with certainty if and only if $G \cong H$. This motivates the definition of graphs G and H being quantum, or non-signalling, isomorphic if there exists a perfect quantum, resp. non-signalling, strategy for this game. These two relations are denoted by $G \cong_q H$ and $G \cong_{ns} H$ respectively. We are able to prove two algebraic characterizations of quantum isomorphism, one of which implies that quantum isomorphic graphs are cospectral. We also show that non-signalling isomorphism is equivalent to the previously studied linear relaxation of isomorphism known as *fractional isomorphism* [22].

Another approach we take is to develop characterizations of isomorphism and quantum isomorphism in terms of conic feasibility programs over the completely positive and completely positive semidefinite cones respectively. This is similar to work done in [13, 24, 25], but in our case the programs can be somewhat simplified due the highly structured form of the isomorphism game. By relaxing to either the doubly nonnegative ($\mathcal{DNN}$) or positive semidefinite ($\mathcal{S}_+$) cones, we are able to use this conic feasibility program to define $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphism, denoted $\cong_{\mathcal{DNN}}$ and $\cong_{\mathcal{S}_+}$ respectively. Interestingly, these semidefinite relaxations of quantum isomorphism are still stronger than non-signalling isomorphism. Therefore, for any graphs G and H we have that $G \cong H \Rightarrow G \cong_q H \Rightarrow G \cong_{\mathcal{DNN}} H \Rightarrow G \cong_{\mathcal{S}_+} H \Rightarrow G \cong_{ns} H$. Moreover, we are able to show that none of these implications can be reversed. In particular, we give a general method for constructing quantum isomorphic graphs that are not isomorphic, based on binary linear systems that are not satisfiable but are *quantum satisfiable*.

Interestingly, the notion of $\mathcal{DNN}$-isomorphism turns out to be equivalent to a previously studied relation in graph theory. This relation, known as graph *equivalence*, is defined in terms of an isomorphism between a certain matrix algebra associated to each of the graphs. To prove this equivalence, the main idea is to use the matrix in the conic feasibility program definition of $\mathcal{DNN}$-isomorphism as the Choi matrix of a linear map from the space of matrices indexed by $V(G)$ to the space of matrices indexed by $V(H)$. Like fractional isomorphism, there exists a polynomial time algorithm for deciding graph equivalence.

We also prove a similar algebraic characterization for $\mathcal{S}_+$-isomorphism, but this appears to be a new relation. However, we are able to prove that this relation is strictly stronger than cospectrality. We also show that classical, quantum, $\mathcal{DNN}$-, and $\mathcal{S}_+$-isomorphism can be characterized in terms of whether the Lovász theta function, or an appropriate generalization, achieves a particular value on a certain product graph. This is similar to the results of [24].

The full version of this work, including all of the proofs, is given in [3] and [16].

2 The Graph Isomorphism Game

Given graphs G and H, the (G, H)-isomorphism game is a nonlocal game whose inputs and outputs are vertices of the graphs G and H. For a detailed explanation of general nonlocal games see the full version of the paper [3]. The (G, H)-isomorphism game is played as follows: A referee/verifier selects uniformly at random a pair of vertices $x_A, x_B \in V(G) \cup V(H)$ and sends x_A to Alice and x_B to Bob respectively. The players respond with vertices $y_A, y_B \in V(G) \cup V(H)$. Throughout, we assume that $V(G)$ and $V(H)$ are disjoint so that players know which graph their vertex is from. As with any nonlocal game, Alice and Bob may agree on a strategy for playing the game beforehand, but they are not allowed to communicate after the game has commenced. In order to concisely state the conditions under which Alice and Bob win the (G, H)-isomorphism game, we let $\mathrm{rel}(g, g')$, for vertices g, g' of some graph G, denote the *relationship* of the vertices g and g', i.e., whether they are equal, adjacent, or distinct and non-adjacent.

The first winning condition is that each player must respond with a vertex from the graph that the vertex they received was *not* from. In other words we require that:

$$x_A \in V(G) \Leftrightarrow y_A \in V(H) \text{ and } x_B \in V(G) \Leftrightarrow y_B \in V(H)\,. \tag{1}$$

If condition (1) is not met, the players lose. Assuming (1) holds we define g_A to be the unique vertex of G among x_A and y_A, and we define g_B, h_A, and h_B similarly. In order to win, the answers of the players must also satisfy the following condition:

$$\mathrm{rel}(g_A, g_B) = \mathrm{rel}(h_A, h_B)\,. \tag{2}$$

In other words, if Alice and Bob are given the same vertex, then they must respond with the same vertex. If they receive (non-)adjacent vertices, they must return (non-)adjacent vertices. Also, assuming that Alice receives g_A and Bob h_B, Alice's output h_A must be related to h_B the same way Bob's output g_B is related to g_A. Note that we do not explicitly require that G and H have the same number of vertices. It is also worth pointing out that the (G, H)-isomorphism game is equivalent to the $(\overline{G}, \overline{H})$-isomorphism game, where $\overline{G}$ denotes the *complement* of G, i.e., the graph obtained by switching edges and non-edges of G.

