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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 cone $\mathcal{CS}_+^n$, a new matrix cone consisting of all $n \times n$ matrices that admit a Gram representation by positive semidefinite matrices (of any size). In particular we study relationships between this cone and the completely positive and doubly nonnegative cones, and between its dual cone and trace positive non-commutative polynomials.

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 can formulate these quantum parameters as conic linear programs over the cone $\mathcal{CS}_+^n$. Using this conic approach we can recover the bounds in terms of the theta number and define further approximations by exploiting the link to trace positive polynomials.

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

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 investigated, 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 $\chi_q(G)$ (introduced in [9]). Given a graph $G = (V, E)$ and an integer $t \geq 1$, consider the following conditions in the variables x_u^i (for $u \in V$ and $i \in [t] = \{1, \ldots, t\}$):

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

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If the variables are 0/1-valued then these conditions are encoding the fact that each vertex of G receives just one out of t possible colors and that 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, $\chi(G) \geq \chi_q(G)$.

It is well known that computing the chromatic number $\chi(G)$ is an NP-hard problem and very recently this hardness result has been extended to the quantum chromatic number $\chi_q(G)$ [27]. Therefore it is of interest to be able to compute good approximations for these parameters. In the classical case, several converging hierarchies of approximations have been proposed for $\chi(G)$ based on semidefinite programming (see [19, 25]). They refine the well known bounds based on the theta number of Lovász [36] and its strengthening by Szegedy [48]: $\chi(G) \geq \vartheta^+(\overline{G}) \geq \vartheta(\overline{G})$. It was shown recently in [45] that the theta number also bounds the quantum chromatic number:

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

This raises naturally the question of constructing further semidefinite programming based bounds for $\chi_q(G)$, strengthening the theta number. The parameter $\chi_q(G)$ derives from a specific nonlocal game and the general problem of finding approximations to the quantum value of any nonlocal game is a very interesting and difficult one. Positive results in this direction have been achieved in [16, 40] where they introduce semidefinite hierarchies converging to a relaxation of the quantum value of the game. The convergence of these hierarchies to the quantum value itself relies on an open problem in mathematical physics, commonly known as Tsirelson's problem.

Here we take a different approach exploiting the particular structure of the quantum graph parameters considered. The main idea is to reformulate the quantum graph parameter $\chi_q(G)$ as a conic optimization problem over a new matrix cone, the cone $\mathcal{CS}_+$, that we call the *completely positive semidefinite cone*. The study of this matrix cone and its use for building approximations is the 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* $x_1, \ldots, x_n \in \mathbb{R}^d$ (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* $x_1, \ldots, x_n \in \mathcal{S}_+^d$ 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 $\mathcal{CS}_+^n$ 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 $\mathcal{DNN}^n$ (consisting of all matrices that are both psd and nonnegative):

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathrm{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{DNN}^n.$$

In what follows we may omit the superscript and write $\mathcal{CP}, \mathcal{CS}_+, \mathcal{DNN}$ when we do not need to explicitly mention the size n of the matrices. As is well known, $\mathcal{DNN}^n = \mathcal{CP}^n$ for $n \leq 4$ and strict inclusion holds for $n \geq 5$ [15, 38]. Fawzi and Parrilo [21] gave recently an example of a 5×5 matrix which is completely positive semidefinite but not completely positive. We construct a class of 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 [19]) where we select the cone $\mathcal{K} = \mathcal{CS}_+$ or its closure, and to apply them for the case when G is the 5-cycle (see Lemma 3.10 and its proof).

Using the completely psd cone $\mathcal{CS}_+$ we can reformulate the quantum chromatic number $\chi_q(G)$ as a linear optimization problem over affine sections of the cone $\mathcal{CS}_+$. The idea is simple and goes as follows: 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 $\mathcal{CS}_+$. By replacing in the conic linear program defining $\chi_q(G)$ the cone $\mathcal{CS}_+$ by its closure $\mathrm{cl}(\mathcal{CS}_+)$, we obtain a new parameter $\widetilde{\chi}_q(G)$, which satisfies $\chi_q(G) \geq \widetilde{\chi}_q(G)$. This new parameter $\widetilde{\chi}_q(G)$ can be equivalently formulated in terms of the dual conic program, since strong duality holds (while we do not know if this is the case for the program defining $\chi_q(G)$). The dual conic program is over the dual cone $\mathcal{CS}_+^*$. As we explain below, $\mathcal{CS}_+^*$ can be interpreted in terms of trace positive polynomials, which naturally opens the way to semidefinite based approximations.

The dual cone $\mathcal{CS}_+^{n*}$ of the completely psd cone $\mathcal{CS}_+^n$ has a useful interpretation in terms of *trace 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 $X_1, \ldots, X_n$. 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 $X_1, \ldots, X_n \in \mathcal{S}^d$ (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 [6, 8]. A sufficient condition for trace positivity of p_M is that p_M belongs to the *tracial quadratic module* $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$ (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.

It is shown in [28, 7, 6] that a celebrated conjecture of Connes in operator algebra is equivalent to showing that, for any non-commutative polynomial p which is trace positive, the polynomial $p + \epsilon$ belongs to $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$ for all $\epsilon > 0$. This motivates our definition of the convex set $\mathcal{K}_{\mathrm{nc},\epsilon}$, which consists of all matrices M for which the perturbed polynomial $p_M + \epsilon$ belongs to the set $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$. Then, the inclusion $\bigcap_{\epsilon>0} \mathcal{K}_{\mathrm{nc},\epsilon} \subseteq \mathcal{CS}_+^*$ holds, with equality if Connes' conjecture holds.

Using these sets $\mathcal{K}_{\mathrm{nc},\epsilon}$, we can define the parameters $\Psi_\epsilon(G)$. Namely, $\Psi_\epsilon(G)$ is obtained by considering the (dual) optimization program over $\mathcal{CS}_+^*$ which defines $\widetilde{\chi}_q(G)$ and replacing in it the cone $\mathcal{CS}_+^*$ by the convex set $\mathcal{K}_{\mathrm{nc},\epsilon}$ (see Definition 4.16). Note that each parameter $\Psi_\epsilon(G)$ can be obtained as the limit of a converging hierarchy of semidefinite programs obtained by introducing degree constraints on the terms in the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$. Unfortunately, as there is no apparent inclusion relationship between $\mathcal{CS}_+^*$ and $\mathcal{K}_{\mathrm{nc},\epsilon}$, we do not know how $\Psi_\epsilon(G)$ compares to $\widetilde{\chi}_q(G)$ (and even less so to $\chi_q(G)$). However, if Connes' conjecture holds, then we have that $\widetilde{\chi}_q(G) \leq \inf_{\epsilon>0} \Psi_\epsilon(G)$. Moreover, $\Psi_\epsilon(G)$ relates to the theta number: $\Psi_\epsilon(G) \geq \vartheta^+(\overline{G})$ (see (4.5)).

Hence devising converging semidefinite approximations for the quantum coloring number is much harder than for its classical counterpart and our results can be seen as a first step in this direction. This difficulty should be put in a broader context and in the light of the general difficulty of approximating the quantum value of nonlocal games as mentioned earlier.

Our main motivation for studying the cone $\mathcal{CS}_+$ comes from its relevance to the quantum graph parameters. There is however a further connection of this cone to the widely studied notion of factorizations of nonnegative matrices. Given a nonnegative $m \times n$ matrix M, a *nonnegative factorization* (resp., a *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* of a factorization (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 by their relevance to linear and semidefinite extended formulations of polytopes, see e.g. [22, 24] 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 $\mathcal{DNN}$. 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 $\mathcal{CS}_+$. We discuss its basic properties (Section 3.1), the links with $\mathcal{CP}$ and $\mathcal{DNN}$ (Section 3.2), the dual cone $\mathcal{CS}_+^*$ and its link to trace positive polynomials (Section 3.3), and the convex sets $\mathcal{K}_{\text{nc},\epsilon}$ (Section 3.4).

