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ON THE CLOSURE OF THE COMPLETELY POSITIVE SEMIDEFINITE CONE AND LINEAR APPROXIMATIONS TO QUANTUM COLORINGS*

SABINE BURGDORF†, MONIQUE LAURENT‡, AND TERESA PIOVESAN§

Abstract. The structural properties of the completely positive semidefinite cone $\mathcal{CS}_+^n$, consisting of all the $n \times n$ symmetric matrices that admit a Gram representation by positive semidefinite matrices of any size, are investigated. This cone has been introduced to model quantum graph parameters as conic optimization problems. Recently it has also been used to characterize the set $\mathcal{Q}$ of bipartite quantum correlations, as projection of an affine section of it. Two main results are shown in this paper concerning the structure of the completely positive semidefinite cone, namely, about its interior and about its closure. On the one hand, a hierarchy of polyhedral cones covering the interior of $\mathcal{CS}_+^n$ is constructed, which is used for computing some variants of the quantum chromatic number by way of a linear program. On the other hand, an explicit description of the closure of the completely positive semidefinite cone is given, by showing that it consists of all matrices admitting a Gram representation in the tracial ultraproduct of matrix algebras.

Key words. Quantum graph parameters, Trace nonnegative polynomials, Copositive cone, Chromatic number, Quantum Entanglement, Nonlocal games, Von Neumann algebra.

AMS subject classifications. 15B48, 81P40, 90C22, 90C27.

1. Introduction.

General background. Entanglement, one of the most peculiar features of quantum mechanics, allows different parties to be correlated in a non-classical way. Properties of entanglement can be studied through the set of bipartite quantum correlations, commonly denoted as $\mathcal{Q}$, consisting of the conditional probabilities that two physically separated parties can generate by performing measurements on a shared entangled state. More formally, a conditional bipartite probability distribution $(P(a,b|x,y))_{a\in A, b\in B, x\in X, y\in Y}$ is called *quantum* if $P(a,b|x,y) = \psi^\dagger(E_x^a \otimes F_y^b)\psi$ for some unit vector ψ in $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A, \mathcal{H}_B$ are finite dimensional Hilbert spaces, and some sets of positive semidefinite matrices (aka positive operator valued measure, POVM for short) $\{E_x^a\}_{a\in A}$ and $\{F_y^b\}_{b\in B}$ satisfying $\sum_{a\in A} E_x^a = I$ and $\sum_{b\in B} F_y^b = I$ for all $x \in X, y \in Y$. Notice that we can equivalently assume that the unit vector ψ is real valued and that E_x^a, F_y^b are real valued positive symmetric operators. We will assume this throughout the paper. We only consider the case of two parties (aka the bipartite setting) and the sets X, Y (respectively, A, B) model the possible inputs (respectively, outputs) of the two parties, assumed throughout to be finite. While the set of classical correlations (those obtained using only local and shared randomness) forms a polytope so that membership can be decided using linear programming, the set $\mathcal{Q}$ of quantum correlations is convex but with infinitely many extreme points and its structure is much harder to characterize. An open question in quantum information theory is whether allowing an infinite amount of entanglement, i.e., allowing the composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$

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in the above definition to be infinite dimensional, gives rise to a probability distribution P which is not quantum [33]. In other words, it is not known whether the set of quantum correlations $\mathcal{Q}$ is closed.

A setting which is frequently used to study the power of quantum correlations is the one of *nonlocal games*. In a nonlocal game a referee gives to each of the two cooperating players a question which, without communication throughout the game, they have to answer. According to some known predicate, which depends on the two questions and on the two answers, the referee determines whether the players have won or lost the game. In a quantum strategy the players can use quantum correlations to answer. The *quantum coloring game* is a particular nonlocal game that has received a substantial amount of attention lately (see [1, 10, 16, 22, 26, 27, 28]). Here, each of the two players receives a vertex of a fixed graph G. They win if they output the same color upon receiving the same vertex or if they output different colors on pairs of adjacent vertices. The *quantum chromatic number* $\chi_q(G)$ is the minimum number of colors that the players must use as output set in order to win the coloring game – with a quantum strategy – on all input pairs. It is not hard to see that if the players are restricted to classical strategies then the minimum number of colors they need to win the game on all input pairs is exactly the classical chromatic number $\chi(G)$.

Like its classical analog the quantum chromatic number is an NP-hard graph parameter [16]. Moreover, it is also lower bounded by the Lovász theta number [28], a parameter that can be efficiently computed with semidefinite programming. With the intention of better understanding $\chi_q(G)$ and other related quantum graph parameters, two of the authors have introduced in [22] the *completely positive semidefinite cone* $\mathcal{CS}_+^n$.

Throughout $\mathcal{S}^n$ is the set of real symmetric $n \times n$ matrices, and $\mathcal{S}_+^n$ is the subset of (real) positive semidefinite matrices; $\langle M, M' \rangle = \mathsf{Tr}(MM')$ is the trace inner product and $\mathsf{Tr}(M) = \sum_{i=1}^n M_{ii}$ for $M, M' \in \mathcal{S}^n$. Then, $\mathcal{CS}_+^n$ consists of all matrices $A \in \mathcal{S}^n$ that admit a Gram representation by positive semidefinite matrices, i.e., such that $A = (\langle X_i, X_j \rangle)_{i,j=1}^n$ for some matrices $X_1, \ldots, X_n \in \mathcal{S}_+^d$ and $d \geq 1$. (When we do not want to specify the size of the matrices in $\mathcal{CS}_+^n$ we omit the superscript and write $\mathcal{CS}_+$.) The structure of the matrix cone $\mathcal{CS}_+$ is still largely unknown. In particular, it is not known whether the cone $\mathcal{CS}_+$ is a closed set.

Using an equivalent formulation of the quantum chromatic number proven in [10], it is shown in [22] that the parameter $\chi_q(G)$ can be rewritten as a feasibility program over the completely positive semidefinite cone:

$$\chi_q(G) = \min t \in \mathbb{N} \ \text{ s.t. } \exists A \in \mathcal{CS}_+^{nt},\ A \in \mathcal{A}^t \text{ and } L_{G,t}(A) = 0. \tag{1.1}$$

Here, n is fixed and equal to the number of vertices of the graph G while t is the variable that triggers the size of the matrix variable A in the above program. Indeed, A is indexed by $V(G) \times [t]$. With $\mathcal{A}^t$ we represent the affine space in $\mathcal{S}^{nt}$ defined by the equations

$$\sum_{i,j \in [t]} A_{ui,vj} = 1 \ \text{ for } u, v \in V(G), \tag{1.2}$$

and with $L_{G,t} : \mathcal{S}^{nt} \to \mathbb{R}$ we denote the linear map defined by

$$L_{G,t}(A) = \sum_{u \in V(G), i \neq j \in [t]} A_{ui,uj} + \sum_{uv \in E(G), i \in [t]} A_{ui,vi}. \tag{1.3}$$

Notice that any matrix in $\mathcal{CS}_+$ is positive semidefinite. Moreover, it has nonnegative entries because the inner product of two positive semidefinite matrices is nonnegative. Hence, the condition $L_{G,t}(A) = 0$ is

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equivalent to requiring that all terms in the sum in (1.3) are equal to zero. The constraint $A \in \mathcal{A}^t$ models that the players are using a conditional probability distribution for their strategy, while $L_{G,t}(A) = 0$ imposes that they have a winning strategy for the coloring game.

By replacing in (1.1) the cone $\mathcal{CS}_+$ by its closure $\mathsf{cl}(\mathcal{CS}_+)$, we get another graph parameter, denoted as $\widetilde{\chi}_q(G)$. Namely,

$$\widetilde{\chi}_q(G) = \min t \in \mathbb{N} \ \text{ s.t. } \exists A \in \mathsf{cl}(\mathcal{CS}_+^{nt}),\ A \in \mathcal{A}^t \text{ and } L_{G,t}(A) = 0. \tag{1.4}$$

Clearly, $\widetilde{\chi}_q(G) \leq \chi_q(G)$, with equality if $\mathcal{CS}_+$ is closed. This parameter, which was introduced in [22], will be studied in this paper.

Mančinska and Roberson [23], and independently Sikora and Varvitsiotis [30], recently showed that the set $\mathcal{Q}$ of quantum bipartite correlations can also be described in terms of the completely positive semidefinite cone. They show that $\mathcal{Q}$ can be obtained as the projection of an affine section of the cone $\mathcal{CS}_+$.

Theorem 1.1. [23, 30] *A conditional probability distribution $P = (P(a, b|x, y))$ with input sets X, Y and output sets A, B is quantum (i.e., $P \in \mathcal{Q}$) if and only if there exists a matrix $R \in \mathcal{CS}_+$ indexed by $(X \times A) \cup (Y \times B)$ satisfying the conditions:*

$$\sum_{a,a' \in A} R_{xa,x'a'} = 1 \ \text{ for all } x, x' \in X, \tag{1.5}$$

$$\sum_{b,b' \in B} R_{yb,y'b'} = 1 \ \text{ for all } y, y' \in Y, \tag{1.6}$$

$$\sum_{a \in A, b \in B} R_{xa,yb} = 1 \ \text{ for all } x \in X, y \in Y, \tag{1.7}$$

$$R_{xa,yb} = P(a, b|x, y) \ \text{ for all } a \in A, b \in B, x \in X, y \in Y. \tag{1.8}$$

In other words,

$$\mathcal{Q} = \pi(\mathcal{CS}_+^N \cap \mathcal{B}^t),$$

where $N = |(X \times A) \cup (Y \times B)|$, $\mathcal{B}^t$ is the affine space defined by the constraints (1.5), (1.6) and (1.7), and π is the projection onto the subspace indexed by $(X \times A) \times (Y \times B)$ (defined by (1.8)).

Notice that any feasible matrix R to the above program has the form $\begin{bmatrix} R_1 & P \\ P^T & R_2 \end{bmatrix}$, where R_1 is indexed by $X \times A$, R_2 is indexed by $Y \times B$ and each entry of P is such that $P_{xa,yb} = P(a, b|x, y)$.

As shown in [23, 30], if the completely positive semidefinite cone is closed then the set $\mathcal{Q}$ of quantum bipartite correlations is also closed. Indeed, the constraints (1.5)-(1.7) imply that the set $\mathcal{CS}_+ \cap \mathcal{B}^t$ is bounded. Hence, if $\mathcal{CS}_+$ is closed then $\mathcal{CS}_+ \cap \mathcal{B}^t$ is compact, and thus, its projection $\mathcal{Q} = \pi(\mathcal{CS}_+ \cap \mathcal{B}^t)$ is also compact.

Our contributions. The results of this paper are twofold. As a first main contribution, in Section 2, we construct a hierarchy of polyhedral cones which asymptotically cover the interior of the completely positive semidefinite cone $\mathcal{CS}_+$. Then in Section 3, we show how this hierarchy can be used to study the quantum chromatic number. In particular, we build a hierarchy of linear programs, among which one of them permits to compute the variant $\widetilde{\chi}_q(G)$ in (1.4) of the parameter $\chi_q(G)$, and we apply a similar reasoning to the variant $\widetilde{\chi}_{qa}(G)$ of the parameter $\chi_{qa}(G)$ considered in [26]. In Section 4, we show how to apply this idea to compute other quantum graph parameters and to more general optimization problems over (the closure

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of) the cone $\mathcal{CS}_+$. Furthermore, we extend this construction to build a polyhedral hierarchy that inner approximates the set $\mathcal{Q}$ of quantum correlations and covers its relative interior.

As a second main contribution, in Section 5, we provide an explicit description of the closure of the cone $\mathcal{CS}_+$ in terms of tracial ultraproducts of matrix algebras. Moreover, we exhibit a larger cone, containing $\mathcal{CS}_+$, which can be interpreted as an infinite dimensional analog of $\mathcal{CS}_+$. This cone consists of the matrices which admit a Gram representation by (a specific class of) positive semidefinite operators on a possibly infinite dimensional Hilbert space instead of Gram representations by *finite dimensional* positive semidefinite matrices. We can show that this larger cone is indeed a closed cone and that it is equal to $\mathsf{cl}(\mathcal{CS}_+)$ if Connes' embedding conjecture holds true. Since the description of these cones involve quite some notation and concepts from operator theory, we skip a preliminary description of the used methods and refer directly to Section 5 which can be read independently of the other part. In summary, our results give structural information about the completely positive semidefinite cone $\mathcal{CS}_+$ which comes in two flavors, depending whether we consider its interior or its boundary.

We now give some more details about our first contribution. In a nutshell, the idea for building the hierarchy of polyhedral cones is to discretize the set of positive semidefinite matrices by rational ones with bounded denominators. Namely, given an integer $r \geq 1$, we define the cone $\mathcal{C}_r^n$ as the conic hull of all matrices A that admit a Gram representation by $r \times r$ positive semidefinite matrices $X_1, \ldots, X_n$ whose entries are rational with denominator at most r and satisfy $\sum_{i=1}^n \mathsf{Tr}(X_i) = 1$. We show that the cones $\mathcal{C}_r^n$ and their dual cones $\mathcal{D}_r^n = \mathcal{C}_r^{n*}$ satisfy the following properties:

$$\mathrm{int}(\mathcal{CS}_+^n) \subseteq \bigcup_{r\geq 1} \mathcal{C}_r^n \subseteq \mathcal{CS}_+^n \quad \text{and} \quad \mathcal{CS}_+^{n*} = \bigcap_{r\geq 1} \mathcal{D}_r^n.$$

Moreover, for any fixed r, linear optimization over the cone $\mathcal{C}_r^n$ can be performed in polynomial time in terms of n. This discretization idea was also used in the classical (scalar) setting, where a hierarchy of polyhedral cones is constructed to approximate the completely positive cone (consisting of all matrices that admit a Gram representation by nonnegative vectors) and its dual, the copositive cone (see [34]). Our construction is in fact inspired by this classical counterpart. Discretization is also widely used in optimization to build good approximations for polynomial optimization problems over the standard simplex or for evaluating tensor norms (see e.g. [3, 20, 7] and references therein).

One of the difficulties in using the cone $\mathcal{CS}_+$ for studying the quantum parameter $\chi_q(G)$ or general quantum correlations in $\mathcal{Q}$ stems from the fact that the additional affine conditions posed on the matrix $A \in \mathcal{CS}_+$ imply that it must lie on the boundary of the cone $\mathcal{CS}_+$. This is the case, for instance, for the conditions that A must belong to the affine space $\mathcal{A}^t$ in (1.2), or the condition $L_{G,t}(A) = 0$ in (1.3), or the conditions (1.5), (1.6) and (1.7). Since we do not know whether the cone $\mathcal{CS}_+$ is closed, we may get different parameters depending on whether we use the cone $\mathcal{CS}_+$ or its closure.

In order to be able to exploit the fact that the cones $\mathcal{C}_r^n$ asymptotically cover the full interior of $\mathcal{CS}_+^n$, we will relax the affine constraints (using a small perturbation) to ensure the existence of a feasible solution in the interior of the cone $\mathcal{CS}_+$. In this way, we will be able to get a hierarchy of parameters that can be computed through linear programming and give the exact value of $\widetilde{\chi}_q(G)$. We remark that this result is existential. We can prove the existence of a linear program permitting to compute the quantum parameter, but we do not know at which stage this happens. This result should be seen in the light of a recent result of the same flavor proved in [26]. The authors of [26] consider yet another variant $\chi_{qc}(G)$ of the quantum parameter $\chi_q(G)$, satisfying $\chi_{qc}(G) \leq \chi_q(G)$, and they show that $\chi_{qc}(G)$ can be computed with a positive

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semidefinite program (also not explicitly known). The definition of $\chi_{qc}(G)$ is given in (1.10) below.