In general one may be interested in the best probability with which Alice and Bob can win this game for some particular G and H. In this work however, we will only be interested in whether or not they can win *perfectly*, i.e., with probability 1. Thus, from henceforth when we say that Alice and Bob cam win the (G, H)-isomorphism game, we mean that they can win with probability 1. Similarly, a *winning* or *perfect strategy* is one that allows them to win with certainty.

Given any fixed strategy for the (G, H)-isomorphism game, we denote by $p(y_A, y_B|x_A, x_B)$ the joint conditional probability of Alice and Bob responding with y_A and y_B upon receiving inputs x_A and x_B respectively. We call such a joint conditional probability distribution a *correlation*. An easy but important observation is that a given strategy for the (G, H)-

isomorphism game is perfect if and only if its corresponding correlation p satisfies

$$p(y_A, y_B|x_A, x_B) = 0, \text{ whenever conditions (1) or (2) fail.} \tag{3}$$

In this work we will focus on three classes of strategies/correlations for the isomorphism game: classical, quantum, and non-signalling.

2.1 Classical strategies

A *deterministic classical strategy* for a nonlocal game is one in which Alice's response is determined by her input, and similarly for Bob. In a general classical strategy, the players may use shared randomness to determine their responses. Once the value that their shared randomness takes is fixed, Alice and Bob's strategy becomes deterministic. This means that the set of (perfect) classical correlations is equal to the convex hull of (perfect) classical deterministic correlations.

Suppose that $\varphi : V(G) \to V(H)$ is an isomorphism of graphs G and H. Then we can construct a perfect strategy for the (G,H)-isomorphism game as follows: if Alice receives $g \in V(G)$ as her input, then she responds with $\varphi(g)$ as her output, and if she receives $h \in V(H)$ as her input, then she responds with $\varphi^{-1}(h)$ as her output. Bob behaves identically. It is not hard to see that this allows Alice and Bob to win the game perfectly. It is not much more difficult to prove the converse (see [3]), and thus we have the following:

▶ **Theorem 1.** *For graphs G and H, the (G,H)-isomorphism game can be won perfectly with a classical strategy if and only if $G \cong H$.*

3 Quantum Isomorphism

In a quantum strategy for the (G,H)-isomorphism game, Alice and Bob are allowed to share and make joint measurements on an entangled state (see [3] for a detailed explanation of shared states and measurements). As any classical post-processing of the outcomes that Alice and Bob perform can be incorporated into the measurements themselves, we may assume that both Alice and Bob have a measurement for each input (an element of $V(G) \cup V(H)$) whose outcomes are indexed by their possible outputs (elements of $V(G) \cup V(H)$). Upon receiving input x, Alice performs her measurement corresponding to x and obtains some outcome y, which she uses as her output, and Bob behaves similarly. Formally, for each $x \in V(G) \cup V(H)$, Alice has a measurement $\mathcal{E}_x = \{E_{xy} \in \mathbb{C}^{d_A \times d_A} : y \in V(G) \cup V(H)\}$ where $E_{xy} \succeq 0$ and $\sum_{y \in V(G) \cup V(H)} E_{xy} = I$, and similarly Bob has measurement $\mathcal{F}_x = \{F_{xy} \in \mathbb{C}^{d_B \times d_B} : y \in V(G) \cup V(H)\}$. They perform these measurements on their shared state $\psi \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$. Note that there are no restrictions on $d_A, d_B \in \mathbb{N}$. The corresponding correlation p for this strategy is given by $p(y,y'|x,x') = \psi^\dagger (E_{xy} \otimes F_{x'y'}) \psi$. If there exists such a strategy that allows Alice and Bob to win the (G,H)-isomorphism game perfectly, then we say that G and H are *quantum isomorphic* and write $G \cong_q H$.

An important property of the isomorphism game is that if Alice and Bob are given the same inputs, they must respond with the same outputs. Games with this property are called *synchronous*, and the perfect quantum strategies for such games are known to have a particular form [14, 23, 15, 8, 21]. Using this we are able to give the following reformulation of quantum isomorphism, the full proof of which is given in [3]:

▶ **Theorem 2.** *Let G and H be graphs. Then $G \cong_q H$ if and only if there exists $d \in \mathbb{N}$ and orthogonal projectors $E_{gh} \in \mathbb{C}^{d \times d}$ for $g \in V(G)$ and $h \in V(H)$ such that*

(i) $\sum_{h\in V(H)} E_{gh} = I$, *for all* $g \in V(G)$*;*
(ii) $\sum_{g\in V(G)} E_{gh} = I$, *for all* $h \in V(H)$*;*
(iii) $E_{gh}E_{g'h'} = 0$, *if* $\mathrm{rel}(g,g') \neq \mathrm{rel}(h,h')$.

The projectors in the above theorem correspond to Alice's (or Bob's) measurement operators in a perfect quantum strategy. One consequence of this is that any winning quantum correlation p for the (G,H)-isomorphism game is *input-output symmetric*, i.e.,

$$p(y,y'|x,x') = p(x,y'|y,x') = p(y,x'|x,y') = p(x,x'|y,y') \text{ for all } x,x',y,y' \in V(G)\cup V(H).$$

Given a set of projectors as in the theorem above, one thing that we could do with them is to make them elements of a block matrix with rows indexed by $V(G)$ and columns indexed by $V(H)$. Investigating the properties of such a matrix leads to the following definition:

▶ **Definition 3.** A block matrix $\mathcal{P}$ with blocks of size d is called a *projective permutation matrix (of block size d)* if it is unitary and all of its blocks are orthogonal projectors.