Section 4 shows how to reformulate the quantum graph parameters using linear optimization over affine sections of the cone $\mathcal{CS}_+$. First, we reformulate the quantum parameters as checking feasibility of a sequence of conic programs over sections of $\mathcal{CS}_+$; this is done in Section 4.1 for the quantum stability numbers and in Section 4.2 for the quantum chromatic numbers. We also show there how to recover the known bounds for the quantum graph parameters in terms of the theta number by replacing the cone $\mathcal{CS}_+$ by the doubly nonnegative cone and establish new bounds given by the parameters $\vartheta^{\mathcal{CS}_+}(G)$ and $\Theta^{\mathcal{CS}_+}(G)$. In Section 4.3, we build a single 'aggregated' optimization program permitting to express the quantum parameter $\chi_q(G)$. The conic dual of this program is then used to define the parameter $\Psi_\epsilon(G)$, which is obtained by replacing in this program the cone $\mathcal{CS}_+^*$ by the convex set $\mathcal{K}_{\text{nc},\epsilon}$.

Section 5 groups some concluding remarks and closes the paper.

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 $S_1, \ldots, S_k$ of G and nonnegative scalars $\lambda_1, \ldots, \lambda_k$ such that $\sum_{h: v \in S_h} \lambda_h = 1$ for all $v \in V(G)$. Clearly, $\omega(G) \le \chi_f(G) \le \chi(G)$.

For $t \in \mathbb{N}$, we set $[t] = \{1, \ldots, t\}$ and K_t denotes the complete graph on $[t]$. 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 ($u = v$ and $i \ne j$) or if ($u \sim v$ and $i = j$).

Cones and matrices. Throughout, $\mathbb{R}^n_+$ denotes the set of (entrywise) nonnegative vectors, $e_1, \ldots, e_n$ 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: $\langle X, Y \rangle = \mathsf{Tr}(XY) = \sum_{i,j=1}^n X_{ij} Y_{ij}$ 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 $\mathcal{DNN}^n$, 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 $x_1, \ldots, x_n \in \mathbb{R}^d$ (for some $d \ge 1$) such that $X_{ij} = \langle x_i, x_j \rangle$ for all $i, j \in [n]$, in which case we say that $x_1, \ldots, x_n$ form a *Gram representation* of X and we call X the *Gram matrix* of $x_1, \ldots, x_n$. Furthermore, $X \in \mathcal{S}^n$ is said to be *completely positive* if X is the Gram matrix of a set of *nonnegative* vectors $x_1, \ldots, x_n \in \mathbb{R}^d_+$ (for some $d \ge 1$). We let $\mathcal{CP}^n$ denote the set of completely positive matrices. $\mathcal{S}^n_+$, $\mathcal{DNN}^n$ and $\mathcal{CP}^n$ are convex cones. We may sometimes omit the superscript and use the notation $\mathcal{S}_+$, $\mathcal{DNN}$ and $\mathcal{CP}$.

For a pair of matrices X, Y, $X \oplus Y = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$ denotes their direct sum, and $X \otimes Y$ their

Kronecker product, defined as the block matrix $X \otimes Y = \begin{pmatrix} X_{11}Y & \dots & X_{1n}Y \\ \vdots & \ddots & \vdots \\ X_{m1}Y & \dots & X_{mn}Y \end{pmatrix}$ 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 $X \in \mathcal{S}^n$ of the form $X = \begin{pmatrix} \alpha & b^T \\ b & A \end{pmatrix}$, where $b \in \mathbb{R}^{n-1}$, $A \in \mathcal{S}^{n-1}$ and $\alpha > 0$,

$$X \succeq 0 \iff A - bb^T/\alpha \succeq 0. \tag{1.2}$$

The matrix $A - bb^T/\alpha$ is called the Schur complement of A in X w.r.t. the entry α.

Given a cone $\mathcal{K} \subseteq \mathcal{S}^n$, its dual cone is the cone $\mathcal{K}^* = \{X \in S^n : \langle X, Y \rangle \geq 0 \quad \forall Y \in \mathcal{K}\}$. Recall that the cone $\mathcal{S}^n_+$ is self-dual, i.e., $\mathcal{S}^{n*}_+ = \mathcal{S}^n_+$. 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 $\mathcal{K}$ (i.e., $\mathcal{K}$ is closed, convex, pointed and full-dimensional):

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

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

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 result of Chvátal [10] which shows how to relate the chromatic number of G to the stability number of the Cartesian product $G \square K_t$.

Theorem 2.1. *[10] For any graph G and any integer $t \geq 1$, $\chi(G) \leq t \iff \alpha(G \square K_t) = |V(G)|$. 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 [30].

Theorem 2.2. *[30] For any graph G, its stability number $\alpha(G)$ is equal to the optimum value of the following program:*

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

In the same vein, Dukanovic and Rendl [19] gave the following reformulation for the fractional chromatic number $\chi_f(G)$.

Theorem 2.3. *[19] For any graph G, its fractional chromatic number $\chi_f(G)$ is equal to the optimum value of the following program:*

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

A well known bound for both the stability and the (fractional) chromatic numbers is provided by the celebrated theta number ϑ of Lovász [36], who showed the following 'sandwich' inequalities:

$$\alpha(G) \leq \vartheta(G) \leq \chi_f(\overline{G}) \leq \chi(\overline{G}). \tag{2.2}$$

Between the many equivalent formulations of the theta number, the following will be appropriate for our setting:

$$\begin{aligned} \vartheta(G) = \max \quad & \langle J, X\rangle & = \min \quad & t \\ \text{s.t.} \quad & X \succeq 0 & \text{s.t.} \quad & Z \succeq 0,\ Z - J \succeq 0 \\ & \mathsf{Tr}(X) = 1 & & Z_{uu} = t \ \ \forall\, u \in V(G) \\ & X_{uv} = 0 \ \ \forall\,\{u,v\} \in E(G); & & Z_{uv} = 0 \ \ \forall\,\{u,v\} \in E(\overline{G}). \end{aligned} \tag{2.3}$$

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 [47] and McEliece et al. [39] and $\vartheta^+(G)$ introduced by Szegedy [48]:

$$\begin{aligned} \vartheta'(G) = \max \quad & \langle J, X\rangle & \vartheta^+(G) = \min \quad & t \\ \text{s.t.} \quad & X \in \mathcal{DNN}^n & \text{s.t.} \quad & Z \in \mathcal{DNN}^n,\ Z - J \succeq 0 \\ & \mathsf{Tr}(X) = 1 & & Z_{uu} = t \ \ \forall\, u \in V(G) \\ & X_{uv} = 0 \ \ \forall\,\{u,v\} \in E(G); & & Z_{uv} = 0 \ \ \forall\,\{u,v\} \in E(\overline{G}). \end{aligned} \tag{2.4}$$

The following inequalities hold, which refine (2.2):

$$\alpha(G) \le \vartheta'(G) \le \vartheta(G) \le \vartheta^+(G) \le \chi_f(\overline{G}) \le \chi(\overline{G}). \tag{2.5}$$

Following [19], we now introduce the following conic programs (2.6), which are obtained by replacing in the above programs (2.3) 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, 4.1 and 4.2:

$$\begin{aligned} \vartheta^{\mathcal{K}}(G) = \sup \ & \langle J, X\rangle & \Theta^{\mathcal{K}}(G) = \inf \ \ & t \\ \text{s.t.} \ & X \in \mathcal{K}^n & \text{s.t.} \ \ & Z \in \mathcal{K}^n,\ Z - J \succeq 0 \\ & \mathsf{Tr}(X) = 1 & & Z_{uu} = t \ \ \forall\, u \in V(G) \\ & X_{uv} = 0 \ \ \forall\ \{u,v\} \in E(G); & & Z_{uv} = 0 \ \ \forall\ \{u,v\} \in E(G). \end{aligned} \tag{2.6}$$

If in the relations from (2.6), 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 $\vartheta'(G)$, $\alpha(G)$, $\vartheta^+(\overline{G})$, $\chi_f(G)$. That is,

$$\vartheta^{\mathcal{DNN}}(G) = \vartheta'(G),\ \vartheta^{\mathcal{CP}}(G) = \alpha(G),\ \Theta^{\mathcal{DNN}}(G) = \vartheta^+(\overline{G}),\ \Theta^{\mathcal{CP}}(G) = \chi_f(G). \tag{2.7}$$

