

# Conic approach to quantum graph parameters using linear optimization over the completely positive semidefinite cone

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## Abstract

We investigate the completely positive semidefinite matrix cone  $\mathcal{CS}_+^n$ , consisting of all  $n \times n$  matrices that admit a Gram representation by positive semidefinite matrices (of any size). We use this new cone to model quantum analogues of the classical independence and chromatic graph parameters  $\alpha(G)$  and  $\chi(G)$ , which are roughly obtained by allowing variables to be positive semidefinite matrices instead of 0/1 scalars in the programs defining the classical parameters.

We study relationships between the cone  $\mathcal{CS}_+^n$  and the completely positive and doubly nonnegative cones, and between its dual cone and trace positive non-commutative polynomials. By using the truncated tracial quadratic module as sufficient condition for trace positivity, we can define hierarchies of cones aiming to approximate the dual cone of  $\mathcal{CS}_+^n$ , which we then use to construct hierarchies of semidefinite programming bounds approximating the quantum graph parameters. Finally we relate their convergence properties to Connes' embedding conjecture in operator theory.

**Keywords:** Quantum graph parameters, Semidefinite programming, Trace positive polynomials, Copositive cone, Chromatic number, Quantum Entanglement, Quantum information, Nonlocal games.

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# 1 Introduction

## 1.1 General overview

Computing the minimum number  $\chi(G)$  of colors needed to properly color a graph  $G$  and computing the maximum cardinality  $\alpha(G)$  of an independent set of vertices in  $G$  are two well studied NP-hard problems in combinatorial optimization. Recently some analogues of these classical graph parameters have been introduced and studied, namely the parameters  $\alpha_q(G)$  and  $\chi_q(G)$  in the context of quantum entanglement in nonlocal games and the parameters  $\alpha^*(G)$  and  $\chi^*(G)$  in the context of quantum information. In a nutshell, while the classical parameters are defined as the optimal values of integer programming problems involving 0/1-valued variables, their quantum analogues are obtained by allowing the variables to be positive semidefinite matrices (of arbitrary size).

To make this precise and simplify our discussion we now focus on the quantum chromatic number  $\chi_q(G)$  of a graph  $G = (V, E)$  (introduced in [18]). For any integer  $t \geq 1$ , consider the the following conditions in the variables  $x_u^i$  (for  $i \in [t]$  and  $u \in V$ ):

$$\sum_{i \in [t]} x_u^i = 1 \quad \forall u \in V, \quad x_u^i x_v^i = 0 \quad \forall \{u, v\} \in E \quad \forall i \in [t], \quad x_u^i x_u^j = 0 \quad \forall u \in V \quad \forall i \neq j \in [t], \quad (1.1)$$

which are encoding the fact that each vertex receives just one color and two adjacent vertices must receive distinct colors. Then the chromatic number  $\chi(G)$  is equal to the smallest integer  $t$  for which the system (1.1) admits a 0/1-valued solution. On the other hand, if we allow the variables  $x_u^i$  to take their values in  $\mathcal{S}_+^d$  (the cone of  $d \times d$  positive semidefinite matrices) for an arbitrary  $d \geq 1$ , and if in the first condition we let 1 denote the identity matrix, then the smallest integer  $t$  for which the system (1.1) is feasible defines the quantum parameter  $\chi_q(G)$ . By construction,

$$\chi_q(G) \leq \chi(G).$$

It is well known that computing the chromatic number  $\chi(G)$  is an NP-hard problem, very recently this hardness result has been extended to the quantum chromatic number  $\chi_q(G)$  [38]. Therefore it is of interest to be able to compute approximations for these parameters. In the classical case, several hierarchies of approximations have been proposed for  $\chi(G)$  based on semidefinite programming (see [27, 35, 36]). They refine the well known bounds based on the theta number of Lovász [49] and its strengthening by Szegedy [65]:  $\chi(G) \geq \vartheta^+(\overline{G}) \geq \vartheta(\overline{G})$ . It was shown recently in [59] that these bounds also hold for the quantum chromatic number:

$$\chi_q(G) \geq \vartheta^+(\overline{G}) \geq \vartheta(\overline{G}).$$

One of the main contributions in this paper is to construct hierarchies of bounds  $\Psi_\epsilon^{(r)}(G)$  for  $\chi_q(G)$  based on solving semidefinite programs of growing sizes. We show that  $\chi_q(G) \geq \Psi_\epsilon^{(r)}(G)$  for any  $r \in \mathbb{N}$  and small  $\epsilon > 0$  (see Proposition 4.17). However, while the hierarchies in [35, 27] are known to converge to  $\chi(G)$  (or to the fractional chromatic number  $\chi_f(G)$ ), it is not known whether there is convergence of the parameters  $\Psi_\epsilon^{(r)}(G)$  to  $\chi_q(G)$ . In fact a positive answer to this question would follow from a positive answer to the celebrated Connes' embedding conjecture in operator theory, as we mention below.

Our construction for the bounds  $\Psi_\epsilon^{(r)}(G)$  relies on developing a new approach to the study of the quantum graph parameters based on conic optimization over a new matrix cone, the cone  $\mathcal{CS}_+$ , that we call the *completely positive semidefinite cone*. This is another main contribution of this paper which we explain below in more detail.

Recall that a matrix  $A \in \mathcal{S}^n$  is positive semidefinite (psd), i.e.,  $A \in \mathcal{S}_+^n$ , precisely when  $A$  admits a Gram representation by *vectors*  $x_1, \dots, x_n \in \mathbb{R}^d$  (for some  $d \geq 1$ ), which means that  $A = (\langle x_i, x_j \rangle)_{i,j=1}^n$ . Moreover,  $A$  is *completely positive* when it admits such a Gram representation by *nonnegative vectors*. We now call  $A$  *completely positive semidefinite* when  $A$  admits a Gram representation by *positive semidefinite matrices*  $x_1, \dots, x_n \in \mathcal{S}_+^d$  for some  $d \geq 1$ . We let  $\mathcal{CP}^n$  and  $\mathcal{CS}_+^n$  denote, respectively, the sets of completely positive and completely psd matrices.

The set  $\mathcal{CS}_+$  is easily seen to be a convex cone, but it is not known whether it is a closed set. A related open question is whether any matrix  $A$  which admits a Gram representation by *infinite* positive semidefinite matrices also admits such a Gram representation by finite ones. (See Theorem 3.3.) It is easy to see that the new cone  $\mathcal{CS}_+^n$  is nested between  $\mathcal{CP}^n$  and the *doubly nonnegative* cone  $\mathcal{DN}\mathcal{N}^n$  (all matrices that are both psd and nonnegative):

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \text{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{DN}\mathcal{N}^n.$$

As is well known,  $\mathcal{DN}\mathcal{N}^n = \mathcal{CP}^n$  for  $n \geq 4$  and strict inclusion holds for  $n \geq 5$  [24, 51]. Fawzi and Parrilo [29] gave recently an example of a  $5 \times 5$  matrix which is completely positive semidefinite but not completely positive. We construct doubly nonnegative matrices that do not lie in the closure of  $\mathcal{CS}_+^5$ . Our first main ingredient for this construction is to show that for matrices supported by a cycle, being completely positive is equivalent to being completely psd (Theorem 3.7). Our second main ingredient is to use the conic analogues  $\vartheta^{\mathcal{K}}(G)$  of the theta number (introduced in [27]) where we select the cone  $\mathcal{K} = \mathcal{CS}_+$  or its closure and apply them for the 5-cycle (see Lemma 3.8 and its proof).

Using the completely psd cone  $\mathcal{CS}_+$  we can reformulate the quantum graph parameters as linear optimization problems over affine sections of the cone  $\mathcal{CS}_+$ . The idea is simple and goes as follows for the quantum chromatic number  $\chi_q(G)$ : linearize the system (1.1) by introducing a matrix  $X$  (defined as the Gram matrix of the psd matrices  $x_u^i$ ), add the condition  $X \in \mathcal{CS}_+$ , and replace the conditions in (1.1) by linear conditions on  $X$  (see Sections 4.1-4.3 for details). In this way the whole complexity of the problem is pushed to the cone  $\mathcal{CS}_+$ .

The dual cone  $\mathcal{CS}_+^{n*}$  of the completely psd cone  $\mathcal{CS}_+^n$  has a useful interpretation in terms of *tracial positive non-commutative polynomials*. For a matrix  $M \in \mathcal{S}^n$ , consider the following polynomial  $p_M = \sum_{i,j=1}^n M_{ij} X_i^2 X_j^2$  in the non-commutative variables  $X_1, \dots, X_n$ . Then,  $M$  belongs to the dual cone  $\mathcal{CS}_+^{n*}$  precisely when  $p_M$  is *trace positive*, which means that one gets a nonnegative value when evaluating  $p_M$  at arbitrary matrices  $X_1, \dots, X_n \in \mathcal{S}^d$  (for any  $d \geq 1$ ) and taking the trace of the resulting matrix. When restricting to commutative variables we find the notion of copositive matrices and the fact that  $\mathcal{CS}_+^{n*}$  is contained in the copositive cone  $\mathcal{COP}^n$  (the dual of the completely positive cone  $\mathcal{CP}^n$ ).

Trace positive polynomials have been studied in the recent years, in particular in [14, 15, 17]. A sufficient condition for trace positivity of  $p_M$  is that  $p_M$  belongs to the *tracial quadratic module*  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}}$  (of the ball), which means that  $p_M$  can

be written as a sum of commutators  $[g, h] = gh - hg$ , Hermitian squares  $gg^*$ , and terms of the form  $g(1 - \sum_{i=1}^n X_i^2)g^*$  where  $g, h$  are non-commutative polynomials. By bounding all degrees by some given  $r$  we get the truncated tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$ .

Klep and Schweighofer [40] (and [16]) have shown that Connes' embedding conjecture is equivalent to showing that for any non-commutative polynomial  $p$  which is trace positive,  $p + \epsilon$  belongs to  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}}$  for any  $\epsilon > 0$ . This motivates our definition of the new cones  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  consisting of all matrices  $M$  for which  $p_M + \epsilon$  belongs to the truncated module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$ . Then,

$$\bigcap_{\epsilon > 0} \bigcup_{r \geq 0} \mathcal{K}_{\text{nc}, \epsilon}^{(r)} \subseteq \mathcal{CS}_+^*,$$

with equality if Connes' conjecture holds. It turns out that, for  $\epsilon = 0$ ,  $\mathcal{K}_{\text{nc}, 0}^{(r)} = \mathcal{DN}\mathcal{N}^*$  for all  $r$  (see Lemma 3.16). Hence the hierarchy of cones  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is interesting only for  $\epsilon > 0$ .

Using these cones  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  we can define semidefinite based parameters approximating the quantum graph parameters, like the parameter  $\Psi_\epsilon^{(r)}(G)$  discussed above. Namely, consider the optimization program over  $\mathcal{CS}_+$  defining  $\chi_q(G)$  and replace in it the cone  $\mathcal{CS}_+$  by the dual cone of  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  to get the parameter  $\Psi_\epsilon^{(r)}(G)$ . Although there is no apparent inclusion relationship between  $\mathcal{CS}_+^*$  and  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  (and thus none between  $\mathcal{CS}_+$  and  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)*}$ ), we yet can show that  $\chi_q(G) \geq \Psi_\epsilon^{(r)}(G)$  for any  $r \in \mathbb{N}$  and any small  $0 < \epsilon < 1/(n-1)$  (see Proposition 4.17). In the paper we also deal with the other quantum graph parameters  $\chi^*(G)$ ,  $\alpha_q(G)$  and  $\alpha^*(G)$  and extend the above results for them.

Our motivation for studying the cone  $\mathcal{CS}_+$  comes from its relevance to the quantum graph parameters. We mention in closing a further connection to the widely studied notion of factorizations of nonnegative matrices. Given a nonnegative  $m \times n$  matrix  $M$ , a *nonnegative factorization* (resp., *psd factorization*) of  $M$  consists of nonnegative vectors  $x_i, y_j \in \mathbb{R}^d$  (resp., psd matrices  $x_i, y_j \in \mathcal{S}_+^d$ ) (for some  $d \geq 1$ ) such that  $M = (\langle x_i, y_j \rangle)_{i \in [m], j \in [n]}$ . Note that asymmetric factorizations are allowed, using  $x_i$  for the rows and  $y_j$  for the columns of  $M$ . In this asymmetric setting, the question is not about the existence (since such a factorization always exists in some dimension  $d$ ), but about the *smallest possible dimension*  $d$  of such a factorization. There is recently a surge of interest in these questions, motivated in particular by their relevance to linear and semidefinite extended formulations of polytopes, see e.g. [30, 34] and further references therein.

## 1.2 Organization of the paper

The paper is organized as follows. In the rest of the Introduction we present some notation and preliminaries about graphs and matrices used throughout. Section 2 introduces all graph parameters considered in the paper. Section 2.1 recalls the classical parameters  $\alpha(G)$ ,  $\chi(G)$ , the theta numbers  $\vartheta(G)$ ,  $\vartheta'(G)$  and  $\vartheta^+(G)$ , and two conic variants  $\vartheta^{\mathcal{K}}(G)$  and  $\Theta^{\mathcal{K}}(G)$  where  $\mathcal{K}$  is a cone nested between  $\mathcal{CP}$  and  $\mathcal{DN}\mathcal{N}$ . Section 2.2 introduces the quantum graph parameters  $\alpha_q(G)$ ,  $\alpha^*(G)$ ,  $\chi_q(G)$ ,  $\chi^*(G)$  and in Section 2.3 we briefly motivate the use of these parameters for analyzing the impact of quantum entanglement in nonlocal games and in quantum information.

Section 3 is devoted to the study of the new cone  $\mathcal{CS}_+$  (Section 3.1), the links with  $\mathcal{CP}$  and  $\mathcal{DN}\mathcal{N}$  (Section 3.2), the dual cone  $\mathcal{CS}_+^*$  and the link to trace positive polynomials and to Parrilo's hierarchy in the commutative case (Section 3.3), the cones  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$  (Section 3.4), and their use to define semidefinite bounds for the parameters  $\nu^{\mathcal{CS}_+}(G)$  and  $\Theta^{\mathcal{CS}_+}(G)$  (Section 3.5).

Section 4 is devoted to the study of the quantum graph parameters using linear optimization over affine sections of the cone  $\mathcal{CS}_+$ . First we give reformulations for the quantum parameters obtained by checking feasibility of a sequence of conic programs over sections of  $\mathcal{CS}_+$ , which is done in Section 4.1 for the quantum stability numbers and in Section 4.2 for the quantum chromatic numbers. Then in Section 4.3, we build a single 'aggregated' optimization program permitting to express each quantum parameter, whose dual will be particularly useful to analyze the relationships between the quantum parameter and its semidefinite approximations. As explained in Section 4.4, these approximations are obtained by replacing in the program defining a given quantum parameter the cone  $\mathcal{CS}_+$  by the cone  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ .

### 1.3 Notation and preliminaries

*Graphs.* Throughout all graphs are assumed to be finite, undirected and without loops. A graph  $G$  has vertex set  $V(G)$  and edge set  $E(G)$ . Given two vertices  $u, v \in V(G)$ , we write  $u \simeq v$  if  $u, v$  are adjacent or equal and we write  $u \sim v$  when  $u$  and  $v$  are adjacent, in which case the corresponding edge is denoted as  $\{u, v\}$  or simply as  $uv$ .  $\overline{G}$  is the complementary graph of  $G$ , with vertex set  $V(G)$  and two distinct vertices are adjacent in  $\overline{G}$  if and only if they are not adjacent in  $G$ .

A stable set of  $G$  is a subset of  $V(G)$  where any two nodes are not adjacent. The *stability number*  $\alpha(G)$  is the maximum cardinality of a stable set in  $G$ . A clique of  $G$  is a set of nodes that are pairwise adjacent and  $\omega(G)$  is the maximum cardinality of a clique; clearly,  $\omega(G) = \alpha(\overline{G})$ . A *proper coloring* of  $G$  is a coloring of the nodes of  $G$  in such a way that adjacent nodes receive distinct colors. The *chromatic number*  $\chi(G)$  is the minimum number of colors needed for a proper coloring. Equivalently,  $\chi(G)$  is the smallest number of stable sets needed to cover all vertices of  $G$ . The *fractional chromatic number*  $\chi_f(G)$  is the fractional analogue, defined as the smallest value of  $\sum_{h=1}^k \lambda_h$  for which there exists stable sets  $S_1, \dots, S_k$  of  $G$  and nonnegative scalars  $\lambda_1, \dots, \lambda_k$  such that  $\sum_{h:v \in S_h} \lambda_h = 1$  for all  $v \in V(G)$ . Clearly,  $\omega(G) \leq \chi_f(G) \leq \chi(G)$ .

$K_t$  denotes the complete graph on  $t$  nodes. The graph  $G \square K_t$  is the *Cartesian product* of  $G$  and  $K_t$ . Its vertex set is  $V(G) \times [t]$  and two nodes  $(u, i)$  and  $(v, j)$  are adjacent in  $G \square K_t$  if  $(u = v \text{ and } i \neq j)$  or if  $(u \sim v \text{ and } i = j)$ .

*Cones and matrices.* Throughout,  $\mathbb{R}_+^n$  denotes the set of (entrywise) nonnegative vectors,  $e_1, \dots, e_n$  denote the standard unit vectors in  $\mathbb{R}^n$ , and  $e$  denotes the all-ones vector.  $\mathbb{R}^n$  is equipped with the standard inner product:  $\langle x, y \rangle = x^T y = \sum_{i=1}^n x_i y_i$  and the corresponding norm  $\|x\| = \sqrt{\langle x, x \rangle}$ .

$\mathcal{S}^n$  denotes the set of  $n \times n$  real symmetric matrices, which is equipped with the standard trace inner product:  $\langle X, Y \rangle = \text{Tr}(XY) = \sum_{i,j=1}^n X_{ij} Y_{ij}$  and the corresponding Frobenius norm  $\|X\| = \sqrt{\langle X, X \rangle}$ .  $\mathcal{S}_+^n$  denotes the set of positive semidefinite matrices in  $\mathcal{S}^n$  and  $\mathcal{DN}\mathcal{N}^n$ , the *double nonnegative cone*, is the set of positive semidefinite matrices in  $\mathcal{S}^n$  with nonnegative entries. For  $X \in \mathcal{S}^n$ ,  $X$  is positive semidefinite (also written as  $X \succeq 0$ ) if all its eigenvalues are nonnegative.

Equivalently,  $X \succeq 0$  if and only if there exist vectors  $x_1, \dots, x_n \in \mathbb{R}^d$  (for some  $d \geq 1$ ) such that  $X_{ij} = \langle x_i, x_j \rangle$  for all  $i, j \in [n]$ , in which case we say that  $x_1, \dots, x_n$  form a *Gram representation* of  $X$  and we call  $X$  the *Gram matrix* of  $x_1, \dots, x_n$ . Furthermore,  $X \in \mathcal{S}^n$  is said to be *completely positive* if  $X$  is the Gram matrix of a set of *nonnegative* vectors  $x_1, \dots, x_n \in \mathbb{R}_+^d$  (for some  $d \geq 1$ ). We let  $\mathcal{CP}^n$  denote the set of completely positive matrices.  $\mathcal{S}_+^n$ ,  $\mathcal{DN}^n$  and  $\mathcal{CP}^n$  are convex cones.

For a pair of matrices  $X, Y$ , we denote with  $X \oplus Y$  the direct sum of  $X$  and  $Y$  and with  $X \otimes Y$  the Kronecker product of the two matrices, i.e.,  $X \oplus Y = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$

and  $X \otimes Y$  is the block matrix  $\begin{pmatrix} X_{11}Y & \dots & X_{1n}Y \\ \vdots & \ddots & \vdots \\ X_{m1}Y & \dots & X_{mn}Y \end{pmatrix}$  if  $X$  is  $m \times n$ .

We will use the following elementary facts. First,  $nI - J \succeq 0$ , where  $I, J$  are the identity and all-ones matrix in  $\mathcal{S}^n$ . If  $X, Y \succeq 0$  then  $\langle X, Y \rangle = 0$  if and only if  $XY = 0$ . Moreover, for a matrix  $X \in \mathcal{S}^n$  of the form

$$X = \begin{pmatrix} \alpha & b^T \\ b & A \end{pmatrix}, \text{ where } b \in \mathbb{R}^{n-1}, A \in \mathcal{S}^{n-1} \text{ and } \alpha > 0,$$

$$X \succeq 0 \iff A - \frac{1}{\alpha}bb^T \succeq 0. \quad (1.2)$$

The matrix  $A - \frac{1}{\alpha}bb^T$  is called the Schur complement of  $A$  in  $X$  w.r.t. the entry  $\alpha$ .

We will also use the following result about conic duality (see e.g. [8]). Given a cone  $\mathcal{K} \subseteq \mathcal{S}^n$ , its dual cone  $\mathcal{K}^*$  is defined as

$$\mathcal{K}^* = \{X \in \mathcal{S}^n : \langle X, Y \rangle \geq 0 \quad \forall Y \in \mathcal{K}\}.$$

Recall that the cone  $\mathcal{S}_+^n$  is self-dual, i.e.,  $\mathcal{S}_+^{n*} = \mathcal{S}_+^n$ . A cone  $\mathcal{K} \subseteq \mathcal{S}^n$  is called *nice* if it is closed, convex, pointed and full-dimensional. If  $\mathcal{K}$  is nice then its dual cone  $\mathcal{K}^*$  is nice as well. As we will see later, we do not know if the cone  $\mathcal{CS}_+$  is closed, but the cone  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is indeed a nice cone. Given  $C, A_j \in \mathcal{S}^n$  and  $b_j \in \mathbb{R}$  for  $j \in [m]$ , consider the following pair of primal and dual conic programs over a nice cone  $\mathcal{K}$ :

$$p^* = \sup \langle C, X \rangle \quad \text{s.t.} \quad \langle A_j, X \rangle = b_j \quad \forall j \in [m], \quad X \in \mathcal{K}, \quad (1.3)$$

$$d^* = \inf \sum_{j=1}^m b_j y_j \quad \text{s.t.} \quad Z = \sum_{j=1}^m y_j A_j - C \in \mathcal{K}^*. \quad (1.4)$$

Weak duality holds:  $p^* \leq d^*$ . Moreover, assume that  $d^* > -\infty$  and (1.4) is strictly feasible (i.e., has a feasible solution  $y, Z$  where  $Z$  lies in the interior of  $\mathcal{K}^*$ ), then strong duality holds:  $p^* = d^*$  and (1.3) attains its supremum.

## 2 Classical and quantum graph parameters

### 2.1 Classical graph parameters

We group here several preliminary results about classical graph parameters that we will need in the paper. In what follows  $G$  is a graph on  $n$  nodes.

We begin with the following (easy to check) result of Chvátal [19] showing how to relate the chromatic number of  $G$  to the stability number of the Cartesian product  $G \square K_t$ .

**Theorem 2.1.** [19] For any graph  $G$ , we have

$$\chi(G) \leq t \iff \alpha(G \square K_t) = |V(G)|.$$

Hence,  $\chi(G)$  is equal to the smallest integer  $t$  for which  $\alpha(G \square K_t) = |V(G)|$  holds.