Link to other variants of the quantum chromatic number. In the papers [27, 26], Paulsen and coauthors have introduced many variants of the quantum chromatic number motivated by the study of quantum correlations. We recall two of them, the parameters $\chi_{qa}(G)$ and $\chi_{qc}(G)$, in order to pinpoint the link to our parameter $\widetilde{\chi}_q(G)$ and to our approach.

Recall that the quantum chromatic number $\chi_q(G)$ is the minimum number of colors that the players must use to always win the corresponding coloring game with a quantum strategy. In other words, this is the minimum integer t for which there exists a conditional probability distribution $P = (P(i,j|u,v)) \in \mathcal{Q}$ with input sets $X = Y = V(G)$ and output sets $A = B = [t]$, such that $P(i,j|u,u) = 0$ for all $i \neq j \in [t]$ and $u \in V(G)$, and $P(i,i|u,v) = 0$ for all $i \in [t]$ and $uv \in E(G)$. For convenience, in the following paragraphs we will omit the dependence of P on t, which should be considered as implicit. Forcing the probability of these combinations of inputs and output to be zero imposes that the players have a winning strategy. We combine those constraints into a single one by defining the linear map $\mathcal{L}_{G,t} : \mathbb{R}^{(nt)^2} \to \mathbb{R}$ by

$$\mathcal{L}_{G,t}(P) = \sum_{i\neq j\in[t],u\in V(G)} P(i,j|u,u) + \sum_{i\in[t],uv\in E(G)} P(i,i|u,v).$$

Then the players have a winning strategy if and only if the probability distribution P satisfies $\mathcal{L}_{G,t}(P) = 0$. The following is the original definition of $\chi_q(G)$ in [10]:

$$\chi_q(G) = \min t \in \mathbb{N} \ \text{ s.t. } \exists P \in \mathcal{Q} \text{ with } \mathcal{L}_{G,t}(P) = 0.$$

In [10] it is shown that the optimal quantum strategy in the coloring game is symmetric: the two players perform the same action upon receiving the same input. This special additional structure of the coloring game is the reason why $\chi_q(G)$ can be equivalently reformulated as in (1.1).

The parameter $\chi_{qa}(G)$ defined in [27] asks the probability distribution P to be in the closure of $\mathcal{Q}$:

$$\chi_{qa}(G) = \min t \in \mathbb{N} \ \text{ s.t. } \exists P \in \mathsf{cl}(\mathcal{Q}) \text{ with } \mathcal{L}_{G,t}(P) = 0.$$

Hence, the following relationship holds: $\chi_{qa}(G) \leq \chi_q(G)$.

The authors of [27] (see also [26]) also consider probability distributions arising from the relativistic point of view. Roughly, instead of assuming that the measurement operators act on different Hilbert spaces so that joint measurements have a tensor product structure, in the relativistic model the measurement operators act on a common Hilbert space and the operators of the two parties commute mutually. In this case, joint measurement operators have a product structure. More formally, a correlation $P = (P(a,b|x,y))_{a,b,x,y}$ is obtained from relativistic quantum field theory if it is of the form $P(a,b|x,y) = \psi^T E_x^a F_y^b \psi$, where ψ is a unit vector in a (possibly infinite dimensional) Hilbert space $\mathcal{H}$, E_x^a and F_y^b are POVM's on $\mathcal{H}$, and $E_x^a F_y^b = F_y^b E_x^a$ for all $a \in A, b \in B, x \in X, y \in Y$. We denote by $\mathcal{Q}_c$ the set of quantum bipartite correlations arising from the relativistic point of view. The set $\mathcal{Q}_c$ is closed (see e.g. [14, Proposition 3.4]) and the following inclusions hold:

$$\mathcal{Q} \subseteq \mathsf{cl}(\mathcal{Q}) \subseteq \mathcal{Q}_c. \tag{1.9}$$

Deciding whether equality $\mathcal{Q}_c = \mathsf{cl}(\mathcal{Q})$ holds is known to be equivalent to Connes' embedding conjecture (see [25, 14, 17]) and deciding whether $\mathcal{Q}_c = \mathcal{Q}$ is known as Tsirelson's problem. Very recently Slofstra [31] answered the latter question in the negative by showing that $\mathcal{Q}$ is strictly contained in $\mathcal{Q}_c$.

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In [27], the parameter $\chi_{qc}(G)$ is defined as

$$\chi_{qc}(G) = \min t \in \mathbb{N} \ \text{ s.t. } \exists P \in \mathcal{Q}_c \text{ with } \mathcal{L}_{G,t}(P) = 0. \tag{1.10}$$

In [26] it is shown that $\chi_{qc}(G)$ can be computed by a positive semidefinite program (after rounding). This result is existential in the sense that the semidefinite program is not explicitly known. For this the authors of [26] use the semidefinite programming hierarchy developed by Navascués, Pironio and Acín [24] for noncommutative polynomial optimization. This technique can be applied since the definition of $\chi_{qc}(G)$ is in terms of products of operators. Note that this technique cannot be applied to the parameters $\chi_{qa}(G)$ and $\chi_q(G)$ whose definitions involve tensor products of operators. It is not known whether the parameters $\chi_{qa}(G)$ and $\chi_q(G)$ can be written as semidefinite programs. As pointed out in [26], in view of the inclusions in (1.9), the following relationships hold between the parameters:

$$\chi_{qc}(G) \leq \chi_{qa}(G) \leq \chi_q(G).$$

Using Theorem 1.1, we can reformulate the parameters $\chi_q(G)$ and $\chi_{qa}(G)$ as feasibility problems over affine sections of the cones $\mathcal{CS}_+$ and $\mathsf{cl}(\mathcal{CS}_+)$, respectively. Namely, we have

$$\begin{aligned} \chi_q(G) &= \min t \ \text{ s.t. } \exists P \in \pi(\mathcal{CS}_+^{2nt} \cap \mathcal{B}^t) \text{ with } \mathcal{L}_{G,t}(P) = 0, \quad \text{and} \\ \chi_{qa}(G) &= \min t \ \text{ s.t. } \exists P \in \mathsf{cl}(\pi(\mathcal{CS}_+^{2nt} \cap \mathcal{B}^t)) \text{ with } \mathcal{L}_{G,t}(P) = 0. \end{aligned}$$

Recall that we introduced the variant $\widetilde{\chi}_q(G)$ by replacing the cone $\mathcal{CS}_+$ by its closure in the definition (1.1) of $\chi_q(G)$. Analogously, we introduce the variant $\widetilde{\chi}_{qa}(G)$ by replacing $\mathcal{CS}_+$ by its closure in the above definition of $\chi_{qa}(G)$. Namely,

$$\widetilde{\chi}_{qa}(G) = \min t \ \text{ s.t. } \exists P \in \pi(\mathsf{cl}(\mathcal{CS}_+^{2nt}) \cap \mathcal{B}^t) \text{ with } \mathcal{L}_{G,t}(P) = 0. \tag{1.11}$$

Note that the set $\mathsf{cl}(\mathcal{CS}_+) \cap \mathcal{B}^t$ is bounded and thus compact, so that its projection $\pi(\mathsf{cl}(\mathcal{CS}_+) \cap \mathcal{B}^t)$ is compact too. (This is the reason why in the above definition (1.11) we have written $P \in \pi(\mathsf{cl}(\mathcal{CS}_+^{2nt}) \cap \mathcal{B}^t)$ instead of $P \in \mathsf{cl}(\pi(\mathsf{cl}(\mathcal{CS}_+^{2nt}) \cap \mathcal{B}^t))$.) The inclusion $\mathcal{CS}_+ \cap \mathcal{B}^t \subseteq \mathsf{cl}(\mathcal{CS}_+) \cap \mathcal{B}^t$ implies:

$$\mathsf{cl}(\pi(\mathcal{CS}_+ \cap \mathcal{B}^t)) \subseteq \pi(\mathsf{cl}(\mathcal{CS}_+) \cap \mathcal{B}^t),$$

and thus, the following relationship: $\widetilde{\chi}_{qa}(G) \leq \chi_{qa}(G)$. In Section 3, we will show that $\widetilde{\chi}_{qa}$ can be computed with a linear program.

Moreover, note that if a matrix A is feasible for the program (1.4) defining $\widetilde{\chi}_q(G)$, then the matrix $R = \left[\begin{smallmatrix} A & A \\ A & A \end{smallmatrix}\right]$ is feasible for the program (1.11) defining $\widetilde{\chi}_{qa}(G)$. Hence, $\widetilde{\chi}_{qa}(G) \leq \widetilde{\chi}_q(G)$ holds.

The relationship between the different parameters $\chi_q(G), \chi_{qc}(G), \chi_{qa}(G)$ and $\widetilde{\chi}_{qa}(G)$, $\widetilde{\chi}_q(G)$ can be summarized as follows:

$$\begin{array}{ccccc} \chi_{qc}(G) & \leq & \chi_{qa}(G) & \leq & \chi_q(G) \\ & & \rotatebox{90}{$\leq$} & & \rotatebox{90}{$\leq$} \\ & & \widetilde{\chi}_{qa}(G) & \leq & \widetilde{\chi}_q(G). \end{array}$$

2. Polyhedral approximations of $\mathcal{CS}_+$ and its dual cone $\mathcal{CS}_+^*$. In this section, we construct hierarchies of polyhedral cones converging asymptotically to the completely positive semidefinite cone and

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its dual. We start in Section 2.1 by recalling the definition of the cone $\mathcal{CS}_+$ and of its dual cone $\mathcal{CS}_+^*$ as well as some useful properties and we introduce the new hierarchy in Section 2.3. The construction of our polyhedral hierarchy for $\mathcal{CS}_+$ is directly inspired from the classical case where analogous hierarchies of polyhedral cones exist for approximating the completely positive cone $\mathcal{CP}^n$ and the copositive cone $\mathcal{COP}^n$; in Section 2.2, we recall this construction.

2.1. The completely positive semidefinite cone and its dual. The completely positive semidefinite cone $\mathcal{CS}_+$ was introduced in [22] to study graph parameters arising from quantum nonlocal games and quantum information theory. It has also been considered implicitly in [15].

Recall that a matrix $A \in \mathcal{S}^n$ is positive semidefinite if and only if it admits a Gram representation by vectors, i.e., if $A = (\langle x_i, x_j \rangle)_{i,j=1}^n$ for some $x_1, \ldots, x_n \in \mathbb{R}^d$ and $d \geq 1$. We write $A \succeq 0$ (resp., $A \succ 0$) when A is positive semidefinite (resp., positive definite) and $\mathcal{S}_+^n$ is the set of positive semidefinite $n \times n$ matrices.

Definition 2.1. The completely positive semidefinite cone $\mathcal{CS}_+^n$ is the set of symmetric matrices A which admit a Gram representation by positive semidefinite matrices, i.e., $A = (\langle X_i, X_j \rangle)_{i,j}$ for some $X_1, \ldots, X_n \in \mathcal{S}_+^d$ and $d \in \mathbb{N}$.

The completely positive cone $\mathcal{CP}^n$ is the set of symmetric matrices that admit a Gram representation by nonnegative vectors: $A \in \mathcal{CP}^n$ if $A = (\langle x_i, x_j \rangle)_{i,j}$ for some $x_1, \ldots, x_n \in \mathbb{R}_+^d$ and $d \in \mathbb{N}$. The cone $\mathcal{CP}^n$ can be considered as the classical analog of $\mathcal{CS}_+^n$. Clearly, every completely positive semidefinite matrix is positive semidefinite and has nonnegative entries, and every completely positive matrix is completely positive semidefinite. That is, we have the following relationships between these cones:

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{S}_+^n \cap \mathbb{R}_+^{n \times n}.$$

In [22] it is shown that all these inclusions are strict for $n \geq 5$ (see also [15]). For $n \leq 4$ it is well-known that $\mathcal{CP}^n = \mathcal{S}_+^n \cap \mathbb{R}_+^{n \times n}$. For this and other properties of $\mathcal{CP}$ we refer to the book [5]. Both $\mathcal{CP}^n$ and $\mathcal{S}_+^n$ are closed cones, while we do not know whether $\mathcal{CS}_+^n$ is closed.

Moving on to the dual side, as noted in [22], the dual cone of $\mathcal{CS}_+^n$ has a simple characterization in terms of trace nonnegative polynomials. Given a matrix $M \in \mathcal{S}^n$, define the polynomial $p_M = \sum_{i,j=1}^n M_{ij} x_i x_j$ in n noncommuting variables. Then M belongs to the dual cone $\mathcal{CS}_+^{n*}$ precisely when $\mathsf{Tr}(p_M(X_1, \ldots, X_n)) \geq 0$ for all n-tuples $\underline{X} = (X_1, \ldots, X_n) \in \bigcup_{d \geq 1} (\mathcal{S}_+^d)^n$. If we require nonnegativity only for all $\underline{X} \in \mathbb{R}_+^n$ (i.e., the case $d = 1$), which amounts to requiring that the polynomial p_M takes nonnegative values when evaluated at any point in $\mathbb{R}_+^n$, then the matrix M is said to be copositive. The cone of copositive matrices is denoted by $\mathcal{COP}^n$. The cones $\mathcal{CP}^n$ and $\mathcal{COP}^n$ are dual to each other: $\mathcal{COP}^n = \mathcal{CP}^{n*}$ and, by duality, we have the inclusions:

$$\mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n \times n}) \subseteq \mathcal{CS}_+^{n*} \subseteq \mathcal{COP}^n.$$

As will be explained in detail in Section 3, in order to be able to use our polyhedral hierarchy, we will need to have matrices that are in the interior of $\mathcal{CS}_+$. Recall that a matrix $A \in \mathcal{CS}_+$ lies in the interior of $\mathcal{CS}_+$ if and only if $\langle A, M \rangle > 0$ for all nonzero matrices $M \in \mathcal{CS}_+^*$. Hence, A lies on the boundary of $\mathcal{CS}_+$ if and only if there exists a nonzero matrix $M \in \mathcal{CS}_+^*$ such that $\langle A, M \rangle = 0$. For further reference, we observe that matrices in $\mathcal{CS}_+$ with a zero entry, or lying in the affine spaces $\mathcal{A}^t$ or $\mathcal{B}^t$, lie on the boundary of $\mathcal{CS}_+$.

Lemma 2.2. *Consider a matrix $A \in \mathcal{CS}_+$ (of appropriate size). Then A lies on the boundary of $\mathcal{CS}_+$ in*

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any of the following cases: (i) A has a zero entry; (ii) A belongs to the affine space $\mathcal{A}^t$ defined by (1.2), or (iii) A belongs to the affine space $\mathcal{B}^t$ defined by the conditions (1.5), (1.6) and (1.7).

Proof. (i) Say $A \in \mathcal{CS}_+^n$ has a zero entry: $A_{ij} = 0$. Then $\langle A, E_{ij}\rangle = 0$, where E_{ij} is the elementary matrix (with all entries zero except entry 1 at positions (i,j) and (j,i)). As E_{ij} is nonnegative it belongs to $\mathcal{CS}_+^{n*}$, and thus, A lies on the boundary of $\mathcal{CS}_+^n$.