We now show that in both programs of (2.6) 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 $\mathcal{DNN}$ and its closure* $\mathrm{cl}(\mathcal{K})$*. For any graph G, we have $\vartheta^{\mathcal{K}}(G) = \vartheta^{\mathrm{cl}(\mathcal{K})}(G)$ and $\Theta^{\mathcal{K}}(G) = \Theta^{\mathrm{cl}(\mathcal{K})}(G)$.*

Proof. We first show equality $\vartheta^{\mathcal{K}}(G) = \vartheta^{\mathrm{cl}(\mathcal{K})}(G)$. The inequality $\vartheta^{\mathcal{K}}(G) \le \vartheta^{\mathrm{cl}(\mathcal{K})}(G)$ is clear. We show the reverse inequality. For this denote by $\mathcal{A}$ the affine space defined by the conditions $\mathsf{Tr}(X) = 1$ and $X_{uv} = 0$ for $\{u,v\} \in E(G)$. Let $A \in \mathrm{cl}(\mathcal{K}) \cap \mathcal{A}$, we show that $A \in \mathrm{cl}(\mathcal{K} \cap \mathcal{A})$. 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 $0 \le \lambda \le 1$. We claim that $A_\lambda \in \mathcal{K}$ if $0 \le \lambda < 1$. 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 $\langle M, A\rangle \ge 0$ since $A \in \mathrm{cl}(\mathcal{K})$ 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 λ go to 1, A_λ 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 $\vartheta^{\mathcal{K}}(G) \geq \vartheta^{\mathrm{cl}(\mathcal{K})}(G)$.

We now show equality $\Theta^{\mathcal{K}}(G) = \Theta^{\mathrm{cl}(\mathcal{K})}(G)$. Analogously, it suffices to show the inequality $\Theta^{\mathcal{K}}(G) \leq \Theta^{\mathrm{cl}(\mathcal{K})}(G)$. 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 $X \in \mathrm{cl}(\mathcal{K})$ 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, $\Theta^{\mathrm{cl}(\mathcal{K})}(G) \leq \lambda t + (1 - \lambda)n$ for all $0 \leq \lambda < 1$. Letting λ tend to 1 we deduce that $\Theta^{\mathrm{cl}(\mathcal{K})}(G) \leq t$ and thus $\Theta^{\mathrm{cl}(\mathcal{K})}(G) \leq \Theta^{\mathcal{K}}(G)$. □

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 [45])**.** *For a graph G, $\alpha_q(G)$ is 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:*

$$\langle \rho, \rho \rangle = 1, \tag{2.8}$$
$$\sum_{u \in V(G)} \rho_i^u = \rho \quad \forall i \in [t], \tag{2.9}$$
$$\langle \rho_i^u, \rho_j^v \rangle = 0 \quad \forall i \neq j \in [t], \forall u \simeq v \in V(G), \tag{2.10}$$
$$\langle \rho_i^u, \rho_i^v \rangle = 0 \quad \forall i \in [t], \forall u \neq v \in V(G). \tag{2.11}$$

Definition 2.6 (Communication entanglement-assisted stability number [13])**.** *For a graph G, $\alpha^\star(G)$ is 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 (2.8), (2.9) and (2.10).*

Definition 2.7 (Game entanglement-assisted chromatic number [9])**.** *For a graph G, $\chi_q(G)$ is 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:*

$$\langle \rho, \rho \rangle = 1, \tag{2.12}$$
$$\sum_{i \in [t]} \rho_u^i = \rho \quad \forall u \in V(G), \tag{2.13}$$
$$\langle \rho_u^i, \rho_v^i \rangle = 0 \quad \forall i \in [t], \forall \{u, v\} \in E(G), \tag{2.14}$$
$$\langle \rho_u^i, \rho_u^j \rangle = 0 \quad \forall i \neq j \in [t], \forall u \in V(G). \tag{2.15}$$

Definition 2.8 (Communication entanglement-assisted chromatic number [5])**.** *For a graph G, $\chi^\star(G)$ is 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 (2.12), (2.13) and (2.14).*

The parameters $\alpha_q(G)$ and $\chi_q(G)$ can, respectively, be equivalently obtained from the definitions of $\alpha^\star(G)$ and $\chi^\star(G)$ if we require ρ 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 [45] and [9]).

The following inequalities follow from the definitions:

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

Recently, several bounds for the quantum parameters have been established in terms of the theta number. Namely, [3, 18] show that $\alpha^*(G) \leq \vartheta(G)$, [14] shows the tighter bound $\alpha^*(G) \leq \vartheta'(G)$, and [5] shows that $\chi^*(G) \geq \vartheta^+(\overline{G})$. Summarizing, the following sandwich inequalities hold:

$$\alpha(G) \leq \alpha_q(G) \leq \alpha^*(G) \leq \vartheta'(G) \text{ and } \vartheta^+(\overline{G}) \leq \chi^*(G) \leq \chi_q(G) \leq \chi(G). \tag{2.16}$$

Using our approach of reformulating the quantum parameters as optimization problems over the cone $\mathcal{CS}_+$, we will recover these bounds (see Section 4, in particular, Corollaries 4.6 and 4.12).

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 $\alpha_q(G)$ and $\chi_q(G)$ are defined in term of *nonlocal games*, which are mathematical abstractions of a physical experiment introduced by [11]. 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 a question to each of the players. The players, without communicating, must each respond 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? Surprisingly, players that share entanglement can (for some games) produce answers correlated in a way that would be impossible in a classical world. (For an introduction to the topic we recommend the book [41].)

Consider a game where two players want to convince a referee that they can color a graph G with t colors. 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 a 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 (see [9] for details and the equivalence with Definition 2.7). This parameter has recently received a notable amount of attention (see among others [1, 9, 23, 37, 45, 27, 43]).

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 [45].

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 (see [32] for a survey and references therein). Recently Cubitt et al. [13] 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 [13, 33, 5]. Without getting into details, the parameters $\alpha^\star(G)$ and $\chi^\star(G)$ arise in this entanglement-assisted information theory setting. For the full description of the problem and its mathematical formulation we refer to [13] and [5] for $\alpha^\star(G)$ and $\chi^\star(G)$, respectively.

We now briefly summarize some known properties of these parameters. 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. Clearly there is no such separation when G is a perfect graph since then the inequalities (2.5) and (2.16) imply $\alpha(G) = \alpha_q(G) = \alpha^\star(G) = \lfloor \vartheta(G) \rfloor$ and $\lceil \vartheta(\overline{G}) \rceil = \chi^\star(G) = \chi_q(G) = \chi(G)$.

A few separation results are known. For instance, there exist a graph for which $\chi^\star(G) = \chi_q(G) = 3$ but $\chi(G) = 4$ [23], and a family of graphs exhibiting an exponential separation between χ_q and χ [1] (and therefore also between $\chi^\star$ and χ). This family is composed by the *orthogonality graphs* Ω_n (where n is a multiple of 4) whose vertices are all $\{\pm 1\}^n$ vectors and two vertices are adjacent if the vectors are orthogonal. In [37, 45] these graphs are used to construct graphs that exhibit an exponential separation, respectively, between $\alpha^\star$ and α and between α_q and α.

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 [45], 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 $\chi^\star(\Omega_n)\alpha^\star(\Omega_n) < |V(\Omega_n)|$. Finally, the chromatic and stability number are NP-hard quantities and only very recently Ji [27] proved that deciding whether $\chi_q(G) \leq 3$ is an NP-hard problem.

3 The completely positive semidefinite cone

In this section we introduce the completely positive semidefinite cone $\mathcal{CS}_+$ and we establish some of its basic properties and its relation with the completely positive cone and with the doubly nonnegative cone. We also investigate its dual cone $\mathcal{CS}_+^{n*}$ and we introduce the convex sets $\mathcal{K}_{\mathrm{nc},\epsilon}$ aiming to approximate it.

3.1 Basic properties

Recall that for any positive semidefinite matrix A there exists a set of vectors $x_1, \ldots, x_n \in \mathbb{R}^d$ 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 $X_1, \ldots, X_n \in \mathcal{S}_+^d$ (for some $d \geq 1$) such that $A = (\langle X_i, X_j \rangle)_{i,j=1}^n$. Then we also say that $X_1, \ldots, X_n$ form a Gram representation of A. We let $\mathcal{CS}_+^n$ denote the set of all $n \times n$ completely positive semidefinite matrices.*

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

Proof. Let $A, B \in \mathcal{CS}_+^n$ and assume that $X_1, \ldots, X_n \in \mathcal{S}_+^d$ and $Y_1, \ldots, Y_n \in \mathcal{S}_+^k$ form a Gram representation of A and B, respectively. Then, the matrices $X_1 \oplus Y_1, \ldots, X_n \oplus Y_n$ are psd and form a Gram representation of $X + Y$, thus showing that $X + Y \in \mathcal{CS}_+^n$.