Note that a projective permutation matrix of block size one is a unitary matrix whose entries square to themselves, *i.e.*, a permutation matrix. The following lemma (see [3] for full proof) shows that projective permutation matrices can be built out of projectors satisfying the first two conditions of Theorem 2.

▶ **Lemma 4.** *A block matrix* $\mathcal{P}$ *with blocks* E_{ij} *for* $i,j \in [n]$ *is a projective permutation matrix if and only if the matrix* E_{ij} *is a projector for all* $i,j \in [n]$ *and*
(i) $\sum_{j=1}^{n} E_{ij} = I$*, for all* $i \in [n]$*;*
(ii) $\sum_{i=1}^{n} E_{ij} = I$*, for all* $j \in [n]$*.*

We note that in the special case where all of the blocks E_{ij} of a projective permutation matrix are of rank one, then the unit vectors that the E_{ij} project onto form a *quantum Latin square*, a notion introduced in [18].

A useful reformulation of graph isomorphism can be stated in terms of the adjacency matrices of the corresponding graphs. Given a graph G, the adjacency matrix of G, denoted A_G, is the symmetric 01-matrix whose gg'-entry is 1 if and only if g is adjacent to g', which we denote by $g \sim g'$. Graphs G and H are isomorphic if and only if there exists a permutation matrix P such that $A_G P = P A_H$, or equivalently $P^T A_G P = A_H$. The motivation for considering projective permutation matrices is that they play the role of permutation matrices in an analogous formulation for quantum isomorphism. This is made precise by the following theorem, whose proof is given in [3]:

▶ **Theorem 5.** *For any two graphs* G *and* H *we have that* $G \cong_q H$ *if and only if there exists* $d \in \mathbb{N}$ *and a projective permutation matrix* $\mathcal{P}$ *of block size* d *such that*

$$(A_G \otimes I_d)\mathcal{P} = \mathcal{P}(A_H \otimes I_d). \tag{4}$$

Since projective permutation matrices are unitary, we can rewrite Equation (4) as $\mathcal{P}^\dagger(A_G \otimes I_d)\mathcal{P} = (A_H \otimes I_d)$. Again, since $\mathcal{P}$ is unitary, this implies that $A_G \otimes I_d$ and $A_H \otimes I_d$, and thus also A_G and A_H, have the same multiset of eigenvalues. Thus we have the following:

▶ **Corollary 6.** *If* $G \cong_q H$*, then* G *and* H *are cospectral with cospectral complements.*

3.1 Separating Classical and Quantum Isomorphism

In order to construct graphs that are quantum isomorphic but not isomorphic, we introduce a type of game investigated by Cleve and Mittal [9] known as *binary constraint system* (BCS) games. We will show that, in the linear case, one can reduce the existence of a perfect classical (quantum) strategy for a BCS game to the existence of a perfect classical (quantum) strategy to a corresponding isomorphism game.

A linear binary constraint system (BCS) $\mathcal{F}$ consists of a family of binary variables $x_1, \dots, x_n$ and *constraints* $C_1, \dots, C_m$, where each C_ℓ is a linear equation over $\mathbb{F}_2$ in some subset of the variables. Thus C_ℓ takes the form $\sum_{x_i \in S_\ell} x_i = b_\ell$ for some $S_\ell \subseteq \{x_1, \dots, x_n\}$ and $b_\ell \in \{0,1\}$. We say that a BCS is *satisfiable* if there is an assignment of values from $\mathbb{F}_2$ to the variables x_i such that every constraint C_ℓ is satisfied. Such an assignment is known as a *satisfying assignment*.

An example of a linear BCS is the following:

$$\begin{aligned} &x_1 + x_2 + x_3 = 0 \qquad\qquad && x_1 + x_4 + x_7 = 0 \\ &x_4 + x_5 + x_6 = 0 && x_2 + x_5 + x_8 = 0 \\ &x_7 + x_8 + x_9 = 0 && x_3 + x_6 + x_9 = 1 \end{aligned} \tag{5}$$

where addition is over $\mathbb{F}_2$. Note that the BCS given above is not satisfiable. Indeed, every variable appears in exactly two constraints and thus summing up all equations modulo 2 we get $0 = 1$.

To any linear BCS $\mathcal{F}$ we associate the following nonlocal game, which we call the *BCS game*. In the BCS game, the verifier gives Alice a constraint C_ℓ and Bob a constraint C_k. In order to win, they must each respond with an assignment of values to the variables in their respective constraints such that those constraints are satisfied. Furthermore, for the variables in $S_\ell \cap S_k$, Alice and Bob must agree on their assignment. Note that if they are given the same constraint, these conditions imply that they must give the same response. We note that in [9], Cleve and Mittal also define a nonlocal game for any linear BCS. This game is very similar, though not identical to the above (Bob is only asked single variables in the game of [9]). However, their results imply that in the quantum and classical cases, these two games are equivalent.

As with the other nonlocal games we have considered in this work, it is not difficult to see that Alice and Bob can win the BCS game classically with probability 1 if and only if the corresponding BCS is satisfiable. This motivates the following definition.