Next we recall the following reformulation for the stability number  $\alpha(G)$  as an optimization problem over the completely positive cone, which was proved by de Klerk and Pasechnik [42] (using a result of Motzkin and Straus [53]).

**Theorem 2.2.** [42] For any graph  $G$ , its stability number  $\alpha(G)$  is equal to the optimum value of the following program:

$$\max \langle J, X \rangle \quad \text{s.t.} \quad X \in \mathcal{CP}^n, \quad \text{Tr}(X) = 1, \quad X_{uv} = 0 \quad \forall \{u, v\} \in E(G). \quad (2.1)$$

Dukanovic and Rendl [27] gave an analogous reformulation for the fractional chromatic number  $\chi_f(G)$ .

**Theorem 2.3.** [27] For any graph  $G$ , its fractional chromatic number  $\chi_f(G)$  is equal to the optimum value of the following program:

$$\begin{aligned} \min t \quad \text{s.t.} \quad & X \in \mathcal{CP}^n, \quad X_{uu} = t \quad \forall u \in V(G), \\ & X_{uv} = 0 \quad \forall \{u, v\} \in E(G), \quad X - J \succeq 0. \end{aligned} \quad (2.2)$$

A well known bound for both the stability and the (fractional) chromatic numbers is provided by the celebrated theta number  $\vartheta$ , introduced by Lovász [49]. The following inequalities hold, known as the ‘sandwich inequalities’:

$$\alpha(G) \leq \vartheta(G) \leq \chi_f(\overline{G}) \leq \chi(\overline{G}) \quad (2.3)$$

(see e.g. [43] for a survey). Between the many equivalent formulations of the theta number, the following will be appropriate for our setting.

$$\begin{aligned} \vartheta(G) = \max \quad & \langle J, X \rangle & = \min \quad & t \\ \text{s.t.} \quad & X \succeq 0 & \text{s.t.} \quad & Z \succeq 0, \quad Z - J \succeq 0 \\ & \text{Tr}(X) = 1 & & Z_{uu} = t \quad \forall u \in V(G) \\ & X_{uv} = 0 \quad \forall \{u, v\} \in E(G), & & Z_{uv} = 0 \quad \forall \{u, v\} \in E(\overline{G}). \end{aligned} \quad (2.4)$$

In view of Theorem 2.2, if in the above maximization program defining  $\vartheta(G)$  we replace the condition  $X \succeq 0$  by the condition  $X \in \mathcal{CP}$ , then the optimal value is equal to  $\alpha(G)$ . Similarly, in view of Theorem 2.3,  $\chi_f(\overline{G})$  is the optimal value of the above minimization program defining  $\vartheta(G)$  when, instead of requiring that  $Z \succeq 0$ , we impose the condition  $Z \in \mathcal{CP}$ .

Several strengthenings of  $\vartheta(G)$  toward  $\alpha(G)$  and  $\chi(G)$  have been proposed, in particular, the following parameters  $\vartheta'(G)$  introduced independently by Schrijver [63] and McEliece et al. [52] and  $\vartheta^+(G)$  introduced by Szegedy [65].

$$\begin{aligned} \vartheta'(G) = \max \quad & \langle J, X \rangle & = \min \quad & t \\ \text{s.t.} \quad & X \in \mathcal{DN}^n & \text{s.t.} \quad & Z \succeq 0, \quad Z - J \succeq 0 \\ & \text{Tr}(X) = 1 & & Z_{uu} = t \quad \forall u \in V(G) \\ & X_{uv} = 0 \quad \forall \{u, v\} \in E(G), & & Z_{uv} \leq 0 \quad \forall \{u, v\} \in E(\overline{G}), \end{aligned} \quad (2.5)$$

$$\begin{aligned}
\vartheta^+(G) &= \min t & & = \max \langle J, Y - M \rangle \\
\text{s.t. } Z - J &\succeq 0, Z \in \mathcal{DNN}^n & & \text{s.t. } Y - M \succeq 0, M \in \mathcal{DNN}^{n*} \\
Z_{uu} &= t \quad \forall u \in V(G) & & \text{Tr}(Y) = 1 \\
Z_{uv} &= 0 \quad \forall \{u, v\} \in E(\overline{G}), & & Y_{uv} = 0 \quad \forall \{u, v\} \in E(G).
\end{aligned} \tag{2.6}$$

The following inequalities hold, which refine (2.3):

$$\alpha(G) \leq \vartheta'(G) \leq \vartheta(G) \leq \vartheta^+(G) \leq \chi_f(\overline{G}) \leq \chi(\overline{G}). \tag{2.7}$$

Following [27] we now introduce some general conic programs obtained by replacing in the above programs defining the theta number the positive semidefinite cone by a general convex cone  $\mathcal{K}$  nested between the cones  $\mathcal{CP}$  and  $\mathcal{DNN}$ . Namely, given a graph  $G$ , we consider the following parameters  $\vartheta^{\mathcal{K}}(G)$  and  $\Theta^{\mathcal{K}}(G)$ , which we will use later in Sections 3.2 and 4.4.

$$\vartheta^{\mathcal{K}}(G) = \max \langle J, X \rangle \quad \text{s.t. } X \in \mathcal{K}^n, \text{Tr}(X) = 1, X_{uv} = 0 \quad \forall \{u, v\} \in E(G), \tag{2.8}$$

$$\begin{aligned}
\Theta^{\mathcal{K}}(G) &= \min t \quad \text{s.t. } Z \in \mathcal{K}^n, \quad Z - J \succeq 0, \quad Z_{uu} = t \quad \forall u \in V(G), \\
&Z_{uv} = 0 \quad \forall \{u, v\} \in E(G).
\end{aligned} \tag{2.9}$$

If in relations (2.8) and (2.9), we set  $\mathcal{K} = \mathcal{DNN}$  or  $\mathcal{K} = \mathcal{CP}$  then, using the above definitions and Theorems 2.2 and 2.3, we find respectively the definitions of  $\vartheta'(G)$ ,  $\alpha(G)$  and of  $\vartheta^+(\overline{G})$ ,  $\chi_f(G)$ . That is,

$$\vartheta^{\mathcal{DNN}}(G) = \vartheta'(G), \quad \vartheta^{\mathcal{CP}}(G) = \alpha(G), \quad \Theta^{\mathcal{DNN}}(G) = \vartheta^+(\overline{G}), \quad \Theta^{\mathcal{CP}}(G) = \chi_f(G).$$

We now observe that in both definitions (2.8) and (2.9) we may replace the cone  $\mathcal{K}$  by its closure, a fact that we will use later in Section 3.2.

**Lemma 2.4.** *Consider a convex cone  $\mathcal{K}$  nested between  $\mathcal{CP}$  and  $\mathcal{DNN}$ . For any graph  $G$ , we have  $\vartheta^{\mathcal{K}}(G) = \vartheta^{\text{cl}(\mathcal{K})}(G)$  and  $\Theta^{\mathcal{K}}(G) = \Theta^{\text{cl}(\mathcal{K})}(G)$ .*

*Proof.* We first show equality  $\vartheta^{\mathcal{K}}(G) = \vartheta^{\text{cl}(\mathcal{K})}(G)$ . The inequality  $\vartheta^{\mathcal{K}}(G) \leq \vartheta^{\text{cl}(\mathcal{K})}(G)$  is clear. We show the reverse inequality. For this denote by  $\mathcal{A}$  the affine space defined by the conditions  $\text{Tr}(X) = 1$  and  $X_{uv} = 0$  for  $\{u, v\} \in E(G)$  in (2.8). Let  $A \in \text{cl}(\mathcal{K}) \cap \mathcal{A}$ , we show that  $A \in \text{cl}(\mathcal{K} \cap \mathcal{A})$ . For this, pick  $B \in \mathcal{A}$  that lies in the interior of  $\mathcal{K}$  (e.g.,  $B = I/n$ ) and set  $A_\lambda = \lambda A + (1 - \lambda)B$  for  $0 \leq \lambda \leq 1$ . We claim that  $A_\lambda \in \mathcal{K}$  if  $0 \leq \lambda < 1$ . If not, there exists a nonzero matrix  $M \in \mathcal{K}^*$  such that  $\langle M, A_\lambda \rangle = 0$ . Then,  $0 = \lambda \langle M, A \rangle + (1 - \lambda) \langle M, B \rangle$ , where  $\langle M, A \rangle \geq 0$  since  $A \in \text{cl}(\mathcal{K})$  and  $\langle M, B \rangle > 0$  since  $B$  lies in the interior of  $\mathcal{K}$ , thus giving a contradiction. Hence,  $A_\lambda \in \mathcal{K} \cap \mathcal{A}$  for all  $0 \leq \lambda < 1$ . When letting  $\lambda$  go to 1,  $A_\lambda$  tends to  $A$ , and thus we can conclude that  $A$  lies in the closure of  $\mathcal{K} \cap \mathcal{A}$ . From this follows the inequality  $\vartheta^{\mathcal{K}}(G) \geq \vartheta^{\text{cl}(\mathcal{K})}(G)$ .

We now show equality  $\Theta^{\mathcal{K}}(G) = \Theta^{\text{cl}(\mathcal{K})}(G)$ . Analogously, it suffices to show the inequality  $\Theta^{\mathcal{K}}(G) \leq \Theta^{\text{cl}(\mathcal{K})}(G)$ . Denote by  $\mathcal{A}_t$  the affine space determined by the conditions  $X_{uu} = t$  for  $u \in V(G)$  and  $X_{uv} = 0$  for  $\{u, v\} \in E(G)$ . Let  $M \in \text{cl}(\mathcal{K})$  such that  $X - J \succeq 0$  and  $X \in \mathcal{A}_t$ . For  $0 \leq \lambda < 1$  define the matrix  $X_\lambda = \lambda X + (1 - \lambda)nI$ . Then,  $X_\lambda \in \mathcal{K}$  (same argument as above),  $M_\lambda \in \mathcal{A}_{\lambda t + (1 - \lambda)n}$ , and  $X_\lambda - J = \lambda(X - J) + (1 - \lambda)(nI - J) \succeq 0$ . Therefore,  $\Theta^{\text{cl}(\mathcal{K})}(G) \leq \lambda t + (1 - \lambda)n$  for all  $0 \leq \lambda < 1$ . Letting  $\lambda$  tend to 1 we deduce that  $\Theta^{\text{cl}(\mathcal{K})}(G) \leq t$  and thus  $\Theta^{\text{cl}(\mathcal{K})}(G) \leq \Theta^{\mathcal{K}}(G)$ .  $\square$



## 2.2 Quantum graph parameters

We now introduce two ‘quantum’ variants  $\alpha_q(G)$  and  $\alpha^*(G)$  of the stability number and two ‘quantum’ variants  $\chi_q(G)$  and  $\chi^*(G)$  of the chromatic number, which have been considered in the literature. Motivation for these parameters will be given in Section 2.3 below.

**Definition 2.5** (Game entanglement-assisted stability number [59]). *For a graph  $G$ ,  $\alpha_q(G)$  is defined as the maximum integer  $t \in \mathbb{N}$  for which there exist positive semidefinite matrices  $\rho, \rho_i^u \in \mathcal{S}_+^d$  for  $i \in [t]$ ,  $u \in V(G)$  (for some  $d \geq 1$ ) satisfying the following conditions:*

$$\langle \rho, \rho \rangle = 1, \quad (2.10)$$

$$\sum_{u \in V(G)} \rho_i^u = \rho \quad \forall i \in [t], \quad (2.11)$$

$$\langle \rho_i^u, \rho_j^v \rangle = 0 \quad \forall i \neq j \in [t], \forall u \simeq v \in V(G), \quad (2.12)$$

$$\langle \rho_i^u, \rho_i^v \rangle = 0 \quad \forall i \in [t], \forall u \neq v \in V(G). \quad (2.13)$$

**Definition 2.6** (Communication entanglement-assisted stability number [22]). *For a graph  $G$ ,  $\alpha^*(G)$  is defined as the maximum  $t \in \mathbb{N}$  for which there exist positive semidefinite matrices  $\rho, \rho_i^u \in \mathcal{S}_+^d$  for  $i \in [t]$ ,  $u \in V(G)$  (for some  $d \geq 1$ ) satisfying the conditions (2.10), (2.11) and (2.12).*

**Definition 2.7** (Game entanglement-assisted chromatic number [18]). *For a graph  $G$ ,  $\chi_q(G)$  is defined as the minimum  $t \in \mathbb{N}$  for which there exist positive semidefinite matrices  $\rho, \rho_u^i \in \mathcal{S}_+^d$  for  $i \in [t]$ ,  $u \in V$  (for some  $d \geq 1$ ) satisfying the following conditions:*

$$\langle \rho, \rho \rangle = 1, \quad (2.14)$$

$$\sum_{i \in [t]} \rho_u^i = \rho \quad \forall u \in V(G), \quad (2.15)$$

$$\langle \rho_u^i, \rho_v^i \rangle = 0 \quad \forall i \in [t], \forall \{u, v\} \in E(G), \quad (2.16)$$

$$\langle \rho_u^i, \rho_u^j \rangle = 0 \quad \forall i \neq j \in [t], \forall u \in V(G). \quad (2.17)$$

**Definition 2.8** (Communication entanglement-assisted chromatic number [12]). *For a graph  $G$ ,  $\chi^*(G)$  is defined as the minimum  $t \in \mathbb{N}$  for which there exist positive semidefinite matrices  $\rho, \rho_u^i \in \mathcal{S}_+^d$  for  $i \in [t]$ ,  $u \in V(G)$  (for some  $d \geq 1$ ) satisfying the conditions (2.14), (2.15) and (2.16).*

The parameters  $\alpha_q(G)$  and  $\chi_q(G)$  can, respectively, be equivalently obtained from the definitions of  $\alpha^*(G)$  and  $\chi^*(G)$  if we require  $\rho$  to be the identity matrix (instead of  $\langle \rho, \rho \rangle = 1$ ) and the other positive semidefinite matrices to be orthogonal projectors, i.e., to satisfy  $\rho^2 = \rho$  (see [59] and [18]).

The following inequalities follow from the definitions:

$$\alpha(G) \leq \alpha_q(G) \leq \alpha^*(G) \quad \text{and} \quad \chi^*(G) \leq \chi_q(G) \leq \chi(G).$$

Recently, several bounds for the quantum parameters have been established in terms of the theta number. Namely, [6, 26] show the bound  $\alpha^*(G) \leq \vartheta(G)$  and [23] shows

the tighter bound  $\alpha^*(G) \leq \vartheta'(G)$ . Moreover, [12] shows the bound  $\chi^*(G) \geq \vartheta^+(\overline{G})$ . Summarizing, the following sandwich inequalities hold:

$$\alpha(G) \leq \alpha_q(G) \leq \alpha^*(G) \leq \vartheta'(G) \text{ and } \vartheta^+(\overline{G}) \leq \chi^*(G) \leq \chi_q(G) \leq \chi(G). \quad (2.18)$$

Using our approach of reformulating the quantum parameters as optimization problems over the cone  $\mathcal{CS}_+$ , we will recover and refine these bounds (see Section 4, in particular, Corollaries 4.6 and 4.11, and Propositions 4.15, 4.17, 4.18 and 4.19).

### 2.3 Motivation

The quantum graph parameters that we have just defined arise in the general context of the study of entanglement, one of the most important features of quantum mechanics. In particular, the parameters  $\alpha_q$  and  $\chi_q$  are defined in term of *nonlocal games*, which are mathematical abstractions of a physical experiment introduced by [20]. In a nonlocal game, two (or more) cooperating players determine a common strategy to answer questions posed by a referee. The question is drawn from a finite set and the referee sends each of the players their questions. The players, without communicating, must respond each to their question and the referee upon collecting all the answers determines according to the rules of the game whether the players win or lose. We can now study properties of quantum mechanics, by asking the following question: does entanglement between the players allow for a better strategy than the best classical one. As it was shown by Bell [7], players that share entanglement can (for some games) produce answers that are correlated in a way that would be impossible in a classical world. Experimental evidence that such peculiar correlations exist in the world we live in was found by Aspect et al. [3]. (For a detailed introduction to the topic we recommend the book [54].)

Consider a game where two players want to convince a referee that they can color a graph  $G$  with  $t$  colors [33, 20]. The players each receive a vertex from the referee and they answer by returning a color from  $[t]$ . They win the game if they answer the same color upon receiving the same vertex and different colors if the vertices are adjacent. The best classical strategy is given by an actual proper coloring of the graph and the players can win using at least  $\chi(G)$  colors. In the entanglement-assisted setting,  $\chi_q(G)$  is the smallest number of colors that the players must use in order to always win the game (we refer to [18] and [60] for the proof that Definition 2.7 is the correct mathematical formulation). This parameter has received a notable amount of attention [4, 18, 32, 50, 60, 59, 38].

Analogously to  $\chi_q(G)$ ,  $\alpha_q(G)$  is the maximum integer  $t$  for which two players sharing an entangled state can convince a referee that the graph  $G$  has a stable set of cardinality  $t$ . For a detailed description of the game and of the correctness of Definition 2.6 we refer to [59] (see also [61]).

Another setting where the properties of entanglement can be studied is zero-error information theory. Here two parties want to perform a communication task (e.g., communicating through a noisy channel) both exactly and efficiently. These problems have led to the development of a new line of research in combinatorics [64, 66, 49, 1, 2] (see [45] for a survey and references therein). Recently Cubitt et al. [22] started studying whether sharing entanglement between the two parties improves the communication. A number of positive results, where entanglement does improve the communication, have been obtained [22, 46, 11, 12]. Without getting

into details, the parameters  $\alpha^*$  and  $\chi^*$  arise in this entanglement-assisted information theory setting. For the full description of the problem and the mathematical characterization we refer to [22] and [12] for  $\alpha^*$  and  $\chi^*$ , respectively.

We now briefly summarize known properties of these parameters. Naturally one of the most interesting questions is to find and characterize graphs for which there is a separation between a quantum parameter and its classical counterpart. An easy observation is that for any perfect graph  $G$  there is no such separation. Indeed, it follows from the inequalities (2.7) and (2.18) that  $\alpha(G) = \alpha_q(G) = \alpha^*(G) = \lfloor \vartheta(G) \rfloor$  and  $\lceil \vartheta(\overline{G}) \rceil = \chi^*(G) = \chi_q(G) = \chi(G)$  hold when  $G$  is a perfect graph. Moreover, for any bipartite graph  $G$  we have  $\chi^*(G) = \chi_q(G) = \chi(G)$ , as  $\chi_q(G) = 2$  if and only if  $\chi(G) = 2$  [18].

On the other hand a few separation results are known. For instance there exists a graph for which  $\chi^*(G) = \chi_q(G) = 3$  but  $\chi(G) = 4$  [32] and a family of graphs exhibiting an exponential separation between  $\chi_q$  and  $\chi$  [10, 13, 4] (and therefore also between  $\chi^*$  and  $\chi$ ). This family is composed by the so-called *orthogonality graphs* (or Hadamard graphs)  $\Omega_n$  whose vertices are the set of  $\{\pm 1\}^n$  vectors and two vertices are adjacent if orthogonal. If  $n$  is a multiple of 4, then  $n = \chi^*(\Omega_n) = \chi_q(\Omega_n) = \vartheta(\overline{\Omega_n})$  [4, 59] while  $\chi(\Omega_n)$  is exponential in  $n$  due to a result of Frankl and Rödl [31]. Using a general technique showing how to construct a graph satisfying  $\alpha_q > \alpha$  from a graph satisfying  $\chi_q < \chi$ , in [50] and [59] the authors show that the graphs  $\Omega_n \square K_n$  exhibit an exponential separation, respectively, between  $\alpha^*$  and  $\alpha$  and between  $\alpha_q$  and  $\alpha$ . In fact, for  $n > 8$  divisible by 4, there exists  $\epsilon > 0$  such that  $\alpha_q(\Omega_n \square K_n) = \alpha^*(\Omega_n \square K_n) = 2^n$  while  $\alpha(\Omega_n \square K_n) \leq n(2 - \epsilon)^n$ . Other examples of graphs with  $\alpha^* > \alpha$  can be found in [22, 46, 11] and see [12] for a graph with  $\alpha^* > \alpha$  and  $\chi^* < \chi$ .

While for the classical parameters the inequality  $\chi(G)\alpha(G) \geq |V(G)|$  holds for any graph  $G$ , interestingly this is not true for the quantum counterparts. As noticed in [59], if  $n$  is a multiple of 4 but not a power of 2, then  $\chi_q(\Omega_n)\alpha_q(\Omega_n) < |V(\Omega_n)|$  and the exact same reasoning implies that  $\chi^*(\Omega_n)\alpha^*(\Omega_n) < |V(\Omega_n)|$ .

It is well known that the chromatic and stability number are NP-hard quantities. Only very recently Ji [38] proved that deciding whether  $\chi_q(G) \leq 3$  is an NP-hard problem. The complexity of computing  $\chi^*, \alpha_q, \alpha^*$  is still open although it might be possible to use the techniques in [38] to prove that also  $\alpha_q$  is NP-hard.

### 3 The completely positive semidefinite cone

In this section we introduce the completely positive semidefinite cone  $\mathcal{CS}_+$  and establish some of its basic properties, also regarding its relation with the completely positive cone and with the doubly nonnegative cone. Moreover, we investigate the dual cone of  $\mathcal{CS}_+^n$  and introduce a hierarchy of cones aiming to approximate the cone  $\mathcal{CS}_+^{n*}$ . We use it to define a hierarchy of semidefinite approximations for the parameters  $\vartheta^{\mathcal{CS}_+(G)}$  and  $\Theta_+^{\mathcal{CS}_+(G)}$ , which converge asymptotically to them when assuming that an open conjecture by Connes in operator theory holds.

#### 3.1 Basic properties

Recall that for any positive semidefinite matrix  $A$  there exists a set of vectors  $x_1, \dots, x_n \in \mathbb{R}^d$  that form its Gram representation, i.e.,  $A = (\langle x_i, x_j \rangle)_{i,j=1}^n$ . We

now consider Gram representations by *positive semidefinite matrices*.

**Definition 3.1.** A matrix  $A \in \mathcal{S}^n$  is said to be *completely positive semidefinite* (completely psd, for short) if there exist matrices  $X_1, \dots, X_n \in \mathcal{S}_+^d$  (for some  $d \geq 1$ ) such that  $A = (\langle X_i, X_j \rangle)_{i,j=1}^n$ . Then we also say that  $X_1, \dots, X_n$  form a *Gram representation* of  $A$ . We let  $\mathcal{CS}_+^n$  denote the set of all completely positive semidefinite matrices.

**Lemma 3.2.**  $\mathcal{CS}_+^n$  is a convex cone.

*Proof.* Let  $A \in \mathcal{CS}_+^n$ ,  $\lambda \geq 0$ , and assume that  $X_1, \dots, X_n \in \mathcal{S}_+^d$  form a Gram representation of  $A$ . Then, the matrices  $\sqrt{\lambda_1}X_1, \dots, \sqrt{\lambda_n}X_n$  are psd and form a Gram representation of  $\lambda A$ , thus showing that  $\lambda A \in \mathcal{CS}_+^n$ .