Moreover, let $\lambda \geq 0$ and consider the psd matrices $\sqrt{\lambda} X_1, \ldots, \sqrt{\lambda} X_n$. These form a Gram representation of λA, thus showing that $\lambda A \in \mathcal{CS}_+^n$. Hence $\mathcal{CS}_+^n$ is a convex cone. □

As is well known, both $\mathcal{S}_+^n$ and $\mathcal{CP}^n$ are closed sets. This is easy 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 $y_1, \ldots, y_N \in \mathbb{R}_+^n$ 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 positive semidefinite matrices of *finite* size?

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 $n \in \mathbb{N}$, $\mathcal{CS}_+^n \subseteq \mathcal{CS}_{\infty+}^n \subseteq \mathrm{cl}(\mathcal{CS}_{\infty+}^n) = \mathrm{cl}(\mathcal{CS}_+^n)$ 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: $\mathcal{CS}_{\infty+}^n \subseteq \mathrm{cl}(\mathcal{CS}_+^n)$. For this, let $A \in \mathcal{CS}_{\infty+}^n$ and $X_1, \ldots, X_n \in \mathcal{S}_+^{\mathbb{N}}$ 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 $X_i^\ell = X_i[\{1, \ldots, l\}]$ be the $\ell \times \ell$ upper left principal submatrix of X_i and let $\widetilde{X}_i^\ell \in \mathcal{S}^{\mathbb{N}}$ be the infinite matrix obtained by adding zero entries to X_i^ℓ. Thus, $X_i^\ell \in \mathcal{S}_+^\ell$ and $\widetilde{X}_i^\ell \in \mathcal{S}_+^{\mathbb{N}}$. Now, let A^ℓ denote the Gram matrix of $X_1^\ell, \ldots, X_n^\ell$, so that $A^\ell \in \mathcal{CS}_+^n$. We show that the sequence $(A^\ell)_{\ell \geq 1}$ converges to A as ℓ tends to ∞, which shows that $A \in \mathrm{cl}(\mathcal{CS}_+^n)$. Indeed, for any $i, j \in [n]$ and $\ell \in \mathbb{N}$, we have:

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

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

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

3.2 Links to completely positive and doubly nonnegative matrices

The following relationships follow from the definitions:

$$\mathcal{CP}^n \subseteq \mathcal{CS}_+^n \subseteq \mathcal{S}_+^n \cap \mathbb{R}_+^{n\times n} =: \mathcal{DNN}^n. \tag{3.1}$$

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 $X, Y \in \mathcal{S}_+$. Taking duals in (3.1) we get the corresponding inclusions:

$$\mathcal{DNN}^{n*} \subseteq \mathcal{CS}_+^{n*} \subseteq \mathcal{CP}^{n*}. \tag{3.2}$$

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 $x^T Mx \geq 0$ for all $x \in \mathbb{R}_+^n$. The dual of $\mathcal{DNN}^n$ 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 [15] and Maxfield and Minc [38] have shown, respectively, that $\mathcal{CP}^{n*} = \mathcal{DNN}^{n*}$ and $\mathcal{CP}^n = \mathcal{DNN}^n$ for any $n \leq 4$. Hence equality holds throughout in (3.1) and (3.2) for $n \leq 4$. Moreover the inclusions $\mathcal{CP}^n \subseteq \mathcal{DNN}^n$ and $\mathcal{DNN}^{n*} \subseteq \mathcal{CP}^{n*}$ are known to be strict for any $n \geq 5$. It suffices to show the strict inclusions for $n = 5$, since $A \in \mathcal{DNN}^5 \setminus \mathcal{CP}^5$ implies $\widetilde{A} \in \mathcal{DNN}^n \setminus \mathcal{CP}^n$, where $\widetilde{A}$ 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., $\mathcal{DNN}^5$, or $\mathcal{CS}_+^5$) if and only if the extended matrix $\tilde{A}$ belongs to $\mathcal{CP}^n$ (resp., $\mathcal{DNN}^n$, or $\mathcal{CS}_+^n$).

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

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

H is the Horn matrix which, as is well known, is copositive but does not lie in the dual of the doubly nonnegative cone (see e.g. [4]). Moreover, the matrix K is doubly nonnegative but is not completely positive (as observed right after Theorem 3.4). Thus,

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

We will show later in this section that K does not belong to the closure of $\mathcal{CS}_+^5$, thus showing the strict inclusion: $\mathrm{cl}(\mathcal{CS}_+^5) \subset \mathcal{DNN}^5$ (see Lemma 3.10).

The strict inclusion: $\mathcal{CP}^5 \subset \mathcal{CS}_+^5$ is shown by the following matrix, found by Fawzi and Parrilo [21]:

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

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 $x_1, \ldots, x_5$ form a Gram representation of $\widehat{L}$, then the psd matrices $x_1x_1^T, \ldots, x_5x_5^T$ 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,

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

In the rest of this section we will show that the inclusion $\mathrm{cl}(\mathcal{CS}_+^5) \subseteq \mathcal{DNN}^5$ is strict and thus, by taking duals, $\mathcal{DNN}^{5*} \subset \mathcal{CS}_+^{5*}$ (see Corollary 3.11). 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 (see Theorem 3.7 below).

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. *[17] (see also [4]) 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, $X_1, \ldots, X_n \in \mathcal{S}_+^d$ 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, in view of Theorem 3.4, $A \in \mathcal{CP}^n$. $\square$

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 [31] 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., the matrix K in (3.3) has $G(K) = C_5$ and $K \in \mathcal{DNN}^5 \setminus \mathcal{CP}^5$) and any bipartite graph is completely positive. By definition, for any matrix A,

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

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 dimension. If $\langle A, B \rangle = 0$ then $\langle A_1, B_1 \rangle = \langle A_3, B_3 \rangle = -\langle A_2, B_2 \rangle$.

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. $\square$

We can now characterize the completely psd matrices supported by a cycle.

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 $X^1, \ldots, X^n \in \mathcal{S}_+^d$ be a psd Gram representation of A. If n is even, then (as in the above proof of Lemma 3.5), the matrices $Y^1 = -X^1, Y^2 = X^2, Y^3 = -X^3, Y^4 = X^4, \ldots, Y^{n-1} = -X^{n-1}, Y^n = X^n$ 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 $Y^1, \ldots, Y^{n-1}$ 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 now show that the matrices $X^1, \ldots, X^n$ 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 $I_1, \ldots, I_{n-2}$. Indeed, without loss of generality we can assume that $X^1 = \begin{pmatrix} X^1_{11} & 0 \\ 0 & 0 \end{pmatrix}$ where X^1_{11} is positive definite and the index set of X^1_{11} defines the index set I_1 of the first block. Next, X^2 has the form $\begin{pmatrix} X^2_{11} & X^2_{12} & 0 \\ X^2_{21} & X^2_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}$, where $X^2_{22} \succ 0$ (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 $X^3 = \begin{pmatrix} X^3_{11} & X^3_{12} & X^3_{13} & 0 \\ X^3_{21} & X^3_{22} & X^3_{23} & 0 \\ X^3_{31} & X^3_{32} & X^3_{33} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$, where $X^3_{33} \succ 0$ and I_3 is the index set of X^3_{33}. As $A_{13} = 0$, we can conclude that $X^3_{11} = 0$ (and thus $X^3_{12} = X^3_{13} = 0$). Hence X^3 has its blocks indexed by I_1, I_2, I_3 and $[d] \backslash (I_1 \cup I_2 \cup I_3)$ with all zero blocks except $X^3_{22}, X^3_{23}, X^3_{32}$ and X^3_{33}. Iterating, we have that, for each $k \in \{2, 3, \ldots, n-3\}$, all blocks of the matrix X^k are equal to zero except its blocks $X^k_{k-1,k-1}$, $X^k_{k-1,k}$, $X^k_{k,k-1}$ and X^k_{kk} and moreover $X^k_{kk} \succ 0$. The index sets of the blocks X^k_{kk} for $1 \leq k \leq n-3$ define the sets $I_1, I_2, \ldots I_{n-3}$ and the set $I_{n-2} := [d] \backslash (I_1 \cup I_2 \cdots \cup I_{n-3})$ collects all the remaining indices. Using the fact that $\langle X^{n-2}, X^k \rangle = 0$ for each $k \in \{1, \ldots, n-4\}$ we obtain that each block X^{n-2}_{kk} is equal to zero. Similarly X^{n-1}_{kk} is the zero matrix for every $k \in \{1, \ldots, n-3\}$ as $\langle X^{n-1}, X^k \rangle = 0$. For the matrix X^n we cannot make any consideration on the presence of zero blocks.