▶ **Definition 7.** A linear BCS is called *quantum satisfiable* if there exists a perfect quantum strategy for the corresponding BCS game.

To any linear BCS $\mathcal{F}$ with m constraints we associate the graph $G_{\mathcal{F}}$ which is defined as follows: For each constraint C_ℓ, and each assignment $f : S_\ell \to \mathbb{F}_2$ that *satisfies* C_ℓ we include a vertex (ℓ, f). Furthermore, we add an edge between two vertices (ℓ, f) and (k, f') if they are *inconsistent*, *i.e.*, if there exists $x_i \in S_\ell \cap S_k$ such that $f(x_i) \neq f'(x_i)$. We remark that this construction is related to the FGLSS reduction from [10], which is well known in approximability literature.

Given any linear BCS $\mathcal{F}$, we define the *homogenization* of $\mathcal{F}$, denoted by $\mathcal{F}_0$, to be the linear BCS obtained from $\mathcal{F}$ by changing the righthand sides of all of the constraints to 0. Note that the homogenization of a linear BCS always has a solution, namely the all-zero assignment. Also note that $G_{\mathcal{F}}$ and $G_{\mathcal{F}_0}$ have the same number of vertices.

Using these constructions, we are able to prove the following (see [3] for proof), where $\alpha(G)$ denotes the independence number of the graph G:

▶ **Theorem 8.** *Let $\mathcal{F}$ be a linear BCS with m constraints. Then the following are equivalent:*
(i) *$\mathcal{F}$ is satisfiable;*
(ii) *The graphs $G_{\mathcal{F}}$ and $G_{\mathcal{F}_0}$ are isomorphic;*
(iii) *$\alpha(G_{\mathcal{F}}) = m$.*

Using the notions of quantum independence number, denoted α_q, and projective packings, we can also prove the following quantum analog of the above (see [3]):

▶ **Theorem 9.** *Let $\mathcal{F}$ be a linear BCS with m constraints. Then the following are equivalent:*
(i) *$\mathcal{F}$ is quantum satisfiable;*
(ii) *The graphs $G_{\mathcal{F}}$ and $G_{\mathcal{F}_0}$ are quantum isomorphic;*
(iii) *There exists a projective packing of $G_{\mathcal{F}}$ of value m;*
(iv) *$\alpha_q(G_{\mathcal{F}}) = m$.*

Thus, to find a pair of graphs that are quantum isomorphic but not isomorphic, it suffices to find a linear BCS that is quantum satisfiable but not satisfiable. One such example is the one given in (5), which corresponds to the well-known Mermin-Peres magic square game. The pair of graphs obtained from this BCS are shown in [3]. In fact, Arkhipov has shown how to construct such a BCS from any non-planar graph [1].

We note here that the first separating example, which was found with the help of Albert Atserias, was slightly different than the one presented above. It was a version of the celebrated CFI construction, named after Cai, Fürer and Immerman [7]. The original CFI construction was designed to produce pairs of non-isomorphic graphs that cannot be distinguished by the d-dimensional Weisfeiler-Lehman algorithm for any fixed d. The CFI construction was reinterpreted by Atserias, Bulatov, and Dawar [2] to view it as an encoding of special systems of linear equations over $\mathbb{Z}_2$, where each variable appears in precisely two equations. Our first separating example was literally the CFI construction corresponding to a system of linear equations as in [2], in which each variable appears in exactly two equations, and that is classically unsatisfiable over $\mathbb{Z}_2$ but quantum satisfiable. The Mermin-Peres magic square game gives rise to such a system of linear equations. The final construction which we described above is a simplified version of this, in which several vertices have been merged together, and several others have been removed, without changing the outcome. The final graphs have a few dozens of vertices. As it turns out, this streamlined version of the construction is quite similar to the FGLSS reduction from the theory of hardness of approximation [10], which interpreted in this context is a reduction from the feasibility problem for arbitrary systems of linear equations over $\mathbb{Z}_2$ to the graph isomorphism problem. As it turns out, the FGLSS construction was also used in the context of the graph isomorphism problem in [19].

4 Non-signalling Isomorphism

An important property of any quantum strategy for the (G, H)-isomorphism game (or any nonlocal game), is that it does not allow the players to communicate any information about their inputs to one another. Formally, this corresponds to

$$\begin{aligned}
&\sum_{y_B} p(y_A, y_B|x_A, x_B) = \sum_{y_B} p(y_A, y_B|x_A, x'_B), \text{ for all } x_A, y_A, x_B, x'_B, \text{ and} \\
&\sum_{y_A} p(y_A, y_B|x_A, x_B) = \sum_{y_A} p(y_A, y_B|x'_A, x_B), \text{ for all } x_B, y_B, x_A, x'_A
\end{aligned} \tag{6}$$

Any correlation which obeys this condition is known as *non-signalling*, and this is known to be a strictly larger class than quantum correlations. Note that this is a condition on correlations rather than strategies, and indeed there may not be any way to physically realize a given non-signalling correlation. Still, there are good reasons for considering this class of correlations. First, they are a linear relaxation of quantum correlations, and so they often allow us to obtain useful bounds on what is possible with quantum strategies, which are notoriously difficult to analyze. Second, they are interesting in their own right since they represent the extreme class of correlations in two senses. In the physical sense, the non-signalling condition can be thought of as encoding the notion that nothing, including information, can travel faster than the speed of light. Thus if Alice and Bob are separated by a great distance and must respond with their answers within a short window of time, then their strategy must be non-signalling. From a mathematical perspective, non-signalling correlations are the most general class of correlations it makes sense to consider for nonlocal games since any larger class would, by definition, allow the parties to communicate to a certain extent. This would essentially violate the definition of a nonlocal game which requires that the parties cannot communicate.