(ii) Assume now that $A \in \mathcal{CS}_+^{nt}$ lies in $\mathcal{A}^t$. Pick two distinct nodes $u, v \in V(G)$ and consider the matrix $M = J \otimes F$, where J is the $t\times t$ all-ones matrix and F is the $n \times n$ matrix with $F_{uu} = F_{vv} = 1$, $F_{uv} = F_{vu} = -1$ and zero elsewhere. Then, $M \succeq 0$ since $J, F \succeq 0$, and thus, $M \in \mathcal{CS}_+^{nt*}$. Moreover, $\langle A, M\rangle = 0$ showing that A lies on the boundary of $\mathcal{CS}_+^{nt}$.

Case (iii) follows with a similar argument. ◻

2.2. Polyhedral approximations of $\mathcal{CP}^n$ and $\mathcal{COP}^n$. As mentioned above, the copositive cone $\mathcal{COP}^n$ consists of all matrices $M \in \mathcal{S}^n$ for which the polynomial $p_M = \sum_{i,j=1}^n M_{ij}x_ix_j$ is nonnegative over $\mathbb{R}_+^n$. Alternatively, a matrix $M \in \mathcal{S}^n$ is copositive if and only if the polynomial p_M is nonnegative over the standard simplex

$$\Delta_n = \left\{ x \in \mathbb{R}_+^n : \sum_{i=1}^n x_i = 1 \right\}.$$

The idea for constructing outer approximations of the copositive cone is simple and relies on requiring nonnegativity of the polynomial p_M over all rational points in the standard simplex with given denominator r and letting r grow. This idea is made explicit in [34] and goes back to earlier work on how to design tractable approximations for quadratic optimization problems over the standard simplex [3, 19] and more general polynomial optimization problems [20]. More precisely, for an integer $r \geq 1$, define the sets

$$\Delta(n,r) = \{x \in \Delta_n : rx \in \mathbb{Z}^n\}, \quad \widetilde{\Delta}(n,r) = \bigcup_{s=1}^r \Delta(n,s)$$

where we restrict to rational points in Δ_n with given denominators. The sets $\widetilde{\Delta}(n,r)$ are nested within the standard simplex: $\widetilde{\Delta}(n,r) \subseteq \widetilde{\Delta}(n,r+1) \subseteq \Delta_n$. Now, following Yildirim [34], define the cone:

$$\mathcal{O}_r^n = \{M \in \mathcal{S}^n : x^{\mathsf{T}}Mx \geq 0, \ \forall x \in \widetilde{\Delta}(n,r)\},$$

and its dual cone $\mathcal{O}_r^{n*}$, which is the conic hull of all matrices of the form vv^{T} for some $v \in \widetilde{\Delta}(n,r)$. By construction, the cones $\mathcal{O}_r^n$ form a hierarchy of outer approximations for $\mathcal{COP}^n$ and their dual cones form a hierarchy of inner approximations for $\mathcal{CP}^n$:

$$\mathcal{COP}^n \subseteq \mathcal{O}_{r+1}^n \subseteq \mathcal{O}_r^n \quad \text{and} \quad \mathcal{O}_r^{n*} \subseteq \mathcal{O}_{r+1}^{n*} \subseteq \mathcal{CP}^n.$$

Yildirim [34] showed the following convergence results.

THEOREM 2.3. [34] *We have: $\mathcal{COP}^n = \bigcap_{r\geq 1} \mathcal{O}_r^n$. Moreover, we have the inclusions* $\mathrm{int}(\mathcal{CP}^n) \subseteq \bigcup_{r\geq 1} \mathcal{O}_r^{n*} \subseteq \mathcal{CP}^n$ *and $\mathcal{CP}^n$ is equal to the closure of the set $\bigcup_{r\geq 1} \mathcal{O}_r^{n*}$.*

2.3. The new cones $\mathcal{C}_r^n$ and $\mathcal{D}_r^n$. We now introduce the cones $\mathcal{C}_r^n$, which will form a hierarchy of inner approximations for the cone $\mathcal{CS}_+^n$, and the cones $\mathcal{D}_r^n$, which will form a hierarchy of outer approximations

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for the dual cone $\mathcal{CS}_+^{n*}$. These cones are in fact dual to each other, so it suffices to define the cones $\mathcal{D}_r^n$. The idea is simple and analogous to the idea used in the classical (scalar) case: instead of requiring trace nonnegativity of the polynomial p_M over the full set $\bigcup_{d\geq 1}(\mathcal{S}_+^d)^n$, we only ask trace nonnegativity over specific finite subsets. We start with defining the set

$$\mathbf{\Delta}_n = \left\{ \underline{X} = (X_1, \ldots, X_n) \in \bigcup_{d\geq 1} (\mathcal{S}_+^d)^n : \sum_{i=1}^n \mathsf{Tr}(X_i) = 1 \right\}, \tag{2.1}$$

which can be seen as a dimension-free matrix analog of the standard simplex Δ_n in $\mathbb{R}^n$. As we now observe, a matrix M belongs to $\mathcal{CS}_+^{n*}$ if and only if its associated polynomial p_M is trace nonnegative on all n-tuples of *rational* matrices in $\mathbf{\Delta}_n$.

LEMMA 2.4. *For $M \in \mathcal{S}^n$ the following assertions are equivalent:*

(i) $M \in \mathcal{CS}_+^{n*}$, *i.e.,* $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ *for all* $\underline{X} \in \bigcup_{d\geq 1}(\mathcal{S}_+^d)^n$.
(ii) $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ *for all* $\underline{X} \in \mathbf{\Delta}_n$.
(iii) $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ *for all* $\underline{X} = (X_1, \ldots, X_n) \in \mathbf{\Delta}_n$ *with* $X_1 \succ 0, \ldots, X_n \succ 0$.
(iv) $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ *for all* $\underline{X} = (X_1, \ldots, X_n) \in \mathbf{\Delta}_n$ *with* $X_1 \succ 0, \ldots, X_n \succ 0$ *and with rational entries.*
(v) $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ *for all* $\underline{X} \in \mathbf{\Delta}_n$ *with rational entries.*

Proof. The implications $(i) \implies (ii) \implies (iii) \implies (iv)$, $(i) \implies (v)$ and $(v) \implies (iv)$ are clear. We will show that $(iv) \implies (iii) \implies (ii) \implies (i)$.

The implication $(ii) \implies (i)$ follows by scaling: Let $\underline{X} \in (\mathcal{S}_+^d)^n$ with the assumption $\lambda = \sum_{i=1}^n \mathsf{Tr}(X_i) > 0$ (else $\underline{X}$ is identically zero and $\mathsf{Tr}(p_M(\underline{X})) = 0$). Then we have $\underline{X}/\lambda \in \mathbf{\Delta}_n$ and thus $\mathsf{Tr}(p_M(\underline{X}/\lambda)) \geq 0$, which implies $\mathsf{Tr}(p_M(\underline{X})) \geq 0$.

The remaining implications follow using continuity arguments. Namely, for the implication $(iv) \implies (iii)$, use the fact that the set of rational positive definite matrices is dense within the set of positive definite matrices. For $(iii) \implies (ii)$, use the fact that the set of positive definite matrices is dense within the set of positive semidefinite matrices. ◻

This motivates introducing the following subset $\mathbf{\Delta}(n,r)$ of the set $\mathbf{\Delta}_n$ obtained by considering only n-tuples of rational positive semidefinite matrices with denominator at most r. This set can be seen as a matrix analog of the rational grid point subsets of the standard simplex Δ_n and it permits to define the new cones $\mathcal{D}_r^n$.

DEFINITION 2.5. Given an integer $r \in \mathbb{N}$, define the set

$$\mathbf{\Delta}(n,r) = \{\underline{X} \in \mathbf{\Delta}_n : \text{ each } X_i \text{ has rational entries with denominator} \leq r\}$$

and define the cone

$$\mathcal{D}_r^n = \{M \in \mathcal{S}^n : \mathsf{Tr}(p_M(\underline{X})) \geq 0, \ \forall \underline{X} \in \mathbf{\Delta}(n,r)\}.$$

Next we show that the cone $\mathcal{D}_r^n$ is a polyhedral cone. Indeed, as we observe in the next lemma, although the set $\mathbf{\Delta}(n,r)$ is not finite, we may without loss of generality replace in the definition of $\mathcal{D}_r^n$ the set $\mathbf{\Delta}(n,r)$

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by its subset $\underline{\mathbf{\Delta}}(n,r)$, obtained by restricting to $r \times r$ matrices $X_1, \ldots, X_n$.

Lemma 2.6. *Define the set*

$$\underline{\mathbf{\Delta}}(n,r) = \left\{ \underline{X} \in (\mathcal{S}^r_+)^n \cap \mathbf{\Delta}_n : \text{ each } X_i \text{ has rational entries with denominator} \leq r \right\}.$$

Then the following equality holds:

$$\mathcal{D}^n_r = \{ M \in \mathcal{S}^n : \mathsf{Tr}(p_M(\underline{X})) \geq 0, \ \forall \underline{X} \in \underline{\mathbf{\Delta}}(n,r) \}.$$

Proof. The inclusion "$\supseteq$" is clear since $\underline{\mathbf{\Delta}}(n,r) \subseteq \mathbf{\Delta}(n,r)$.

To show the reverse inclusion, take a matrix M such that $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ for all $\underline{X} \in \underline{\mathbf{\Delta}}(n,r)$. Consider a n-tuple $\underline{X} = (X_1, \ldots, X_n) \in \mathbf{\Delta}(n,r)$, we now prove that $\mathsf{Tr}(p_M(\underline{X})) \geq 0$. By assumption, the matrices $X_1, \ldots, X_n$ are rational with denominator at most r, $\sum_{i=1}^n \mathsf{Tr}(X_i) = 1$ and $X_1, \ldots, X_n \in \mathcal{S}^d_+$ with $d > r$ (else there is nothing to prove). For each $i \in [n]$, set $I_i = \{k \in [d] : X_i(k,k) \neq 0\}$ and notice that $\mathsf{Tr}(X_i) \geq |I_i|/r$ (since each diagonal entry $X_i(k,k)$ indexed by $k \in I_i$ is at least $1/r$). Hence, we have $1 = \sum_{i=1}^n \mathsf{Tr}(X_i) \geq \sum_{i=1}^n |I_i|/r$, implying $\sum_{i=1}^n |I_i| \leq r$. Then we can find a set I containing $\bigcup_{i \in [n]} I_i$ with cardinality $|I| = r$. As each matrix X_i has only zero entries outside of its principal submatrix $X_i[I]$ indexed by I, then $\mathsf{Tr}(p_M(X_1, \ldots, X_n)) = \mathsf{Tr}(p_M(X_1[I], \ldots, X_n[I])) \geq 0$, where the last inequality follows from the fact that $(X_1[I], \ldots, X_n[I])$ belongs to the set $\underline{\mathbf{\Delta}}(n,r)$. ∎

The cardinality of the set $\underline{\mathbf{\Delta}}(n,r)$ is clearly finite. Moreover, in the following lemma we provide a simple upper bound on the cardinality of $\underline{\mathbf{\Delta}}(n,r)$. The proof is straightforward and thus omitted.

Lemma 2.7. *For any fixed r, the cardinality of the set $\underline{\mathbf{\Delta}}(n,r)$ is polynomial in terms of n. More precisely, let γ_r denote the number of $r \times r$ positive semidefinite matrices whose entries are rational with denominator at most r and whose trace is at most one. Then, $|\underline{\mathbf{\Delta}}(n,r)| \leq (\gamma_r)^r$ if $n \leq r$, and $|\underline{\mathbf{\Delta}}(n,r)| \leq \binom{n}{r}(\gamma_r)^r$ if $n > r$.*

Notice that $\mathsf{Tr}(p_M(\underline{X})) = \sum_{i,j} M_{ij} \langle X_i, X_j \rangle$ for any $\underline{X} = (X_1, \ldots, X_n)$. Hence, the cone $\mathcal{D}^n_r$ can be equivalently defined as the set of matrices $M \in \mathcal{S}^n$ satisfying the (finitely many) linear inequalities: $\sum_{i,j=1}^n M_{ij} \langle X_i, X_j \rangle \geq 0$ for all $(X_1, \ldots, X_n) \in \underline{\mathbf{\Delta}}(n,r)$. This implies the following corollary.

Corollary 2.8. *The cone $\mathcal{D}^n_r$ is a polyhedral cone.*

As $\underline{\mathbf{\Delta}}(n,r) \subseteq \underline{\mathbf{\Delta}}(n,r+1)$, the sets $\mathcal{D}^n_r$ form a hierarchy of outer approximations for $\mathcal{CS}^{n*}_+$:

$$\mathcal{CS}^{n*}_+ \subseteq \mathcal{D}^n_{r+1} \subseteq \mathcal{D}^n_r \subseteq \cdots \subseteq \mathcal{D}^n_1.$$

Hence, $\mathcal{CS}^{n*}_+ \subseteq \bigcap_{r \geq 1} \mathcal{D}^n_r$. In fact, as a direct application of the equivalence of (i) and (v) in Lemma 2.4, equality holds. The proof of the following theorem is thus omitted.

Theorem 2.9. $\mathcal{CS}^{n*}_+ = \bigcap_{r \geq 1} \mathcal{D}^n_r$.

We will also use the following property of the cones $\mathcal{D}^n_r$.

Lemma 2.10. *Consider a sequence of matrices $(M_r)_{r \geq 1}$ in $\mathcal{S}^n$ converging to a matrix $M \in \mathcal{S}^n$. If $M_r \in \mathcal{D}^n_r$ for all $r \in \mathbb{N}$, then $M \in \mathcal{CS}^{n*}_+$.*

Proof. In view of Lemma 2.4, it suffices to show that $\mathsf{Tr}(p_M(\underline{X})) \geq 0$ whenever $\underline{X} \in \mathbf{\Delta}_n$ is rational valued. Fix a rational valued $\underline{X} \in \mathbf{\Delta}_n$ and say that $\underline{X} \in (\mathcal{S}^d_+)^n$ and all its entries have denominator at most

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t. Then $\underline{X} \in \underline{\mathbf{\Delta}}(n,r)$ for all $r \geq r_0 = \max\{d,t\}$. Hence, $\mathsf{Tr}(p_{M_r}(\underline{X})) \geq 0$ for all M_r with $r \geq r_0$. When r tends to infinity, $\mathsf{Tr}(p_{M_r}(\underline{X}))$ tends to $\mathsf{Tr}(p_M(\underline{X}))$, and thus, we obtain that $\mathsf{Tr}(p_M(\underline{X})) \geq 0$. □

We now turn to the description of the dual cone $\mathcal{C}_r^n = \mathcal{D}_r^{n*}$. As a direct application of Lemma 2.6, we can conclude that $\mathcal{C}_r^n$ is the set of conic combinations of matrices which have a Gram representation by matrices in $\underline{\mathbf{\Delta}}(n,r)$; i.e.,

$$\mathcal{C}_r^n = \text{cone}\left\{A \in \mathcal{S}^n : A = (\langle X_i, X_j\rangle)_{i,j=1}^n \text{ for some } (X_1,\ldots,X_n) \in \underline{\mathbf{\Delta}}(n,r)\right\}.$$

By construction, the cones $\mathcal{C}_r^n$ are polyhedral and they form a hierarchy of inner approximations of $\mathcal{CS}_+^n$: $\mathcal{C}_1^n \subseteq \cdots \subseteq \mathcal{C}_r^n \subseteq \mathcal{C}_{r+1}^n \subseteq \mathcal{CS}_+^n$. Moreover, as it is proven in the following lemma, strict inclusion holds.