We now indicate how to construct the (non-symmetric) matrix Y^n from X^n: we just resign its two blocks $X^n_{n-3,n-2}$ and $X^n_{n-2,n-2}$. In other words, we let Y^n be the $(n-2) \times (n-2)$ block matrix with blocks $Y^n_{n-3,n-2} = -X^n_{n-3,n-2}$, $Y^n_{n-2,n-2} = -X^n_{n-2,n-2}$ and $Y^n_{rs} = X^n_{rs}$ for all other blocks. Let us stress that in particular we do not change the sign of the block $X^n_{n-2,n-3}$. 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 $Y^1, \ldots, Y^n$ 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 $Y^i_{r,n-2}$ 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

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

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

$$\langle Y^{n-2}, Y^n \rangle = \langle \begin{pmatrix} -X^{n-2}_{n-3,n-3} & -X^{n-2}_{n-3,n-2} \\ -X^{n-2}_{n-2,n-3} & -X^{n-2}_{n-2,n-2} \end{pmatrix}, \begin{pmatrix} X^n_{n-3,n-3} & -X^n_{n-3,n-2} \\ X^n_{n-2,n-3} & -X^n_{n-2,n-2} \end{pmatrix} \rangle$$

is equal to 0. ◻

Consequently, the matrix K in (3.3) is not completely psd (using Theorem 3.7, since $G(K) = C_5$ and $K \notin \mathcal{CP}^5$). Furthermore, Lemma 3.9 below gives a class of matrices in $\mathcal{DNN}^n \setminus \mathcal{CS}^n_+$ obtained by combining Theorem 3.7 with the next result.

Theorem 3.8. *[26] Assume $n \geq 5$ is odd and consider a matrix $A \in \mathcal{DNN}^n$ with rank $n-2$. Then, A lies on an extreme ray of $\mathcal{DNN}^n$ if and only if $G(A) = C_n$.*

Lemma 3.9. *For odd $n \geq 5$, any matrix A lying on an extreme ray of $\mathcal{DNN}^n$ with rank $n-2$ is not completely positive semidefinite.*

Proof. Assume A lies on an extreme ray of $\mathcal{DNN}^n$, $\operatorname{rank} A = n-2$ and $A \in \mathcal{CS}^n_+$. Then, $G(A) = C_n$ by Theorem 3.8 and thus $A \in \mathcal{CP}^n$ by Theorem 3.7. Moreover, A lies on an extreme ray of $\mathcal{CP}^n$, so that $\operatorname{rank} A = 1$, a contradiction. ◻

For instance, the following matrix

$$A = \begin{pmatrix} 6 & 3 & 0 & 0 & 3 \\ 3 & 6 & 3 & 0 & 0 \\ 0 & 3 & 3 & 4 & 0 \\ 0 & 0 & 4 & 16 & 4 \\ 3 & 0 & 0 & 4 & 3 \end{pmatrix} \tag{3.5}$$

satisfies the conditions of Theorem 3.8 and thus $A \in \mathcal{DNN}^5 \setminus \mathcal{CS}_+^5$. As any matrix lying on an extreme ray of $\mathcal{DNN}^5$ has rank 1 or 3 [26], Lemma 3.9 gives a broad class of matrices in $\mathcal{DNN}^5 \setminus \mathcal{CS}_+^5$.

We now show that the matrix K in (3.3) does not belong to the closure of $\mathcal{CS}_+^5$. For this we use the parameter $\vartheta^{\mathcal{K}}(G)$ introduced earlier in (2.6), selecting for $\mathcal{K}$ the cones $\mathcal{CS}_+$, $\mathrm{cl}(\mathcal{CS}_+)$ and $\mathcal{CP}$, and we prove the next result.

Lemma 3.10. *Let $X \in \mathcal{DNN}^5$ and assume that the support of X is the cycle C_5 and that $\langle J - 2I, X\rangle > 0$. Then, $X \notin \mathrm{cl}(\mathcal{CS}_+^5)$.*

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 (2.6) of $\vartheta^{\mathcal{CS}_+}(C_5)$ is completely positive. Assume that there exists a matrix $X \in \mathrm{cl}(\mathcal{CS}_+^5)$ whose support is C_5 and such that $\langle J-2I, X\rangle > 0$. Then the matrix $X/\operatorname{Tr}(X)$ is feasible for the definition of the parameter $\vartheta^{\mathrm{cl}(\mathcal{CS}_+)}(C_5)$ and thus $\vartheta^{\mathrm{cl}(\mathcal{CS}_+)}(C_5) \geq \langle J, X\rangle/\operatorname{Tr}(X) > 2$. Applying Lemma 2.4, we obtain that $\vartheta^{\mathcal{CS}_+}(C_5) = \vartheta^{\mathrm{cl}(\mathcal{CS}_+)}(C_5) > 2$, thus reaching a contradiction. □

As an application, the matrix K in (3.3) does not belong to $\mathrm{cl}(\mathcal{CS}_+^5)$, since $K \in \mathcal{DNN}^5$ with $G(K) = C_5$ and $\langle J-2I, K\rangle > 0$. This does not apply to the matrix A in (3.5) since $\langle J-2I, A\rangle = 0$, so we do not know whether $A \in \mathrm{cl}(\mathcal{CS}_+^5)$ or not.

Corollary 3.11. *The inclusions $\mathrm{cl}(\mathcal{CS}_+^n) \subseteq \mathcal{DNN}^n$ 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 $M \in \mathcal{S}^n$ for which the n-variate polynomial $p_M = \sum_{i,j=1}^n M_{ij} x_i^2 x_j^2$ is nonnegative over $\mathbb{R}^n$, i.e., $\sum_{i,j=1}^n M_{ij} x_i^2 x_j^2 \geq 0$ for all $x_1, \ldots, x_n \in \mathbb{R}^n$. We now consider the dual of the cone $\mathcal{CS}_+^n$.

Lemma 3.12. *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* $X_1, \ldots, X_n \in \mathcal{S}_+^d$ *and* $d \in \mathbb{N}$.

(ii) $\operatorname{Tr}(\sum_{i,j=1}^n M_{ij} X_i^2 X_j^2) \geq 0$ *for all* $X_1, \ldots, X_n \in \mathcal{S}^d$ *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 $Y = P\sqrt{D}P^T$. □

In other words, $M \in \mathcal{CS}_+^{n*}$ if the associated polynomial $p_M = \sum_{i,j=1}^n M_{ij} X_i^2 X_j^2$ in the non-commutative variables $X_1, \ldots, X_n$ is *trace positive*, which means that the evaluation of p_M at any symmetric matrices $X_1, \ldots, X_n$ (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 Connes' embedding conjecture [12], one of the most important conjectures in von Neumann algebra. A reformulation of the conjecture that shows this connection is given by Klep and Schweighofer [28], see Conjecture 3.13 below. 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 $x_1, \ldots, x_n$ (resp., in the non-commutative variables $X_1, \ldots, X_n$). $\mathbb{R}\langle \underline{X}\rangle$ is endowed with the involution $* : \mathbb{R}\langle \underline{X}\rangle \to \mathbb{R}\langle \underline{X}\rangle$ that sends each variable to itself, 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; e.g., $(X_1X_2 + X_2X_3^2)^* = X_2X_1 + X_3^2X_2$. 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 $\mathsf{Tr}(f(X_1, \ldots, X_n)) \geq 0$ for all $(X_1, \ldots, X_n) \in \cup_{d\geq 1}(\mathcal{S}^d)^n$. Note that f^* evaluated at $(X_1, \ldots, X_n) \in (\mathcal{S}^d)^n$ is equal to $f(X_1, \ldots, X_n)^T$; hence, any Hermitian square ff^* is trace positive. Moreover, the trace of any commutator vanishes when evaluated at symmetric matrices.