Let  $B \in \mathcal{CS}_+^n$  with Gram representation  $Y_1, \dots, Y_n \in \mathcal{S}_+^k$ . Then, the matrices  $X_1 \oplus Y_1, \dots, X_n \oplus Y_n$  are psd and form a Gram representation of  $X + Y$ , thus showing that  $X + Y \in \mathcal{CS}_+^n$ . Hence  $\mathcal{CS}_+^n$  is a convex cone.  $\square$

As is well known, both  $\mathcal{S}_+^n$  and  $\mathcal{CP}^n$  are closed sets. This is easy to see for  $\mathcal{S}_+^n$ , since it is a self-dual cone. For the cone  $\mathcal{CP}^n$ , this can be seen as follows: any matrix in  $\mathcal{CP}^n$  can be written as a sum of rank 1 matrices  $\sum_{i=1}^N y_i y_i^T$ , where  $y_1, \dots, y_N \in \mathbb{R}_+^n$  and where  $N \leq \binom{n}{2}$  (using Caratheory's theorem) and thus closeness follows using a compactness argument. Interestingly, we do not know whether the cone  $\mathcal{CS}_+^n$  is closed as well.

What we can show is that deciding whether the cone  $\mathcal{CS}_+$  is closed is related to the following question: Does the existence of a Gram representation by *infinite* positive semidefinite matrices imply the existence of another Gram representation by finite ones?

More precisely, let  $\mathcal{S}^{\mathbb{N}}$  denote the set of all infinite symmetric matrices  $X = (X_{ij})_{i,j \geq 1}$  with finite norm:  $\sum_{i,j \geq 1} X_{ij}^2 < \infty$ . Thus  $\mathcal{S}^{\mathbb{N}}$  is a Hilbert space, equipped with the inner product  $\langle X, Y \rangle = \sum_{i,j \geq 1} X_{ij} Y_{ij}$ . Call a matrix  $X \in \mathcal{S}^{\mathbb{N}}$  psd (again denoted as  $X \succeq 0$ ) when all its finite principal submatrices are psd, i.e.,  $X[I] \in \mathcal{S}_+^{|I|}$  for all finite subsets  $I \subseteq \mathbb{N}$ , and let  $\mathcal{S}_+^{\mathbb{N}}$  denote the set of all psd matrices in  $\mathcal{S}^{\mathbb{N}}$ .

Finally, let  $\mathcal{CS}_{\infty+}^n$  denote the set of matrices  $A \in \mathcal{S}^n$  having a Gram representation by elements of  $\mathcal{S}_+^{\mathbb{N}}$ . As for  $\mathcal{CS}_+^n$ , one can verify that  $\mathcal{CS}_{\infty+}^n$  is a convex cone. Moreover we can show the following relationships between these two cones.

**Theorem 3.3.** For any  $n \in \mathbb{N}$ ,  $\mathcal{CS}_+^n \subseteq \mathcal{CS}_{\infty+}^n \subseteq \text{cl}(\mathcal{CS}_{\infty+}^n) = \text{cl}(\mathcal{CS}_+^n)$  holds.

*Proof.* The inclusion  $\mathcal{CS}_+^n \subseteq \mathcal{CS}_{\infty+}^n$  is clear, since any matrix  $X \in \mathcal{S}_+^d$  can be viewed as an element of  $\mathcal{S}_+^{\mathbb{N}}$  by adding zero entries.

We now prove the inclusion:  $\mathcal{CS}_{\infty+}^n \subseteq \text{cl}(\mathcal{CS}_+^n)$ . For this, let  $A \in \mathcal{CS}_{\infty+}^n$  and  $X_1, \dots, X_n \in \mathcal{S}_+^{\mathbb{N}}$  be a Gram representation of  $A$ , i.e.,  $A_{ij} = \langle X_i, X_j \rangle$  for  $i, j \in [n]$ . For any  $\ell \in \mathbb{N}$  and  $i \in [n]$ , let  $X_i^\ell = X_i[\{1, \dots, \ell\}]$  be the  $\ell \times \ell$  upper left principal submatrix of  $X_i$  and let  $\tilde{X}_i^\ell \in \mathcal{S}^{\mathbb{N}}$  be the infinite matrix obtained by adding zero entries to  $X_i^\ell$ . Thus,  $X_i^\ell \in \mathcal{S}_+^\ell$  and  $\tilde{X}_i^\ell \in \mathcal{S}_+^{\mathbb{N}}$ . Now, let  $A^\ell$  denote the Gram matrix of  $X_1^\ell, \dots, X_n^\ell$ , so that  $A^\ell \in \mathcal{CS}_+^n$ . We show that the sequence  $(A^\ell)_{\ell \geq 1}$  converges to  $A$  as  $\ell$  tends to  $\infty$ , which shows that  $A \in \text{cl}(\mathcal{CS}_+^n)$ . Indeed, for any  $i, j \in [n]$  and

$\ell \in \mathbb{N}$ , we have:

$$\begin{aligned} |A_{i,j} - A_{i,j}^\ell| &= |\langle X_i, X_j \rangle - \langle X_i^\ell, X_j^\ell \rangle| \\ &\leq |\langle X_i - \tilde{X}_i^\ell, X_j \rangle| + |\langle \tilde{X}_i^\ell, X_j - \tilde{X}_j^\ell \rangle| \\ &\leq \|X_i - \tilde{X}_i^\ell\| \|X_j\| + \|\tilde{X}_i^\ell\| \|X_j - \tilde{X}_j^\ell\|, \end{aligned}$$

using the Cauchy-Schwarz inequality in the last step. Clearly,  $\|X_i^\ell\| \leq \|X_i\| = \sqrt{A_{ii}}$  for all  $\ell \in \mathbb{N}$  and  $i \in [n]$ . Hence  $\lim_{\ell \rightarrow \infty} |A_{i,j} - A_{i,j}^\ell| = 0$  for all  $i, j \in [n]$ , concluding the proof.

Taking the closure in the inclusions:  $\mathcal{CS}_+^n \subseteq \mathcal{CS}_{\infty+}^n \subseteq \text{cl}(\mathcal{CS}_+^n)$ , we conclude that  $\text{cl}(\mathcal{CS}_{\infty+}^n) = \text{cl}(\mathcal{CS}_+^n)$  holds.  $\square$   $\square$

### 3.2 Links to completely positive and doubly nonnegative matrices

The following relationships follow from the definitions:

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{S}_+^n \cap \mathbb{R}_+^{n \times n} =: \mathcal{DN}\mathcal{N}^n. \quad (3.1)$$

Hence, the cone  $\mathcal{CS}_+^n$  is full-dimensional and pointed. That every completely positive matrix is entrywise nonnegative follows from the fact that  $\langle X, Y \rangle \geq 0$  for all  $X, Y \in \mathcal{S}_+^d$ . Taking duals in (3.1) we get the corresponding inclusions:

$$\mathcal{DN}\mathcal{N}^{n*} \subseteq \mathcal{CS}_+^{n*} \subseteq \mathcal{CP}^{n*}. \quad (3.2)$$

The dual of  $\mathcal{CP}^n$  is the *copositive cone*, which consists of all matrices  $M \in \mathcal{S}^n$  that are *copositive*, i.e., satisfy  $x^T M x \geq 0$  for all  $x \in \mathbb{R}_+^n$ . The dual of  $\mathcal{DN}\mathcal{N}^n$  is the cone  $\mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n \times n})$ . We will investigate the dual of  $\mathcal{CS}_+^n$  in detail in the next section.

We now present some results regarding the inclusions in (3.1) and (3.2). Remarkably, Diananda [24] and Maxfield and Minc [51] have shown, respectively, that  $\mathcal{CP}^{n*} = \mathcal{DN}\mathcal{N}^{n*}$  and  $\mathcal{CP}^n = \mathcal{DN}\mathcal{N}^n$  for any  $n \leq 4$ . Hence equality holds throughout in (3.1) and (3.2) for  $n \leq 4$ . Moreover the inclusions  $\mathcal{CP}^n \subseteq \mathcal{DN}\mathcal{N}^n$  and  $\mathcal{DN}\mathcal{N}^{n*} \subseteq \mathcal{CP}^{n*}$  are known to be strict for any  $n \geq 5$ . It suffices to show the strict inclusions for  $n = 5$ , since  $A \in \mathcal{DN}\mathcal{N}^5 \setminus \mathcal{CP}^5$  implies  $\tilde{A} \in \mathcal{DN}\mathcal{N}^n \setminus \mathcal{CP}^n$ , where  $\tilde{A}$  is obtained by adding a border of zero entries to  $A$ . This extends to the cone  $\mathcal{CS}_+$ . Indeed, the matrix  $A$  belongs to  $\mathcal{CP}^5$  (resp.,  $\mathcal{DN}\mathcal{N}^5$ , or  $\mathcal{CS}_+^5$ ) if and only if the extended matrix  $\tilde{A}$  belongs to  $\mathcal{CP}^n$  (resp.,  $\mathcal{DN}\mathcal{N}^n$ , or  $\mathcal{CS}_+^n$ ).

To show strict inclusion, we will use the following two matrices:

$$H = \begin{pmatrix} 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{pmatrix}, \quad K = \begin{pmatrix} 4 & 0 & 2 & 2 & 0 \\ 0 & 4 & 0 & 2 & 2 \\ 2 & 0 & 4 & 0 & 3 \\ 2 & 2 & 0 & 4 & 0 \\ 0 & 2 & 3 & 0 & 4 \end{pmatrix}. \quad (3.3)$$

$H$  is the Horn matrix which, as is well known, is copositive but does not lie in the dual of the doubly nonnegative cone [37]. Moreover, the matrix  $K$  is doubly nonnegative but is not completely positive (as observed right after Theorem 3.4). Thus,

$$H \in \mathcal{CP}^{5*} \setminus \mathcal{DN}\mathcal{N}^{5*} \quad \text{and} \quad K \in \mathcal{DN}\mathcal{N}^5 \setminus \mathcal{CP}^5.$$

We will show later in this section that  $K$  does not belong to the closure of  $\mathcal{CS}_+^5$ , thus showing the strict inclusion:  $\text{cl}(\mathcal{CS}_+^5) \subset \mathcal{DNN}^5$  (see Lemma 3.8).

The strict inclusion:  $\mathcal{CP}^5 \subset \mathcal{CS}_+^5$  is shown by the following matrix, found by Fawzi and Parillo [29]:

$$L = \begin{pmatrix} 1 & \cos^2(\frac{2\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{2\pi}{5}) \\ \cos^2(\frac{2\pi}{5}) & 1 & \cos^2(\frac{2\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{4\pi}{5}) \\ \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{2\pi}{5}) & 1 & \cos^2(\frac{2\pi}{5}) & \cos^2(\frac{4\pi}{5}) \\ \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{2\pi}{5}) & 1 & \cos^2(\frac{2\pi}{5}) \\ \cos^2(\frac{2\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{4\pi}{5}) & \cos^2(\frac{2\pi}{5}) & 1 \end{pmatrix}. \quad (3.4)$$

To see that  $L \in \mathcal{CS}_+^5$ , observe that the entrywise square root matrix  $\widehat{L} = (\sqrt{L_{ij}})_{i,j}$  is positive semidefinite. Indeed, if the vectors  $x_1, \dots, x_5$  form a Gram representation of  $\widehat{L}$ , then the psd matrices  $x_1 x_1^T, \dots, x_5 x_5^T$  form a Gram representation of  $L$ . However  $L$  is not completely positive, since its inner product with the Horn matrix is negative:  $\langle H, L \rangle = 5(2 - \sqrt{5})/2 < 0$ . Therefore,

$$L \in \mathcal{CS}_+^5 \setminus \mathcal{CP}^5 \quad \text{and} \quad H \in \mathcal{CP}^{5*} \setminus \mathcal{CS}_+^{5*}.$$

In the rest of this section we will show that the inclusion  $\text{cl}(\mathcal{CS}_+^5) \subseteq \mathcal{DNN}^5$  is strict and thus, by taking duals,  $\mathcal{DNN}^{5*} \subset \mathcal{CS}_+^{5*}$  (see Corollary 3.9). For this we consider matrices whose pattern of nonzero entries forms a cycle and we show that for such matrices being completely positive is equivalent to being completely psd. Given a matrix  $A \in \mathcal{S}^n$ , its *support graph* is the graph  $G(A) = ([n], E)$  where there is an edge  $\{i, j\}$  when  $A_{ij} \neq 0$ . Moreover, the *comparison matrix* of  $A$  is the matrix  $C(A) \in \mathcal{S}^n$  with entries  $C(A)_{ii} = A_{ii}$  for all  $i \in [n]$  and  $C(A)_{ij} = -A_{ij}$  for all  $i \neq j \in [n]$ . We will use the following result characterizing completely positive matrices whose support graph is triangle-free.

**Theorem 3.4.** [25] (see also [9]) *Let  $A \in \mathcal{S}^n$  and assume that its support graph is triangle-free. Then,  $A$  is completely positive if and only if its comparison matrix  $C(A)$  is positive semidefinite.*

As a first application, we obtain that the matrix  $K$  from (3.3) is not completely positive, since its support graph is  $C_5$  and its comparison matrix is not positive semidefinite. Moreover, we have the following easy result for matrices supported by bipartite graphs.

**Lemma 3.5.** *Let  $A \in \mathcal{S}^n$  and assume that  $G(A)$  is a bipartite graph. Then,  $A \in \mathcal{CS}_+^n$  if and only if  $A \in \mathcal{CP}^n$ .*

*Proof.* Assume  $A \in \mathcal{CS}_+^n$ ; we show that  $A \in \mathcal{CP}^n$  (the reverse implication holds trivially). Say,  $X_1, \dots, X_n \in \mathcal{S}_+^d$  form a Gram representation of  $A$ . As  $G(A)$  is bipartite, consider a bipartition of its vertex set as  $U \cup W$  so that all edges of  $G(A)$  are of the form  $\{i, j\}$  with  $i \in U$  and  $j \in W$ . Now, observe that the matrices  $X_i$  for  $i \in U$ , and  $-X_j$  for  $j \in W$  form a Gram representation of the comparison matrix  $C(A)$ . This shows that  $C(A) \succeq 0$  and thus  $A \in \mathcal{CP}^n$  in view of Theorem 3.4.  $\square$

The above result also follows from the known characterization of *completely positive graphs*. Recall that a graph  $G$  is *completely positive* if every doubly nonnegative matrix with support  $G$  is completely positive. Kogan and Berman [44] show that

a graph  $G$  is completely positive if and only if it does not contain an odd cycle of length at least 5 as a subgraph. In particular, odd cycles are not completely positive graphs (e.g., because the matrix  $K$  has  $G(K) = C_5$  and  $K \in \mathcal{DN}\mathcal{N}^5 \setminus \mathcal{CP}^5$ ) and any bipartite graph is completely positive. By definition, for any matrix  $A$ ,

$$\text{if } G(A) \text{ is completely positive then: } A \in \mathcal{DN}\mathcal{N}^n \iff A \in \mathcal{CS}_+^n \iff A \in \mathcal{CP}^n.$$

We will also use the following elementary result about psd matrices.

**Lemma 3.6.** *Let  $A$  and  $B$  be positive semidefinite matrices with block-form:*

$$A = \begin{pmatrix} A_1 & A_2 \\ A_2^T & A_3 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} B_1 & B_2 \\ B_2^T & B_3 \end{pmatrix},$$

where  $A_i$  and  $B_i$  have the same dimensions. Then,  $\langle A, B \rangle = 0$  implies that  $\langle A_1, B_1 \rangle = \langle A_3, B_3 \rangle = -\langle A_2, B_2 \rangle$ .

*Proof.* As  $A, B \succeq 0$ ,  $\langle A, B \rangle = 0$  implies  $AB = 0$  and thus  $A_1B_1 + A_2B_2^T = 0$  and  $A_2^TB_2 + A_3B_3 = 0$ . Taking the trace we obtain the desired identities.  $\square$

**Theorem 3.7.** *Let  $A \in \mathcal{S}^n$  and assume that  $G(A)$  is a cycle. Then,  $A \in \mathcal{CS}_+^n$  if and only if  $A \in \mathcal{CP}^n$ .*

*Proof.* One direction is obvious since  $\mathcal{CP}^n \subseteq \mathcal{CS}_+^n$ . Assume now that  $A \in \mathcal{CS}_+^n$  with  $G(A) = C_n$ ; we show that  $A \in \mathcal{CP}^n$ . We consider only the non-trivial case when  $n \geq 5$ . In view of Theorem 3.4, it suffices to show that the comparison matrix  $C(A)$  is positive semidefinite.

Let  $X^1, \dots, X^n \in \mathcal{S}_+^d$  be a psd Gram representation of  $A$ . If  $n$  is even, then (as in the above proof of Lemma 3.5), the matrices  $Y^1 = -X^1, Y^2 = X^2, Y^3 = -X^3, Y^4 = X^4, \dots, Y^{n-1} = -X^{n-1}, Y^n = X^n$  form a Gram representation of  $C(A)$ , thus showing that  $C(A) \succeq 0$  and concluding the proof in the case  $n$  even.

We now consider the case when  $n$  is odd. As we will see, in order to construct a Gram representation of  $C(A)$ , we can choose the same matrices  $Y^1, \dots, Y^{n-1}$  as above but we need to look in more detail into the structure of the  $X^i$ 's in order to be able to tell how to define the last matrix  $Y^n$ . For this, we observe that the matrices  $X^1, \dots, X^n$  can be assumed to be  $(n-2) \times (n-2)$  block-matrices, where we denote the blocks of  $X^k$  as  $X_{rs}^k$  for  $r, s \in [n-2]$  (with  $X_{sr}^k = (X_{rs}^k)^T$ ) and the index sets of the blocks as  $I_1, \dots, I_{n-2}$ . Indeed, without loss of generality we can assume that  $X^1$  is diagonal and we let  $X_{11}^1$  denote its nonzero diagonal principal submatrix, so that  $X^1 = \begin{pmatrix} X_{11}^1 & 0 \\ 0 & 0 \end{pmatrix}$  and the index set of  $X_{11}^1$  defines the index set

$I_1$  of the first block. Next,  $X^2$  has the form  $\begin{pmatrix} X_{11}^2 & X_{12}^2 & 0 \\ X_{21}^2 & X_{22}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ , where  $X_{22}^2 \succ 0$  (since

$A_{13} = 0$  while  $A_{23} \neq 0$ ) and its index set defines the index set  $I_2$  of the second

block. Next, we can write  $X^3 = \begin{pmatrix} X_{11}^3 & X_{12}^3 & X_{13}^3 & 0 \\ X_{21}^3 & X_{22}^3 & X_{23}^3 & 0 \\ X_{31}^3 & X_{32}^3 & X_{33}^3 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ , where  $I_3$  is the index set

of  $X_{33}^3$ . As  $A_{13} = 0$ , we can conclude that  $X_{11}^3 = 0$  (and thus  $X_{12}^3 = X_{13}^3 = 0$ ). Iterating, we see that, for each  $k \in \{2, 3, \dots, n-2\}$ , all blocks of the matrix  $X^k$

are equal to 0 except its blocks  $X_{k-1,k-1}^k$ ,  $X_{k-1,k}^k$ ,  $X_{k,k-1}^k$  and  $X_{kk}^k$ . Moreover, all blocks of the matrix  $X^{n-1}$  are equal to 0 except its last diagonal block  $X_{n-2,n-2}^{n-1}$  and for the matrix  $X^n$  all the blocks might be present.

We now indicate how to construct the matrix  $Y^n$  from  $X^n$ : we just resign its two blocks  $X_{n-3,n-2}^n$  and  $X_{n-2,n-2}^n$ . In other words, we let  $Y^n$  be the  $(n-2) \times (n-2)$  block matrix with blocks  $Y_{n-3,n-2}^n = -X_{n-3,n-2}^n$ ,  $Y_{n-2,n-2}^n = -X_{n-2,n-2}^n$  and  $Y_{rs}^n = X_{rs}^n$  for all other blocks. Let us stress that in particular we do not change the sign of the block  $X_{n-2,n-3}^n$ . As in the case  $n$  even, for any  $1 \leq i \leq n-1$ , we set  $Y^i = -X^i$  for odd  $i$  and  $Y^i = X^i$  for even  $i$ .

We claim that  $Y^1, \dots, Y^n$  form a Gram representation of the comparison matrix  $C(A)$ . It is clear that  $\langle Y^i, Y^j \rangle = C(A)_{ij}$  for all  $i, j \in [n-1]$  and that  $\langle Y^1, Y^n \rangle = -A_{1n} = C(A)_{1n}$  and  $\langle Y^i, Y^n \rangle = 0$  for  $2 \leq i \leq n-3$  (since the blocks indexed by  $[n-3]$  in  $Y^n$  are the same as in  $X^n$  and each block  $Y_{r,n-2}^i$  is equal to 0). Moreover,  $\langle Y^n, Y^n \rangle = \langle X^n, X^n \rangle = C(A)_{nn}$  and  $\langle Y^{n-1}, Y^n \rangle = -A_{n-1,n} = C(A)_{n-1,n}$ . Finally, we use Lemma 3.6 to verify that  $\langle Y^{n-2}, Y^n \rangle = 0$ . Indeed, we have that

$$0 = A_{n-2,n} = \langle X^{n-2}, X^n \rangle = \left\langle \begin{pmatrix} X_{n-3,n-3}^{n-2} & X_{n-3,n-2}^{n-2} \\ X_{n-2,n-3}^{n-2} & X_{n-2,n-2}^{n-2} \end{pmatrix}, \begin{pmatrix} X_{n-3,n-3}^n & X_{n-3,n-2}^n \\ X_{n-2,n-3}^n & X_{n-2,n-2}^n \end{pmatrix} \right\rangle$$

which, by Lemma 3.6, implies that  $\langle X_{n-3,n-3}^{n-2}, X_{n-3,n-3}^n \rangle = \langle X_{n-2,n-2}^{n-2}, X_{n-2,n-2}^n \rangle$ . Therefore,

$$\langle Y^{n-2}, Y^n \rangle = \left\langle \begin{pmatrix} -X_{n-3,n-3}^{n-2} & -X_{n-3,n-2}^{n-2} \\ -X_{n-2,n-3}^{n-2} & -X_{n-2,n-2}^{n-2} \end{pmatrix}, \begin{pmatrix} X_{n-3,n-3}^n & -X_{n-3,n-2}^n \\ X_{n-2,n-3}^n & -X_{n-2,n-2}^n \end{pmatrix} \right\rangle$$

is equal to 0.  $\square$

We can now already deduce that the matrix  $K$  in (3.3) is not completely psd (by applying Theorem 3.7, since the support of  $K$  is  $C_5$  and  $K \notin \mathcal{CP}^5$ ). In order to show that  $K$  does not belong to the closure of  $\mathcal{CS}_+^5$  we need to do a bit more work. For this we use the parameter  $\vartheta^{\mathcal{K}}(G)$  introduced earlier in relation (2.8), selecting for  $\mathcal{K}$  the cones  $\mathcal{CS}_+$ ,  $\text{cl}(\mathcal{CS}_+)$  and  $\mathcal{CP}$ , for proving the next result.