Using the non-signalling condition and the winning conditions of the isomorphism game, one can prove the following lemma (proof given in [3]):

▶ **Lemma 10.** *Let p be a winning non-signalling correlation for the (G, H)-isomorphism game. Then $p(h, h|g, g) = p(g, h|h, g) = p(h, g|g, h) = p(g, g|h, h)$, for all $g \in V(G)$, $h \in V(H)$.*

Note that for a winning correlation p for the (G, H)-isomorphism game, for $g \in V(G)$ we have that $p(y, y'|g, x') = 0$ unless $y \in V(H)$, and similarly with Alice and Bob or G and H switched. This, along with the above lemma allows us to take any winning non-signalling correlation for the (G, H)-isomorphism game and construct the following *doubly stochastic* matrix: $D_{gh} = p(h, h|g, g)$.

It turns out that this matrix has the interesting property that $A_G D = DA_H$. Whenever such a doubly stochastic matrix exists, one says that G and H are *fractionally isomorphic*, denoted $G \cong_f H$. Thus, non-signalling isomorphic graphs are always fractionally isomorphic.

To prove the converse of the above, we need a result of Ramana, Scheinerman, and Ullman [22] which shows that fractional graph isomorphism is equivalent to deciding whether the graphs have a common equitable partition. To explain this result we first need to introduce some definitions.

Let $\mathcal{C} = \{C_1, \dots, C_k\}$ be a partition of $V(G)$ for some graph G. The partition $\mathcal{C}$ is called *equitable* if there exist numbers c_{ij} for $i, j \in [k]$ such that any vertex in C_i has exactly c_{ij} neighbors in C_j. Note that c_{ij} and c_{ji} are not necessarily equal, but $c_{ij}|C_i| = c_{ji}|C_j|$. We refer to the numbers c_{ij} as the *partition numbers* of an equitable partition $\mathcal{C}$. A trivial example of this is the partition where each part has size 1. Less trivially, if G is regular, the partition with only one cell is equitable.

Equivalently, a partition $\mathcal{C} = \{C_1, \dots, C_k\}$ is equitable if for any $i \in [k]$, the subgraph induced by the vertices in C_i is regular, and for any $i \neq j \in [k]$ the subgraph with vertex set $C_i \cup C_j$ and containing the edges between C_i and C_j is a semiregular bipartite graph.

We say that $\mathcal{C}$ and $\mathcal{D}$ have a *common equitable partition* if there exist equitable partitions $\mathcal{C} = \{C_1, \dots, C_k\}$ and $\mathcal{D} = \{D_1, \dots, D_{k'}\}$ for G and H respectively, satisfying $k = k'$, $|C_i| = |D_i|$ for all $i \in [k]$, and lastly, $c_{ij} = d_{ij}$ for all $i, j \in [k]$. As an example, if G and H are both d-regular and have the same number of vertices, then the single cell partitions form a common equitable partition, and thus, by Theorem 11, any such graphs are fractionally isomorphic. This makes it seem like fractional isomorphism is a weak condition, but in fact it is known [6] that asymptotically almost surely no graphs are fractionally isomorphic to any graphs that they are not isomorphic to. Since non-signalling/fractional isomorphism is the coarsest relation we will consider in this work, the same holds for all the other relations we will see. As mentioned above, common equitable partitions characterize fractional isomorphism.

▶ **Theorem 11** ([22]). *Two graphs are fractionally isomorphic if and only if they have a common equitable partition.*

Given a common equitable partition $\mathcal{C} = \{C_1, \ldots, C_k\}$ and $\mathcal{D} = \{D_1, \ldots, D_k\}$ for graphs G and H respectively, one can construct a perfect non-signalling strategy for the (G, H)-isomorphism game. The details are given in [3], but the idea is that if Alice is given $g \in C_i$ and Bob given $g' \in C_j$ and g and g' are adjacent/non-adjacent/equal, then they respond uniformly at random with $h \in D_i$ and $h' \in D_j$ that are adjacent/non-adjacent/equal. The fact that the corresponding correlation is non-signalling follows from the fact that $\mathcal{C}$ and $\mathcal{D}$ form a common equitable partition of G and H. Therefore, we have the following:

▶ **Theorem 12.** *For any graphs G and H we have that $G \cong_f H$ if and only if $G \cong_{ns} H$.*

5 Conic Formulations

Given graphs G and H and a winning correlation p for the (G, H)-isomorphism game, define the matrix M^p to be the matrix with rows and columns indexed by $V(G) \times V(H)$ to have entries $M^p_{gh,g'h'} = p(h, h'|g, g')$.