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

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

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

Klep and Schweighofer [28] (see also [7]) showed that Connes' embedding conjecture is equivalent to the following conjecture characterizing the trace positive polynomials on Q_{nc}.

Conjecture 3.13. *[28] Let $f \in S\mathbb{R}\langle \underline{X} \rangle$. The following are equivalent:*

- *(i) f is trace positive on Q_{nc}, i.e., $\mathsf{Tr}(f(X_1, \ldots, X_n)) \geq 0$ for all $(X_1, \ldots, X_n) \in Q_{\mathrm{nc}}$.*
- *(ii) For any $\epsilon > 0$, $f + \epsilon \in \mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{cube}}$, i.e., $f + \epsilon = g + h$, where h is a sum of commutators and $g = \sum_{j=1}^{m_0} f_j f_j^* + \sum_{i=1}^n \sum_{j_i=1}^{m_i} g_{j_i}(1 - X_i^2) g_{j_i}^*$ for some $f_j, g_{j_i} \in \mathbb{R}\langle \underline{X} \rangle$ and $m_0, m_i \in \mathbb{N}$.*

In fact, Connes' embedding conjecture is also equivalent to Conjecture 3.13 where we restrict f to have degree at most 4 (see [6]). Note that the polynomials p_M involve only monomials of the form $X_i^2 X_j^2$. Interestingly, in the proof that Conjecture 3.13 is equivalent to Connes' embedding conjecture, these monomials $X_i^2 X_j^2$ play a fundamental role (due to a result of Rădulescu [44]). Finally, let us point out that, as observed by Burgdorf [6, Remark 2.8], Connes' conjecture is also equivalent to Conjecture 3.13 where the ball is used instead of the hypercube, i.e., replacing the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{cube}}$ by the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$.

While Conjecture 3.13 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. This gives:

Lemma 3.14. *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_{nc} or, equivalently, over the ball B_{nc}.*

3.4 Approximating the dual cone of $\mathcal{CS}_+$

For a matrix $M \in \mathcal{S}^n$, if its associated polynomial p_M belongs to the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$ then M belongs to the dual cone $\mathcal{CS}_+^{n*}$. We now define the set $\mathcal{K}_{\mathrm{nc},\epsilon}$ consisting of all matrices M for which the perturbed polynomial $p_M + \epsilon$ belongs to $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$. To simplify the notation, in $\mathcal{K}_{\mathrm{nc},\epsilon}$ we omit the dependence on the size n of the matrices.

Definition 3.15. *For $\epsilon \geq 0$, let $\mathcal{K}_{\mathrm{nc},\epsilon}$ denote the set of matrices $M \in \mathcal{S}^n$ for which the polynomial $p_M + \epsilon$ belongs to the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$.*

Lemma 3.16. *For any $\epsilon \geq 0$, $\mathcal{K}_{\mathrm{nc},\epsilon}$ is a convex set. Moreover, the inclusion $\bigcap_{\epsilon>0} \mathcal{K}_{\mathrm{nc},\epsilon} \subseteq \mathcal{CS}_+^{n*}$ holds, with equality if Connes' embedding conjecture holds.*

Proof. Convexity follows from the fact that $p_{\lambda M+(1-\lambda)M'} + \epsilon = \lambda(p_M + \epsilon) + (1-\lambda)(p_{M'} + \epsilon)$ for $M, M' \in \mathcal{S}^n$ and $\lambda \in [0,1]$. The inclusion $\bigcap_{\epsilon>0} \mathcal{K}_{\mathrm{nc},\epsilon} \subseteq \mathcal{CS}_+^{n*}$ follows by a continuity argument and the equality under Connes' conjecture follows from the fact that Connes' conjecture is equivalent to Conjecture 3.13 (also when the ball is used instead of the hypercube). □

We now point out a connection between the set $\mathcal{K}_{\mathrm{nc},\epsilon}$ and the following set $\mathcal{K}_{\mathrm{c}}$, used in the commutative setting. Let Σ denote the set of sums of squares of (commutative) polynomials and following [42] define the cone

$$\mathcal{K}_{\mathrm{c}} := \left\{ M \in \mathcal{S}^n : \exists r \in \mathbb{N}\; p_M(\sum_{i=1}^n x_i^2)^r \in \Sigma \right\} = \left\{ M \in \mathcal{S}^n : p_M \in \Sigma + (1 - \sum_{i=1}^n x_i^2)\mathbb{R}[\underline{x}] \right\} \quad (3.6)$$

(see [29, Prop. 2] for the equivalence between both definitions). The inclusion $\mathcal{K}_{\mathrm{c}} \subseteq \mathcal{COP}$ is clear and Parrilo [42] showed that $\mathcal{K}_{\mathrm{c}}$ covers the interior of $\mathcal{COP}$. Moreover, by adding degree constraints on the terms entering the decomposition of p_M, he defined a hierarchy of subcones of $\mathcal{COP}$ whose first level is the cone

$$\mathcal{K}_{\mathrm{c}}^{(0)} := \{M \in \mathcal{S}^n : p_M \in \Sigma\} = \mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n\times n}) = \mathcal{DNN}^{n*}.$$

It turns out that the set $\mathcal{K}_{\mathrm{nc},0}$ is equal to $\mathcal{K}_{\mathrm{c}}^{(0)}$.

Lemma 3.17. *We have: $\mathcal{DNN}^{n*} = \mathcal{K}_{\mathrm{c}}^{(0)} = \mathcal{K}_{\mathrm{nc},0} \subseteq \mathcal{K}_{\mathrm{nc},\epsilon}$ for any $\epsilon > 0$.*

Proof. The inclusion $\mathcal{K}_{\mathrm{nc},0} \subseteq \mathcal{K}_{\mathrm{nc},\epsilon}$ is clear.

First we show the inclusion $\mathcal{K}_{\mathrm{nc},0} \subseteq \mathcal{K}_{\mathrm{c}}^{(0)}$. For this, assume $M \in \mathcal{K}_{\mathrm{nc},0}$, i.e., $p_M = h + g$, where h is a sum of commutators and $g = \sum_{j=1}^{m_0} f_j f_j^* + \sum_{j=1}^{m_1} g_j(1 - \sum_{i=1}^n X_i^2)g_j^*$ with $f_j, g_j \in \mathbb{R}\langle \underline{X} \rangle$. If we evaluate p_M at commutative variables x, we see that $h(x)$ vanishes and thus we obtain $p_M(x) = g(x) \in \Sigma + (1 - \sum_{i=1}^n x_i^2)\Sigma$. As p_M is a homogeneous polynomial it follows (using [29, Prop. 4]) that $p_M \in \Sigma$ and thus $M \in \mathcal{K}_{\mathrm{c}}^{(0)}$.

We now show the reverse inclusion $\mathcal{K}_{\mathrm{c}}^{(0)} \subseteq \mathcal{K}_{\mathrm{nc},0}$. As $\mathcal{K}_{\mathrm{c}}^{(0)} = \mathcal{DNN}^{n*} = \mathcal{S}_+^n + (\mathcal{S}^n \cap \mathbb{R}_+^{n\times n})$, it suffices to show that if $M \succeq 0$ or if $M \geq 0$ then p_M is a sum of commutators and of Hermitian squares, which implies that $M \in \mathcal{K}_{\mathrm{nc},0}$. Assume first that $M \succeq 0$ and let $u_1, \ldots, u_n \in \mathbb{R}^d$ be vectors forming a Gram representation of M. Then, $p_M(\underline{X}) = \sum_{i,j=1}^n \sum_{h=1}^d u_i(h)u_j(h)X_i^2X_j^2 = \sum_{h=1}^d (\sum_{i=1}^n u_i(h)X_i^2)^2$ is a sum of Hermitian squares. Assume now that $M \geq 0$. Then each $M_{ij}X_i^2X_j^2 = [X_i^2X_j, X_j] + X_jX_i^2X_j$ is sum of a commutator and a Hermitian square and thus p_M is sum of commutators and Hermitian squares. □

We conclude with some remarks concerning how well $\mathcal{K}_{\mathrm{c}}$ and $\mathcal{K}_{\mathrm{nc},\epsilon}$ approximate the cones $\mathcal{COP}$ and $\mathcal{CS}_+^*$, respectively. As mentioned above, Parrilo [42] showed that $\mathcal{K}_{\mathrm{c}}$ covers the interior of the copositive cone, i.e., $\mathrm{int}(\mathcal{COP}) \subseteq \mathcal{K}_{\mathrm{c}} \subseteq \mathcal{COP}$, which can also be derived using the following result of Schmüdgen [46].