**Lemma 3.8.** *Let  $X \in \mathcal{DNN}^5$  and assume that the support of  $X$  is the cycle  $C_5$ . If  $\langle J - 2I, X \rangle > 0$  then  $X \notin \text{cl}(\mathcal{CS}_+^5)$ .*

*Proof.* Consider the parameter  $\vartheta^{\mathcal{CS}_+}(C_5)$ . By combining Theorems 2.2 and 3.7, we deduce that  $\vartheta^{\mathcal{CS}_+}(C_5) = \vartheta^{\mathcal{CP}}(C_5) = \alpha(C_5) = 2$ , since any matrix feasible for the definition (2.8) of  $\vartheta^{\mathcal{CS}_+}(C_5)$  is completely positive. Assume that there exists a matrix  $X \in \text{cl}(\mathcal{CS}_+^5)$  whose support is  $C_5$  and such that  $\langle J - 2I, X \rangle > 0$ . Then the matrix  $X/\text{Tr}(X)$  is feasible for the definition of the parameter  $\vartheta^{\text{cl}(\mathcal{CS}_+)}(C_5)$  and thus  $\vartheta^{\text{cl}(\mathcal{CS}_+)}(C_5) \geq \langle J, X \rangle / \text{Tr}(X) > 2$ . Applying Lemma 2.4, we obtain that  $\vartheta^{\mathcal{CS}_+}(C_5) = \vartheta^{\text{cl}(\mathcal{CS}_+)}(C_5) > 2$ , thus reaching a contradiction.  $\square$

As a direct application, the matrix  $K$  in (3.3) does not belong to  $\text{cl}(\mathcal{CS}_+^5)$ , since  $K \in \mathcal{DNN}^5$ , its support is  $C_5$  and  $\langle J - 2I, K \rangle > 0$ .

**Corollary 3.9.** *The inclusions  $\text{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{DNN}^n$  and  $\mathcal{DNN}^{n*} \subseteq \mathcal{CS}_+^{n*}$  are strict for any  $n \geq 5$ .*



### 3.3 The dual cone of the completely positive semidefinite cone

The dual of the completely positive cone  $\mathcal{CP}^n$  is the copositive cone  $\mathcal{COP}^n$ , consisting of the matrices  $M \in \mathcal{S}^n$  satisfying  $\sum_{i,j=1}^n M_{ij}x_i^2x_j^2 \geq 0$  for all  $x_1, \dots, x_n \in \mathbb{R}^n$  or, equivalently, the  $n$ -variate polynomial  $p_M = \sum_{i,j=1}^n M_{ij}x_i^2x_j^2$  is nonnegative over  $\mathbb{R}^n$ . We now consider the dual of the cone  $\mathcal{CS}_+^n$ .

**Lemma 3.10.** *Given a matrix  $M \in \mathcal{S}^n$ , the following assertions are equivalent:*

- (i)  $M \in \mathcal{CS}_+^{n*}$ , i.e.,  $\sum_{i,j=1}^n M_{ij}\langle X_i, X_j \rangle \geq 0$  for all  $X_1, \dots, X_n \in \mathcal{S}_+^d$  and  $d \in \mathbb{N}$ .
- (ii)  $\text{Tr}(\sum_{i,j=1}^n M_{ij}X_i^2X_j^2) \geq 0$  for all  $X_1, \dots, X_n \in \mathcal{S}^d$  and  $d \in \mathbb{N}$ .

*Proof.* Use the fact that any matrix  $X \in \mathcal{S}_+^d$  can be written as  $X = Y^2$  for some  $Y \in \mathcal{S}^d$ . Indeed, write  $X = PDP^T$ , where  $P$  is orthogonal and  $D$  is the diagonal matrix containing the eigenvalues of  $X$ , and set  $Y = P\sqrt{D}P^T$ .  $\square$

In other words,  $M \in \mathcal{CS}_+^{n*}$  if the associated polynomial  $p_M = \sum_{i,j=1}^n M_{ij}X_i^2X_j^2$  in the non-commutative variables  $X_1, \dots, X_n$  is *trace positive*, which means that the evaluation of  $p_M$  at any symmetric matrices  $X_1, \dots, X_n$  (of the same arbitrary size  $d \geq 1$ ) produces a matrix with nonnegative trace. Hence copositivity corresponds to restricting to symmetric matrices  $X_i$  of size  $d = 1$ , i.e., to real numbers.

Interestingly, describing the matrices in  $\mathcal{CS}_+^{n*}$  is deeply connected with one of the most important conjectures in von Neumann algebra: Connes' embedding conjecture [21]. A reformulation of the conjecture that shows this connection is given by Klep and Schweighofer [40]. In order to state it, we need to introduce some notation.

We let  $\mathbb{R}[\underline{x}]$  (resp.,  $\mathbb{R}\langle \underline{X} \rangle$ ) denote the set of real polynomials in the commutative variables  $x_1, \dots, x_n$  (resp., in the non-commutative variables  $X_1, \dots, X_n$ ). Then,  $\mathbb{R}[\underline{x}]_k$  and  $\mathbb{R}\langle \underline{X} \rangle_k$  denote the subsets of all polynomials of degree at most  $k$ .  $\mathbb{R}\langle \underline{X} \rangle$  is endowed with the involution  $*$ :  $\mathbb{R}\langle \underline{X} \rangle \rightarrow \mathbb{R}\langle \underline{X} \rangle$  that sends each variable  $X_i$  to  $X_i$ , each monomial  $X_{i_1}X_{i_2} \cdots X_{i_t}$  to its reverse  $X_{i_t} \cdots X_{i_2}X_{i_1}$  and extending linearly to arbitrary polynomials; for instance,  $(X_1X_2 + X_2X_3)^* = X_2X_1 + X_3X_2$ . A polynomial  $f \in \mathbb{R}\langle \underline{X} \rangle$  is *symmetric* if  $f^* = f$  and  $S\mathbb{R}\langle \underline{X} \rangle$  denotes the set of symmetric polynomials in  $\mathbb{R}\langle \underline{X} \rangle$ . A polynomial of the form  $ff^*$  is called a *Hermitian square* and a polynomial of the form  $[f, g] = fg - gf$  is called a *commutator*.

A polynomial  $f \in \mathbb{R}\langle \underline{X} \rangle$  is said to be *trace positive* if  $\text{Tr}(f(X_1, \dots, X_n)) \geq 0$  for all  $(X_1, \dots, X_n) \in \cup_{d \geq 1} (\mathcal{S}^d)^n$ . Note that  $f^*$  evaluated at  $(X_1, \dots, X_n) \in (\mathcal{S}^d)^n$  is equal to  $f(X_1, \dots, X_n)^T$ ; hence, any Hermitian square  $ff^*$  is trace positive. Moreover, the trace of any commutator vanishes when evaluated at symmetric matrices.

The *quadratic module*  $\mathcal{M}$  generated by a set of polynomials  $p_1, \dots, p_m \in S\mathbb{R}\langle \underline{X} \rangle$  consists of all polynomials of the form  $\sum_{j=1}^{m_0} f_j f_j^* + \sum_{i=1}^m \sum_{j_i=1}^{m_i} g_{j_i} p_i g_{j_i}^*$  for some  $f_i, g_{j_i} \in \mathbb{R}\langle \underline{X} \rangle$  and  $m_0, m_i \in \mathbb{N}$ . The *tracial quadratic module*  $\text{tr}\mathcal{M}$  consists of all polynomials of the form  $g + h$ , where  $g \in \mathcal{M}$  and  $h$  is a sum of commutators. We consider here the quadratic module generated by the polynomials  $1 - X_1^2, \dots, 1 - X_n^2$ , which we denote by  $\mathcal{M}_{\text{nc}}^{\text{cube}}$ , and the corresponding tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{cube}}$ . Clearly any polynomial in  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{cube}}$  is trace positive on the (non-commutative version of the) hypercube:

$$Q_{\text{nc}} = \bigcup_{d \geq 1} \{(X_1, \dots, X_n) \in (\mathcal{S}^d)^n : I - X_i^2 \succeq 0 \forall i \in [n]\}.$$

We also consider trace positivity over the (non-commutative) ball:

$$B_{\text{nc}} = \bigcup_{d \geq 1} \{(X_1, \dots, X_n) \in (\mathcal{S}^d)^n : I - \sum_{i=1}^n X_i^2 \succeq 0\}$$

and the corresponding quadratic module  $\mathcal{M}_{\text{nc}}^{\text{ball}}$ , which is generated by the polynomial  $1 - \sum_{i=1}^n X_i^2$ , and the tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}}$ .

Klep and Schweighofer [40] (see [16] for the corrected version of the proof) showed the following reformulation of Connes' embedding conjecture [21] in terms of characterizing all trace positive polynomials on  $Q_{\text{nc}}$ .

**Conjecture 3.11.** [40] *Let  $f \in S\mathbb{R}\langle \underline{X} \rangle$ . The following are equivalent:*

- (i)  *$f$  is trace positive on  $Q_{\text{nc}}$ .*
- (ii) *For any  $\epsilon > 0$ ,  $f + \epsilon \in \text{tr}\mathcal{M}_{\text{nc}}^{\text{cube}}$ , i.e.,  $f + \epsilon = g + h$ , where  $g$  belongs to the quadratic module  $\mathcal{M}_{\text{nc}}^{\text{cube}}$  and  $h$  is a sum of commutators.*

Note that the implication: (ii)  $\Rightarrow$  (i) is easy. Klep and Schweighofer [40] (see also [14]) proved that Connes' embedding conjecture is also equivalent to Conjecture 3.11 where we restrict  $f$  to have degree at most 4. The polynomials  $p_M$  involve only monomials of the form  $X_i^2 X_j^2$ . Interestingly, in the proof that Conjecture 3.11 is equivalent to Connes' embedding conjecture, these monomials  $X_i^2 X_j^2$  play a fundamental role (due to a result of Rădulescu [58]).

While Conjecture 3.11 involves trace positive polynomials on the hypercube, membership of a matrix  $M$  in  $\mathcal{CS}_+^{n*}$  requires that the polynomial  $p_M$  is trace positive on *all* symmetric matrices. To make the link between both settings, the key (easy to check) observation is that, since  $p_M$  is a homogeneous polynomial, trace positivity over the hypercube, over the full space and over the ball are all equivalent properties.

**Lemma 3.12.** *A matrix  $M \in \mathcal{S}^n$  belongs to  $\mathcal{CS}_+^{n*}$  if and only if the associated polynomial  $p_M$  is trace positive over the cube  $Q_{\text{nc}}$  or, equivalently, over the ball  $B_{\text{nc}}$ .*

Let us point out that, as observed by Burgdorf [14, Remark 2.8], Connes' conjecture is also equivalent to Conjecture 3.11 where the ball is used instead of the hypercube, i.e., replacing the quadratic module  $\mathcal{M}_{\text{nc}}^{\text{cube}}$  by the quadratic module  $\mathcal{M}_{\text{nc}}^{\text{ball}}$ .

### 3.4 Hierarchies of cones

Consider a matrix  $M \in \mathcal{S}^n$  and assume that the non-commutative polynomial  $p_M$  belongs to the tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}}$  (of the ball), i.e., that it can be written as  $p_M = g + h$ , where  $h$  is a sum of commutators and  $g$  has a decomposition of the form:

$$g = \sum_{j=1}^{m_0} f_j f_j^* + \sum_{j=1}^{m_1} g_j \left(1 - \sum_{i=1}^n X_i^2\right) g_j^* \quad (3.5)$$

with  $f_j, g_j \in \mathbb{R}\langle \underline{X} \rangle$  and  $m_0, m_1 \geq 0$ . Then  $p_M$  is trace positive and thus  $M \in \mathcal{CS}_+^{n*}$ . By imposing degree constraints on the polynomials entering the decomposition (3.5) and considering a small perturbation  $p_M + \epsilon$ , we can define a hierarchy of convex sets  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  aiming to approximate the cone  $\mathcal{CS}_+^{n*}$ . (We omit the dependence on the size  $n$  of the matrices to simplify notation.)

**Definition 3.13.** For  $r \in \mathbb{N}$ , let  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$  denote the truncated tracial quadratic module consisting of all polynomials  $g + h$ , where  $h$  is a sum of commutators and  $g$  has a decomposition (3.5) with all polynomials  $f_j f_j^*$  and  $g_j(1 - \sum_{i=1}^n X_i^2)g_j^*$  having degree at most  $2r + 4$ .

For  $r \in \mathbb{N}$  and  $\epsilon \geq 0$ , let  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  denote the set of matrices  $M \in \mathcal{S}^n$  for which the polynomial  $p_M + \epsilon$  belongs to the truncated tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$ .

**Lemma 3.14.** The set  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is a nice cone, i.e., it is closed, convex, pointed and full-dimensional. Moreover, both  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  and its dual cone  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)*}$  are closed under the operations of taking principal submatrices and of extending matrices by adding zero entries. That is, given matrices

$$M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}, \quad M' = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix},$$

$$M \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)} \implies A, M' \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)} \quad \text{and} \quad M \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)*} \implies A, M' \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)*}.$$

*Proof.* Convexity is easy and that  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is a cone follows the fact that  $p_{\lambda M}(\underline{X}) = p_M(\sqrt[4]{\lambda}\underline{X})$  for any  $\lambda > 0$ . To see that  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is closed, use the fact that the truncated tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$  is closed, which can be shown in the same way as done for the truncated tracial quadratic module of the cube in [40, Prop. 5.1]. Finally,  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is full-dimensional since it contains  $\mathcal{DN}\mathcal{N}^{n*}$  (see Lemma 3.16 below).

Say,  $M \in \mathcal{S}^n$ ,  $A \in \mathcal{S}^m$ ,  $M' \in \mathcal{S}^N$  with  $m \leq n \leq N$  and consider variables  $(X_i)_{i \in [N]}$ . Assume  $M \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)}$ , i.e.,  $p_M(X_1, \dots, X_n) + \epsilon \in \text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$ . By setting  $X_i = 0$  for  $m + 1 \leq i \leq n$ , we obtain that  $A \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)}$ . Moreover, the polynomial  $p_{M'}(X_1, \dots, X_N) + \epsilon = p_M(X_1, \dots, X_n) + \epsilon$  belongs to the truncated module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$  in the variables  $X_1, \dots, X_n$ , and thus also to the truncated module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}, r}$  in the variables  $X_1, \dots, X_N$ . Here we use the identity:  $g(1 - \sum_{i=1}^n X_i^2)g^* = g(1 - \sum_{i=1}^N X_i^2)g^* + \sum_{i=n+1}^N gX_i^2g^*$  for any  $g \in \mathbb{R}\langle \underline{X} \rangle$ . Hence  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  is closed under taking principal submatrices and extending matrices by zero entries, and thus the same holds for its dual.  $\square$

We have the chain of inclusions:

$$\mathcal{DN}\mathcal{N}^* \subseteq \mathcal{K}_{\text{nc}, \epsilon}^{(0)} \subseteq \dots \subseteq \mathcal{K}_{\text{nc}, \epsilon}^{(r)} \subseteq \mathcal{K}_{\text{nc}, \epsilon}^{(r+1)} \quad (3.6)$$

for any  $\epsilon \geq 0$  (see Lemma 3.16 below). Furthermore,  $\bigcap_{\epsilon > 0} \bigcup_{r \geq 0} \mathcal{K}_{\text{nc}, \epsilon}^{(r)} \subseteq \mathcal{CS}_+^{n*}$ , with equality if Connes' embedding conjecture holds.

We now point out a connection between the hierarchy  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  and the hierarchy  $\mathcal{K}^{(r)}$  introduced by Parrilo [55] as inner approximations of the copositive cone

$\mathcal{COP}^n = \mathcal{CP}^{n*}$ . Let  $\Sigma$  denote the set of (commutative) sum of squares of polynomials and  $\Sigma_k = \Sigma \cap \mathbb{R}[\underline{x}]_k$ . Clearly all polynomials in  $\Sigma$  are nonnegative. Exploiting this idea, Parrilo [55] introduced, for any integer  $r \geq 0$ , the following cones:

$$\mathcal{K}^{(r)} = \left\{ M \in \mathcal{S}^n : p_M \left( \sum_{i=1}^n x_i^2 \right)^r \in \Sigma \right\}, \quad (3.7)$$

that satisfy the following inclusions:

$$\mathcal{K}^{(0)} \subseteq \dots \subseteq \mathcal{K}^{(r)} \subseteq \mathcal{K}^{(r+1)} \subseteq \dots \subseteq \mathcal{COP}^n. \quad (3.8)$$

Parrilo [55] showed that  $\mathcal{K}^{(0)} = \mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n \times n}) = \mathcal{DN}\mathcal{N}^{n*}$  and the exact description of  $\mathcal{K}^{(1)}$  can be found in [42].

The link to the non-commutative setting becomes more transparent if we observe that the cone  $\mathcal{K}^{(r)}$  can be alternatively reformulated as

$$\mathcal{K}^{(r)} = \left\{ M \in \mathcal{S}^n : p_M \in \Sigma_{2r+4} + \left( 1 - \sum_{i=1}^n x_i^2 \right) \mathbb{R}[\underline{x}] \right\}, \quad (3.9)$$

which follows by using the following result.

**Proposition 3.15.** [41] *Let  $f \in \mathbb{R}[\underline{x}]$  be a homogeneous polynomial of even degree  $2d$  and let  $r \geq 0$  be an integer. Then, the polynomial  $f(x) \left( \sum_{i=1}^n x_i^2 \right)^r$  is a sum of squares of polynomials if and only if  $f \in \Sigma_{2r+2d} + \left( 1 - \sum_{i=1}^n x_i^2 \right) \mathbb{R}[\underline{x}]$ .*

It turns out that the hierarchy  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$  is interesting only when selecting  $\epsilon > 0$ , since it collapses when  $\epsilon = 0$ .

**Lemma 3.16.** *For any  $r \in \mathbb{N}$  and  $\epsilon \geq 0$ , we have:  $\mathcal{DN}\mathcal{N}^{n*} = \mathcal{K}^{(0)} = \mathcal{K}_{\text{nc},0}^{(r)} \subseteq \mathcal{K}_{\text{nc},\epsilon}^{(r)}$ .*

*Proof.* We first show the inclusion  $\mathcal{K}_{\text{nc},0}^{(r)} \subseteq \mathcal{K}^{(0)}$ . For this, assume  $M \in \mathcal{K}_{\text{nc},0}^{(r)}$ , i.e.,  $p_M = g + h$  where  $g \in \mathcal{M}_{\text{nc}}^{\text{ball}}$  and  $h$  is a sum of commutators. If we now evaluate  $p_M$  at commutative variables  $x$ , we see that  $h(x)$  vanishes and thus we obtain  $p_M(x) = g(x) \in \Sigma + \left( 1 - \sum_{i=1}^n x_i^2 \right) \Sigma$ . As  $p_M$  is homogeneous of degree 4 it follows, using [41, Prop. 4], that  $p_M \in \Sigma$  and thus  $M \in \mathcal{K}^{(0)}$ .

For the reverse inclusion, as  $\mathcal{K}^{(0)} = \mathcal{DN}\mathcal{N}^{n*} = \mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n \times n})$ , it suffices to show that if  $M \succeq 0$  or  $M \geq 0$  then  $M \in \mathcal{K}_{\text{nc},0}^{(0)}$ , i.e.,  $p_M$  is a sum of commutators and Hermitian squares of degree 4. Assume that  $M \succeq 0$  and let  $u_1, \dots, u_n \in \mathbb{R}^d$  be vectors forming a Gram representation of  $M$ . Then,  $p_M(\underline{X}) = \sum_{i,j=1}^n \sum_{h=1}^d u_i(h) u_j(h) X_i^2 X_j^2 = \sum_{h=1}^d \left( \sum_{i=1}^n u_i(h) X_i^2 \right)^2$  is a sum of Hermitian squares of degree 4. If  $M \geq 0$ , then each  $M_{ij} X_i^2 X_j^2 = [X_i^2 X_j, X_j] + X_j X_i^2 X_j$  is sum of a commutator and a Hermitian square of degree 4 and therefore  $p_M(\underline{X}) = \sum_{i,j} M_{ij} X_i^2 X_j^2 \in \text{tr} \mathcal{M}_{\text{nc}}^{\text{ball},0}$ , so that  $M \in \mathcal{K}_{\text{nc},0}^{(0)}$ .

The inclusion  $\mathcal{K}_{\text{nc},0}^{(r)} \subseteq \mathcal{K}_{\text{nc},\epsilon}^{(r)}$  clearly holds.  $\square$

We conclude with some remarks concerning the convergence of the hierarchies (3.8) and (3.6) to the cones  $\mathcal{COP}^n$  and  $\mathcal{CS}_+^{n*}$ . Parrilo [55] shows that the hierarchy  $\mathcal{K}^{(r)}$  covers the interior of the copositive cone  $\mathcal{COP}^n$ . That is,

$$\text{int}(\mathcal{COP}^n) \subseteq \bigcup_{r \geq 0} \mathcal{K}^{(r)} \subseteq \mathcal{COP}^n. \quad (3.10)$$

Parrilo [55] shows this by using the definition (3.7) and a result of Pólya (Theorem 3.17 below). Alternatively this can be shown by using the definition (3.9) and a result of Schmüdgen (Theorem 3.18 below).

**Theorem 3.17.** [57] *Let  $f \in \mathbb{R}[\underline{x}]$  be a homogeneous polynomial. Assume that  $f(x) > 0$  for all nonzero  $x \in \mathbb{R}_+^n$ . Then there exists  $r \in \mathbb{N}$  such that the polynomial  $(\sum_{i=1}^n x_i)^r f(x)$  has nonnegative coefficients.*

**Theorem 3.18.** [62] *If  $f \in \mathbb{R}[\underline{x}]$  is positive on the sphere, i.e.,  $f(x) > 0$  for all  $x \in \mathbb{R}^n$  with  $\sum_{i=1}^n x_i^2 = 1$ , then  $f \in \Sigma + (1 - \sum_{i=1}^n x_i^2)\mathbb{R}[\underline{x}]$ .*

In the non-commutative case, membership of a matrix  $M$  in  $\bigcup_{r \geq 0} \mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  means that the polynomial  $p_M + \epsilon$  belongs to the tracial quadratic module  $\text{tr}\mathcal{M}_{\text{nc}}^{\text{ball}}$ , but there is no clear link between this and membership in the interior of the cone  $\mathcal{CS}_+^{n*}$ .

To explain this difference of behavior between the two hierarchies of cones let us point out that, in the commutative (scalar) case, working with the ball is in some sense equivalent to working with the sphere. Indeed, as  $p_M$  is homogeneous, it is nonnegative over  $\mathbb{R}^n$  if and only if it is nonnegative over the ball or, equivalently, over the sphere, because one can *rescale* any non-zero  $x \in \mathbb{R}^n$  so that  $\sum_{i=1}^n x_i^2 = 1$ . However, when working with matrices  $X_1, \dots, X_n$ , one can rescale them to ensure that  $I - \sum_{i=1}^n X_i^2 \succeq 0$  but not ensure equality:  $\sum_{i=1}^n X_i^2 = I$ . Hence, in the non-commutative case one cannot equivalently switch between the ball and the sphere.