Note that the matrix M^p does not contain all of the probabilities of p, only those corresponding to inputs from $V(G)$ and outputs from $V(H)$. Thus, in general the matrix M^p may not completely determine the correlation p. However, if p is input-output symmetric, as in the case of classical or quantum correlations, then p is determined by the matrix M^p. Also note that in the classical and quantum cases Alice and Bob are symmetric, i.e., $p(y, y'|x, x') = p(y', y|x', x)$ for all $x, x', y, y' \in V(G) \cup V(H)$, and thus M^p is symmetric.

Since p is a correlation, sums of certain entries of M^p must be 1. Furthermore, since p is winning, certain entries of M^p must be 0. This motivates the following definition:

▶ **Definition 13.** Let G and H be graphs and $\mathcal{K}$ a matrix cone. We say that a matrix M with rows and columns indexed by $V(G) \times V(H)$ is a *$\mathcal{K}$-isomorphism matrix for G to H* if $M \in \mathcal{K}$ and

$$\sum_{h,h' \in V(H)} M_{gh,g'h'} = 1 \text{ for all } g, g' \in V(G) \tag{7}$$

$$\sum_{g,g' \in V(G)} M_{gh,g'h'} = 1 \text{ for all } h, h' \in V(H) \tag{8}$$

$$M_{gh,g'h'} = 0 \text{ if } \operatorname{rel}(g, g') \neq \operatorname{rel}(h, h'). \tag{9}$$

We will say that graphs G and H are $\mathcal{K}$-isomorphic, and write $G \cong_{\mathcal{K}} H$, whenever there exists a $\mathcal{K}$-isomorphism matrix for G to H.

Though we have defined them for any matrix cone $\mathcal{K}$, we will mainly be interested in just four cones in this work. The first cone is the positive semidefinite cone, denoted $\mathcal{S}_+$. Recall that a matrix M is positive semidefinite if and only if it is the Gram matrix of a set of vectors $v_1, \ldots, v_n$, i.e., $M_{ij} = v_i^T v_j$. We will also be interested in the *doubly nonnegative cone*, denoted $\mathcal{DNN}$, which consists of all positive semidefinite matrices that are also entrywise nonnegative. The next cone we will consider is the recently introduced [13] *completely positive semidefinite* *cone*, denoted $\mathcal{CS}_+$, which will correspond to quantum correlations. A matrix M is completely positive semidefinite if it is the Gram matrix of positive semidefinite matrices $\rho_1, \dots, \rho_n$, i.e., $M_{ij} = \langle \rho_i, \rho_j \rangle := \mathrm{Tr}(\rho_i^\dagger \rho_j)$. Note that this inner product is equal to the usual inner product if we think of the matrices ρ_i as vectors, and thus $\mathcal{CS}_+ \subseteq \mathcal{S}_+$. Moreover, $\mathrm{Tr}(AB) \geq 0$ for any positive semidefinite matrices A and B, with equality if and only if $AB = 0$, and thus $\mathcal{CS}_+ \subseteq \mathcal{DNN}$. Lastly, the *completely positive cone*, denoted $\mathcal{CP}$, will correspond to the classical correlations. A matrix is completely positive if it is the Gram matrix of entrywise nonnegative vectors $v_1, \dots, v_n$. Note that if D_i is the diagonal matrix with diagonal entries equal to the entries of v_i, then D_i is positive semidefinite and $v_i^T v_j = \mathrm{Tr}(D_i D_j)$. Therefore, $\mathcal{CP} \subseteq \mathcal{CS}_+$. Altogether we have that $\mathcal{CP} \subseteq \mathcal{CS}_+ \subseteq \mathcal{DNN} \subseteq \mathcal{S}_+$. Moreover, it is known that these containments are all strict for square matrices of dimension at least 5. With the above notions, we can prove the following (full proof given in [16]):

▶ **Theorem 14.** *Suppose G and H are graphs and p is a correlation for the (G, H)-isomorphism game. Then p is winning classical correlation if and only if p is input-output symmetric and M^p is a $\mathcal{CP}$-isomorphism matrix.*

▶ **Theorem 15.** *Suppose G and H are graphs and p is a correlation for the (G, H)-isomorphism game. Then p is a winning quantum correlation if and only if p is input-output symmetric and M^p is a $\mathcal{CS}_+$-isomorphism matrix.*

The above motivates us to investigate the notions of $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphism. In order to do this, we need to define something we call an isomorphism map.

After submission of this work, a referee informed us that the graph isomorphism problem has been formulated as a completely positive program previously in [11].

5.1 Isomorphism Maps

Given a $\mathcal{K}$-isomorphism matrix M for G to H, the *isomorphism map* Φ_M is a linear map from the space of complex matrices indexed by $V(G)$ to the space of complex matrices indexed by $V(H)$ defined as $(\Phi_M(X))_{h,h'} = \sum_{g,g'} M_{gh,g'h'} X_{g,g'}$.