Theorem 3.18. *[46] 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 $\mathcal{K}_{\mathrm{nc},\epsilon}$ means that the polynomial $p_M + \epsilon$ belongs to the tracial quadratic module $\mathrm{tr}\mathcal{M}_{\mathrm{nc}}^{\mathrm{ball}}$, 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 $\mathcal{K}_{\mathrm{c}}$ and $\mathcal{K}_{\mathrm{nc},\epsilon}$ 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 nonzero $x \in \mathbb{R}^n$ so that $\sum_{i=1}^n x_i^2 = 1$. However, when working with matrices $X_1, \ldots, X_n$, one can rescale them to ensure that $I - \sum_{i=1}^n X_i^2 \succeq 0$ but one cannot 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.

4 Conic programs for the quantum graph parameters

In this section we show how to reformulate the quantum graph parameters as conic optimization problems using the completely positive semidefinite cone $\mathcal{CS}_+$. We first express each quantum graph parameter as a sequence of feasibility conic optimization programs over the cone $\mathcal{CS}_+$ (Propositions 4.1 and 4.9) and then as a single 'aggregated' optimization program over $\mathcal{CS}_+$ (Proposition 4.15). Moreover we show that, if in these conic programs we replace the cone $\mathcal{CS}_+$ by its subcone $\mathcal{CP}$ or by its supercone $\mathcal{DNN}$, then we find respectively the classical graph parameters and their corresponding bounds in terms of the theta number (Corollaries 4.5 and 4.11). In Section 4.3, we use the convex sets $\mathcal{K}_{\mathrm{nc},\epsilon}$ to define the new parameters $\Psi_\epsilon(G)$.

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 $t \in \mathbb{N}$ for which there exists a matrix $X \in \mathcal{CS}_+^{|V(G)|t+1}$ (indexed by $V(G) \times [t] \cup \{0\}$) 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 ρ, ρ_i^u (for $u \in V(G)$, $i \in [t]$) satisfying (2.8)-(2.11). Let X denote the Gram matrix of ρ, ρ_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 (2.8), (2.10) and (2.11). Next, using (2.8), (2.9) and (2.11), 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 ρ, ρ_i^u forming a Gram representation of X; we show that the matrices ρ, ρ_i^u satisfy the conditions of Definition 2.5. It is clear that (2.8), (2.10) and (2.11) hold. Next, for any $i \in [t]$, we have: $\|\rho - \sum_{u \in V(G)} \rho_i^u\|^2 = 1 - 2\sum_{u \in V(G)} X_{0,ui} + \sum_{u,v \in V(G)} X_{ui,vi} = 0$, using (C2a) and (C2c). This shows (2.9) and thus concludes the proof for $\alpha_q(G)$.

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

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 $\mathrm{Sym}(t)$ (consisting of all permutations of $[t] = \{1, \ldots, t\}$). We sketch this well known symmetry reduction, which has been used in particular for the study of the chromatic number in [25].

Given $Y \in \mathcal{S}^{|V|t+1}$ and a permutation $\pi \in \text{Sym}(t)$, define the new matrix $\pi(Y)$ with entries $\pi(Y)_{00} = Y_{00}$, $\pi(Y)_{0,ui} = Y_{0,u\pi(i)}$ and $\pi(Y)_{ui,vj} = Y_{u\pi(i),v\pi(j)}$ for $i,j \in [t], u,v \in V$, and the matrix $Y' = \frac{1}{|\text{Sym}(t)|}\sum_{\pi\in\text{Sym}(t)} \pi(Y)$, called the *symmetrization* of Y under action of Sym(t). Then, Y' is invariant under action of Sym(t), i.e., $\pi(Y') = Y'$ for all $\pi \in \text{Sym}(t)$, and thus Y' has the following block-form:

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

Notice that the programs described in Proposition 4.1 are invariant under action of Sym(t); that is, if Y is feasible for one of them then any permutation $\pi(Y)$ is feasible too and thus its symmetrization Y' as well. Therefore both programs have a feasible solution in block-form (4.1) (assuming some exists).

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

Lemma 4.2. *(see e.g. [25]) Let Y be a $t \times t$ block-matrix, of the form:*

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

having A as diagonal blocks and B as off-diagonal blocks, where $A, B \in \mathcal{S}^k$ (for some $k \geq 1$). Then, $Y \succeq 0 \Longleftrightarrow A - B \succeq 0$ 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 $\mathcal{DNN}$. We show that when using $\mathcal{CP}$ we find the classical stability number $\alpha(G)$ while, when using the cone $\mathcal{DNN}$, we find the parameter $\lfloor \vartheta'(G) \rfloor$ (see Corollary 4.5 below). To show this we will use the following property of completely positive matrices.

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

The following result is crucial for showing Corollary 4.5 and for its proof we will use Theorem 4.3 for the choice of B having $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ as its 2×2 nonzero principal submatrix.

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

(i) There exists a matrix $X \in \mathcal{K}^{|V(G)|}$ satisfying $\lfloor \langle J, X \rangle \rfloor = t$, $\mathsf{Tr}(X) = 1$ 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 $\mathcal{K} = \mathcal{DNN}$. 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 ϑ' 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 $u_1, \ldots, u_n$. As $X \in \mathcal{DNN}$, $X \geq 0$ and X is the Gram matrix of some vectors $x_{u_1}, \ldots, x_{u_n}$. 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 $e_1, \ldots, e_n$ 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 program in (2.4) which defines $\vartheta'(G_n)$. Indeed, $Y \in \mathcal{DNN}$ 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: $\mathsf{Tr}(Y) = \sum_{i,j=1}^n \|y_{u_i}^j\|^2 = \sum_{i,j=1}^n \|x_{u_i}\|^2 = n \,\mathsf{Tr}(X) = n$. 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 program in (2.4) for $\vartheta'(G_t)$), there exists a matrix $Y \in \mathcal{DNN}^{|V(G)|t}$ satisfying $\langle J, Y \rangle = t^2$, $\mathsf{Tr}(Y) = t$, and $Y_{(u,i),(v,j)} = 0$ for all edges $\{(u,i),(v,j)\}$ of G_t. Moreover, (after symmetrization by $\mathrm{Sym}(t)$) 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, $t = \mathsf{Tr}(Y) = t\,\mathsf{Tr}(A) = t\langle J, A \rangle$ and $t^2 = \langle J, Y \rangle = t\langle J, A \rangle + t(t-1)\langle J, B \rangle$, implying $\mathsf{Tr}(A) = \langle J, A \rangle = \langle J, B \rangle = 1$.

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, $\langle y, y \rangle = \sum_{v \in V(G)} \langle y, y_v^{i_0} \rangle = \langle J, A \rangle = \mathsf{Tr}(A) = 1$ 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 $Y' \in \mathcal{DNN}$ 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 $\mathsf{Tr}(X) = \sum_{u \in V(G)} \|x_u\|^2 = \sum_{i,j \in [t]} \sum_{u \in V(G)} \langle y_i^u, y_j^u \rangle = \sum_{i \in [t]} \sum_{u \in V(G)} Y_{ui,ui} = t$. 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 $\mathcal{K} = \mathcal{DNN}$.