In the next section we use the hierarchy  $\mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  to define approximations for the parameters  $\vartheta^{\mathcal{CS}_+}(G)$  and  $\Theta^{\mathcal{CS}_+}(G)$  and we use it again later in Section 4.4 to approximate the quantum stability and chromatic parameters.

### 3.5 Semidefinite approximations for $\vartheta^{\mathcal{CS}_+}(G)$ and $\Theta^{\mathcal{CS}_+}(G)$

We start with a simple but useful result that we will need below.

**Lemma 3.19.** *Consider two matrices  $M, Z \in \mathcal{S}^n$  and  $\epsilon > 0$ . Assume that  $p_M + \epsilon$  is trace positive and that the following condition holds:*

$$\text{For any } d \in \mathbb{N} \text{ and } \underline{X} = (X_1, \dots, X_n) \in (\mathcal{S}^d)^n, \quad \text{Tr}(p_Z(\underline{X})) = 0 \implies \underline{X} = 0. \quad (3.11)$$

*Then,  $p_{M+\epsilon Z}$  is trace positive. Condition (3.11) holds e.g. for  $Z = I$  and  $Z = J$ .*

*Proof.* Let  $\underline{X} = (X_1, \dots, X_n) \in (\mathcal{S}^d)^n$ , not all zero. We define the new matrices  $X'_i = \lambda X_i$  for  $i \in [n]$ , where we select  $\lambda > 0$  such that  $\text{Tr}(p_Z(\underline{X}') - I) = 0$ , i.e.,  $\lambda = \sqrt[4]{d / \text{Tr}(p_Z(\underline{X}))}$  (which is well defined since  $Z$  satisfies (3.11)).

By assumption, we know that  $\text{Tr}(p_M(\underline{X}') + \epsilon I) \geq 0$ . Therefore, we obtain that  $\text{Tr}(p_{M+\epsilon Z}(\underline{X}')) = \text{Tr}(p_M(\underline{X}') + \epsilon I) + \epsilon \text{Tr}(p_Z(\underline{X}') - I) = \text{Tr}(p_M(\underline{X}') + \epsilon I) \geq 0$ . As the polynomial  $p_{M+\epsilon Z}$  is homogeneous of degree 4, it follows that  $\text{Tr}(p_{M+\epsilon Z}(\underline{X})) = \text{Tr}(p_{M+\epsilon Z}(\underline{X}')) / \lambda^4 \geq 0$ . This shows that  $p_{M+\epsilon Z}$  is trace positive.

For  $Z = I$ , we have  $\text{Tr}(p_Z(\underline{X})) = \sum_{i=1}^n \text{Tr}(X_i^4)$  and, for  $Z = J$ ,  $\text{Tr}(p_Z(\underline{X})) = \text{Tr}((\sum_{i=1}^n X_i^2)^2)$ . In both cases  $\text{Tr}(p_Z(\underline{X})) = 0$  implies  $X_1 = \dots = X_n = 0$ .  $\square$

Let us first consider the parameter  $\vartheta^{\mathcal{CS}_+}(G)$ . As shown in Lemma 2.4 we have equality  $\vartheta^{\mathcal{CS}_+}(G) = \vartheta^{\text{cl}(\mathcal{CS}_+)}(G)$ . As the conic program defining  $\vartheta^{\text{cl}(\mathcal{CS}_+)}(G)$  admits a strictly feasible matrix (e.g.,  $I/n$ ), we can conclude that strong duality holds:

$$\vartheta^{\mathcal{CS}_+}(G) = \min t \text{ s.t. } M \in \mathcal{CS}_+^*, M_{uu} = t-1 \forall u \in V(G), M_{uv} = -1 \forall \{uv\} \in E(\overline{G}). \quad (3.12)$$

We now define new parameters that we obtain by replacing the cone  $\mathcal{CS}_+^*$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$  in (3.12) and investigate their link to the parameter  $\vartheta^{\mathcal{CS}_+}(G)$ :

$$\varphi_\epsilon^{(r)}(G) = \min t \text{ s.t. } M \in \mathcal{K}_{\text{nc},\epsilon}^{(r)}, M_{uu} = t-1 \forall u \in V(G), M_{uv} = -1 \forall \{uv\} \in E(\overline{G}). \quad (3.13)$$

**Lemma 3.20.** *For any  $\epsilon > 0$  and  $r \in \mathbb{N}$ , we have  $\varphi_\epsilon^{(r)}(G) \leq \varphi_0^{(r)}(G) = \vartheta'(G)$ .*

*Proof.* We use the dual formulation of  $\vartheta'(G)$  from (2.5). Namely,  $\vartheta'(G)$  is the minimum scalar  $t$  for which there exists  $M \in \mathcal{S}_+^n$  such that  $M_{uu} = t-1$  for  $u \in V(G)$  and  $M_{uv} \leq -1$  for  $uv \in E(\overline{G})$ . By adding nonnegative scalars to the entries indexed by nonedges we get a matrix  $M' \in \mathcal{DN}\mathcal{N}^{n*} = \mathcal{K}_{\text{nc},0}^{(r)}$  such that  $M'_{uu} = t-1$  for  $u \in V(G)$  and  $M'_{uv} = -1$  for  $uv \in E(\overline{G})$ . This shows that  $t = \vartheta'(G) \geq \varphi_0^{(r)}(G)$ . The reverse inequality is clear and the inequality  $\varphi_\epsilon^{(r)}(G) \leq \varphi_0^{(r)}(G)$  follows from Lemma 3.16.  $\square$

**Proposition 3.21.** *For any  $1 > \epsilon > 0$  and  $r \in \mathbb{N}$  we have*

$$\vartheta^{\mathcal{CS}_+}(G) \leq \frac{1}{1-\epsilon} \varphi_\epsilon^{(r)}(G).$$

*Proof.* Let  $t, M$  be optimum for the definition of  $\varphi_\epsilon^{(r)}(G)$ , i.e.,  $p_M + \epsilon$  lies in the tracial quadratic module of order  $r$ ,  $M_{uu} = t-1$  for  $u \in V(G)$ , and  $M_{uv} = -1$  for  $uv \in E(\overline{G})$ . Define the new matrix  $M' = \frac{M+\epsilon J}{1-\epsilon}$ . As  $p_M + \epsilon$  is trace positive, Lemma 3.19 implies that  $p_{M+\epsilon J}$  is trace positive and thus  $p_{M'}$  as well, i.e.,  $M' \in \mathcal{CS}_+^{n*}$ . Moreover,  $M'_{uu} = \frac{t-1+\epsilon}{1-\epsilon} = \frac{t}{1-\epsilon} - 1$  for  $u \in V(G)$  and  $M'_{uv} = \frac{-1+\epsilon}{1-\epsilon} = -1$  for  $uv \in E(\overline{G})$ . Thus the pair  $(t' = \frac{t}{1-\epsilon}, M')$  is feasible for the definition of  $\vartheta^{\mathcal{CS}_+}(G)$ , which shows  $\vartheta^{\mathcal{CS}_+}(G) \leq \frac{t}{1-\epsilon} = \frac{1}{1-\epsilon} \varphi_\epsilon^{(r)}(G)$ .  $\square$

**Lemma 3.22.** *Assume that Connes' embedding conjecture holds. Then,*

$$\text{for any } \epsilon > 0 \text{ there exists } r \in \mathbb{N} \text{ such that } \varphi_\epsilon^{(r)}(G) \leq \vartheta^{\mathcal{CS}_+}(G).$$

*Proof.* Directly since  $\mathcal{CS}_+ \subseteq \cup_{r \geq 0} \mathcal{K}_{\text{nc},\epsilon}^{(r)}$  if Connes' conjecture holds.  $\square$

By combining the above two results, we see that, under Connes' conjecture, the parameters  $\varphi_\epsilon^{(r)}(G)$  tend to  $\vartheta_+^{\mathcal{CS}}(G)$ . More precisely, consider a sequence  $(\epsilon_l)_{l \geq 1}$  tending to 0 as  $l$  tends to  $\infty$  and integers  $r_l \in \mathbb{N}$  such that  $\varphi_{\epsilon_l}^{(r_l)}(G) \leq \vartheta_+^{\mathcal{CS}}(G)$  for all  $l$  (which exist by Lemma 3.22). Then, in view of Proposition 3.21, we can conclude that any accumulation point of the sequence  $(\varphi_{\epsilon_l}^{(r_l)}(G))_{l \geq 1}$  is equal to  $\vartheta^{\mathcal{CS}_+}(G)$ . Moreover, there is at least one accumulation point since all parameters  $\varphi_{\epsilon_l}^{(r_l)}(G)$  lie in a bounded interval.

We now extend the above results to the parameter  $\Theta^{\mathcal{CS}^+}(G)$ . We begin with recalling the primal and the dual programs defining this parameter:

$$\Theta^{\mathcal{CS}^+}(G) = \min t \quad \text{s.t.} \quad \begin{aligned} Z &\in \mathcal{CS}_+^n, \quad Z - J \succeq 0, \quad Z_{uu} = t \quad \forall u \in V(G), \\ Z_{uv} &= 0 \quad \forall \{u, v\} \in E(G), \end{aligned} \quad (3.14)$$

$$\Theta^{\mathcal{CS}^+}(G) = \max \langle J, Y - M \rangle \quad \text{s.t.} \quad \begin{aligned} M &\in \mathcal{CS}_+^{n*}, \quad Y - M \succeq 0, \quad \text{Tr}(Y) = 1, \\ Y_{uv} &= 0 \quad \forall \{u, v\} \in E(\overline{G}). \end{aligned} \quad (3.15)$$

Indeed there is no duality gap since the matrix  $X = (n+1)I$  is strictly feasible for the primal program (3.14). Analogously, we define the parameters  $\Phi_\epsilon^{(r)}(G)$  obtained by replacing the condition  $M \in \mathcal{CS}_+^*$  by  $M \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)}$  in the definition (3.15). For  $\epsilon = 0$ ,  $\mathcal{K}_{\text{nc}, 0}^{(r)} = \mathcal{DN}\mathcal{N}^*$  and thus  $\Phi_0^{(r)}(G) = \vartheta^+(\overline{G}) \leq \Phi_\epsilon^{(r)}(G)$  for any  $\epsilon > 0$  and  $r \in \mathbb{N}$ .

**Proposition 3.23.** *For any  $1 > \epsilon > 0$ ,  $r \in \mathbb{N}$  and graph  $G$  on  $n$  nodes, we have*

$$\Theta^{\mathcal{CS}^+}(G) \geq \frac{1}{1 + \epsilon n} \Phi_\epsilon^{(r)}(G).$$

*Proof.* Let  $(Y, M)$  be an optimal solution for the program defining  $\Phi_\epsilon^{(r)}(G)$ , i.e.,  $M \in \mathcal{K}_{\text{nc}, \epsilon}^{(r)}$ ,  $Y - M \succeq 0$ ,  $Y_{uv} = 0$  if  $\{u, v\} \in E(\overline{G})$ , and  $\text{Tr}(Y) = 1$ . We consider the following matrices  $M' = \frac{M + \epsilon I}{1 + \epsilon n}$  and  $Y' = \frac{Y + \epsilon I}{1 + \epsilon n}$ . Then,  $Y' - M' \succeq 0$ ,  $Y'_{uv} = 0$  if  $\{u, v\} \in E(\overline{G})$ , and  $\text{Tr}(Y') = 1$ . Moreover, as  $p_M + \epsilon$  is trace positive we deduce from Lemma 3.19 that  $p_{M + \epsilon I}$  is trace positive and thus  $M' \in \mathcal{CS}_+^{n*}$ . Hence, the pair  $(Y', M')$  is feasible for the program (3.15) and thus  $\Theta^{\mathcal{CS}^+}(G) \geq \langle J, Y' - M' \rangle = \frac{\langle J, Y - M \rangle}{1 + \epsilon n} = \frac{1}{1 + \epsilon n} \Phi_\epsilon^{(r)}(G)$ .  $\square$

The analogue of Lemma 3.22 holds: If Connes' embedding conjecture holds then for any  $\epsilon > 0$  there exists  $r \in \mathbb{N}$  such that  $\Theta^{\mathcal{CS}^+}(G) \leq \Phi_\epsilon^{(r)}(G)$ . Therefore, as for the parameter  $\vartheta^{\mathcal{CS}^+}(G)$ , the parameter  $\Theta^{\mathcal{CS}^+}(G)$  can be obtained as the limit of sequences of parameters  $\Phi_\epsilon^{(r)}(G)$ .

It is not clear what is the complexity of computing the parameters  $\vartheta^{\mathcal{CS}^+}(G)$  and  $\Theta^{\mathcal{CS}^+}(G)$  (although we expect these parameters to be hard to compute). On the other hand, the bounds  $\varphi_\epsilon^{(r)}(G)$  and  $\Phi_\epsilon^{(r)}(G)$  can be computed using semidefinite programming in polynomial time to any precision, for any fixed  $r$ . This is based on the fact that testing whether a polynomial can be written as sum of Hermitian squares can be done with semidefinite programming (see [14]) and it is also easy to test whether a polynomial is a sum of commutators (see [40, Remark 1.3]).

## 4 Conic programs for quantum graph parameters

In this section we show how to reformulate the quantum graph parameters as a sequence of conic feasibility optimization programs over the cone  $\mathcal{CS}_+$  of completely positive semidefinite matrices (Propositions 4.1 and 4.8) and as single optimization programs over  $\mathcal{CS}_+$  (Lemmas 4.13 and 4.14). Then we investigate these programs when replacing the cone  $\mathcal{CS}_+$  by its subcone  $\mathcal{CP}$  or by its supercone  $\mathcal{DN}\mathcal{N}$  and show that we respectively find the classical graph parameters and their corresponding bounds in terms of the theta number (Corollaries 4.5 and 4.10). In Section 4.4,

we define and study semidefinite based approximations for the quantum graph parameters that we obtain by replacing the cone  $\mathcal{CS}_+^*$  by the approximate cones  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$  in their definitions.

#### 4.1 Conic reformulation for quantum stability numbers

We begin with providing an equivalent reformulation for the two quantum stability numbers  $\alpha_q(G)$  and  $\alpha^*(G)$  as conic feasibility programs over the completely positive semidefinite cone  $\mathcal{CS}_+$ .

**Proposition 4.1.** *For a graph  $G$ , the parameter  $\alpha_q(G)$  is equal to the maximum integer  $t$  for which there exists a matrix  $X \in \mathcal{CS}_+^{|V(G)|t+1}$  satisfying the following conditions:*

$$X_{0,0} = 1, \tag{C1}$$

$$\sum_{u \in V(G)} X_{0,ui} = 1 \quad \forall i \in [t], \tag{C2a}$$

$$\sum_{u \in V(G)} X_{ui,ui} = 1 \quad \forall i \in [t], \tag{C2b}$$

$$X_{ui,vj} = 0 \quad \forall i \neq j \in [t], \forall u \simeq v \in V(G), \tag{O1}$$

$$X_{ui,vi} = 0 \quad \forall i \in [t], \forall u \neq v \in V(G). \tag{O2}$$

Moreover, the parameter  $\alpha^*(G)$  is equal to the maximum integer  $t$  for which there exists a matrix  $X \in \mathcal{CS}_+^{|V(G)|t+1}$  satisfying (C1), (C2a), (O1) and the condition

$$\sum_{u,v \in V(G)} X_{ui,vi} = 1 \quad \forall i \in [t]. \tag{C2c}$$

*Proof.* Observe that, if  $X$  satisfies (O2), then both conditions (C2b) and (C2c) are equivalent. We first consider the parameter  $\alpha_q(G)$ .

By Definition 2.5, there exist positive semidefinite matrices  $\rho, \rho_i^u$  (for  $u \in V(G)$ ,  $i \in [t]$ ) satisfying (2.10)-(2.13). Let  $X$  denote the Gram matrix of  $\rho, \rho_i^u$ , i.e.,  $X_{0,0} = \langle \rho, \rho \rangle$ ,  $X_{0,ui} = \langle \rho, \rho_i^u \rangle$  and  $X_{ui,vj} = \langle \rho_i^u, \rho_j^v \rangle$  for all  $u, v \in V(G)$ ,  $i, j \in [t]$ . By construction,  $X$  belongs to the cone  $\mathcal{CS}_+^{|V(G)|t+1}$ . Moreover,  $X$  satisfies the conditions (C1), (O1) and (O2) which correspond, respectively, to (2.10), (2.12) and (2.13). Next, using (2.10), (2.11) and (2.13), we obtain that for any  $i \in [t]$ :

$$1 = \langle \rho, \rho \rangle = \langle \rho, \sum_u \rho_i^u \rangle = \langle \sum_u \rho_i^u, \sum_v \rho_i^v \rangle = \sum_u \langle \rho_i^u, \rho_i^u \rangle$$

which shows that  $X$  also satisfies (C2a) and (C2b).

Conversely, assume that  $X \in \mathcal{CS}_+^{|V(G)|t+1}$  satisfies the conditions (C1), (C2a), (C2b), (O1), (O2) (and thus (C2c)). As  $X$  is completely positive semidefinite, there exist positive semidefinite matrices  $\rho, \rho_i^u$  forming a Gram representation of  $X$ ; we show that the matrices  $\rho, \rho_i^u$  satisfy the conditions of Definition 2.5. It is clear that (2.10), (2.12) and (2.13) hold. Next, for any  $i \in [t]$ , we have:

$$\left\| \rho - \sum_{u \in V(G)} \rho_i^u \right\|^2 = 1 - 2 \sum_{u \in V(G)} X_{0,ui} + \sum_{u,v \in V(G)} X_{ui,vi} = 0,$$



using (C2a) and (C2c). This shows (2.11) and thus concludes the proof for  $\alpha_q(G)$ .

The proof is analogous for the parameter  $\alpha^*(G)$  and thus omitted.  $\square$

Next we observe that, in Proposition 4.1, we can restrict without loss of generality to solutions that are invariant under action of the permutation group  $\text{Sym}(t)$  (consisting of all permutations of  $[t] = \{1, \dots, t\}$ ).

We sketch this well known symmetry reduction, which has been used in particular for the study of the chromatic number in [35, 36]. Given  $Y \in \mathcal{S}^{|V|t+1}$  and a permutation  $\pi \in \text{Sym}(t)$ , set  $\pi(Y)_{00} = Y_{00}$ ,  $\pi(Y)_{0,ui} = Y_{0,u\pi(i)}$  and  $\pi(Y) = (Y_{u\pi(i),v\pi(j)})_{i,j \in [t], u,v \in V}$  and define the new matrix  $Y' = \frac{1}{|\text{Sym}(t)|} \sum_{\pi \in \text{Sym}(t)} \pi(Y)$ , called the *symmetrization* of  $Y$  under action of  $\text{Sym}(t)$ . Then,  $Y'$  is invariant under action of  $\text{Sym}(t)$ , i.e.,  $\pi(Y') = Y'$  for all  $\pi \in \text{Sym}(t)$ , and thus  $Y'$  has the following block-form:

$$\begin{pmatrix} \alpha & a^T & \dots & a^T \\ a & A & \dots & B \\ \vdots & \vdots & \ddots & \vdots \\ a & B & \dots & A \end{pmatrix} \quad \text{for some } \alpha \in \mathbb{R}, a \in \mathbb{R}^{|V|}, A, B \in \mathcal{S}^{|V|}. \quad (4.1)$$

Notice that the programs described in Proposition 4.1 are invariant under action of  $\text{Sym}(t)$ ; that is, if  $Y$  is feasible for one of them then any permutation  $\pi(Y)$  is feasible as well. If we choose  $Y$  to be an optimal solution of a program (assuming some exists), we can conclude that its symmetrization  $Y'$  is again an optimal solution. Therefore both programs have an optimal solution in block-form (4.1).

This invariance property, which holds not only for the cone  $\mathcal{CS}_+$  but also for the cones  $\mathcal{S}_+$ ,  $\mathcal{CP}$  and  $\mathcal{DN}$ , will be useful, together with the following lemma, for proving Proposition 4.4 below.

**Lemma 4.2.** (see e.g. [35]) *Let  $Y$  be a  $t \times t$  block-matrix, of the form:*

$$Y = \underbrace{\begin{pmatrix} A & B & \dots & B \\ B & A & \dots & B \\ \vdots & \vdots & \ddots & \vdots \\ B & B & \dots & A \end{pmatrix}}_{t \text{ blocks}}, \quad (4.2)$$

having  $A$  as diagonal blocks and  $B$  as off-diagonal blocks, where  $A, B \in \mathcal{S}^k$  (for some  $k \geq 1$ ). Then,

$$Y \succeq 0 \iff A - B \succeq 0 \text{ and } A + (t-1)B \succeq 0.$$

Next we consider again the programs introduced in Proposition 4.1 for defining the parameters  $\alpha_q(G)$  and  $\alpha^*(G)$ , and we investigate what is their optimum value when replacing the cone  $\mathcal{CS}_+$  by any of the two cones  $\mathcal{CP}$  or  $\mathcal{DN}$ . We show that when using  $\mathcal{CP}$  we find the classical stability number  $\alpha(G)$  while, when using the cone  $\mathcal{DN}$ , we find the parameter  $\lfloor \vartheta'(G) \rfloor$ .

In the proof we will use the following property of completely positive matrices, with  $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$  as the  $2 \times 2$  nonzero principal submatrix of  $B$ .

**Theorem 4.3.** [5] Let  $A, B \in \mathcal{S}^n$ . Suppose that  $A$  is completely positive,  $B$  is positive semidefinite with all entries equal to zero except for a  $2 \times 2$  principal submatrix and that  $A + B$  is a nonnegative matrix. Then  $A + B$  is completely positive.

**Proposition 4.4.** Let  $G$  be a graph and let  $\mathcal{K}$  denote the cone  $\mathcal{DN}\mathcal{N}$  or  $\mathcal{CP}$ . The following statements are equivalent.

- (i) There exists a matrix  $X \in \mathcal{K}^{|V(G)|}$  satisfying  $[\langle J, X \rangle] = t$ ,  $\text{Tr}(X) = 1$  and  $X_{uv} = 0$  for all  $\{u, v\} \in E(G)$ .
- (ii) There exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C2a), (C2b), (O1) and (O2).
- (iii) There exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C2a), (C2c), and (O1).

*Proof.* Assume first  $\mathcal{K} = \mathcal{DN}\mathcal{N}$ . For convenience, we introduce the graph  $G_t$ , which models the orthogonality conditions (O1) and (O2), i.e., its vertex set is  $V(G) \times [t]$  and two distinct nodes  $(u, i)$  and  $(v, j)$  are adjacent in  $G_t$  if  $i \neq j$  and  $u \simeq v$ , or if  $i = j$  and  $u \neq v$ . Moreover, let  $|V(G)| = n$ . We introduce an intermediary step:  $\vartheta'(G_t) \geq t$  and show the implications: (i)  $\Rightarrow [\vartheta'(G_t) \geq t] \Rightarrow (iii) \Rightarrow (ii) \Rightarrow (i)$ .