Lemma 2.11. *For any $n \geq 2$ and $r \geq 1$, we have strict inclusions: $C_r^n \subsetneq C_{r+1}^n \subsetneq \mathcal{CS}_+^n$.*

Proof. The only fact which needs a proof is that each inclusion is strict. It suffices to show this for $n = 2$ since one can extend a matrix A in $\mathcal{C}_r^2$ to a matrix in $\mathcal{C}_r^n$ by adding all zero coordinates, and similar for $\mathcal{CS}_+$. For this we consider a rank 1 matrix $A = vv^T$, where $v = (1\ a)^T$ and a is a nonnegative scalar. Then $A \in \mathcal{CS}_+^2$. If we choose a to be an irrational number, A cannot belong to any cone $\mathcal{C}_r^2$, and if we choose $a = 1/(r+1)$, A belongs to $\mathcal{C}_{r+1}^2$ but not to $\mathcal{C}_r^2$. □

We now show that the union of the cones $\mathcal{C}_r^n$ covers the interior of the cone $\mathcal{CS}_+^n$.

Theorem 2.12. *We have the inclusions:*

$$\text{int}(\mathcal{CS}_+^n) \subseteq \bigcup_{r\geq 1} \mathcal{C}_r^n \subseteq \mathcal{CS}_+^n.$$

Proof. We only need to show the first inclusion. For a contradiction consider a matrix A in the interior of the cone $\mathcal{CS}_+^n$ and assume that A does not belong to $\bigcup_{r\geq 1}\mathcal{C}_r^n$. Then, for each $r \geq 1$, there exists a hyperplane strictly separating A from the (closed convex) cone $\mathcal{C}_r^n$. That is, there exists a matrix $M_r \in \mathcal{D}_r^n$ such that $\langle M_r, A\rangle < 0$ and $\|M_r\| = 1$. Since all matrices M_r lie in a compact set, the sequence $(M_r)_r$ admits a converging subsequence $(M_{r_i})_{i\geq 1}$ which converges to a matrix $M \in \mathcal{S}^n$. By Lemma 2.10, we know that the matrix M then belongs to the cone $\mathcal{CS}_+^{n*}$, and thus, $\langle A, M\rangle \geq 0$. On the other hand, as $\langle A, M_{r_i}\rangle < 0$ for all i, by taking the limit as i tends to infinity, we get that $\langle A, M\rangle \leq 0$. Hence, we obtain $\langle A, M\rangle = 0$, which contradicts the assumption that A lies in the interior of $\mathcal{CS}_+^n$. □

It is easy to give an explicit description of the cones $\mathcal{C}_r^n$ for small r. For example, $\mathcal{C}_1^n$ is the set of $n \times n$ diagonal nonnegative matrices and $\mathcal{C}_2^n$ is the convex hull of the matrices E_{ii} and $E_{ii} + E_{ij} + E_{jj}$ (for $i, j \in [n]$), where E_{ij} denote the elementary matrices in $\mathcal{S}^n$.

3. LP lower bounds to the quantum chromatic number. In this section, we use the polyhedral hierarchy $\mathcal{C}_r^n$ $(r \geq 1)$ to show that the parameter $\widetilde{\chi}_q(G)$ in (1.4) can be written as a linear program. We recall the definition of $\widetilde{\chi}_q(G)$:

$$\widetilde{\chi}_q(G) = \min t \in \mathbb{N} \text{ s.t. } \exists A \in \mathsf{cl}(\mathcal{CS}_+^{nt}),\ A \in \mathcal{A}^t \text{ and } L_{G,t}(A) = 0, \tag{3.1}$$

where the affine space $\mathcal{A}^t$ is defined in (1.2) and the map $L_{G,t}$ in (1.3). A first natural approach for building a linear relaxation of $\widetilde{\chi}_q(G)$ is to replace the cone $\mathsf{cl}(\mathcal{CS}_+^{nt})$ in the definition of $\widetilde{\chi}_q(G)$ by the subcone $\mathcal{C}_r^{nt}$ leading to the parameter

$$\ell_r(G) = \min t \in \mathbb{N} \text{ s.t. } \exists A \in \mathcal{C}_r^{nt},\ A \in \mathcal{A}^t \text{ and } L_{G,t}(A) = 0.$$

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As $\mathcal{C}_r^{nt} \subseteq \mathcal{CS}_+^{nt}$, we have $\widetilde{\chi}_q(G) \leq \chi_q(G) \leq \ell_r(G)$. Moreover, the sequence $(\ell_r(G))_{r\in\mathbb{N}}$ of natural numbers is monotonically nonincreasing and thus has a limit (it even becomes stationary). However, it is not clear whether the limit is equal to $\chi_q(G)$. If one could claim that for $t = \chi_q(G)$ there is a feasible matrix A for the program (3.1) which lies in the interior of $\mathcal{CS}_+^{nt}$ then, by Theorem 2.12, A would belong to some cone $\mathcal{C}_r^{nt}$ which would imply the equality $\chi_q(G) = \ell_r(G)$. But this idea cannot work because, as observed in Lemma 2.2, any matrix feasible for (3.1) lies on the boundary of $\mathcal{CS}_+^{nt}$. To go around this difficulty, our strategy is to relax the affine constraints in (3.1) so as to allow feasible solutions in the interior of $\mathcal{CS}_+^{nt}$.

More precisely, given an integer $k \geq 1$, we consider the affine space $\mathcal{A}_k^t$ defined by the equations: $|\sum_{i,j} A_{ui,vj} - 1| \leq 1/k$ for all $u, v \in V(G)$. We define the parameter:

$$\lambda_k(G) = \min t \ \text{ s.t. } \exists A \in \mathsf{cl}(\mathcal{CS}_+^{nt}),\ A \in \mathcal{A}_k^t \text{ and } L_{G,t}(A) \leq \frac{1}{k}. \tag{3.2}$$

In a first step we show that $\lambda_k(G) = \widetilde{\chi}_q(G)$ for k large enough.

Lemma 3.1. *For any graph G, there exists an integer $k_0 \in \mathbb{N}$ such that $\widetilde{\chi}_q(G) = \lambda_k(G)$ holds for all $k \geq k_0$.*

Proof. Notice that $\lambda_k(G) \leq \widetilde{\chi}_q(G)$ holds for every $k \in \mathbb{N}$. Indeed, any matrix solution for $\widetilde{\chi}_q(G)$ is also a solution for $\lambda_k(G)$. Moreover, as the sequence $(\lambda_k(G))_{k\in\mathbb{N}}$ is a monotone nondecreasing sequence of natural numbers upper bounded by $\widetilde{\chi}_q(G)$, there exists a k_0 such that $\lambda_k(G) = \lambda_{k_0}(G)$ for all $k \geq k_0$. Let $t = \lambda_{k_0}(G)$. For all $k \geq k_0$, there exists a matrix $A_k \in \mathsf{cl}(\mathcal{CS}_+^{nt})$ with $A_k \in \mathcal{A}_k^t$ and $L_{G,t}(A_k) \leq 1/k$. Consider the sequence $(A_k)_{k\geq k_0}$, which is bounded as all A_k lie in $\mathcal{A}_{k_0}^t$. Therefore, the sequence has a converging subsequence to, say, A where $A \in \mathsf{cl}(\mathcal{CS}_+^{nt})$, $A \in \mathcal{A}^t$ and $L_{G,t}(A) = 0$. Hence, A is a feasible solution for $\widetilde{\chi}_q(G)$ and $\widetilde{\chi}_q(G) \leq t = \lambda_{k_0}(G) = \lambda_k(G)$ for all $k \geq k_0$. □

In a second step we show that the new parameter $\lambda_k(G)$ can be computed by a linear program. For this we replace in the definition of $\lambda_k(G)$ the cone $\mathsf{cl}(\mathcal{CS}_+^{nt})$ by the polyhedral cone $\mathcal{C}_r^{nt}$, leading to the following parameter:

$$\lambda_k^r(G) = \min t \ \text{ s.t. } \exists A \in \mathcal{C}_r^{nt},\ A \in \mathcal{A}_k^t \text{ and } L_{G,t}(A) \leq \frac{1}{k}. \tag{3.3}$$

Notice that this parameter $\lambda_k^r(G)$ can be computed through a linear program since $\mathcal{C}_r^{nt}$ is polyhedral. We will show that for any graph G there exist integers k_0 and r_0 such that $\widetilde{\chi}_q(G) = \lambda_{k_0}^{r_0}(G)$. We emphasize that this is an existential result: we do not know for which integers k_0 and r_0 such a convergence happens. One of the ingredients to prove the result is to show the existence of a matrix in the interior of $\mathcal{CS}_+$ satisfying certain constraints. To this end, we will use the matrix $Z = I + J \in \mathcal{S}^{nt}$ where I and J are, respectively, the identity and the all-ones matrix.

Lemma 3.2. *The matrix $Z = I + J \in \mathcal{S}^{nt}$ lies in the interior of $\mathcal{CS}_+$. Moreover, we have that $\sum_{i,j\in[t]} Z_{ui,uj} = t^2 + t$ for all $u \in V(G)$, $\sum_{i,j\in[t]} Z_{ui,vj} = t^2$ for all $u \neq v \in V(G)$ and $L_{G,t}(Z) = nt^2 - nt + 2mt$, where m is the number of edges of the graph G.*

Proof. We only show that $I + J$ lies in the interior of $\mathcal{CS}_+^{nt}$, the other claims are direct verification. Assume that there exists a matrix $M \in \mathcal{CS}_+^{nt*}$ such that $\langle M, I + J\rangle = 0$; we show that $M = 0$. Indeed, as both I and J lie in $\mathcal{CS}_+^{nt}$ we get that $\mathsf{Tr}(M) = 0$ and $\langle J, M\rangle = 0$. Observe that, since M is copositive with zero diagonal entries, all entries of M must be nonnegative. Combining with $\langle J, X\rangle = 0$, we deduce that M is identically zero. □

Theorem 3.3. *For any graph G, there exist k_0 and $r_0 \in \mathbb{N}$ such that $\widetilde{\chi}_q(G) = \lambda_k^r(G)$ for all $k \geq k_0$ and*

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$r \geq r_0$. Moreover, $\lambda_{k_0}^{r_0}(G)$, and thus, $\widetilde{\chi}_q(G)$ can be computed via a linear program.

Proof. From Lemma 3.1 we know that there exists $k_0 \in \mathbb{N}$ such that $\lambda_k(G) = \widetilde{\chi}_q(G)$ for all $k \geq k_0$. In view of this, we just need to show that for this k_0 there exists an integer $r_0 \in \mathbb{N}$ for which $\lambda_{k_0}^{r_0}(G) = \lambda_{k_0}(G)$. Let $t = \lambda_{k_0}(G) = \widetilde{\chi}_q(G)$.

By the definitions (3.2) and (3.3) and the inclusion relationships between the cones $\mathcal{C}_r^{nt}$, we have that the sequence $(\lambda_{k_0}^r)_{r\in\mathbb{N}}$ of natural numbers is nonincreasing and it is lower bounded by $\lambda_{k_0}(G)$. Hence, there exists an $r_0 \in \mathbb{N}$ such that $\lambda_{k_0}^r(G) = \lambda_{k_0}^{r_0}(G) \geq \lambda_{k_0}(G)$ for all $r \geq r_0$. We are left to prove that $\lambda_{k_0}^{r_0}(G) \leq \lambda_{k_0}(G) = t$.

To this end, we show that there exists a matrix $Y_{k_0} \in \operatorname{int}(\mathcal{CS}_+^{nt})$ with $Y_{k_0} \in \mathcal{A}_{k_0}^t$ and $L_{G,t}(Y_{k_0}) \leq 1/k_0$. This will suffice since then by Theorem 2.12, $Y_{k_0} \in \mathcal{C}_{r_0}^{nt}$ for some r_0. Therefore, Y_{k_0} satisfies the conditions in program (3.3), and thus, $\lambda_{k_0}^{r_0}(G) \leq t = \lambda_{k_0}(G)$. To show the existence of such a matrix Y_{k_0}, let $A \in \mathsf{cl}(\mathcal{CS}_+^{nt})$ be a feasible solution of the program (3.1) defining $\widetilde{\chi}_q(G) = t$ and consider the matrix $Z = I + J$ which belongs to $\operatorname{int}(\mathcal{CS}_+^{nt})$ by Lemma 3.2. Then any convex combination $Z_\varepsilon = (1-\varepsilon)A + \varepsilon Z$ (for $0 < \varepsilon < 1$) lies in the interior of $\mathcal{CS}_+^{nt}$. If we can tune ε so that the new matrix Z_ε satisfies the conditions in program (3.3), then we can choose $Y_{k_0} = Z_\varepsilon$ and we are done. We claim that selecting $\varepsilon = \min\left\{\frac{1}{k_0(t^2+t-1)}, \frac{1}{k_0(nt^2-nt+2mt)}\right\}$ will do the trick. Indeed, for this choice of ε we have $Z_\varepsilon \in \operatorname{int}(\mathcal{CS}_+^{nt})$ and $L_{G,t}(Z_\varepsilon) = \varepsilon L_{G,t}(Z) \leq 1/k_0$ (use Lemma 3.2). Moreover, $Z_\varepsilon \in \mathcal{A}_{k_0}^t$ since for all $u, v \in V(G)$ the following holds

$$
\begin{aligned}
\Big|\sum_{i,j\in[t]} Y_{k_0}(ui,vj) - 1\Big| &= \Big|(1-\varepsilon) + \varepsilon \sum_{i,j\in[t]} Z_{ui,vj} - 1\Big| \\
&\leq \Big| -\varepsilon + \varepsilon \sum_{i,j\in[t]} Z_{ui,uj}\Big| = \big|\varepsilon(t^2+t-1)\big| \leq \frac{1}{k_0}.
\end{aligned}
$$

Summarizing, from Lemma 3.1 we know that there exists an integer $k_0 \in \mathbb{N}$ such that $\lambda_{k_0}(G) = \widetilde{\chi}_q(G)$ and we just proved that for this k_0 there exists an integer $r_0 \in \mathbb{N}$ with the property that $\lambda_{k_0}^{r_0}(G) = \lambda_{k_0}(G) = \widetilde{\chi}_q(G)$. ∎

The same result holds for the parameter $\widetilde{\chi}_{qa}(G)$ introduced in (1.11). For clarity we rewrite its definition in the following form:

$$
\widetilde{\chi}_{qa}(G) = \min t \in \mathbb{N} \;\text{ s.t. }\; \exists A \in \mathsf{cl}(\mathcal{CS}_+^{2nt}), A \in \mathcal{B}^t \text{ with } \mathcal{L}_{G,t}(\pi(A)) = 0.
$$

Note the analogy with the definition (3.1) of $\widetilde{\chi}_q(G)$. The only difference is that we now work with matrices A of size $2nt$ (instead of nt) lying in the affine space $\mathcal{B}^t$ (instead of $\mathcal{A}^t$) and satisfying $\mathcal{L}_{G,t}(\pi(A)) = 0$ (instead of $L_{G,t}(A) = 0$). In analogy to the parameter $\lambda_k(G)$ we can define the parameter $\Lambda_k(G)$ by doing these replacements and defining the relaxed affine space $\mathcal{B}_k^t$ in the same way as $\mathcal{A}_k^t$ was defined from $\mathcal{A}^t$. Then the analog of Lemma 3.1 holds: there exists an integer k_0 such that $\widetilde{\chi}_{qa}(G) = \Lambda_k(G)$ for all $k \geq k_0$. Next, replacing the cone $\mathsf{cl}(\mathcal{CS}_+^{2nt})$ by $\mathcal{C}_r^{2nt}$, we get the parameter $\Lambda_k^r(G)$ (the analog of $\lambda_r^k(G)$):

$$
\Lambda_k^r(G) = \min t \in \mathbb{N} \;\text{ s.t. }\; A \in \mathcal{C}_r^{2nt}, A \in \mathcal{B}_k^t \text{ with } \mathcal{L}_{G,t}(\pi(A)) \leq \frac{1}{k}.
$$

The analog of Theorem 3.3 holds, whose proof is along the same lines and thus omitted.