For $\mathcal{K} \subseteq \mathcal{S}_+$, this map has some remarkable properties. In particular, it is completely positive, meaning that $\Phi_M \otimes \mathrm{id}$ maps psd matrices to psd matrices, where id can be an identity map of any size. This is not related to the completely positive cone, an unfortunate ambiguity. The map Φ_M is trace-preserving and unital, meaning that $\Phi_M(I) = I$. It also preserves the sum of the entries of a matrix, and maps the all ones matrix J to itself. If $\mathcal{K} \in \mathcal{DNN}$, then Φ_M maps entrywise nonnegative matrices to entrywise nonnegative matrices. These last three properties define a notion of being doubly stochastic purely in terms of linear maps. The adjoint of an isomorphism map from G to H is an isomorphism map from H to G. Lastly, one can show that $\Phi_M(A_G) = A_H$ and $\Phi_M^*(A_H) = A_G$, where Φ_M^* is the adjoint of Φ_M which will be an isomorphism map for H to G. Since the eigenvalues of a Hermitian matrix X majorize those of a Hermitian matrix Y if and only if there exists a completely positive, trace-preserving, unital map taking X to Y, this last property implies Lemma 16 below. None of these properties are difficult to show, and the details are given in [16].

▶ **Lemma 16.** *If G and H are $\mathcal{S}_+$-isomorphic graphs, then they are cospectral.*

The idea of isomorphism maps is borrowed from Ortiz and Paulsen who constructed similar linear maps from winning correlations for the *homomorphism* game in [20]. These isomorphism maps will allow us to give characterizations of $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphisms in terms of certain algebras associated to graphs. But first we must introduce these algebras.

5.2 Coherent and Partially Coherent Algebras

A subspace of $\mathbb{C}^{n\times n}$ which is also closed under matrix multiplication is an *algebra*. If $\mathcal{A}$ is a subalgebra of $\mathbb{C}^{n\times n}$, then $\mathcal{A}$ is a *coherent algebra* if it contains the identity and the all ones matrix, is closed under Schur (entrywise) product, and is closed under conjugate transpose, *i.e.*, is self-adjoint. The simplest example of a coherent algebra is $\text{span}\{I, J-I\}$. Of course, $\mathbb{C}^{n\times n}$ is itself a coherent algebra. Less trivially, if A is the adjacency matrix of any *strongly regular graph*, then $\text{span}\{I, A, J-I-A\}$ is a coherent algebra.

It follows from the fact that a coherent algebra $\mathcal{A}$ is closed under Schur product that it must have an orthogonal (with respect to the Hilbert-Schmidt inner product) basis of 01 matrices $A_1, \ldots, A_r$. To each of the matrices A_i, we can associate a subset of $V(G)\times V(G)$, namely the set of ordered pairs (g, g') such that the gg'-entry of A_i is 1. This gives a partition of the ordered pairs of vertices of G. One can reformulate the properties of being a coherent algebra in terms of this partition, and a partition with these properties is known as a *coherent configuration*. Conversely, any coherent configuration corresponds to some coherent algebra. The parts in a coherent configuration are usually referred to as its *classes*.

Coherent algebras of graphs

It is not hard to see that the intersection of two coherent algebras is a coherent algebra. We can therefore define the *coherent algebra of a graph* G, denoted $\mathcal{A}_G$, to be the intersection of all coherent algebras containing its adjacency matrix A_G, *i.e.*, the smallest coherent algebra containing A_G. Equivalently, this is the set of all matrices that can be written as a finite expression involving I, A, J, and the operations of addition, scalar multiplication, matrix multiplication, Schur multiplication, and conjugate transpose.

An *isomorphism* between coherent algebras $\mathcal{A}$ and $\mathcal{B}$ is a bijective linear map $\phi : \mathcal{A} \to \mathcal{B}$ that preserves all operations of a coherent algebra, *i.e.*,

- $\phi(M^\dagger) = \phi(M)^\dagger$ for all $M \in \mathcal{A}$;
- $\phi(MN) = \phi(M)\phi(N)$ for all $M, N \in \mathcal{A}$;
- $\phi(M \bullet N) = \phi(M) \bullet \phi(N)$ for all $M, N \in \mathcal{A}$.

As a consequence of the above, we must have that $\phi(I) = I$ and $\phi(J) = J$. More generally, if ϕ is an isomorphism of coherent algebras $\mathcal{A}$ and $\mathcal{B}$, then ϕ maps the elements of the unique 01 basis of $\mathcal{A}$ to those of $\mathcal{B}$ in a manner that preserves how the basis elements relate to one another (this is made precise in [16]).

▶ **Definition 17.** If G and H are two graphs with respective adjacency matrices A_G and A_H and coherent algebras $\mathcal{A}_G$ and $\mathcal{A}_H$, then we say that G and H are *equivalent* if there exists an isomorphism ϕ from $\mathcal{A}_G$ to $\mathcal{A}_H$ such that $\phi(A_G) = A_H$. We refer to the map ϕ as an *equivalence* of G and H.

Note that the condition $\phi(A_G) = A_H$ completely determines the function ϕ on $\mathcal{A}_G$. In Section 5.4, we show that two graphs are $\mathcal{DNN}$-isomorphic if and only if they are equivalent.

5.3 Partially Coherent Algebras

Suppose that S is some subset of $\mathbb{C}^{n\times n}$. We say that an algebra $\mathcal{A}$ is an *S-partially coherent algebra* if $\mathcal{A}$ contains the identity, is self-adjoint, contains the all ones matrix, and is closed under Schur multiplication by any matrix in S.

As with coherent algebras, it is easy to see that the intersection of two S-partially coherent algebras is an S-partially coherent algebra. Therefore, there is some minimal S-partially coherent algebra for any S. This will be equal to the set of matrices that can be expressed using the elements of $S \cup \{I, J\}$ and a finite number of the operations of addition, scalar multiplication, matrix multiplication, conjugate transposition, and Schur multiplication where at least one of the factors is an element of S.