(i)  $\Rightarrow [\vartheta'(G_t) \geq t]$ : As  $G_t$  is a subgraph of  $G_n$  and the parameter  $\vartheta'$  is monotone nondecreasing under taking subgraphs, we have  $\vartheta'(G_t) \geq \vartheta'(G_n)$  and thus it suffices to show that  $\vartheta'(G_n) \geq t$ . For this, consider a matrix  $X$  satisfying (i). Say, the nodes of  $G$  are ordered as  $u_1, \dots, u_n$ . As  $X \in \mathcal{DN}\mathcal{N}$ ,  $X \geq 0$  and  $X$  is the Gram matrix of some vectors  $x_{u_1}, \dots, x_{u_n}$ . Then,  $t = \lfloor \|\sum_{i=1}^n x_{u_i}\|^2 \rfloor$ ,  $\sum_{i=1}^n \|x_{u_i}\|^2 = 1$ , and  $x_{u_i}^T x_{u_{i'}} = 0$  if  $\{u_i, u_{i'}\} \in E(G)$ .

With  $e_1, \dots, e_n$  denoting the standard unit vectors in  $\mathbb{R}^n$ , we define the new vectors  $y_{u_i}^j = x_{u_i} \otimes e_{i+j}$  for  $i, j \in [n]$ , where we take indices modulo  $n$  in  $e_{i+j}$ . Let  $Y$  denote the Gram matrix of the vectors  $y_{u_i}^j$ , i.e.,  $Y_{u_i j, u_{i'} j'} = \langle y_{u_i}^j, y_{u_{i'}}^{j'} \rangle$  for all  $i, i', j, j' \in [n]$ ; we show that  $Y/n$  is feasible for the maximization program in (2.5) which defines  $\vartheta'(G_n)$ . Indeed,  $Y \in \mathcal{DN}\mathcal{N}$  and  $Y$  satisfies the required orthogonality relations since  $\langle y_{u_i}^j, y_{u_{i'}}^{j'} \rangle = \langle x_{u_i}, x_{u_{i'}} \rangle \langle e_{i+j}, e_{i'+j'} \rangle = 0$  if  $\{u_i, u_{i'}\} \in E(G)$  or if  $i + j \neq i' + j'$  modulo  $n$ . We have:  $\text{Tr}(Y) = \sum_{i,j=1}^n \|y_{u_i}^j\|^2 = \sum_{i,j=1}^n \|x_{u_i}\|^2 = n \text{Tr}(X) = n$ . Moreover,  $\sum_{i,j=1}^n y_{u_i}^j = \sum_{i,j=1}^n x_{u_i} \otimes e_{i+j} = (\sum_{i=1}^n x_{u_i}) \otimes e$ , where  $e$  is the all-ones vector, so that  $\langle J, Y \rangle = \|(\sum_{i=1}^n x_{u_i}) \otimes e\|^2 = \|\sum_{i=1}^n x_{u_i}\|^2 \|e\|^2 = \langle J, X \rangle n$ . This implies that  $\vartheta'(G_n) \geq \langle J, Y/n \rangle = \langle J, X \rangle \geq t$ . Hence we have shown that  $\vartheta'(G_t) \geq t$ .

$[\vartheta'(G_t) \geq t] \Rightarrow (iii)$ : By assumption,  $\vartheta'(G_t) \geq t$ . Hence (after scaling by  $t$  a psd matrix solution for the maximization program in (2.5) for  $\vartheta'(G_t)$ ), there exists a matrix  $Y \in \mathcal{DN}\mathcal{N}^{|V(G)|t}$  satisfying  $\langle J, Y \rangle = t^2$ ,  $\text{Tr}(Y) = t$ , and  $Y_{(u,i),(v,j)} = 0$  for all edges  $\{(u, i), (v, j)\}$  of  $G_t$ . Moreover, (after symmetrization by  $\text{Sym}(t)$ ) we can assume that  $Y$  has the block-form (4.2), where  $A$  is a diagonal matrix and  $B_{uv} = 0$  for all edges  $\{u, v\}$  of  $G$ . Then,  $t = \text{Tr}(Y) = t \text{Tr}(A) = t \langle J, A \rangle$  and  $t^2 = \langle J, Y \rangle = t \langle J, A \rangle + t(t-1) \langle J, B \rangle$ , implying  $\text{Tr}(A) = \langle J, A \rangle = \langle J, B \rangle = 1$ .

Let  $\{y_u^i : u \in V(G), i \in [t]\}$  be a Gram factorization of  $Y$ , i.e.,  $Y_{ui,vj} = \langle y_u^i, y_v^j \rangle$  for all  $i, j \in [t]$  and  $u, v \in V(G)$ . Fix  $i_0 \in [t]$  and define the vector  $y = \sum_{u \in V(G)} y_u^{i_0}$ . Then,  $\langle y, y \rangle = \sum_{v \in V(G)} \langle y, y_v^{i_0} \rangle = \langle J, A \rangle = \text{Tr}(A) = 1$  and for any  $j \in [t] \setminus \{i_0\}$   $\sum_{v \in V(G)} \langle y, y_v^j \rangle = \sum_{u,v \in V(G)} \langle y_u^{i_0}, y_v^j \rangle = \langle J, B \rangle = 1$ . Define  $Y'$  to be the Gram matrix of the vectors  $\{y, y_u^i : u \in V(G), i \in [t]\}$ . From the properties just explained, we see that  $Y' \in \mathcal{DN}\mathcal{N}$  is a feasible matrix for (iii).

(iii)  $\Rightarrow$  (ii): Assume that  $Y'$  satisfies (iii); we construct a new matrix  $Y$  satisfying (ii). Without loss of generality,  $Y'$  has the block-form (4.1). If  $A_{uv} = 0$  for all  $u \neq v$ , then  $Y'$  satisfies (O2) and we are done. Assume now that  $A_{uv} > 0$  for some  $u \neq v$ . For any  $u \neq v \in V(G)$ , let  $F^{uv}$  be the matrix indexed by  $V(G)$  with  $F_{uu}^{uv} = F_{vv}^{uv} = 1$ ,  $F_{uv}^{uv} = F_{vu}^{uv} = -1$ , and all other entries are equal to 0. Moreover, let  $\tilde{F}^{uv}$  be the square matrix of size  $(|V(G)|t + 1)$  with the block-form (4.1), where the first row/column is zero and all blocks are zero except the diagonal blocks which are equal to  $F^{uv}$ . Finally, define  $F = \sum_{u,v \in V(G), u \neq v} A_{uv} \tilde{F}^{uv}$  and  $Y = Y' + F$ . We claim that the new matrix  $Y$  satisfies (ii). As both  $F^{uv}$  and  $\tilde{F}^{uv}$  are positive semidefinite,  $Y$  is positive semidefinite. Moreover, by construction,  $Y \geq 0$  and  $Y$  satisfies (C1), (C2a), (O1) and (O2). Furthermore,  $Y$  also satisfies (C2c) (and therefore (C2b)) since  $\langle J, \tilde{F}^{uv} \rangle = 0$  for all  $u \neq v$ . Hence,  $Y$  satisfies (ii).

(ii)  $\Rightarrow$  (i): Let  $Y$  be a matrix satisfying (ii). As  $Y \succeq 0$ , there exists vectors  $y, y_i^u$  ( $u \in V(G), i \in [t]$ ) forming a Gram representation of  $Y$ . For  $i \in [t]$ , we have:  $\|y - \sum_{u \in V(G)} y_i^u\|^2 = Y_{0,0} - 2 \sum_{u \in V(G)} Y_{0,ui} + \sum_{u,v \in V(G)} Y_{ui,vi} = 0$  (using (C1),(C2a),(C2c)), which implies that  $y = \sum_{u \in V(G)} y_i^u$  for all  $i \in [t]$ . Define the vectors  $x_u = \sum_{i \in [t]} y_i^u$  for all  $u \in V(G)$  and let  $X \in \mathcal{S}^{|V(G)|}$  denote their Gram matrix. Then,  $X \succeq 0$ ,  $\langle J, X \rangle = \|\sum_{u \in V(G)} \sum_{i=1}^t y_i^u\|^2 = \|ty\|^2 = t^2$ , and  $\text{Tr}(X) = \sum_{u \in V(G)} \|x_u\|^2 = \sum_{i,j \in [t]} \sum_{u \in V(G)} \langle y_i^u, y_j^u \rangle = \sum_{i \in [t]} \sum_{u \in V(G)} Y_{ui,ui} = t$ . Moreover,  $X_{uv} = \langle x_u, x_v \rangle = \sum_{i,j \in [t]} \langle y_i^u, y_j^v \rangle = \sum_{i,j \in [t]} Y_{ui,vj} \geq 0$  for any  $u, v \in V(G)$ , with equality for  $\{u, v\} \in E(G)$ . Rescaling the matrix  $X$  by  $1/t$ , we obtain a feasible solution for (i). This concludes the proof in the case  $\mathcal{K} = \mathcal{DN}\mathcal{N}$ .

Assume now  $\mathcal{K} = \mathcal{CP}$ . We show: (i)  $\Rightarrow$  (iii)  $\Rightarrow$  (ii)  $\Rightarrow$  (i).

(i)  $\Rightarrow$  (iii): Let  $X$  be a matrix that satisfies (i). Applying Theorem 2.2, we obtain that  $\alpha(G) \geq t$ . Let  $S \subseteq V(G)$  be a stable set of cardinality  $t$ . Say,  $V(G) = [n]$  and  $S = \{1, \dots, t\}$ . Define the vector  $y \in \mathbb{R}^{nt+1}$  with block-form  $y = (1, e_1, \dots, e_t)$ , where  $e_1, \dots, e_t$  are the first  $t$  standard unit vectors in  $\mathbb{R}^n$ . Define the matrix  $Y' = yy^T$  which, by construction, belongs to  $\mathcal{CP}^{nt+1}$ . It is easy to verify that  $Y'$  satisfies (iii).

(iii)  $\Rightarrow$  (ii): We can mimic the above proof of this implication in the case of the cone  $\mathcal{DN}\mathcal{N}$ . The only thing to notice is that the new matrix  $Y = Y' + \sum_{u,v \in V(G), u \neq v} A_{uv} \tilde{F}^{uv}$  is completely positive, which can be proved by applying Theorem 4.3. Indeed,  $X \in \mathcal{CP}$ , each  $A_{uv} \tilde{F}^{uv}$  is positive semidefinite and can be easily decomposed in a sum of positive semidefinite matrices with only a  $2 \times 2$  nonzero principal submatrix, and one gets a nonnegative matrix at each intermediate step of the summation. Hence, Theorem 4.3 can be applied at every step and one can conclude that  $Y \in \mathcal{CP}$ .

(ii)  $\Rightarrow$  (i): The proof is analogous to the above proof of this implication in the case of  $\mathcal{DN}\mathcal{N}$ .  $\square$

As an application, if in Proposition 4.1 we replace the cone  $\mathcal{CS}_+$  by the cone  $\mathcal{DN}\mathcal{N}$  in the definition of  $\alpha_q(G)$  or of  $\alpha^*(G)$ , then we obtain the parameter  $\lfloor \vartheta^l(G) \rfloor$ ; analogously, if we replace the cone  $\mathcal{CS}_+$  by the cone  $\mathcal{CP}$  then we obtain  $\alpha(G)$ .

**Corollary 4.5.** *For any graph  $G$ , the maximum integer  $t$  for which there exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C2a), (C2b), (O1) and (O2) (or, equivalently, the conditions (C1), (C2a), (C2c) and (O1)) is equal to the*

parameter  $\lfloor \vartheta'(G) \rfloor$  when  $\mathcal{K} = \mathcal{DNN}$  and it is equal to the stability number  $\alpha(G)$  when  $\mathcal{K} = \mathcal{CP}$ .

*Proof.* This follows by applying Proposition 4.4 combined with the definition of  $\vartheta'$  as maximization program in (2.5) when  $\mathcal{K} = \mathcal{DNN}$  and with Theorem 2.2 when  $\mathcal{K} = \mathcal{CP}$ .  $\square$

In turn this permits to derive the following ‘sandwich inequalities’ for the quantum analogues of the stability number.

**Corollary 4.6.** *For any graph  $G$ ,  $\alpha(G) \leq \alpha_q(G) \leq \alpha^*(G) \leq \lfloor \vartheta'(G) \rfloor$ .*

The bound  $\alpha^*(G) \leq \lfloor \vartheta'(G) \rfloor$  was shown recently, with a different method, by Cubitt et al. [23]. The inequality  $\alpha(G) \leq \alpha_q(G)$  can be tight [59]. It is not known whether the other two inequalities can be tight.

Observe that, if one could prove that the two conditions (ii) and (iii) in Proposition 4.4 are equivalent also when setting  $\mathcal{K} = \mathcal{CS}_+$ , then this would imply that equality  $\alpha_q(G) = \alpha^*(G)$  holds. This would work if we could show the analogue of Theorem 4.3 when replacing the condition of being ‘completely positive’ by the condition of being ‘completely positive semidefinite’, since then the reasoning used in the proof of Proposition 4.4 for the implication (iii)  $\Rightarrow$  (ii) would extend to the case of  $\mathcal{CS}_+$ . However, the following example shows that Theorem 4.3 does not extend to the cone  $\mathcal{CS}_+$ .

**Example 4.7.** *Let  $L \in \mathcal{CS}_+^5$  be the matrix defined in relation (3.4). For  $i \neq j \in [5]$ , let  $F^{ij} \in \mathcal{S}_+^5$  be the matrix with all zero entries except  $F_{ii}^{ij} = F_{jj}^{ij} = 1$  and  $F_{ij}^{ij} = F_{ji}^{ij} = -1$ . Define the matrix  $L' = L + \cos^2(\frac{2\pi}{5})(F^{12} + F^{23} + F^{34} + F^{45} + F^{15})$ . Then,  $L'$  is not completely positive, since its inner product with the Horn matrix is negative. Indeed,  $\langle H, L' \rangle = 5(1 + 2 \cos^2(\frac{2\pi}{5})) - 10 \cos^2(\frac{4\pi}{5}) = 5(2 - \sqrt{5})/2 < 0$ . As the support of  $L'$  is equal to the 5-cycle, we can conclude using Theorem 3.7 that  $L'$  is not completely positive semidefinite.*

*Thus, although one gets nonnegative matrices at each step of the summation defining  $L'$  starting from  $L \in \mathcal{CS}_+^5$ , the final matrix  $L'$  does not belong to the cone  $\mathcal{CS}_+^5$ . This shows that the result of Theorem 4.3 does not extend to the cone  $\mathcal{CS}_+$ .*

## 4.2 Conic reformulation for quantum chromatic numbers

Analogously to what we did for the quantum stability numbers, we can reformulate the two quantum variants  $\chi_q(G)$  and  $\chi^*(G)$  of the chromatic number as conic feasibility programs over the cone  $\mathcal{CS}_+$ . The proof is omitted since it is easy and along the same lines as for Proposition 4.1.

**Proposition 4.8.** *For a graph  $G$ ,  $\chi_q(G)$  is equal to the minimum integer  $t$  for*

which there exists a matrix  $X \in \mathcal{CS}_+^{|V(G)|t+1}$  satisfying the following conditions:

$$X_{0,0} = 1, \quad (\text{C1})$$

$$\sum_{i \in [t]} X_{0,ui} = 1 \quad \forall u \in V(G), \quad (\text{C3a})$$

$$\sum_{i \in [t]} X_{ui,ui} = 1 \quad \forall u \in V(G), \quad (\text{C3b})$$

$$X_{ui,vi} = 0 \quad \forall i \in [t], \forall \{u, v\} \in E(G), \quad (\text{O3})$$

$$X_{ui,uj} = 0 \quad \forall i \neq j \in [t], \forall u \in V(G). \quad (\text{O4})$$

Moreover, the parameter  $\chi^*(G)$  is equal to the minimum integer  $t$  for which there exists a matrix  $X \in \mathcal{CS}_+^{|V(G)|t+1}$  satisfying (C1), (C3a), (O3) and

$$\sum_{i,j \in [t]} X_{ui,uj} = 1 \quad \forall u \in V(G). \quad (\text{C3c})$$

**Proposition 4.9.** *Let  $G$  be a graph and let  $\mathcal{K}$  denote the cone  $\mathcal{DNN}$  or  $\mathcal{CP}$ . Consider the following three assertions.*

- (i) *There exists a matrix  $X \in \mathcal{K}^{|V(G)|}$  such that  $[X_{uu}] = t$  for every  $u \in V(G)$ ,  $X_{uv} = 0$  for all  $\{u, v\} \in E(G)$  and  $X - J \succeq 0$ .*
- (ii) *There exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C3a), (C3b), (O3) and (O4).*
- (iii) *There exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C3a), (C3c) and (O3).*

Then, (i)  $\iff$  (ii)  $\iff$  (iii) if  $\mathcal{K} = \mathcal{DNN}$ , and (iii)  $\iff$  (ii)  $\implies$  (i) if  $\mathcal{K} = \mathcal{CP}$ .

*Proof.* Assume first  $\mathcal{K} = \mathcal{DNN}$ . We show: (i)  $\implies$  (iii)  $\implies$  (ii)  $\implies$  (i).

(i)  $\implies$  (iii): Let  $X$  be a matrix that satisfies the conditions of (i). By adding a nonnegative diagonal matrix to  $X$  we can assume that  $X_{uu} = t$  for every  $u \in V(G)$ . Define the matrix  $X' = X - J \in \mathcal{S}^{|V(G)|}$ . Then,  $X' \succeq 0$ ,  $X'_{uu} = t - 1$  for all  $u \in V(G)$  and, for  $u \neq v$ ,  $X'_{uv} = X_{uv} - 1 \geq -1$  with equality when  $\{u, v\} \in E(G)$ . Moreover,  $X'_{uv} \geq -(t - 1)$  since  $X' \succeq 0$  with diagonal entries equal to  $t - 1$ . (Although we do not need it, observe that this shows that  $\vartheta^+(G) \leq t$ .)

Next, we define the matrices  $A = \frac{1}{t^2}(X' + J)$ ,  $B = \frac{1}{t^2}(J - \frac{1}{t-1}X') \in \mathcal{S}^{|V(G)|}$ , and we let  $Y \in \mathcal{S}^{|V(G)|t}$  be the block-matrix as in (4.2) with  $A$  as diagonal blocks and  $B$  as off-diagonal blocks. By construction,  $A, B \geq 0$  and thus  $Y \geq 0$ . Moreover,  $A + (t - 1)B = \frac{1}{t}J \succeq 0$  and  $A - B = \frac{1}{t(t-1)}X' \succeq 0$  and thus, by Lemma 4.2, we deduce that  $Y \succeq 0$ . Next we show how to construct from  $Y$  a matrix  $Y' \in \mathcal{S}^{|V(G)|t+1}$  satisfying (iii).

As  $Y \succeq 0$ , there exists a set of vectors  $y_u^i$  (for  $u \in V(G)$  and  $i \in [t]$ ) forming a Gram representation of  $Y$ . Fix  $u_0 \in V(G)$  and define the vector  $y = \sum_{i \in [t]} y_{u_0}^i$ . Then, define  $Y'$  as the Gram matrix of the vectors  $y$  and  $y_u^i$  for  $u \in V(G)$  and  $i \in [t]$ . We claim that  $Y'$  satisfies (iii). For this, we use the properties of  $A$  and  $B$ . Observe that for all  $\{u, v\} \in E(G)$  and  $i \in [t]$ ,  $Y'_{ui,vi} = \langle y_u^i, y_v^i \rangle = A_{uv} = 0$ , and that for all  $u \in V(G)$  and  $i \neq j$ ,  $Y'_{ui,uj} = \langle y_u^i, y_u^j \rangle = B_{uu} = 0$ , thus showing (O3) and (O4). Moreover, for every  $u \in V(G)$  and  $i \in [t]$ ,  $\langle y_u^i, y_u^i \rangle = A_{uu} = \frac{1}{t}$  and therefore

$Y'_{00} = \langle y, y \rangle = \sum_{i,j \in [t]} \langle y_{u_0}^i, y_{u_0}^j \rangle = \sum_{i \in [t]} \langle y_{u_0}^i, y_{u_0}^i \rangle = \text{Tr}(A) = 1$ , showing (C1). Next, (C3a),(C3c) follow from the identity  $tA + t(t-1)B = J$ , since  $\sum_{i \in [t]} Y'_{0,ui} = \sum_{i,j \in [t]} \langle y_{u_0}^j, y_{u_0}^i \rangle = (tA + t(t-1)B)_{u_0u}$  and  $\sum_{i,j \in [t]} Y'_{ui,uj} = (tA + t(t-1)B)_{uu}$ . Thus we have shown that  $Y'$  satisfies (iii).

(iii)  $\Rightarrow$  (ii): Let  $Y'$  be a feasible matrix for (iii). We may assume without loss of generality that  $Y'$  is invariant under permutations of the symmetric group  $\text{Sym}(t)$ , i.e., that  $Y'$  has the block-form (4.1) where  $B$  is the off-diagonal block. If  $B_{uu} = 0$  holds for all  $u \in V(G)$ , then  $Y'$  satisfies (O4) and thus (ii) and we are done. Otherwise, there is some  $u \in V(G)$  for which  $B_{uu} > 0$ . We show how to construct from  $Y'$  a new matrix  $Y$  satisfying (ii). For this, define the matrix  $F^u \in \mathcal{S}^{|V(G)|t+1}$  whose entries are all 0 except  $F^u_{ui,ui} = t-1$  for  $i \in [t]$  and  $F^u_{ui,uj} = -1$  for  $i \neq j \in [t]$ , and observe that  $F^u \succeq 0$ . Now we set  $Y = Y' + \sum_{u \in V(G)} B_{uu} F^u$ . Hence,  $Y$  satisfies (O4) by construction. Moreover,  $Y \succeq 0$ ,  $Y \geq 0$  and  $Y$  still respects (C1), (C3a) and (O3). Finally,  $Y$  also satisfies (C3c) since  $\langle J, F^u \rangle = 0$  for all  $u \in V(G)$ . Hence we have shown that  $Y \in \mathcal{DN}\mathcal{N}$  satisfies (ii).