Theorem 3.4. *For any graph G, there exist k_0 and $r_0 \in \mathbb{N}$ such that $\widetilde{\chi}_{qa}(G) = \Lambda_k^r(G)$ for all $k \geq k_0$ and $r \geq r_0$. Hence, the parameter $\widetilde{\chi}_{qa}(G)$ can be computed by a linear program.*

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4. Further applications of the polyhedral approximations. In the previous section, we showed how to use the polyhedral hierarchy $\mathcal{C}_r^n$ to study the quantum chromatic number. This is, however, only one illustrative application. In this section, we explain how a similar approach can be used to study other quantum graph parameters, general optimization problems over the cone $\mathcal{CS}_+$ and the set $\mathcal{Q}$ of quantum bipartite correlations.

4.1. Quantum graph parameters. The quantum chromatic number $\chi_q(G)$ is only one example of a quantum graph parameter that can be written as a conic program over an affine section of the cone $\mathcal{CS}_+$. As shown in [22], the same holds for the parameter $\chi^\star(G)$, a variant of the chromatic number that arises in the entangled-assisted communication setting [8], and for $\alpha_q(G)$ [28] and $\alpha^\star(G)$ [12], two analogous quantum variants of the classical stability number $\alpha(G)$. For example, the parameter $\alpha_q(G)$ can be expressed via the following program

$$\alpha_q(G) = \max t \in \mathbb{N} \text{ s.t. } \exists A \in \mathcal{CS}_+^{nt},\ A \in \mathcal{A}'^t \text{ and } L'_{G,t}(A) = 0, \tag{4.1}$$

where $\mathcal{A}'^t$ is the affine space in $\mathcal{S}^{nt}$ defined by the equations

$$\sum_{u,v \in V(G)} A_{ui,vi} = 1 \text{ for } i \in [t],$$

and $L'_{G,t} : \mathcal{S}^{nt} \to \mathbb{R}$ denotes the linear map defined by

$$L'_{G,t}(A) = \sum_{u \neq v \in V(G), i \in [t]} A_{ui,vi} + \sum_{u \simeq v \in V(G), i \neq j \in [t]} A_{ui,vj},$$

where $u \simeq v$ means that u, v are either adjacent or equal.

By relaxing these programs to optimization over the closure of $\mathcal{CS}_+$, the relaxed parameters can be expressed by means of a linear program, resulting in LP bounds for the original quantum graph parameters. In the case of the quantum stability number $\alpha_q(G)$ one derives a linear program to compute the parameter

$$\widetilde{\alpha}_q(G) = \max t \in \mathbb{N} \text{ s.t. } \exists A \in \mathsf{cl}(\mathcal{CS}_+^{nt}),\ A \in \mathcal{A}'^t \text{ and } L'_{G,t}(A) = 0,$$

which is an upper bound on $\alpha_q(G)$, and $\widetilde{\alpha}_q(G) = \alpha_q(G)$ holds if the cone $\mathcal{CS}_+$ is closed.

This method can also be applied to a more general setting. Sikora and Varvitsiotis [30] showed that a nonlocal game admits a quantum strategy that wins the game with probability one if and only if a certain conic program over an affine section of the cone $\mathcal{CS}_+$ is feasible. The constraints of this program only impose that some entries of the matrix are equal to zero. Thus, the conic program has a form similar to, for example, (4.1) and we can apply the procedure explained above.

4.2. Optimization over the cone $\mathcal{CS}_+$. Our discretization LP-based approach can also be applied to the following class of optimization problems over the (closure of the) cone $\mathcal{CS}_+^n$:

$$\mathsf{opt} = \min\ \langle C, A \rangle \text{ s.t. } A \in \mathsf{cl}(\mathcal{CS}_+^n),\ A \in \mathcal{A} \text{ and } \mathcal{L}(A) = 0,$$

where $C \in \mathcal{S}^n$, $\mathcal{L}$ a linear functional on $\mathcal{S}^n$, and $\mathcal{A} \subseteq \mathcal{S}^n$ is an affine subspace of $\mathcal{S}^n$ with the property that $\mathcal{A} \cap \mathcal{CS}_+^n$ is bounded. Then a double hierarchy can be defined in an analogous manner, yielding a sequence

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of two-parameters LP-based bounds, which converges *asymptotically* to the optimum value of the above optimization program. More concretely, for any integer $k \geq 1$ define the parameter

$$\lambda_k = \min \ \langle C, A\rangle \ \text{ s.t. } \ A \in \mathsf{cl}(\mathcal{CS}_+^n), A \in \mathcal{A}_k \text{ and } |\mathcal{L}(A)| \leq \frac{1}{k},$$

where, assuming that $\mathcal{A}$ is defined by the affine equations $\langle B_j, A\rangle = b_j$ (for $j \in [m]$), the set $\mathcal{A}_k$ is the perturbed affine space defined by the constraints $|\langle B_j, A\rangle - b_j| \leq 1/k$ (for $j \in [m]$). Using similar arguments as for Lemma 3.1, one can show that the sequence $(\lambda_k)_{k\in\mathbb{N}}$ is monotone non-decreasing and converges to opt as $k \to \infty$, but, in contrast to Lemma 3.1, we cannot guarantee finite convergence in general (finite convergence in Lemma 3.1 followed from the fact that the parameter $\lambda_k(G)$ is integer valued, which is generally the case). Next, for any integer $r \geq 1$ define the parameter

$$\lambda_k^r = \min \ \langle C, A\rangle \ \text{ s.t. } \ A \in \mathcal{C}_r, A \in \mathcal{A}_k \text{ and } |\mathcal{L}(A)| \leq \frac{1}{k}.$$

Using similar arguments as for the proof of Theorem 3.3, one can show that the sequence $(\lambda_k^r)_{r\in\mathbb{N}}$ is monotone non-increasing and converges to λ_k. Hence, in contrast to the finite convergence result of Theorem 3.3, we obtain only asymptotic convergence $\lambda_k^r \to \mathsf{opt}$ as k, r tend to infinity.

4.3. Polyhedral approximations for the set of quantum correlations. We use the polyhedral approach to define a hierarchy of polytopes which form an inner approximation to the set of quantum bipartite correlations $\mathcal{Q}$ and cover its relative interior.

As we previously mentioned, the set $\mathcal{Q}$ consists of the conditional probability distributions

$$P = (P(a,b|x,y))_{a\in A, b\in B, x\in X, y\in Y}$$

of the form $P(a,b|x,y) = \langle \psi, (E_x^a \otimes F_y^b)\psi\rangle$, where $\psi \in \mathcal{H}_A \otimes \mathcal{H}_B$ is a unit vector, $\mathcal{H}_A$, $\mathcal{H}_B$ are finite dimensional Hilbert spaces, E_x^a and F_y^b are positive operators forming a POVM with outcomes a and b for measurements x and y, respectively. More precisely, for each $x \in X$, there is a set of positive semidefinite matrices $\{E_x^a\}_{a\in A}$ acting on $\mathcal{H}_A$ such that $\sum_{a\in A} E_x^a = I$. Analogously, for every $y \in Y$, there is a POVM $\{F_y^b\}_{b\in B}$ acting on $\mathcal{H}_B$. Moreover, without loss of generality we can assume that all positive semidefinite matrices E_x^a, F_y^b are real valued and with the same dimension d, and that the vector ψ is in $\mathbb{R}^{d^2}$, for some $d \in \mathbb{N}$.

We introduce some notation. For $x \in X$, we let $\underline{E}_x$ denote the tuple $(E_x^a)_{a\in A}$ and then the tuple $\underline{E} = (\underline{E}_x)_{x\in X}$ contains all matrices E_x^a for $a \in A, x \in X$. Analogously, for $y \in Y$, $\underline{F}_y$ denotes the tuple $(F_y^b)_{b\in B}$ and $\underline{F} = (\underline{F}_y)_{y\in Y}$ contains all matrices F_y^b for $b \in B, y \in Y$. We let Γ' denote the set of all triples $(\underline{E}, \underline{F}, \psi)$, where $\underline{E} = (\underline{E}_x)_{x\in X}$, $\underline{F} = (\underline{F}_y)_{y\in Y}$ and each $\underline{E}_x, \underline{F}_y$ is a POVM, and where ψ is a unit vector. By definition the elements of $\mathcal{Q}$ are characterized by triples in the set Γ'. We define the sets

$$\begin{aligned}\Gamma_d = \{(\underline{E}, \underline{F}, \psi) : \ & \underline{E} = (\underline{E}_x)_{x\in X} \text{ where each } \underline{E}_x = (E_x^a)_{a\in A} \in (\mathcal{S}_+^d)^{|A|} \text{ is a POVM},\\ & \underline{F} = (\underline{F}_y)_{y\in Y} \text{ where each } \underline{F}_y = (F_y^b)_{b\in B} \in (\mathcal{S}_+^d)^{|B|} \text{ is a POVM}\\ & \text{and } \psi \in \mathbb{R}^{d^2}, \psi \neq 0, \|\psi\|^2 \leq 1\}\end{aligned}$$

and

$$\Gamma = \bigcup_{d\geq 1} \Gamma_d.$$

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The elements of $\mathcal{Q}$ can, then, be equivalently described as

$$\mathcal{Q} = \left\{ P = \left(\frac{1}{\|\psi\|^2} \langle \psi, (E_a^x \otimes F_b^y)\psi \rangle \right)_{a,b,x,y} \text{ for some } (\underline{E}, \underline{F}, \psi) \in \Gamma \right\}.$$

We introduce a discretization of the set Γ which we then use to define the polyhedral inner approximations of $\mathcal{Q}$.

Definition 4.1. Given an integer $r \in \mathbb{N}$, define the sets

$$\Gamma(r) = \{(\underline{E}, \underline{F}, \psi) \in \Gamma_d : d \leq r \text{ and each element has rational entries with} \\ \text{denominator at most } r\}$$

and

$$\mathcal{Q}(r) = \text{Conv} \left\{ P = \left(\frac{1}{\|\psi\|^2} \langle \psi, (E_a^x \otimes F_b^y)\psi \rangle \right)_{a,b,x,y} \text{ for some } (\underline{E}, \underline{F}, \psi) \in \Gamma(r) \right\}.$$

By construction, the set $\Gamma(r)$ is finite, and thus, the set $\mathcal{Q}(r)$ is a polytope. Clearly, $\mathcal{Q}(r) \subseteq \mathcal{Q}(r+1) \subseteq \mathcal{Q}$ holds for every $r \in \mathbb{N}$, and therefore, the polytopes $\mathcal{Q}(r)$ form a hierarchy of inner approximations for $\mathcal{Q}$. Moreover, as we see below, the union of the sets $\mathcal{Q}(r)$ covers the relative interior of $\mathcal{Q}$.

Theorem 4.2. *The relative interior of the set $\mathcal{Q}$ is contained in the union $\bigcup_{r\geq 1} \mathcal{Q}(r)$.*

While in Section 2 we considered the set $\boldsymbol{\Delta}_n$ as a dimension-free matrix analog of the standard simplex Δ_n, consisting of the n-tuples of positive semidefinite matrices such that $\mathsf{Tr}(\sum_{i=1}^n X_i) = 1$ (see (2.1)), here we will use a different normalization. Indeed, we will study the set of n-tuples $\underline{X} = (X_1, \ldots, X_n)$ forming a POVM, i.e., a collection of positive semidefinite matrices such that $\sum_{i=1}^n X_i = I$. Notice that this is another possible way to define the dimension-free matrix analog of the standard simplex Δ_n.

The rest of the section will be devoted to the proof of Theorem 4.2. For this, we will first prove that for any triple $(\underline{E}, \underline{F}, \psi) \in \Gamma$ we can find a triple $(\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi}) \in \Gamma(r)$ (for some $r \in \mathbb{N}$) which is arbitrarily close to it and then we will prove some useful geometric properties of the set $\mathcal{Q}$.

In what follows, the norm of a matrix X will be the operator norm $\|X\|$, while for a n-tuple of matrices $\underline{X} = (X_1, \ldots, X_n)$ we define $\|\underline{X}\| = \sqrt{\sum_{i=1}^n \|X_i\|^2}$.

Lemma 4.3. *Given a n-tuple $\underline{X} = (X_1, \ldots, X_n) \in (\mathcal{S}_+^d)^n$ such that $\sum_{i=1}^n X_i = I$ and a constant $\varepsilon > 0$, there exists a n-tuple $\underline{Y} = (Y_1, \ldots, Y_n) \in (\mathcal{S}_+^d)^n$ of rational valued matrices with $\sum_{i=1}^n Y_i = I$ and such that $\|\underline{X} - \underline{Y}\| < \varepsilon$.*

Proof. Let $\underline{X} = (X_1, \ldots, X_n)$ be a POVM, i.e., $\sum_{i=1}^n X_i = I$ and $X_i \succeq 0$ for all $i \in [n]$, and fix $\varepsilon > 0$. We will prove the statement in two steps: we first build a n-tuple $\underline{Z}$ of positive definite matrices such that $\sum_{i=1}^n Z_i = I$ and $\|\underline{X} - \underline{Z}\| < \varepsilon/2$ and then a n-tuple of rational valued positive semidefinite matrices $\underline{Y}$ such that $\sum_{i=1}^n Y_i = I$ and $\|\underline{Z} - \underline{Y}\| < \varepsilon/2$. Combining these two results, we get the statement of the lemma.

Let $0 < \lambda < 1$ be a constant and, for all $i \in [n]$, define $Z_i = (1-\lambda)X_i + \lambda/nI$. Then $\sum_{i=1}^n Z_i = I$, each Z_i is a positive definite matrix, and $\|X_i - Z_i\| = \lambda \|X_i + I/n\|$. Hence, we can choose λ to be small enough such that the n-tuples $\underline{X}$ and $\underline{Z}$ are arbitrarily close.