We define the *partially coherent algebra of a graph G*, denoted $\hat{\mathcal{A}}_G$, to be the minimal S-partially coherent algebra where $S = \{I, A_G\}$. Note that this will also be S'-partially coherent for $S' = \{I, A_G, A_{\overline{G}}\}$ since $A_{\overline{G}} = J - I - A_G$ and J is the Schur identity.

▶ **Definition 18.** Let G and H be graphs with adjacency matrices A_G and A_H and partially coherent algebras $\hat{\mathcal{A}}_G$ and $\hat{\mathcal{A}}_H$ respectively. We say that G and H are *partially equivalent* if there exists a linear bijection $\phi : \hat{\mathcal{A}}_G \to \hat{\mathcal{A}}_H$ such that

1. $\phi(M^\dagger) = \phi(M)^\dagger$ for all $M \in \hat{\mathcal{A}}_G$;
2. $\phi(MN) = \phi(M)\phi(N)$ for all $M, N \in \hat{\mathcal{A}}_G$;
3. $\phi(I) = I$, $\phi(A_G) = A_H$, and $\phi(J) = J$;
4. $\phi(M \bullet N) = \phi(M) \bullet \phi(N)$ for all $M \in \{I, A_G\}$ and $N \in \hat{\mathcal{A}}_G$.

We refer to ϕ as a *partial equivalence* of G and H.

5.4 Characterizations of $\mathcal{DNN}$- and $\mathcal{S}_+$-Isomorphisms

Using the ideas from the previous sections we can now give our characterizations of $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphisms (full proof given in [16]):

▶ **Theorem 19.** *Let G and H be graphs. Then $G \cong_{\mathcal{DNN}} H$ if and only if G and H are equivalent. Also, $G \cong_{\mathcal{S}_+} H$ if and only if G and H are partially equivalent.*

The proof of the above goes roughly as follows: If $G \cong_{\mathcal{DNN}} H$, then there exists a $\mathcal{DNN}$-isomorphism matrix M and corresponding isomorphism map Φ_M. When restricted to the coherent algebra $\mathcal{A}_G$, the map Φ_M is an equivalence of G and H. Conversely, suppose ϕ is an equivalence of G and H, and let Π be the orthogonal projection of $\mathbb{C}^{V(G)\times V(G)}$ to $\mathcal{A}_G$, then the Choi matrix of the map $\phi \circ \Pi$ is a $\mathcal{DNN}$-isomorphism matrix for G to H. The proof for $\mathcal{S}_+$-isomorphism is similar.

There is a well known algorithm, known as the Weisfeiler-Lehman algorithm, that determines whether two graphs are equivalent. Thus $\mathcal{DNN}$-isomorphism is polynomial time decidable. We do not yet know the complexity of $\mathcal{S}_+$-isomorphism, but we suspect it is also polynomial time decidable.

We can use the above characterizations of $\mathcal{DNN}$- and $\mathcal{S}_+$-isomorphisms to prove the following results for 1-walk-regular and distance regular graphs (proofs given in [16]):

▶ **Theorem 20.** *Let G be a connected 1-walk-regular graph. If H is a graph, then $G \cong_{\mathcal{S}_+} H$ if and only if H is a connected 1-walk-regular graph that is cospectral to G.*

▶ **Theorem 21.** *Let G be a distance regular graph. If H is a graph, then $G \cong_{\mathcal{DNN}} H$ if and only if H is a distance regular graph that is cospectral to G.*

▶ **Lemma 22.** *If $G \cong_{\mathcal{DNN}} H$, then G and H have the same radius and diameter.*

6 Separations

In Section 3.1 we saw that isomorphism and quantum isomorphism are distinct relations. In this section we show that the rest of relations we have defined are distinct from one another. Here we give examples and brief explanations, but the full details are in [16].

Quantum vs. $\mathcal{DNN}$-Isomorphism. The 4×4 rook's graph and the Shrikhande graph are cospectral distance regular graphs. Therefore, they are $\mathcal{DNN}$-isomorphic by Theorem 21. However, we show that their complements have different quantum chromatic numbers, a parameter that is preserved by quantum isomorphism (see [3] for details).

$\mathcal{DNN}$-Isomorphism vs. $\mathcal{S}_+$-Isomorphism. The 4-cube graph has the binary strings of length 4 as its vertices, two being adjacent if they differ in exactly one bit. The Hoffman graph is the unique cospectral mate of the 4-cube, and they are both connected and 1-walk-regular. Therefore they are $\mathcal{S}_+$-isomorphic by Theorem 20. However, the 4-cube has radius 4 and the Hoffman graph has radius 3, thus they are not $\mathcal{DNN}$-isomorphic by Lemma 22.

$\mathcal{S}_+$-Isomorphism vs. Non-signalling Isomorphism. By Lemma 16, any pair of k-regular graphs on n vertices for some n and k that are not cospectral will work for this. For example, the 6-cycle and two disjoint 3-cycles will do.

Acknowledgements. The authors would like to especially thank Albert Atserias who was instrumental in finding the first separation between isomorphism and quantum isomorphism.

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