(ii)  $\Rightarrow$  (i): Let  $Y \in \mathcal{DN}\mathcal{N}$  satisfy (ii). Without loss of generality, we can assume that  $Y$  has the block-form (4.1). Then,  $\alpha = Y_{00} = 1$  by (C1),  $a = \frac{1}{t}e$  by (C3a),  $A_{uu} = \frac{1}{t}$  for all  $u \in V(G)$  by (C3b),  $A_{uv} = 0$  for  $\{u, v\} \in E(G)$  by (O3), and  $B_{uu} = 0$  for  $u \in V(G)$  by (O4). Let  $Z \in \mathcal{S}^{|V(G)|t}$  denote the principal submatrix of  $Y$  obtained by deleting its first row and column indexed by the index 0, so that  $Z$  has the block-form (4.2). Let  $Z'$  denote the Schur complement of  $Z$  in  $Y$  w.r.t. its  $(0,0)$ -th entry (recall (1.2)). Using the fact that  $a = e/t$ , we obtain that  $Z' = Z - \frac{1}{t^2}J$ . Moreover,  $Y \succeq 0$  implies  $Z' \succeq 0$ . Now,  $Z'$  has again the block-form (4.2) with diagonal blocks  $A' = A - \frac{1}{t^2}J$  and with off-diagonal blocks  $B' = B - \frac{1}{t^2}J$ . Applying Lemma 4.2, we deduce that  $A' - B' \succeq 0$  and  $A' + (t-1)B' \succeq 0$ , which implies  $A - B \succeq 0$  and  $A + (t-1)B - \frac{1}{t}J \succeq 0$ . Now observe that  $\text{Tr}(A + (t-1)B - \frac{1}{t}J) = \text{Tr}(A - \frac{1}{t}J) = 0$  and that this implies  $A + (t-1)B - \frac{1}{t}J = 0$  as  $A + (t-1)B - \frac{1}{t}J \succeq 0$ .

We can now construct a matrix  $X \in \mathcal{S}^{|V(G)|}$  satisfying (i). Namely, set  $X = t^2A$ . Thus,  $X \in \mathcal{DN}\mathcal{N}$ ,  $X_{uu} = t$  for  $u \in V(G)$ , and  $X_{uv} = 0$  for  $\{u, v\} \in E(G)$ . Moreover,  $X - J \succeq 0$ , since  $A - B \succeq 0$  and  $X - J = t^2A - J = t(t-1)(A - B)$  follows from the identity  $A + (t-1)B = \frac{1}{t}J$ . This concludes the proof in the case  $\mathcal{K} = \mathcal{DN}\mathcal{N}$ .

We now consider the case  $\mathcal{K} = \mathcal{CP}$ . The implication (ii)  $\Rightarrow$  (iii) is clear.

(iii)  $\Rightarrow$  (ii): We can mimic the above proof of this implication in the  $\mathcal{DN}\mathcal{N}$  cone. In order to do so, we need to observe that the new matrix  $Y = Y' + \sum_{u \in V(G)} B_{uu} F^u$  is completely positive. This is so because, for every  $u \in V(G)$ , the matrix  $F^u$  can be written as a sum of positive semidefinite matrices with only a  $2 \times 2$  non-zero principal submatrix. Moreover, Theorem 4.3 can be applied at every step of the summation, since one gets a nonnegative matrix at each step.

(ii)  $\Rightarrow$  (i): Again we can mimic the above proof of this implication in the case of  $\mathcal{DN}\mathcal{N}$ . Indeed, we can assume that there exists a matrix  $Y \in \mathcal{CP}^{|V(G)|t+1}$  satisfying (ii) and with block-form (4.1), where  $A, B$  satisfy the identity:  $A + (t-1)B = \frac{1}{t}J$ . Then, the matrix  $X = t^2A$  belongs to  $\mathcal{CP}^{|V(G)|}$  and satisfies (i).  $\square$

**Corollary 4.10.** *For any graph  $G$ , the minimum integer  $t$  for which there exists a matrix  $X \in \mathcal{K}^{|V(G)|t+1}$  satisfying the conditions (C1), (C3a), (C3b), (O3) and*

(O4) (or, equivalently, the conditions (C1), (C3a), (C3c) and (O3)) is equal to the parameter  $\lceil \vartheta^+(\overline{G}) \rceil$  when  $\mathcal{K} = \mathcal{DN}\mathcal{N}$  and it is equal to the chromatic number  $\chi(G)$  when  $\mathcal{K} = \mathcal{CP}$ .

*Proof.* In the case  $\mathcal{K} = \mathcal{DN}\mathcal{N}$ , the result follows using Proposition 4.9 combined with the minimization program definition of  $\vartheta^+(G)$  from (2.6).

Consider now the case  $\mathcal{K} = \mathcal{CP}$ . In view of Proposition 4.9, we know that the two conditions (ii) and (iii) are equivalent. Let  $t$  denote the minimum integer for which the condition (ii) of Proposition 4.9 holds; we show that  $\chi(G) = t$ . First, we show that  $\chi(G) \leq t$ . For this, consider a matrix  $Y \in \mathcal{CP}^{|V(G)|^{t+1}}$  satisfying (ii) which has block-form (4.1) and let  $Z$  be its principal submatrix obtained by deleting its first row and column indexed by 0. Then,  $Z \in \mathcal{CP}^{|V(G)|^t}$ . Moreover,  $\text{Tr}(Z) = |V(G)|$  and  $\langle J, Z \rangle = |V(G)|^2$  (see the proof of the implication (ii)  $\Rightarrow$  (i) in Proposition 4.9). Now we use the result of Theorem 2.2 for computing the value of  $\alpha(G \square K_t)$ . For this, set  $Z' = \frac{1}{|V(G)|} Z \in \mathcal{CP}^{|V(G)|^t}$ . We see that  $Z'$  satisfies the conditions of the program (2.1) applied to the graph  $G \square K_t$ . Indeed the orthogonality conditions (O3) and (O4) correspond exactly to the edges of  $G \square K_t$ . Therefore, we can deduce that  $\alpha(G \square K_t) \geq |V(G)|$ . As the reverse inequality also holds (since  $G$  can be covered by  $|V(G)|$  cliques  $K_t$ ), we have  $\alpha(G \square K_t) = |V(G)|$ . Using the reduction of Chvátal in Theorem 2.1, we can conclude that  $\chi(G) \leq t$ .

We now prove the reverse inequality:  $t \leq \chi(G) =: s$ . It is easy to see that  $G \square K_s$  can be properly colored with  $s = \chi(G)$  colors. Therefore,  $\chi(G \square K_s) = s$  holds. We construct a matrix  $Y \in \mathcal{CP}^{|V(G)|^{s+1}}$  satisfying the conditions of (ii), which will imply  $t \leq s$  and thus conclude the proof. For this, select  $s$  subsets  $S_1, \dots, S_s \subseteq V(G \square K_s)$  which are stable sets in  $G \square K_s$  and partition the vertex set of  $G \square K_s$ . For  $k \in [s]$ , let  $x^k \in \mathbb{R}^{|V(G)|^s}$  denote the incidence vector of  $S_k$  and set  $y^k = (1, x^k) \in \mathbb{R}^{|V(G)|^{s+1}}$ . Finally, define the matrix  $Y = \frac{1}{s} \sum_{k=1}^s y^k (y^k)^T$ . By construction,  $Y \in \mathcal{CP}^{|V(G)|^{s+1}}$  and  $Y$  satisfies conditions (O3) and (O4). Moreover  $Y_{0,0} = 1$ ,  $Y_{0,ui} = Y_{ui,ui} = \frac{1}{s}$  for every  $u \in V(G)$  and  $i \in [s]$  and thus  $Y$  also satisfies (C1), (C3a) and (C3b). Hence  $Y$  is feasible for (ii). This concludes the proof.  $\square$

As an application we obtain the following ‘sandwich inequalities’ for the quantum variants of the chromatic number.

**Corollary 4.11.** *For any graph  $G$ ,  $\lceil \vartheta^+(\overline{G}) \rceil \leq \chi^*(G) \leq \chi_q(G) \leq \chi(G)$ .*

The inequality  $\lceil \vartheta^+(\overline{G}) \rceil \leq \chi^*(G)$  was shown recently in [12]. In the above chain of inequalities, only the right most one is known to be tight [18]. Note also that the quantum chromatic numbers are not upper bounded by the fractional chromatic number. For instance, for  $G = C_5$ ,  $\chi_f(G) = 5/2$  while  $\chi_q(G) = 3$ . Indeed, [18] shows that  $\chi_q(G) \leq 2$  if and only if  $G$  is a bipartite graph.

We conclude with observing that, in Proposition 4.9, the implication (i)  $\Rightarrow$  (ii) does not hold when selecting the cone  $\mathcal{K} = \mathcal{CP}$ .

**Remark 4.12.** *As we just saw in Corollary 4.10, the smallest integer  $t$  for which there exists a matrix  $X \in \mathcal{CP}^{|V(G)|^{t+1}}$  satisfying Proposition 4.9 (ii) is equal to the chromatic number  $\chi(G)$ . On the other hand, as a direct application of Theorem 2.3, we see that the smallest integer  $t$  for which there exists a matrix  $X \in \mathcal{CP}^{|V(G)|}$  satisfying Proposition 4.9 (i) is equal to  $\lceil \chi_f(G) \rceil$ , where  $\chi_f(G)$  is the fractional*

chromatic number of  $G$ . The inequality  $\lceil \chi_f(G) \rceil \leq \chi(G)$  is consistent with the inequality  $t \leq s$  corresponding to the implication (ii)  $\Rightarrow$  (i) in Proposition 4.9.

Moreover, the parameters  $\lceil \chi_f(G) \rceil$  and  $\chi(G)$  can differ significantly. For  $n \geq 2r$ , consider the Kneser graph  $K(n, r)$ , whose vertices are the subsets of size  $r$  of  $[n]$  and where two vertices are adjacent if the sets are disjoint. Then,  $\chi_f(K(n, r)) = \frac{n}{r}$  [49] and  $\chi(K(n, r)) = n - 2r + 2$  [48]. This shows that the implication: (i)  $\Rightarrow$  (ii) does not hold in Proposition 4.9 in the case  $\mathcal{K} = \mathcal{CP}$ .

### 4.3 Optimization programs for the quantum parameters

In this section we reformulate each of the quantum parameters  $\chi_q(G)$ ,  $\chi^*(G)$ ,  $\alpha_q(G)$  and  $\alpha^*(G)$  as a single optimization program over an affine section of the cone  $\mathcal{CS}_+$ , which we will then use in the next section for defining semidefinite approximations. As deciding whether  $\chi_q(G) \leq 3$  is NP-hard [38], it follows that linear optimization over affine sections of the completely positive semidefinite cone is NP-hard.

We begin with the parameters  $\chi_q(G)$  and  $\chi^*(G)$ .

For convenience, we introduce the matrix  $A_u^t \in \mathcal{S}^{nt+1}$  (for  $u \in V(G)$ ,  $t \in [n]$ ), with entries  $A_u^t(0, 0) = A_u^t(ui, uj) = 1 \ \forall i, j \in [t]$ ,  $A_u^t(0, ui) = -1 \ \forall i \in [t]$  and zero elsewhere, and we set  $A^t = \sum_{u \in V(G)} A_u^t$ . Observe that each matrix  $A_u^t$  is positive semidefinite (with rank 1). These matrices are useful to formulate the constraints defining  $\chi_q(G)$  and  $\chi^*(G)$  in a bit more compact way. Indeed, observe that if the condition (O4) (from Proposition 4.8) holds, then both conditions (C3b) and (C3c) are equivalent. Moreover, if (C1) holds then the two conditions (C3a), (C3c) are equivalent to  $\langle A^t, X \rangle = 0$ . Therefore,  $\chi_q(G)$  is equal to the smallest  $t \in \mathbb{N}$  for which there exists  $X \in \mathcal{CS}_+^{nt+1}$  satisfying the conditions (C1), (O3), (O4) and  $\langle A^t, X \rangle = 0$ . Analogously,  $\chi^*(G)$  is equal to the smallest  $t \in \mathbb{N}$  for which there exists  $X \in \mathcal{CS}_+^{nt+1}$  satisfying the conditions (C1), (O3) and  $\langle A^t, X \rangle = 0$ .

**Lemma 4.13.** *Let  $G$  be a graph and set  $n = |V(G)|$ . The quantum chromatic number  $\chi_q(G)$  is equal to the optimal value of the following program:*

$$\begin{aligned} \min \sum_{t \in [n]} t X_{0,0}^t \quad \text{s.t.} \quad & X^t \in \mathcal{CS}_+^{nt+1} \quad \forall t \in [n], \\ & \sum_{t \in [n]} X_{0,0}^t = 1, \quad \sum_{t \in [n]} \langle A^t, X^t \rangle = 0 \\ & X_{ui,vi}^t = 0 \quad \forall i \in [t], \forall \{u, v\} \in E(G), \forall t \in [n], \\ & X_{ui,uj}^t = 0 \quad \forall i \neq j \in [t], \forall u \in V(G), \forall t \in [n]. \end{aligned} \quad (4.3)$$

Moreover,  $\chi^*(G)$  is equal to the optimum value of the program (4.3) where we omit the last condition:  $X_{ui,uj}^t = 0$  for all  $i \neq j \in [t]$ ,  $u \in V(G)$  and  $t \in [n]$ .

*Proof.* We prove the result for  $\chi_q(G)$  and the same proof applies for  $\chi^*(G)$ . Set  $t = \chi_q(G)$  and let  $\mu$  denote the optimal value of the program (4.3).

Let  $(t, X)$  be a solution for the program from Proposition 4.8 defining  $\chi_q(G)$ . We obtain a solution  $X^1, \dots, X^n$  to the program (4.3) by setting  $X^t = X$  and  $X^i = 0$  if  $i \neq t$ . This shows that  $\mu \leq t$ .

Conversely, let  $X^1, \dots, X^n$  be an optimal solution for the program (4.3) and let  $s$  be the minimum  $i \in [n]$  such that  $X_{0,0}^i \neq 0$ . Then, the matrix  $X = X^s / X_{0,0}^s$  is feasible for the program in Proposition 4.8. This implies that  $t \leq s = s \sum_{i \geq s} X_{0,0}^i \leq \sum_{i \geq s} i X_{0,0}^i = \mu$ . Hence, we have shown that  $\chi_q(G) = \mu$ .  $\square$



We now turn to the parameters  $\alpha_q(G)$  and  $\alpha^*(G)$ . Again it is convenient to introduce the matrices  $D_i^t \in \mathcal{S}^{nt+1}$  (for  $t \in [n]$  and  $i \in [t]$ ), with entries  $(D_i^t)_{0,0} = 1$ ,  $(D_i^t)_{0,ui} = -1$ ,  $(D_i^t)_{ui,vi} = 1$  for  $u, v \in V(G)$  (thus the analogues of the above matrices  $A_u^t$ , interchanging the role of nodes  $u \in V(G)$  and indices  $i \in [t]$ ). Set  $D^t = \sum_{i=1}^t D_i^t$  and note that  $D_i^t, D \succeq 0$ . Then,  $\alpha_q(G)$  is equal to the maximum  $t \in \mathbb{N}$  for which there exists a matrix  $X \in \mathcal{CS}_+^{nt+1}$  satisfying the conditions (C1), (O1), (O2) and  $\langle D^t, X \rangle = 0$ , and  $\alpha^*(G)$  is the maximum  $t \in \mathbb{N}$  for which there exists  $X \in \mathcal{CS}_+^{nt+1}$  satisfying (C1), (O1) and  $\langle D^t, X \rangle = 0$ . We now formulate these parameters as linear optimization problems over the cone  $\mathcal{CS}_+^N$ , we omit the proof which is analogous to the one of Lemma 4.13.

**Lemma 4.14.** *Let  $G$  be a graph and set  $n = |V(G)|$ . The quantum stability number  $\alpha_q(G)$  is equal to the optimal value of the program:*

$$\begin{aligned} \max \sum_{t=1}^n t X_{0,0}^t \quad \text{s.t.} \quad & X^t \in \mathcal{CS}_+^{nt+1} \quad \forall t \in [n], \\ & \sum_{t \in [n]} X_{0,0}^t = 1, \quad \sum_{t \in [n]} \langle D^t, X^t \rangle = 0 \quad \forall t \in [n], \\ & X_{ui,vj}^t = 0 \quad \forall i \neq j \in [t], \forall u \simeq v \in V(G), \forall t \in [n], \\ & X_{ui,vi}^t = 0 \quad \forall i \in [t], \forall u \neq v \in V(G), \forall t \in [n]. \end{aligned} \tag{4.4}$$

Moreover,  $\alpha^*(G)$  is equal to the optimal value of the program (4.4), where we omit the last condition  $X_{ui,vi}^t = 0$  for all  $i \in [t]$ ,  $u \neq v \in V(G)$  and  $t \in [n]$ .

#### 4.4 Semidefinite approximations for the quantum graph parameters

As computing the parameter  $\chi_q(G)$  is NP-hard it is interesting to find good bounds that can be computed in polynomial time. As mentioned earlier, one such bound is provided by the theta number:  $\vartheta^+(\overline{G}) \leq \chi_q(G)$ . We now see how to design tighter semidefinite programming bounds by using the reformulation of  $\chi_q(G)$  as an optimization problem over the cone  $\mathcal{CS}_+$  and the hierarchy of cones  $\mathcal{K}_{nc,\epsilon}^{(r)}$ . We also do this for the other quantum parameters.

In a first step we show how to relate the quantum chromatic and stability numbers with the parameters  $\vartheta^{\mathcal{CS}_+}$  and  $\Theta^{\mathcal{CS}_+}$ . These relationships follow by revisiting the proofs of Propositions 4.4 and 4.9.

**Proposition 4.15.** *For any graph  $G$ , we have:*

$$\alpha_q(G) \leq \lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor \leq \lfloor \vartheta'(G) \rfloor \quad \text{and} \quad \lceil \vartheta^+(\overline{G}) \rceil \leq \lceil \Theta^{\mathcal{CS}_+}(G) \rceil \leq \chi^*(G) \leq \chi_q(G).$$

*Proof.* From the simple observation that  $\vartheta^{\mathcal{DN}\mathcal{N}}(G) = \vartheta'(G)$  and the fact that  $\mathcal{CS}_+ \subseteq \mathcal{DN}\mathcal{N}$ , we have  $\vartheta^{\mathcal{CS}_+}(G) \leq \vartheta'(G)$  and thus  $\lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor \leq \lfloor \vartheta'(G) \rfloor$ .

We now show the inequality  $\alpha_q(G) \leq \lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor$ . For this, we use Proposition 4.4. First we observe that the implication (ii)  $\Rightarrow$  (i) remains true in Proposition 4.4 if we select the cone  $\mathcal{K} = \mathcal{CS}_+$ . (Indeed, the same proof applies as in the case  $\mathcal{K} = \mathcal{DN}\mathcal{N}$ , except that  $y, y_i^u$  are now psd matrices.) By definition,  $\alpha_q(G)$  is the largest integer  $t$  for which Proposition 4.4 (ii) holds with  $\mathcal{K} = \mathcal{CS}_+$ . In turn, by the above, this largest integer is at most the largest integer  $t$  for which Proposition 4.4 (i) holds with  $\mathcal{K} = \mathcal{CS}_+$ , the latter being equal to  $\lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor$ . Thus  $\alpha_q(G) \leq \lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor$  holds.

Similarly, as  $\Theta^{\mathcal{DN}\mathcal{N}}(G) = \vartheta^+(\overline{G})$ , then  $\lceil \vartheta^+(\overline{G}) \rceil \leq \lceil \Theta^{\mathcal{CS}_+}(G) \rceil$ . Moreover,  $\lceil \Theta^{\mathcal{CS}_+}(G) \rceil$  is the minimum integer  $t$  for which Proposition 4.9 (i) holds when selecting  $\mathcal{K} = \mathcal{CS}_+$ . As  $\chi^*(G)$  is by definition the minimum integer  $t$  for which Proposition 4.9 (iii) holds with  $\mathcal{K} = \mathcal{CS}_+$ , in order to prove that  $\lceil \Theta^{\mathcal{CS}_+}(G) \rceil \leq \chi^*(G)$  holds, it suffices to show that Proposition 4.9 (iii) implies Proposition 4.9 (i) also in the case  $\mathcal{K} = \mathcal{CS}_+$ . This is what we do next.

Let  $Y \in \mathcal{CS}_+$  satisfy Proposition 4.9 (iii) with  $\mathcal{K} = \mathcal{CS}_+$ . Again we may assume without loss of generality that  $Y$  has the block-form (4.1). First we observe that we can use the initial part of the proof (ii)  $\Rightarrow$  (i) to show that  $A + (t-1)B - \frac{1}{t}J = 0$ . The key observation is that condition (C3c) still implies that  $\text{Tr}(A + (t-1)B - \frac{1}{t}J) = 0$ . Next, following the proof of (ii)  $\Rightarrow$  (i), we consider the matrix  $X = t^2A$ . Then  $X \in \mathcal{CS}_+$ ,  $X_{uv} = 0$  for every  $\{u, v\} \in E(G)$  and  $X - J \succeq 0$ . Since we started with a solution  $Y$  of (iii) (instead of a solution for (ii)), we can only derive that  $X_{uu} \leq t$  for any  $u \in V(G)$ . We now build a solution  $X'$  by adding to  $X$  a diagonal matrix  $D$  with entries  $D_{uu} = t - X_{uu} \geq 0$  for any  $u \in V(G)$ . Hence  $X' \in \mathcal{CS}_+$  and satisfies all the conditions of (i). This concludes the proof.  $\square$

We do not know whether  $\theta^{\mathcal{CS}_+}(G)$  provides an upper bound for  $\alpha^*(G)$ , since we cannot show that Proposition 4.4 (iii) implies Proposition 4.4 (i) in the case  $\mathcal{K} = \mathcal{CS}_+$ . The proof used for the case  $\mathcal{K} = \mathcal{DN}\mathcal{N}$  and  $\mathcal{CP}$  indeed does not extend to the case  $\mathcal{K} = \mathcal{CS}_+$  since Theorem 4.3 does not hold if we consider matrices in  $\mathcal{CS}_+$  (as shown in Example 4.7).

As an application of Proposition 4.15, the bounds  $\varphi_\epsilon^{(r)}(G)$  for  $\vartheta^{\mathcal{CS}_+}(G)$  and  $\Phi_\epsilon^{(r)}(G)$  for  $\Theta^{\mathcal{CS}_+}(G)$  from Section 3.5 also provide bounds for the quantum stability and chromatic numbers. However these bounds might be weak if  $\Theta^{\mathcal{CS}_+}(G)$  (resp.,  $\vartheta^{\mathcal{CS}_+}(G)$ ) is far from the quantum chromatic (resp. stability) number. In what follows we formulate new hierarchies of bounds  $\psi_\epsilon^{(r)}(G)$ ,  $\psi_\epsilon^{(r)*}(G)$  for the quantum stability numbers  $\alpha_q(G)$ ,  $\alpha^*(G)$ , and bounds  $\Psi_\epsilon^{(r)}(G)$ ,  $\Psi_\epsilon^{(r)*}(G)$  for the quantum chromatic numbers  $\chi_q(G)$ ,  $\chi^*(G)$ . Moreover, we will show that the bounds  $\Psi_\epsilon^{(r)}(G)$  strengthen the bounds  $\Phi_\epsilon^{(r)}(G)$ . These new bounds are obtained by replacing the cone  $\mathcal{CS}_+$  by the (dual) cone  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  in the definitions of the quantum parameters from Propositions 4.1 and 4.8.

**Definition 4.16.** For  $r \in \mathbb{N}$  and  $\epsilon \geq 0$ , let  $\psi_\epsilon^{(r)}(G)$  (resp.,  $\psi_\epsilon^{(r)*}(G)$ ) denote the maximum integer  $t$  for which there exists a matrix  $X \in \mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  satisfying the conditions (C1), (C2a), (C2b), (O1), (O2) (resp., the conditions (C1), (C2a), (C2c), (O1)) from Proposition 4.1.