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As the set of rational positive semidefinite matrices is dense within the set of positive definite matrices, for each $i \in [n-1]$ and $0 < \gamma < 1$, we can pick a rational valued positive semidefinite matrix Y_i such that $\|Z_i - Y_i\| < \gamma$. We show that, for γ small enough, the matrix $Y_n = I - \sum_{i=1}^{n-1} Y_i$ is also positive semidefinite. Since $Z_n = I - \sum_{i=1}^{n-1} Z_i \succ 0$, we have $\|\sum_{i=1}^{n-1} Z_i\| < 1$. Therefore, $\|\sum_{i=1}^{n-1} Y_i\| - \|\sum_{i=1}^{n-1} Z_i\| \leq \|\sum_{i=1}^{n-1}(Y_i - Z_i)\|$, which implies that $\|\sum_{i=1}^{n-1} Y_i\| \leq \gamma(n-1) + \|\sum_{i=1}^{n-1} Z_i\|$. For any $0 < \gamma < (1 - \|\sum_{i=1}^{n-1} Z_i\|)/(n-1)$ we then have that $\|\sum_{i=1}^{n-1} Y_i\| < 1$, equivalently that $Y_n \succ 0$. Hence, we have constructed a rational valued POVM n-tuple $\underline{Y}$ which is arbitrarily close to $\underline{Z}$. □

The above lemma says that we can approximate any POVM by a rational valued one of the same dimension. Moreover, as the set of rational numbers is dense in the set of real numbers, any nonzero vector can be approximated by a rational valued one. By noticing that any element of the set Γ is composed of a collection of POVM's and a nonzero vector, we get the following corollary.

Corollary 4.4. *Given a triple $(\underline{E}, \underline{F}, \psi) \in \Gamma_d$ (for some $d \in \mathbb{N}$) and a constant $\varepsilon > 0$, there exist an integer $r \in \mathbb{N}$ and a triple $(\underline{\widetilde{E}}, \underline{\widetilde{F}}, \widetilde{\psi}) \in \Gamma(r)$ satisfying the inequality $\|(\underline{E}, \underline{F}, \psi) - (\underline{\widetilde{E}}, \underline{\widetilde{F}}, \widetilde{\psi})\| < \varepsilon$.*

We now prove some useful geometrical properties of the set $\mathcal{Q}$. As is well-known, the set $\mathcal{Q}$ is a convex bounded subset of the space $\mathbb{R}^{A\times X\times B\times Y}$, which for convenience is denoted below as $\mathcal{V}$ and can be seen as the set of all $(X \times A) \times (Y \times B)$ matrices. For $x \in X, y \in Y$, let $H_{x,y}$ denote the hyperplane:

$$H_{x,y} = \left\{ P \in \mathcal{V} : \sum_{a\in A, b\in B} P(a,b|x,y) = 1 \right\} = \{P \in \mathcal{V} : \langle J_{xy}, P\rangle = 1\},$$

where $J_{xy} \in \mathcal{V}$ is the matrix whose entries are equal to 1 at the positions within the block $(\{x\}\times A)\times(\{y\}\times B)$ and zero otherwise. Since any $P \in \mathcal{Q}$ is a conditional probability distribution, we have that the inclusion $\mathcal{Q} \subseteq \bigcap_{x\in X, y\in Y} H_{x,y}$ holds and that any $P \in \mathcal{Q}$ is entrywise nonnegative. The combination of these two simple observations gives that the set $\mathcal{Q}$ is bounded. We show that the hyperplanes $H_{x,y}$ are (essentially) the only ones containing $\mathcal{Q}$.

Lemma 4.5. *Assume that the hyperplane $\{P \in \mathcal{V} : \langle M, P\rangle = \alpha\}$ contains the set $\mathcal{Q}$. Then there exist scalars $\lambda_{x,y}$ such that $M = \sum_{x\in X, y\in Y} \lambda_{x,y} J_{xy}$ and $\sum_{x\in X, y\in Y} \lambda_{x,y} = \alpha$.*

Proof. We start by observing that if for any $a \in A$, $b \in B$ the entries $M_{xa,yb}$ are all equal to a common value depending only on (x,y), denoted by $\lambda_{x,y}$, then $\alpha = \sum_{x\in X, y\in Y} \lambda_{x,y}$ and this gives the wanted statement.

Fix $\hat{x} \in X$, $\hat{y} \in Y$ and let $a', a'' \in A$, $b', b'' \in B$; we show that $M_{\hat{x}a',\hat{y}b'} = M_{\hat{x}a'',\hat{y}b''}$. For this we first consider a deterministic conditional probability distribution P (i.e., $P \in \mathcal{V}$ and has exactly one entry equal to 1 in each of its (x,y)-blocks and all other entries equal to zero) such that $P(a', b'|\hat{x}, \hat{y}) = 1$. We also consider a second deterministic conditional probability distribution P' satisfying $P'(a'', b''|\hat{x}, \hat{y}) = 1$ and $P'(a, b|x, y) = P(a, b|x, y)$ for all $x \in X, y \in Y$ with $(x, y) \neq (\hat{x}, \hat{y})$ and all $a \in A, b \in B$. Clearly, P and P' lie in $\mathcal{Q}$. Hence, we have $\langle M, P\rangle = \langle M, P'\rangle$, which implies $M_{\hat{x}a',\hat{y}b'} = M_{\hat{x}a'',\hat{y}b''}$ and thus concludes the proof. □

As $\mathcal{Q}$ is not full-dimensional, any linear inequality $\langle M, P\rangle \leq \alpha$ that is valid for $\mathcal{Q}$ admits several possible forms obtained by adding a linear combination of the equations $\langle J_{xy}, P\rangle = 1$ to it. We say that the inequality $\langle M, P\rangle \leq \alpha$ is *non-trivial* if $\langle M, P\rangle < \alpha$ for some $P \in \mathcal{Q}$, i.e., if $\mathcal{Q}$ is not contained in the hyperplane $\langle M, P\rangle = \alpha$. In the following lemma, we observe that any non-trivial valid linear inequality for

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$\mathcal{Q}$ can be assumed to have a unique representation of a special form.

LEMMA 4.6. *Any linear inequality which is valid for $\mathcal{Q}$ and non-trivial has, without loss of generality, the form:*

$$\langle M, P\rangle \leq 1, \quad \textit{where} \quad M \geq 0 \quad \textit{and} \quad \min{}_{a\in A, b\in B} M_{xa,yb} = 0 \ \forall x \in X, y \in Y. \tag{4.2}$$

Moreover, the same holds for any valid non-trivial inequality for $\mathcal{Q}(r)$ with $r \in \mathbb{N}$.

Proof. Let $\langle M, P\rangle \leq \alpha$ be a non-trivial valid inequality for $\mathcal{Q}$. Up to adding suitable scalar multiples of the matrices J_{xy} and modifying accordingly the right hand side α, we can assume M to be nonnegative and that $\alpha > 0$. Scaling by α we thus can assume that $\alpha = 1$. Finally, let $\mu_{x,y}$ denote the smallest of the entries $M_{xa,yb}$ for $x \in X, y \in Y$ and suppose that $\mu_{x,y} > 0$ for some x, y. Now, if we replace M by $M' = (M - \sum_{x,y} \mu_{x,y} J_{xy})/(1 - \sum_{x,y} \mu_{x,y})$, then we obtain a reformulation of the form $\langle M', P\rangle \leq 1$ as desired. This can be done since the inequality $\langle M, P\rangle \leq 1$ being non-trivial implies that $1 - \sum_{x,y} \mu_{x,y} > 0$. Indeed, by definition of $\mu_{x,y}$ we have that $M - \sum_{x,y} \mu_{x,y} J_{xy} \geq 0$. So, $1 = \sum_{x,y} \mu_{x,y}$ implies that for all $P \in \mathcal{Q}$ we have $\langle M, P, \rangle \geq \sum_{x,y} \mu_{x,y} \langle J_{xy}, P\rangle = 1$, and thus, that $\langle M, P\rangle \leq 1$ is a trivial inequality, which is a contradiction of the assumption.

The same reasoning proves that, for any $r \in \mathbb{N}$, one may assume that any non-trivial valid linear inequality for $\mathcal{Q}(r)$ has the form (4.2). □

The following corollary can be deduced directly from Lemma 4.6.

COROLLARY 4.7. *The set $\mathcal{Q}$ can be defined as the solution set of all its valid inequalities, which can be assumed to be of the form (4.2). Moreover, an element $P \in \mathcal{Q}$ lies in the relative interior of $\mathcal{Q}$ precisely when $\langle M, P\rangle < 1$ for all the non-trivial valid inequalities for $\mathcal{Q}$.*

For the proof of Theorem 4.2 we will also need the following lemma.

LEMMA 4.8. *Assume $\langle M_r, P\rangle \leq 1$ is valid for $\mathcal{Q}(r)$ for all $r \geq 1$ and assume that the sequence $(M_r)_{r\in\mathbb{N}}$ converges to M. Then the inequality $\langle M, P\rangle \leq 1$ is valid for $\mathcal{Q}$.*

Proof. For any fixed $d \in \mathbb{N}$, consider the function $f_d : \Gamma_d \to \mathcal{Q}$ that maps $(\underline{E}, \underline{F}, \psi)$ to $P = (\langle\psi, (\underline{E}_x^a \otimes \underline{F}_y^b)\psi\rangle/\|\psi\|^2)_{a,b,x,y}$. Notice that each f_d is a continuous function.

Consider a $P \in \mathcal{Q}$, then there exist a $d \in \mathbb{N}$ and a triple $(\underline{E}, \underline{F}, \psi) \in \Gamma_d$ such that $f_d(\underline{E}, \underline{F}, \psi) = P$. As f_d is continuos, for any fixed $\varepsilon > 0$ there exists a $\eta > 0$ with the property that for all $(\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi}) \in \Gamma_d$ such that $\|(\underline{E}, \underline{F}, \psi) - (\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi})\| < \eta$ then we have $\|P - \widetilde{P}\| < \varepsilon$ where $\widetilde{P} = f_d(\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi})$. Moreover, from Corollary 4.4 we know that there exists a triple $(\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi})$ with these properties and that is rational valued. Suppose that the denominator of the entries of all the matrices in $\widetilde{\underline{E}}, \widetilde{\underline{F}}$ and in the vector $\widetilde{\psi}$ is at most ℓ and let $r_0 = \max\{\ell, d\}$. Then, $\widetilde{P} = f_d(\widetilde{\underline{E}}, \widetilde{\underline{F}}, \widetilde{\psi}) \in \mathcal{Q}(r)$, and thus, $\langle M_r, \widetilde{P}\rangle \leq 1$ holds for all $r \geq r_0$ by assumption. We have the following chain of inequalities:

$$\begin{aligned}\langle M, P\rangle &= \langle M, P - \widetilde{P}\rangle + \langle M_r, \widetilde{P}\rangle + \langle -M_r + M, \widetilde{P}\rangle \\ &\leq 1 + \|M\|\|P - \widetilde{P}\| + \|\widetilde{P}\|\|M - M_r\| < 1 + \varepsilon\|M\| + \|\widetilde{P}\|\|M - M_r\|,\end{aligned}$$

using the Cauchy-Schwarz inequality. As M_r tends to M, for any r large enough also $\|M - M_r\| \leq \varepsilon$ holds. Hence, for any fixed $\varepsilon > 0$ there exist a $r \in \mathbb{N}$ and a $\widetilde{P} \in \mathcal{Q}(r)$ such that $\langle M, P\rangle < 1 + \varepsilon(\|M\| + \|\widetilde{P}\|)$. As $\mathcal{Q}$ is bounded, $\|M\| + \|\widetilde{P}\|$ is upper bounded by an absolute constant. Therefore, by letting ε tend to zero, we deduce that the inequality $\langle M, P\rangle \leq 1$ is valid for $\mathcal{Q}$. □

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We can finally prove the statement of Theorem 4.2.

Proof of Theorem 4.2. Consider an element P_0 lying in the relative interior of $\mathcal{Q}$ and, for a contradiction, assume that it does not belong to any of the sets $\mathcal{Q}(r)$. Then, for each $r \geq 1$, there exists a non-trivial inequality valid for $\mathcal{Q}(r)$ which separates P_0 from the closed convex set $\mathcal{Q}(r)$, i.e., there exist matrices M_r and $\alpha_r > 0$ such that $\langle M_r, P\rangle \leq \alpha_r$ for all $P \in \mathcal{Q}(r)$ while $\langle M_r, P_0\rangle \geq \alpha_r$. By Lemma 4.6, the inequalities can be chosen of the form $\langle M_r, P\rangle \leq 1$ and satisfying (4.2). Since all the entries of M_r lie in $[0, 1]$, the sequence $(M_r)_{r\in\mathbb{N}}$ admits a converging subsequence $(M_{r_i})_{i\geq 1}$ that converges to, say, M. Moreover, $\langle M_{r_i}, P\rangle \leq 1$ for all $P \in \mathcal{Q}(r_i)$ $(i \geq 1)$ and, from Lemma 4.8, we deduce that the inequality $\langle M, P\rangle \leq 1$ is valid for $\mathcal{Q}$. Hence, we have $\langle M, P_0\rangle \leq 1$. At the same time, $\langle M_r, P_0\rangle \geq 1$ holds for all r by construction. Taking the limit as i tends to infinity, we obtain that $\langle M, P_0\rangle \geq 1$. Therefore, the equality $\langle M, P_0\rangle = 1$ holds. However, since P_0 lies in the relative interior of $\mathcal{Q}$, by Corollary 4.7 the inequality $\langle M, P\rangle \leq 1$ must be trivial for $\mathcal{Q}$ and it thus defines a hyperplane that contains the set $\mathcal{Q}$. Using Lemma 4.5 we know that $M = \sum_{x,y} \lambda_{x,y} J_{xy}$ for some scalars $\lambda_{x,y}$. We now show that for all x, y the scalar $\lambda_{x,y}$ is equal to zero. This means that $M = 0$ and gives a contradiction.

Fix some $x \in X, y \in Y$. As $\langle M_r, P\rangle \leq 1$ is a valid non-trivial inequality for $\mathcal{Q}(r)$, by Lemma 4.6 it follows that each M_r has at least one zero entry within the block indexed by $(\{x\} \times A) \times (\{y\} \times B)$. Hence, there must exist a pair $(a, b) \in A \times B$ and an infinite subsequence $(M_{r_j})_{j\geq 1}$ of the sequence $(M_r)_{r\in\mathbb{N}}$ such that all M_{r_j} have a zero entry at the same position (xa, yb). Taking the limit as j tends to infinity, we obtain that the (xa, yb)-entry of M must be equal to 0. However, this entry is equal to $\lambda_{x,y}$, which implies that $\lambda_{x,y} = 0$, as desired. □

5. The closure of $\mathcal{CS}_+$. In the introduction, we have mentioned that if the completely positive semidefinite cone is closed, then the set of quantum correlations would be closed as well (see also [23, 30]). Although we still do not know whether $\mathcal{CS}_+$ is closed, in this section, we make a small progress by giving a new description of the closure of $\mathcal{CS}_+$ using the tracial ultraproduct of matrix algebras $\mathbb{R}^{k\times k}$. More precisely, the closure $\mathsf{cl}(\mathcal{CS}_+)$ consists of the symmetric matrices having a Gram representation by positive semidefinite operators which belong to the above mentioned tracial ultraproduct. This ultraproduct will be an algebra of bounded operators on an infinite dimensional Hilbert space.

A connection between $\mathsf{cl}(\mathcal{CS}_+)$ and the Gram matrices of operators on infinite dimensional Hilbert spaces has already been made by two of the authors in [22]. Namely, let $\mathcal{S}^{\mathbb{N}}$ denote the vector space of all infinite symmetric matrices $X = (X_{ij})_{i,j}$, indexed by $i, j \in \mathbb{N}$, with finite norm $\sum_{i,j\geq 1} X_{ij}^2 < \infty$, equipped with the inner product $\langle X, Y\rangle = \sum_{i,j\geq 1} X_{ij}Y_{ij}$. Using this notation, we let $\mathcal{CS}^n_{\infty+}$ denote the convex cone of matrices $A \in \mathcal{S}^n$ having a Gram representation by positive semidefinite matrices in $S^{\mathbb{N}}$. Then it is shown in [22] that $\mathcal{CS}_+ \subseteq \mathcal{CS}_{\infty+} \subseteq \mathsf{cl}(\mathcal{CS}_{\infty+}) = \mathsf{cl}(\mathcal{CS}_+)$ holds. In particular, the closure of $\mathcal{CS}_+$ a priori contains matrices having a Gram representation by infinite dimensional matrices.

Tracial ultraproducts of matrix algebras, or more generally of finite von Neumann algebras, are an adapted version of classical ultraproducts from model theory. Since the methods used might not be familiar to the reader, we recap the construction of tracial ultraproducts in Section 5.1. In Section 5.3, we introduce the new cone $\mathcal{CS}_{\mathcal{U}+}$ and show that it is equal to the closure of $\mathcal{CS}_+$. Finally, we present a possibly larger cone $\mathcal{CS}_{\mathrm{vN}+}$, containing $\mathcal{CS}_+$, which can be seen as an infinite dimensional analog of the completely positive semidefinite cone. This cone turns out to be closed. Furthermore, $\mathcal{CS}_{\mathrm{vN}+}$ would be equal to $\mathsf{cl}(\mathcal{CS}_+)$ if the embedding problem of Connes has an affirmative answer. More details about the algebras involved in the general case as well as on the embedding problem of Connes are given in Section 5.2.

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5.1. Tracial ultraproducts. The construction of tracial ultraproducts is a standard technique in von Neumann algebras, see e.g. the appendix of [4]. Usually one considers complex Hilbert spaces but the construction works similarly over real Hilbert spaces. Alternatively one can use the complex construction and 'realify' the resulting algebra afterwards, see for instance [2, 21]. Ultraproducts are constructions with respect to an ultrafilter. We will only consider ultrafilters on $\mathbb{N}$. Throughout $\mathcal{P}(\mathbb{N})$ is the collection of all subsets of $\mathbb{N}$.

Definition 5.1. An ultrafilter on the set $\mathbb{N}$ is a subset $\mathcal{U} \subseteq \mathcal{P}(\mathbb{N})$ satisfying the conditions:

(a) $\emptyset \notin \mathcal{U}$,
(b) if $A \subseteq B \subseteq \mathbb{N}$ and $A \in \mathcal{U}$ then $B \in \mathcal{U}$,
(c) if $A, B \in \mathcal{U}$ then $A \cap B \in \mathcal{U}$,
(d) for every $A \in \mathcal{P}(\mathbb{N})$ either $A \in \mathcal{U}$ or $\mathbb{N} \setminus A \in \mathcal{U}$.

In particular, any two elements in $\mathcal{U}$ need to have non-empty intersection (from (a) and (c)). This allows only two kinds of ultrafilters: either every element of $\mathcal{U}$ contains a common element $n_0 \in \mathbb{N}$ or $\mathcal{U}$ contains the cofinite sets of $\mathbb{N}$. We are only interested in the second kind of ultrafilters, which are called *free ultrafilters*. For a given free ultrafilter $\mathcal{U}$ on $\mathbb{N}$ we can define the *ultralimit* $\lim_{\mathcal{U}} a_k$ of a bounded sequence $(a_k)_{k\in\mathbb{N}}$ of real numbers as follows:

$$\lim_{\mathcal{U}} a_k = a \quad \text{if } \{k \in \mathbb{N} : |a_k - a| < \varepsilon\} \in \mathcal{U} \quad \text{for all } \varepsilon > 0.$$

Let us have a look at ultralimits in a less formal way. If we have a non-free ultrafilter, i.e., $\mathcal{U} = \{A \in \mathcal{P}(\mathbb{N}) : k_0 \in A\}$ for some $k_0 \in \mathbb{N}$, then $\lim_{\mathcal{U}} a_k = a_{k_0}$ for any sequence $(a_k)_{k\in\mathbb{N}} \subseteq \mathbb{R}$. The case of a free ultrafilter is more interesting. Then the ultralimit of a bounded sequence $(a_k)_{k\in\mathbb{N}}$ will be one of its accumulation points. For example, the sequence given by $a_k = (-1)^k$ for all $k \in \mathbb{N}$ has two accumulation points and both can be attained as an ultralimit depending on the choice of the ultrafilter $\mathcal{U}$. In fact, considering the set $2\mathbb{N}$ of even numbers, we get by conditions (c) and (d) that any ultrafilter contains either $2\mathbb{N}$ or its complement (the odd numbers $2\mathbb{N}+1$) but not both. Hence, there is an ultrafilter $\mathcal{U}$ (containing $2\mathbb{N}$) with $\lim_{\mathcal{U}} a_k = 1$ and an ultrafilter $\mathcal{U}'$ (containing $2\mathbb{N}+1$) with $\lim_{\mathcal{U}'} a_k = -1$.

Remark 5.2. Any bounded sequence of real numbers has an ultralimit and this is unique for fixed $\mathcal{U}$. In particular, if $\lim_{k\to\infty} a_k = a$ then $\lim_{\mathcal{U}} a_k = a$ for any free ultrafilter $\mathcal{U}$ on $\mathbb{N}$.

We can use ultralimits to construct the tracial ultraproduct of a sequence of matrix algebras $(\mathbb{R}^{d_k\times d_k})_{k\in\mathbb{N}}$ for $d_k \in \mathbb{N}$. To simplify notation we let $\mathcal{M}_k = \mathbb{R}^{k\times k}$ denote the matrix algebra of all $k \times k$ matrices and we consider the full sequence $(\mathcal{M}_k)_{k\in\mathbb{N}}$, but the same construction would work for the sequence $(\mathcal{M}_{d_k})_{k\in\mathbb{N}}$. Here we assume that each $\mathcal{M}_k$ is endowed with the normalized trace $\mathsf{tr}_k = \frac{1}{k}\,\mathsf{Tr}$ (if the dimension k is clear we might simply write tr) and the corresponding inner product, so that $\|I\|_2 = \mathsf{tr}(I) = 1$ for the identity matrix. For $T \in \mathcal{M}_k$, $\|T\|$ denotes its operator norm and $\|T\|_2$ its L_2-norm. They satisfy $\|ST\|_2 \le \|S\|\|T\|_2$ for $S, T \in \mathcal{M}_k$. Define the C^*-algebra

$$\ell^\infty(\mathbb{N}, (\mathcal{M}_k)_k) = \left\{ (T_k)_{k\in\mathbb{N}} \in \prod_{k\in\mathbb{N}} \mathcal{M}_k : \sup_{k\in\mathbb{N}} \|T_k\| < \infty \right\}.$$

Every free ultrafilter $\mathcal{U}$ on $\mathbb{N}$ defines a two-sided ideal

$$\mathcal{I}_{\mathcal{U}} = \left\{ (T_k)_{k\in\mathbb{N}} \in \ell^\infty(\mathbb{N}, (\mathcal{M}_k)_k) : \lim_{\mathcal{U}} \|T_k\|_2 = 0 \right\},$$

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which is well-defined since sequences in $\ell^\infty(\mathbb{N},(\mathcal{M}_k)_k)$ are also bounded in the Hilbert-Schmidt norm. The ideal $\mathcal{I}_\mathcal{U}$ is a maximal ideal, and therefore, it is closed with respect to the operator norm. The quotient algebra

$$\mathcal{M}_\mathcal{U} = \ell^\infty(\mathbb{N},(\mathcal{M}_k)_k)/\mathcal{I}_\mathcal{U}$$

is called the *tracial ultraproduct* of $(\mathcal{M}_k)_k$ along $\mathcal{U}$. Using the Cauchy-Schwarz inequality it is easy to show that the map

$$\tau_\mathcal{U} : \mathcal{M}_\mathcal{U} \to \mathbb{R}, \quad (T_k)_{k\in\mathbb{N}} + \mathcal{I}_\mathcal{U} \mapsto \lim_{\mathcal{U}} \mathsf{tr}_k(T_k)$$

defines a tracial state (or trace) on $\mathcal{M}_\mathcal{U}$, i.e., $\tau_\mathcal{U}$ is a normalized positive linear map satisfying $\tau_\mathcal{U}(T^*T) = \tau_\mathcal{U}(TT^*)$ for any $T \in \mathcal{M}_\mathcal{U}$. In fact, $\mathcal{M}_\mathcal{U}$ is a finite von Neumann algebra of type II_1 (see below for definitions). In particular, $\mathcal{M}_\mathcal{U}$ is a subalgebra of bounded operators on an infinite dimensional Hilbert space. As von Neumann algebras are in particular C^*-algebras, positive semidefinite operators are exactly squares of (symmetric) operators.

5.2. Von Neumann algebras and Connes' embedding problem. We give a short overview of what is needed for our purpose; for details we refer to the book [32].

A von Neumann algebra $\mathcal{N}$ is a unital $*$-subalgebra of the $*$-algebra $\mathcal{B}(\mathcal{H})$ of bounded operators on a Hilbert space $\mathcal{H}$ that is closed in the weak operator topology. The weak operator topology is the weakest topology on $\mathcal{B}(\mathcal{H})$ such that the functional $\mathcal{B}(\mathcal{H}) \to \mathbb{C}$ which maps $T \mapsto \langle Tx, y\rangle$ is continuous for any $x, y \in \mathcal{H}$. In other words, a sequence $(T_k)_{k\in\mathbb{N}} \in \mathcal{B}(\mathcal{H})$ converges to $T \in \mathcal{B}(\mathcal{H})$ if for all $x, y \in \mathcal{H}$ the sequence $(\langle T_k x, y\rangle)_{k\in\mathbb{N}}$ converges to $\langle Tx, y\rangle$ as k tends to infinity.

A factor is a von Neumann algebra with trivial center. Every von Neumann algebra on a separable Hilbert space is isomorphic to a direct integral of factors, which is the appropriate analog of matrix block decomposition.

A factor $\mathcal{F}$ is finite if it possesses a normal, faithful, tracial state $\tau : \mathcal{F} \to \mathbb{C}$. In particular, we can always assume that $\tau(I) = 1$. This tracial state τ is unique and gives rise to the Hilbert-Schmidt norm on $\mathcal{F}$ given by $\|T\|_2^2 = \tau(T^*T)$ for $T \in \mathcal{F}$. A von Neumann algebra is finite if it decomposes into finite factors. Every finite von Neumann algebra comes with a trace, which might not be unique.

Von Neumann algebras can be classified into two types depending on the behavior of their projections (i.e., the elements $P \in \mathcal{N}$ satisfying $P = P^* = P^2$). If for a given finite factor $\mathcal{F}$ with trace τ the range of τ over all projections $P \in \mathcal{F}$ is discrete, then $\mathcal{F}$ is of type I. A von Neumann algebra is of type I if it consists only of type I factors. Any finite type I von Neumann algebra is isomorphic to a matrix algebra over $\mathbb{C}$. The only other possibility for a finite factor is that τ maps projections (surjectively) onto $[0, 1]$. Those are II_1 factors, and a von Neumann algebra is of type II_1 if it is finite and contains at least one II_1 factor.

Connes' embedding problem asks to which extent II_1 factors are close to matrix algebras. Murray and von Neumann showed that there is a unique II_1 factor $\mathcal{R}$ which contains an ascending sequence of finite-dimensional von Neumann subalgebras, i.e., matrix algebras, with dense union. This factor $\mathcal{R}$ is called the *hyperfinite* II_1 *factor*. There are several constructions of $\mathcal{R}$, e.g., as infinite tensor product $\overline{\bigotimes}_{n\in\mathbb{N}} M_2(\mathbb{C})$ of the von Neumann algebras $M_2(\mathbb{C})$, which is the weak closure of the algebraic tensor product $\bigotimes_{n\in\mathbb{N}} M_2(\mathbb{C})$. In fact, any infinite countable sequence of matrix algebras will do.

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Connes conjectured that all separable II_1 factors embed (in a trace-preserving way) into an ultrapower $\mathcal{R}^{\mathcal{U}}$ of the hyperfinite II_1 factor $\mathcal{R}$, where the ultrapower $\mathcal{R}^{\mathcal{U}}$ is just a short-hand notation for the ultraproduct $\ell^\infty(\mathbb{N},(\mathcal{R})_k)/\mathcal{I}_{\mathcal{U}}$. Since $\mathcal{R}$ contains ascending sequences of matrix algebras with dense union, any matrix algebra $\mathcal{M}_k$ embeds into $\mathcal{R}$. One can extend these embeddings of $\mathcal{M}_k$ into $\mathcal{R}$ to an embedding of the tracial ultraproduct $\mathcal{M}_{\mathcal{U}}$ into $\mathcal{R}^{\mathcal{U}}$ (using a more general construction of ultralimits). Hence, the finite von Neumann algebra $M_{\mathcal{U}}$ satisfies Connes' embedding conjecture.

This conjecture is equivalent to a huge variety of other important conjectures in, e.g., operator theory, noncommutative real algebraic geometry and quantum information theory. In particular, as we already mentioned in the introduction, it is equivalent to deciding whether $\mathsf{cl}(\mathcal{Q}) = \mathcal{Q}_c$ holds.

For an alternative description of $\mathsf{cl}(\mathcal{CS}_+)$ in the case that Connes' embedding conjecture is a true statement, we will use the following result on finite von Neumann algebras which embed into $\mathcal{R}^{\mathcal{U}}$. The claim is that tracial moments of an embeddable finite factor can be approximated up to arbitrary precision by matricial tracial moments. This is stated more formally in the next proposition, for a proof see e.g. [11].

Proposition 5.3. *[11] Let $(\mathcal{F},\tau)$ be a II_1 factor which embeds into $\mathcal{R}^{\mathcal{U}}$ for some free ultrafilter $\mathcal{U}$. Then $\mathcal{F}$ has matricial microstates, i.e., for any $n \in \mathbb{N}$ and given self-adjoint $T_1,\dots,T_n \in \mathcal{F}$ the following holds: for every $k \in \mathbb{N}$ and $\varepsilon > 0$ there exists $d \in \mathbb{N}$ and $B_1,\dots,B_n \in \mathcal{S}^d$ such that*

$$|\tau(T_{i_1}\cdots T_{i_t}) - \mathsf{tr}(B_{i_1}\cdots B_{i_t}))| < \varepsilon \quad \text{for all } i_1,\dots,i_t \in [n],\ t \le k.$$

5.3. Ultraproduct description of $\mathsf{cl}(\mathcal{CS}_+)$. We are now ready to define the new cone $\mathcal{CS}_{\mathcal{U}+}$ which will turn out to be equal to the closure of $\mathcal{CS}_+$. For this, we fix a free ultrafilter $\mathcal{U}$ on $\mathbb{N}$ and consider the tracial ultraproduct $\mathcal{M}_{\mathcal{U}} = \ell^\infty(\mathbb{N},(\mathcal{M}_k)_k)/\mathcal{I}_{\mathcal{U}}$ where again $\mathcal{M}_k$ denotes the full matrix algebra $\mathbb{R}^{k\times k}$ for any $k \in \mathbb{N}$. Using this we define

$$\mathcal{CS}_{\mathcal{U}+} = \{A \in \mathcal{S}_+ :\ A = (\tau_{\mathcal{U}}(X_iX_j))_{i,j} \quad \text{for some positive semidefinite } X_1,\dots,X_n \in \mathcal{M}_{\mathcal{U}}\}.$$

We note that the trace $\tau_{\mathcal{U}}$ is normalized (i.e., $\tau_{\mathcal{U}}(I) = 1$) whereas we used the (not normalized) trace Tr in the definition of $\mathcal{CS}_+$. However, both descriptions agree up to rescaling of the X_i's.