Analogously, let  $\Psi_\epsilon^{(r)}(G)$  (resp.,  $\Psi_\epsilon^{(r)*}(G)$ ) denote the minimum integer  $t$  for which there exists a matrix  $X \in \mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  satisfying the conditions (C1), (C3a), (C3b), (O3), (O4) (resp., the conditions (C1), (C3a), (C3c), (O3)) from Proposition 4.8.

We will show below that the parameters  $\Psi_\epsilon^{(r)}(G)$  provide lower bounds for  $\chi_q(G)$  (for any small enough  $\epsilon$ ). It is not clear how to show this directly from the above definition of  $\Psi_\epsilon^{(r)}(G)$ , since there is no inclusion relationship between the two cones  $\mathcal{CS}_+$  and  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ . Our strategy will be as follows: first we reformulate  $\Psi_\epsilon^{(r)}(G)$  as the minimum value of a single optimization program (in analogy with Lemma 4.13), then we consider the dual program, and finally we relate the optimal value of this dual program with the optimal value of the corresponding program for  $\chi_q(G)$ .

We start with rewriting the optimization program (4.3) defining  $\chi_q(G)$  in a more compact way. For this, recall the matrices  $A^t$  introduced in Section 4.3 and set  $A = \bigoplus_{t=1}^n A^t \in \mathcal{S}^N$ , setting  $N = \sum_{t=1}^n (nt + 1)$ ,  $n = |V(G)|$ . Let  $E_{0,ui}^t, E_{ui,vj}^t$  denote the elementary matrices in  $\mathcal{S}^{nt+1}$  and let  $\tilde{E}_{0,ui}^t, \tilde{E}_{ui,vj}^t$  denote their extensions to  $\mathcal{S}^N$  obtained by adding zero entries. Moreover, set  $C = \bigoplus_{t=1}^n tE_{0,0}^t$  and  $B = \bigoplus_{t=1}^n E_{0,0}^t \in \mathcal{S}^N$ . Then we can rewrite the program (4.3) as follows:

$$\begin{aligned} \chi_q(G) = \min \langle C, X \rangle \quad \text{s.t.} \quad & X \in \mathcal{CS}_+^N, \quad \langle B, X \rangle = 1, \quad \langle A, X \rangle = 0, \\ & \langle \tilde{E}_{ui,vi}^t, X \rangle = 0 \quad \forall i \in [t], \quad \forall \{u, v\} \in E(G), \quad \forall t \in [n], \\ & \langle \tilde{E}_{ui,uj}^t, X \rangle = 0 \quad \forall i \neq j \in [t], \quad \forall u \in V(G), \quad \forall t \in [n]. \end{aligned} \quad (4.5)$$

The dual program reads:

$$\max \lambda \quad \text{s.t.} \quad M = C - \lambda B - \mu A - \sum y_{u,v,i}^t \tilde{E}_{ui,vi}^t - \sum z_{u,i,j}^t \tilde{E}_{ui,uj}^t \in \mathcal{CS}_+^{N*}, \quad (4.6)$$

where the variables are  $\lambda, \mu, y_{u,v,i}^t$  and  $z_{u,i,j}^t$ , the first summation is over  $t \in [n]$ ,  $i \in [t]$ ,  $\{u, v\} \in E(G)$ , and the second summation is over  $t \in [n]$ ,  $i \neq j \in [t]$ ,  $u \in V(G)$ . The dual program is strictly feasible, hence there is no duality gap and the optimal value of (4.6) is equal to  $\chi_q(G)$ .

To see that (4.6) is strictly feasible, define the matrix  $M = \bigoplus_{t=1}^n M^t$ , where  $M^t = (t + n^2)E_{0,0}^t + A^t - \sum_{u \in V(G)} \sum_{i \neq j \in [t]} E_{ui,uj}^t$ . Then,  $M$  lies in the interior of  $\mathcal{CS}_+^*$ , since  $M^t \succ 0$  (as its entries are  $(M^t)_{0,0} = n + t + n^2$ ,  $(M^t)_{0,ui} = -1$ ,  $(M^t)_{ui,ui} = 1$  and all other entries are zero, and take a Schur complement to see that  $M^t \succ 0$ ). Observe that the primal program (4.5) is not strictly feasible. Indeed any feasible solution  $X$  lies on the boundary of the cone  $\mathcal{CS}_+$ , since it satisfies  $\langle A, X \rangle = 0$  where  $A \in \mathcal{CS}_+^*$  (as  $A \succeq 0$ ).

The analogue of Lemma 4.13 holds when replacing the cone  $\mathcal{CS}_+$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  (the proof is similar and uses the fact that the cone  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  is closed under taking principal submatrices and extensions by zero, recall Lemma 3.14). Therefore, the parameter  $\Psi_\epsilon^{(r)}(G)$  is equal to the optimum value of the program (4.5), where we replace  $\mathcal{CS}_+$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ , and also to the optimum value of the program (4.6), where we replace  $\mathcal{CS}_+^*$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$ . We are now in a position to compare the parameters  $\chi_q(G)$ ,  $\Phi_\epsilon^{(r)}(G)$  and  $\Psi_\epsilon^{(r)}(G)$ .

**Proposition 4.17.** *For  $\epsilon > 0$ ,  $r \in \mathbb{N}$  and any graph  $G$  (with  $n = |V(G)|$ ), we have*

$$\Psi_\epsilon^{(r)}(G) \geq \Phi_\epsilon^{(r)}(G), \quad (4.7)$$

$$\chi_q(G) \geq \frac{1}{1 + \epsilon} \Psi_\epsilon^{(r)}(G). \quad (4.8)$$

Moreover,  $\Psi_0^{(r)}(G) = \lceil \Phi_0^{(r)}(G) \rceil = \lceil \vartheta^+(\overline{G}) \rceil$ , and  $\chi_q(G) \geq \Psi_\epsilon^{(r)}(G)$  for any  $\epsilon < \frac{1}{n-1}$ .

*Proof.* To show (4.7), we use the formulation of  $\Psi_\epsilon^{(r)}(G)$  via the program (4.5) and the formulation of  $\Phi_\epsilon^{(r)}(G)$  via the program (3.14), where in both programs we replace  $\mathcal{CS}_+$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ . The inequality (4.7) now follows since we can use the same proof as for the implication (ii)  $\Rightarrow$  (i) in Proposition 4.9.

The equality  $\Psi_0^{(r)}(G) = \lceil \vartheta^+(\overline{G}) \rceil$  follows from Corollary 4.10 as  $\mathcal{K}_{\text{nc},0}^{(r)} = \mathcal{DN}\mathcal{N}^*$  (Lemma 3.16). The inequality  $\chi_q(G) \geq \Psi_\epsilon^{(r)}(G)$  when  $\epsilon < 1/(n-1)$  follows directly

from (4.8) and the fact that both  $\chi_q(G)$  and  $\Psi_\epsilon^{(r)}(G)$  are integers upper bounded by  $n$ . Hence it suffices to show (4.8).

For this, let  $M, \lambda, \mu, y, z$  be a feasible solution to the program (4.6) (with  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$  instead of  $\mathcal{CS}_+^*$ ) defining  $\psi_\epsilon^{(r)}$ . We construct a feasible solution  $M', \lambda', \mu', y', z'$  for the program (4.6) defining  $\chi_q(G)$  with  $\lambda' = \lambda/(1 + \epsilon)$ , which will show (4.8). It suffices to define the diagonal blocks  $(M')^t$  and then we set  $M' = \bigoplus_{t=1}^n (M')^t$ . We start with  $(M')^t = \frac{t}{t+\epsilon}(M^t + \epsilon E_{0,0}^t + \epsilon A^t)$ , which we will modify a bit thereafter.

In a first step we claim that  $(M')^t \in \mathcal{CS}_+^*$ , i.e., that  $p_{(M')^t}$  is trace positive. For this we use Lemma 3.19. Hence it suffices to show that the matrix  $Z = E_{0,0}^t + A^t$  satisfies the condition (3.11). We have  $p_Z = p_{E_{0,0}^t} + p_{A^t} = p_{E_{0,0}^t} + \sum_{u \in V(G)} p_{A_u^t}$ , where all matrices  $E_{0,0}^t$  and  $A_u^t$  are positive semidefinite. Assume that  $\underline{X} \in (\mathcal{S}^d)^n$  satisfies  $\text{Tr}(p_Z(\underline{X})) = 0$ . Then,  $\text{Tr}(p_{E_{0,0}^t}(\underline{X})) = \text{Tr}(p_{A_u^t}(\underline{X})) = 0$  for all  $t, u$ .  $\text{Tr}(p_{E_{0,0}^t}(\underline{X})) = \text{Tr}(X_0^4) = 0$  implies  $X_0 = 0$ . Moreover, using the fact that  $A_u^t$  has rank 1 we see that the condition  $\text{Tr}(p_{A_u^t}(\underline{X})) = 0$  implies  $\text{Tr}((X_0^2 - \sum_{i=1}^t X_{ui}^2)^2) = 0$  and thus  $X_0^2 = \sum_{i=1}^t X_{ui}^2$ . Combining both relations we deduce that  $X_{ui} = 0$  for all  $u, i$ , i.e.,  $\underline{X} = 0$ . Thus we can conclude that  $(M')^t \in \mathcal{CS}_+^*$ .

Next, observe that  $(M')^t = tE_{0,0}^t - \lambda_t E_{0,0}^t - \mu_t A^t - \sum y_{u,v,i}^t E_{ui,vi}^t - \sum z_{u,i,j}^t E_{ui,vi}^t$ , where  $\lambda_t = t - \frac{t}{t+\epsilon}(t - \lambda + \epsilon) = \frac{t}{t+\epsilon}\lambda$ , and  $\mu_t = \frac{t}{t+\epsilon}(\mu - \epsilon)$ . We now need to modify each  $(M')^t$  in order to replace  $\lambda_t$  by  $\lambda'$  (not depending on  $t$ ) and to replace  $\mu_t$  by  $\mu'$  (not depending on  $t$ ).

As  $\lambda_t \geq \frac{\lambda}{1+\epsilon}$ , we can add to  $(M')^t$  the matrix  $(\lambda_t - \frac{\lambda}{1+\epsilon})E_{0,0}^t \in \mathcal{CS}_+^*$  to get a new matrix  $(M'')^t$  where the coefficient of  $-E_{0,0}^t$  is equal to  $\lambda' := \frac{\lambda}{1+\epsilon}$ .

If  $\mu - \epsilon \leq 0$ , we add to  $(M'')^t$  the matrix  $-\mu_t A^t \in \mathcal{CS}_+^*$ , and in that case we can choose  $\mu' = 0$ . If  $\mu - \epsilon \geq 0$ , then  $\mu_t \geq \frac{\mu - \epsilon}{1+\epsilon}$  and we add to  $(M'')^t$  the matrix  $(\mu_t - \frac{\mu - \epsilon}{1+\epsilon})A^t \in \mathcal{CS}_+^*$ , and in that case we can choose  $\mu' = \frac{\mu - \epsilon}{1+\epsilon}$ .

Hence we now have constructed a solution to the program (4.6) with value  $\lambda' = \frac{\lambda}{1+\epsilon}$ . This shows that  $\chi_q(G) \geq \frac{\lambda}{1+\epsilon}$  and thus  $\chi_q(G) \geq \frac{\Psi_\epsilon^{(r)}(G)}{1+\epsilon}$ .  $\square$

The above discussion for  $\chi_q(G)$  extends directly to the parameter  $\chi^*(G)$ : Rewrite  $\chi^*(G)$  as the optimal value of the program (4.5), where we omit the last set of conditions:  $\langle \tilde{E}_{ui,uj}^t, X \rangle = 0$  (for  $u \in V(G)$ ,  $i \neq j \in [t]$ ,  $t \in [n]$ ), or equivalently as the optimal value of the dual program (4.6), where we set all variables  $z_{u,i,j}^t$  to 0. Denote by  $\Psi_\epsilon^{*(r)}(G)$  the optimal value of this modified dual program where we replace  $\mathcal{CS}_+^*$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$ . Then the following partial analogue of Proposition 4.17 holds.

**Proposition 4.18.** *For  $\epsilon > 0$ ,  $r \in \mathbb{N}$  and any graph  $G$  (with  $n = |V(G)|$ ), we have*

$$\chi^*(G) \geq \frac{1}{1+\epsilon} \Psi_\epsilon^{*(r)}(G). \quad (4.9)$$

Moreover,  $\Psi_0^{*(r)}(G) = \lceil \vartheta^+(\overline{G}) \rceil$  and  $\chi^*(G) \geq \Psi_\epsilon^{*(r)}(G)$  for any  $\epsilon < 1/(n-1)$ .

It is not clear whether the inequality (4.7) extends to the parameter  $\chi^*(G)$ , i.e., whether  $\Psi^{*(r)} \geq \Phi_\epsilon^{(r)}(G)$  holds. Indeed we do not know if the implication (iii)  $\Rightarrow$  (i) from Proposition 4.9 still holds when using the cone  $\mathcal{K} = \mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  (because for this we would need the analogue of Theorem 4.3 with  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$  instead of  $\mathcal{CP}$ ).

We now turn to the parameters  $\alpha_q(G)$  and  $\alpha^*(G)$ . As above, consider the matrices  $D_i^t \in \mathcal{S}^{nt+1}$  (for  $t \in [n]$ ,  $i \in [t]$ ), with entries  $(D_i^t)_{0,0} = 1$ ,  $(D_i^t)_{0,ui} = -1$ ,

$(D_i^t)_{ui,vi} = 1$  for  $u, v \in V(G)$  (thus the analogues of the matrices  $A_u^t$ , interchanging the role of nodes  $u \in V(G)$  and indices  $i \in [t]$ ). Set  $D^t = \sum_{i=1}^t D_i^t$  and  $D = \bigoplus_{t=1}^n D^t$ . Then we can rewrite the program (4.4) as follows:

$$\begin{aligned} \alpha_q(G) = \max \langle C, X \rangle \quad \text{s.t.} \quad & X \in \mathcal{CS}_+^N, \quad \langle B, X \rangle = 1, \quad \langle D, X \rangle = 0, \\ & \langle \tilde{E}_{ui,vj}^t, X \rangle = 0 \quad \forall i \neq j \in [t], \forall u \simeq v \in V(G), \forall t \in [n], \\ & \langle \tilde{E}_{ui,vi}^t, X \rangle = 0 \quad \forall i \in [t], \forall u \neq v \in V(G), \forall t \in [n], \end{aligned} \quad (4.10)$$

with dual formulation:

$$\alpha_q(G) = \min \lambda \quad \text{s.t.} \quad M = C - \lambda B - \mu D - \sum y_{u,v,i,j}^t \tilde{E}_{ui,vj}^t - \sum z_{u,i,j}^t \tilde{E}_{ui,uj}^t \in \mathcal{CS}_+^{N*} \quad (4.11)$$

(with the obvious summations). Here we have used the fact that strong duality holds since (4.11) is strictly feasible (analogous argument as for  $\chi_q(G)$ ).

The analogue of Lemma 4.14 holds when replacing  $\mathcal{CS}_+$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ . Therefore, the parameter  $\psi_\epsilon^{(r)}(G)$  is equal to the optimal value of the program (4.10), where we replace  $\mathcal{CS}_+$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)}$ , and also to the optimal value of (4.11), where we replace  $\mathcal{CS}_+^*$  by  $\mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ . The analogue statement holds for the parameter  $\alpha^*(G)$ , omitting in (4.10) the conditions  $\langle \tilde{E}_{ui,vi}^t, X \rangle = 0$  (for  $i \in [t], u \neq v \in V(G), t \in [n]$ ), and setting the variables  $z$  to 0 in program (4.11). (It is now not clear if strong duality holds, however this does not impact the result of Lemma 4.19 below.) As for the quantum chromatic number we can show the following relationship to the quantum stability numbers (whose proof is omitted since it is along the same lines as above).

**Proposition 4.19.** *For  $\epsilon > 0$ ,  $r \in \mathbb{N}$  and any graph  $G$  (with  $n = |V(G)|$ ), we have*

$$\alpha_q(G) \leq \alpha^*(G) \leq \frac{1}{1+\epsilon} \psi_\epsilon^{(r)}(G). \quad (4.12)$$

Therefore,  $\alpha_q(G) \leq \alpha^*(G) \leq \psi_\epsilon^{(r)}(G)$  for any  $\epsilon < \frac{1}{n-1}$ . Moreover,  $\psi_0^{(r)}(G) = \psi_0^{*(r)}(G) = \lfloor \vartheta'(G) \rfloor$ .

Finally, we cannot show the inequality  $\psi_\epsilon^{(r)}(G) \leq \varphi_\epsilon^{(r)}(G)$ , since we do not know whether the implication (ii)  $\Rightarrow$  (i) from Proposition 4.4 extends to the case  $\mathcal{K} = \mathcal{K}_{\text{nc},\epsilon}^{(r)*}$ .

## 5 Concluding remarks

We have introduced the cone  $\mathcal{CS}_+$  of completely positive semidefinite matrices and studied some first basic properties. However, the structure of this cone remains largely unknown. The first fundamental open question is to settle whether the cone  $\mathcal{CS}_+$  is closed. A closely related open question is whether the existence of a Gram representation by *infinite* psd matrices in  $\mathcal{S}^{\mathbb{N}}$  implies the existence of another Gram representation by *finite* psd matrices. The answer is positive if  $\mathcal{CS}_+$  is closed (in view of Theorem 3.3). This question is quite similar in spirit to several open problems in the quantum information literature (see e.g. [47, 56]).

To fix ideas (but the same would apply to the other quantum graph parameters), consider the definition of the quantum chromatic number  $\chi_q(G)$  from Definition 2.7

where, instead of requiring that  $\rho, \rho_u^i$  lie in  $\mathcal{S}_+^d$  (for some  $d \geq 1$ ), we require that  $\rho, \rho_u^i$  lie in  $\mathcal{S}_+^{\mathbb{N}}$ , and denote by  $\chi_q^\infty(G)$  the resulting parameter. Then,  $\chi_q^\infty(G)$  can be formulated as linear optimization over an affine section of the cone  $\mathcal{CS}_{\infty+}$  (the analogue of the fact that  $\chi_q(G)$  can be formulated as linear optimization over an affine section of  $\mathcal{CS}_+$ ). Hence,  $\chi_q^\infty(G) \leq \chi_q(G)$ , with equality if  $\mathcal{CS}_+ = \mathcal{CS}_{\infty+}$ . Moreover, observe that if in the definition of  $\chi_q(G)$  we would require that  $\rho, \rho_u^i$  are positive compact operators on a Hilbert space  $H$  and we rewrite the orthogonality conditions as  $\rho_u^i \rho_v^i = 0$  (for  $\{u, v\} \in E(G), i \in [t]$ ) and  $\rho_u^i \rho_u^j = 0$  (for  $i \neq j \in [t], u \in V(G)$ ), then we would get again the parameter  $\chi_q^\infty(G)$ .

Indeed, by the first Hilbert-Schmidt theorem (see e.g. [28, Thm 6.2.3]), the Hilbert space  $H$  can be decomposed as  $H = \ker \rho \oplus H'$ , where  $H'$  is the closure of the image of  $\rho$  and admits an orthonormal base  $\{e_k : k \in \mathbb{N}\}$  consisting of the eigenvectors of  $\rho$ . Let  $\rho', \rho_u^i$  denote the restrictions of  $\rho, \rho_u^i$  to  $H'$ . Then,  $\rho' \neq 0$  and  $\rho', \rho_u^i$  are positive operators on  $H'$ . Moreover, the operators  $\rho_u^i$  satisfy the same orthogonality conditions as the operators  $\rho_u^i$  (since  $\ker \rho \subseteq \ker \rho_u^i$  for all  $u, i$ , which follows from positivity and the fact that  $\rho = \sum_i \rho_u^i$  for all  $u$ ). Finally, using the base  $\{e_k : k \in \mathbb{N}\}$  of  $H'$ , the operators  $\rho', \rho_u^i$  can be identified with matrices in  $\mathcal{S}_+^{\mathbb{N}}$ .

We saw earlier that in the definition of the parameters  $\vartheta^{\mathcal{K}}(G)$  and  $\Theta^{\mathcal{K}}(G)$  we can replace the cone  $\mathcal{K}$  by its closure without changing the value of the parameter; this applies in particular to the cone  $\mathcal{K} = \mathcal{CS}_+$  (see Lemma 2.4). In contrast, we point out that we do not know whether we can replace the cone  $\mathcal{CS}_+$  by its closure, for instance in Lemma 4.13. Denoting by  $\mathcal{A}$  the affine space defined by the affine conditions in program (4.3),  $\chi_q(G)$  is the minimum value of the objective function taken over  $\mathcal{CS}_+ \cap \mathcal{A}$ , which in turn is equal to the minimum value taken over the closure of  $\mathcal{CS}_+ \cap \mathcal{A}$ . Clearly,  $\text{cl}(\mathcal{CS}_+ \cap \mathcal{A}) \subseteq \mathcal{A} \cap \text{cl}(\mathcal{CS}_+)$ . However we cannot prove that equality holds. If we could prove equality then this would imply that the two parameters  $\chi_q(G)$  and  $\chi_q^\infty(G)$  coincide.

A different but equally interesting problem is, given a matrix  $A \in \mathcal{CS}_+$ , to find upper bounds on the smallest dimension  $d$  of the matrices forming a Gram representation of  $A$ . This corresponds to giving an upper bound on the amount of entanglement needed to perform certain protocols [20].

We have studied quantum analogues of several classical graph parameters and introduced some hierarchies of approximations that can be computed using semidefinite programming. These hierarchies of approximations represent the first strengthenings of the known bounds (in terms of the theta number) for the quantum graph parameters.

In particular, we have extended the well known lower bound  $\chi(G) \geq \vartheta^+(\overline{G})$  to the quantum setting. We showed that  $\chi_q(G) \geq \Theta^{\mathcal{CS}_+}(G)$  and we could relate their respective hierarchical bounds:  $\Psi_\epsilon^{(r)}(G) \geq \Phi_\epsilon^{(r)}(G)$  for any  $\epsilon \geq 0$  and  $r \in \mathbb{N}$ , the case  $\epsilon = 0$  giving back the theta number:  $\Psi_0^{(r)}(G) = \Phi_0^{(r)}(G) = \vartheta^+(\overline{G})$ . We have introduced analogous hierarchical bounds for the other quantum parameters, however the exact links between the various bounds remain elusive. Finally, while in the classical (commutative) setting the hierarchical bounds are known to converge to the classical graph parameters (thanks to results about positive polynomials of Pólya and Schmüdgen), the convergence in the non-commutative setting of these approximations to the quantum graph parameters is open and relies on the celebrated Connes' embedding conjecture. At last let us mention that this is not the

first result that connects this conjecture to a problem related to quantum information theory. As shown in [39], a fundamental physical problem posed by Tsirelson regarding two mathematical models of quantum mechanics is essentially equivalent to Connes' embedding conjecture.

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