To show that the closure of $\mathcal{CS}_+$ is a subset of $\mathcal{CS}_{\mathcal{U}+}$, we will consider a sequence of matrices $A^{(k)} \in \mathcal{CS}^n_+$ converging to some $A \in \mathcal{S}^n$, i.e., $\lim_{k\to\infty} A^{(k)}_{ij} = A_{ij}$ for all $i,j \in [n]$. A priori, for each k, there exist an integer d_k and matrices $X^{(k)}_1,\dots,X^{(k)}_n \in \mathcal{S}^{d_k}_+$ such that $A^{(k)} = (\mathsf{tr}(X^{(k)}_iX^{(k)}_j))$. The following technical lemma says that without loss of generality we can assume $d_k = k$ for all $k \in \mathbb{N}$.

Lemma 5.4. *If the sequences $(X_k)_k,(Y_k)_k \in \prod_{k\in\mathbb{N}} \mathcal{S}^{d_k}_+$ are such that the sequence $(\mathsf{tr}_{d_k}(X_kY_k))_{k\in\mathbb{N}}$ converges to some $a \in \mathbb{R}$, then there exist $(X'_k)_k,(Y'_k)_k \in \prod_{k\in\mathbb{N}} \mathcal{S}^k_+$ with $\mathsf{tr}_k(X'_kY'_k) \to a$ as k tends to infinity.*

Proof. By possibly reordering the indices, we can assume that the sequence $(d_k)_{k\in\mathbb{N}}$ is monotonically nondecreasing. First, we modify the sequence $(X_k)_k$ in such a way that $d_k \le k$ holds for all $k \in \mathbb{N}$. For this, if there is some $k \in \mathbb{N}$ with $d_k > k$ we repeat the preceding element X_{k-1} exactly $d_k - k$ times before the element X_k. For instance, if $X_1 \in \mathbb{R}_+$ and $X_2 \in \mathcal{S}^3_+$ (i.e., $d_1 = 1$ and $d_2 = 3$), we replace the sequence $(X_1,X_2,X_3,\dots)$ by $(X_1,X_1,X_2,X_3,\dots)$ Then the position of X_k is shifted by $d_k - k$ to $k + d_k - k = d_k$.

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If $k = 1$ we simply add $d_1 - 1$ zero matrices before X_1. We do the same with the sequence $(Y_k)_k$. Now, the new sequence of inner products is obtained from the original sequence $(\mathsf{tr}_{d_k}(X_kY_k))_{k\in\mathbb{N}}$ by replacing each $\mathsf{tr}_{d_k}(X_kY_k)$ by $d_k - k + 1$ copies of it if $d_k > k$, and thus still converges to the limit a.

Thus, we can assume that $d_k \le k$ for all $k \in \mathbb{N}$. We set $X'_k = \sqrt{\frac{k}{d_k}}(X_k \oplus 0_{k-d_k}) \in \mathcal{S}^k_+$ and $Y'_k = \sqrt{\frac{k}{d_k}}(Y_k \oplus 0_{k-d_k}) \in \mathcal{S}^k_+$ for every $k \in \mathbb{N}$. Then we have

$$\mathsf{tr}_k(X'_kY'_k) = \frac{1}{k}\,\mathsf{Tr}(X'_kY'_k) = \frac{1}{k}\frac{k}{d_k}\,\mathsf{Tr}(X_kY_k) = \mathsf{tr}_{d_k}(X_kY_k)$$

for every $k \in \mathbb{N}$. Hence, the final sequence $(\mathsf{tr}_k(X'_kY'_k))_{k\in\mathbb{N}}$ still converges to a. ☐

We proceed by showing that the closure of $\mathcal{CS}_+$ is a subset of $\mathcal{CS}_{\mathcal{U}+}$. The main ingredient will be Remark 5.2 together with the result of Lemma 5.4.

Lemma 5.5. *For any free ultrafilter $\mathcal{U}$ on $\mathbb{N}$, we have $\mathsf{cl}(\mathcal{CS}_+) \subseteq \mathcal{CS}_{\mathcal{U}+}$.*

Proof. Let $A \in \mathsf{cl}(\mathcal{CS}_+)$ be given. Then there is a sequence of matrices $A^{(k)} \in \mathcal{CS}_+$ converging to A: $\lim_{k\to\infty} A^{(k)}_{ij} = A_{ij}$ for all $i, j \in [n]$. For each k, there exist positive semidefinite matrices $X^{(k)}_1, \dots, X^{(k)}_n$ such that $A^{(k)} = (\mathsf{tr}(X^{(k)}_i X^{(k)}_j))$. By Lemma 5.4 we can assume that $X^{(k)}_1, \dots, X^{(k)}_n \in \mathcal{S}^k_+$. As the matrices $A^{(k)}$ are bounded the matrices $X^{(k)}_i$ are bounded as well. Hence, the sequence $(X^{(k)}_i)_{k\in\mathbb{N}}$ belongs to $\ell^\infty(\mathbb{N}, (\mathcal{M}_k)_k)$ and we can consider its image X_i in the tracial ultrapower $\mathcal{M}_{\mathcal{U}}$. By the theorem of Łos (see e.g. [13, Prop. 4.3] and references therein) the operators X_i are positive semidefinite since all $X^{(k)}_i$ are positive semidefinite. It suffices now to show that $A = (\tau_{\mathcal{U}}(X_iX_j))$ since then we can conclude that $A \in \mathcal{CS}_{\mathcal{U}+}$. For this observe that, by the definition of $\tau_{\mathcal{U}}$, we have: $\tau_{\mathcal{U}}(X_iX_j) = \lim_{\mathcal{U}} \mathsf{tr}(X^{(k)}_i X^{(k)}_j) = \lim_{\mathcal{U}} A^{(k)}_{ij}$. On the other hand, as the sequence $(A^{(k)}_{ij})_{k\in\mathbb{N}}$ converges to A_{ij}, in view of Remark 5.2, we have that $\lim_{\mathcal{U}} A^{(k)}_{ij} = A_{ij}$. This concludes the proof. ☐

Theorem 5.6. *For any free ultrafilter $\mathcal{U}$ on $\mathbb{N}$ $\mathsf{cl}(\mathcal{CS}_+) = \mathcal{CS}_{\mathcal{U}+}$ holds.*

Proof. In view of Lemma 5.5 we only have to show the inclusion $\mathcal{CS}_{\mathcal{U}+} \subseteq \mathsf{cl}(\mathcal{CS}_+)$. Let $A \in \mathcal{CS}_{\mathcal{U}+}$. By assumption, $A = (\tau_{\mathcal{U}}(X_iX_j))$ for some positive semidefinite operators $X_1, \dots, X_n \in \mathcal{M}_{\mathcal{U}}$. As the operators X_i are positive semidefinite, there exist operators $Y_i \in \mathcal{M}_{\mathcal{U}}$ such that $X_i = Y_i^2$ for $i \in [n]$, where each element Y_i is given by a sequence of symmetric matrices $(Y^{(k)}_i)_{k\in\mathbb{N}} \in \prod_{k\in\mathbb{N}} \mathcal{M}_k$. Further, by definition of $\tau_{\mathcal{U}}$, for any $s \in \mathbb{N}$ the index set $I_s = \{k \in \mathbb{N} : |\tau_{\mathcal{U}}(Y_i^2Y_j^2) - \mathsf{tr}((Y^{(k)}_i)^2(Y^{(k)}_j)^2)| \le 1/s \text{ for all } i, j \in [n]\}$ belongs to $\mathcal{U}$ and is therefore non-empty. Thus, we find for any $s \in \mathbb{N}$ an index $k_s \in I_s$. Hence, the operators $X^{(s)}_i = (Y^{(k_s)}_i)^2$ belong to $\mathcal{S}^{k_s}_+$ and satisfy

$$\left|\tau_{\mathcal{U}}(X_iX_j) - \mathsf{tr}(X^{(s)}_i X^{(s)}_j)\right| < \frac{1}{s} \quad \text{for all } i, j \in [n] \text{ and all } s \ge 1. \tag{5.1}$$

For each $s \in \mathbb{N}$, the matrix $A^{(s)} = (\mathsf{tr}(X^{(s)}_i X^{(s)}_j))$ belongs to the cone $\mathcal{CS}_+$. Moreover, it follows from (5.1) that the sequence $(A^{(s)})_{s\in\mathbb{N}}$ converges to the matrix A as s tends to infinity. This shows that A belongs to the closure of $\mathcal{CS}_+$, which concludes the proof. ☐

We would like to conclude with a possible other description of the closure of $\mathcal{CS}_+$ in the case that Connes' embedding conjecture turns out to be true.

As mentioned at the beginning of the section, the closure of $\mathcal{CS}_+$ contains the cone $\mathcal{CS}_{\infty+}$, i.e., it contains symmetric matrices which have a Gram representation by some class of positive semidefinite infinite

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dimensional matrices. Also the given description of $\mathsf{cl}(\mathcal{CS}_+)$ as $\mathcal{CS}_{\mathcal{U}+}$ involves Gram representations by operators on an infinite dimensional Hilbert space. In regard to the relativistic model of quantum correlations, where one allows *all* (possibly infinite dimensional) Hilbert spaces, one might ask for the most general infinite dimensional version of $\mathcal{CS}_+$. Since one is restricted to operators for which one can define an inner product (or a trace), a decent candidate for the infinite dimensional analog of $\mathcal{CS}_+$ is given by the following:

Definition 5.7.

$$\mathcal{CS}_{\mathrm{vN}+} = \{A \in \mathcal{S}_+ : A = (\tau_{\mathcal{N}}(X_iX_j))_{i,j} \text{ for a finite von Neumann algebra } \mathcal{N} \\ \text{and positive semidefinite } X_1, \ldots, X_n \in \mathcal{N}\},$$

where we allow any finite von Neumann algebra $\mathcal{N}$ (with trace $\tau_{\mathcal{N}}$).

Obviously we have the chain of inclusions $\mathcal{CS}_+ \subseteq \mathcal{CS}_{\mathcal{U}+} \subseteq \mathcal{CS}_{\mathrm{vN}+}$. Moreover, using the general theory of tracial ultraproducts of von Neumann algebras (instead of just matrix algebras), one can show with a similar line of reasoning as in Lemma 5.5 that $\mathcal{CS}_{\mathrm{vN}+}$ is closed. Indeed, take a sequence of matrices $A^{(k)} \in \mathcal{CS}^n_{\mathrm{vN}+}$ converging to some $A \in \mathcal{S}^n$. Then $\lim_{k\to\infty} A^{(k)}_{ij} = A_{ij}$ for all $i, j \in [n]$, and for each k there exist a finite von Neumann algebra $\mathcal{N}_k$ with trace τ_k and bounded positive operators $X^{(k)}_1, \ldots, X^{(k)}_n \in \mathcal{N}_k$ such that $A^{(k)} = (\tau_k(X^{(k)}_i X^{(k)}_j))$. Fixing a free ultrafilter $\mathcal{U}$ one can conclude that the images X_i of the sequences $(X^{(k)}_i)_{k\in\mathbb{N}}$ in the tracial ultraproduct $\mathcal{N}_{\mathcal{U}} = \ell^\infty(\mathbb{N}, (\mathcal{N}_k)_k)/\mathcal{I}_{\mathcal{U}}$ of the corresponding finite von Neumann algebras provide a Gram representation for A in the von Neumann algebra $\mathcal{N}_{\mathcal{U}}$. Hence, the following statement holds.

Theorem 5.8. *$\mathcal{CS}_{\mathrm{vN}+}$ is a closed cone.*

In this context, we would like to mention a result in [15] showing the strict inclusion $\mathcal{CS}^n_{\mathrm{vN}+} \subsetneq \mathcal{S}^n_+ \cap \mathbb{R}^{n\times n}_+$ for any $n \geq 5$. Summarizing we have the inclusions:

$$\mathsf{cl}(\mathcal{CS}^n_+) = \mathcal{CS}^n_{\mathcal{U}+} \subseteq \mathcal{CS}^n_{\mathrm{vN}+} \subseteq \mathcal{S}^n_+ \cap \mathbb{R}^{n\times n}_+.$$

Finally, if Connes' embedding conjecture is true then the cone $\mathcal{CS}_{\mathrm{vN}+}$ coincides with the closure of $\mathcal{CS}_+$.

Theorem 5.9. *If Connes' embedding conjecture is true, then $\mathsf{cl}(\mathcal{CS}_+) = \mathcal{CS}_{\mathrm{vN}+}$.*

Proof. We only have to show the inclusion $\mathcal{CS}_{\mathrm{vN}+} \subseteq \mathsf{cl}(\mathcal{CS}_+)$. As the line of reasoning is similar to the one in the proof of Theorem 5.6, we will only give a sketch of the proof. For this, fix a matrix $A \in \mathcal{CS}_{\mathrm{vN}+}$ and let $Y_1^2, \ldots, Y_n^2 \in \mathcal{F}$ be its Gram representation, where $\mathcal{F}$ is a finite II_1 factor. Since by assumption Connes' embedding conjecture holds, $\mathcal{F}$ embeds into an ultrapower $\mathcal{R}^{\mathcal{U}}$ of the hyperfinite II_1 factor $\mathcal{R}$ for some free ultrafilter $\mathcal{U}$. Hence, we can apply Proposition 5.3 and find for every $k \in \mathbb{N}$ finite dimensional matrices $(Y^{(k)}_1)^2, \ldots, (Y^{(k)}_n)^2$ approximating the tracial moments $A_{ij} = \tau(Y_i^2 Y_j^2)$ for $i, j \in [n]$ within a distance $1/k$. The corresponding Gram matrices $A^{(k)}$ of $(Y^{(k)}_1)^2, \ldots, (Y^{(k)}_n)^2$ then belong to $\mathcal{CS}_+$, and hence, the limit point $\lim_{k\to\infty} A^{(k)} = A$ lies in $\mathsf{cl}(\mathcal{CS}_+)$. The general case where $A \in \mathcal{CS}_{\mathrm{vN}+}$ is a Gram matrix of operators Y_i^2 in a finite von Neumann algebra $\mathcal{N}$ follows from this since any finite von Neumann algebra can be decomposed into finite factors. $\square$

We conclude with mentioning that a hierarchy of semidefinite outer approximations of the cone $\mathcal{CS}_+$ was recently formulated in [6]. These in fact also form outer approximations for the larger cone $\mathcal{CS}_{\mathrm{vN}+}$.

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2015) (see [9]). We thank an anonymous referee of TQC for pointing out that the original proof of Theorem 5.6 could be simplified to the elementary proof given above. S. B. and T. P. were funded by the SIQS European project. S. B. was also funded by the NWO TOP project 617.001.351.

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