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 $S = \{1, \ldots, t\}$. Define the vector $y \in \mathbb{R}^{nt+1}$ with block-form $y = (1, e_1, \ldots, e_t)$, where $e_1, \ldots, e_t$ 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 $\mathcal{DNN}$. 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 proved by applying Theorem 4.3. Indeed, $Y' \in \mathcal{CP}$, each $A_{uv}\tilde{F}^{uv}$ is positive semidefinite and can be easily decomposed in a sum of positive semidefinite matrices with only a 2×2 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 for $\mathcal{DNN}$. □

As an application, if in Proposition 4.1 we replace the cone $\mathcal{CS}_+$ by the cone $\mathcal{DNN}$ in the definition of $\alpha_q(G)$ or of $\alpha^*(G)$, then we obtain the parameter $\lfloor \vartheta'(G) \rfloor$; 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 ϑ' in (2.4) when $\mathcal{K} = \mathcal{DNN}$ and with Theorem 2.2 when $\mathcal{K} = \mathcal{CP}$. □

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, $\alpha(G) \leq \alpha_q(G) \leq \alpha^\star(G) \leq \lfloor \vartheta'(G) \rfloor$.*

The bound $\alpha^\star(G) \leq \lfloor \vartheta'(G) \rfloor$ was shown recently, with a different method, by Cubitt et al. [14]. The inequality $\alpha(G) \leq \alpha_q(G)$ can be tight [45]. 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 $\alpha_q(G) = \alpha^\star(G)$ 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 $F^{ij}_{ii} = F^{ij}_{jj} = 1$ and $F^{ij}_{ij} = F^{ij}_{ji} = -1$. 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 $\mathcal{CS}_+^5$. Moreover, L' does not even belong to the closure of $\mathcal{CS}_+^5$, since $\langle J - 2I, L' \rangle = -\langle H, L' \rangle > 0$ (using Lemma 3.10). This shows that the result of Theorem 4.3 does not extend to the cone $\mathcal{CS}_+$ or to its closure $\mathrm{cl}(\mathcal{CS}_+)$.

Finally, we relate the quantum stability number $\alpha_q(G)$ with the generalized theta number $\vartheta^{\mathcal{CS}_+}(G)$, obtained when selecting the cone $\mathcal{K} = \mathcal{CS}_+$ in the definition (2.6).

Proposition 4.8. *For any graph G, we have: $\alpha_q(G) \leq \lfloor \vartheta^{\mathcal{CS}_+}(G) \rfloor \leq \lfloor \vartheta'(G) \rfloor$.*

Proof. Using the equality $\vartheta^{\mathcal{DNN}}(G) = \vartheta'(G)$ (from (2.7)) and the fact that $\mathcal{CS}_+ \subseteq \mathcal{DNN}$, we obtain $\vartheta^{\mathcal{CS}_+}(G) \leq \vartheta'(G)$ 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 revisit the proof of 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 $\mathcal{K} = \mathcal{DNN}$, 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. □

We do not know whether $\vartheta^{\mathcal{CS}_+}(G)$ also provides an upper bound for $\alpha^\star(G)$, 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 $\mathcal{K} = \mathcal{DNN}$ 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).

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 4.9. *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:*

$$X_{0,0} = 1, \tag{C1}$$
$$\sum_{i\in[t]} X_{0,ui} = 1 \quad \forall u \in V(G), \tag{C3a}$$
$$\sum_{i\in[t]} X_{ui,ui} = 1 \quad \forall u \in V(G), \tag{C3b}$$
$$X_{ui,vi} = 0 \quad \forall i \in [t], \forall \{u,v\} \in E(G), \tag{O3}$$
$$X_{ui,uj} = 0 \quad \forall i \neq j \in [t], \forall u \in V(G). \tag{O4}$$

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

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

Proposition 4.10. *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 $\lceil X_{uu} \rceil = t$ 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) ⇒ (iii) ⇒ (ii) ⇒ (i)*.

(i) ⇒ (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 $\vartheta^+(\overline{G}) \leq t$.)

Next, we define the matrices $\tilde{A} = \frac{1}{t^2}X'$, $\tilde{B} = -\frac{1}{t^2(t-1)}X'$, $A = \tilde{A} + \frac{1}{t^2}J$ and $B = \tilde{B} + \frac{1}{t^2}J \in \mathcal{S}^{|V(G)|}$. 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 and $Y' = \begin{pmatrix} 1 & \frac{1}{t}e^T \\ \frac{1}{t}e & Y \end{pmatrix}$. We now show that $Y' \in \mathcal{S}^{|V(G)|t+1}$ satisfies (iii).

By construction, (C1), (C3a) and (O3) hold. (C3c) follows from the simple observation that $tA + t(t-1)B = J$ and thus $\sum_{i,j\in[t]} Y'_{ui,uj} = tA_{uu} + t(t-1)B_{uu} = 1$ for every $u \in V(G)$. At last we argue that $Y' \in \mathcal{DNN}$. Notice that $A, B \geq 0$ and thus $Y, Y' \geq 0$. Moreover, doing the Schur complement of Y in Y' w.r.t. its $(0,0)$-th entry (recall (1.2)), we obtain that $Y' \succeq 0$ if and only if $\tilde{Y} = Y - \frac{1}{t^2}J \succeq 0$. Now, $\tilde{Y}$ has the block structure of (4.2) with $\tilde{A}$ and $\tilde{B}$ as diagonal and off-diagonal blocks, respectively. Moreover, $\tilde{A} + (t-1)\tilde{B} = 0$ and $\tilde{A} - \tilde{B} = \frac{1}{t(t-1)}X' \succeq 0$ and thus, by Lemma 4.2, we deduce that $\tilde{Y} \succeq 0$ and therefore $Y' \succeq 0$.

(iii) ⇒ (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 $Y \in \mathcal{DNN}$ satisfies (ii).

(ii) ⇒ (i): Let $Y \in \mathcal{DNN}$ 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 $\mathsf{Tr}(A + (t-1)B - \frac{1}{t}J) = \mathsf{Tr}(A - \frac{1}{t}J) = 0$ 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, $X \in \mathcal{DNN}$, $X_{uu} = t$ 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 $\mathcal{K} = \mathcal{DNN}$.

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

(iii) ⇒ (ii): We can mimic the above proof of this implication in the $\mathcal{DNN}$ cone. In order to do so, we only 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 2×2 nonzero 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) ⇒ (i): Again we can mimic the above proof of this implication in the case of $\mathcal{DNN}$. 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). □

Corollary 4.11. *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 $\mathcal{K} = \mathcal{DNN}$ and it is equal to the chromatic number $\chi(G)$ when $\mathcal{K} = \mathcal{CP}$.*

Proof. In the case $\mathcal{K} = \mathcal{DNN}$, the result follows using Proposition 4.10 combined with the definition of $\vartheta^+(G)$ from (2.4).

Consider now the case $\mathcal{K} = \mathcal{CP}$. In view of Proposition 4.10, we know that the two conditions (ii) and (iii) are equivalent. Let t denote the minimum integer for which the condition (ii) of Proposition 4.10 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, $\mathsf{Tr}(Z) = |V(G)|$ and $\langle J, Z\rangle = |V(G)|^2$ (see the proof of the implication $(ii) \Rightarrow (i)$ in Proposition 4.10). 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. □

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

Corollary 4.12. *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 [5]. In the above chain of inequalities, only the right most one is known to be tight [9]. 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, [9] shows that $\chi_q(G) \leq 2$ if and only if G is a bipartite graph.

We further observe that, in Proposition 4.10, the implication $(i) \Rightarrow (ii)$ does not hold when selecting the cone $\mathcal{K} = \mathcal{CP}$.

Remark 4.13. *As we just saw in Corollary 4.11, the smallest integer t for which there exists a matrix $X \in \mathcal{CP}^{|V(G)|t+1}$ satisfying Proposition 4.10 (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 4.10 (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 4.10.*

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, $\chi_f(K(n,r)) = \frac{n}{r}$ [36] and $\chi(K(n,r)) = n - 2r + 2$ [35]. This shows that the implication: $(i) \Rightarrow (ii)$ does not hold in Proposition 4.10 in the case $\mathcal{K} = \mathcal{CP}$.

We conclude with a comparison of the quantum chromatic numbers with the generalized theta number $\Theta^{\mathcal{CS}_+}(G)$, obtained by selecting the cone $\mathcal{K} = \mathcal{CS}_+$ in the definition (2.6).

Proposition 4.14. *For any graph G, we have: $\lceil \vartheta^+(\overline{G}) \rceil \leq \lceil \Theta^{\mathcal{CS}_+}(G) \rceil \leq \chi^\star(G) \leq \chi_q(G)$.*

Proof. Combining the equality $\Theta^{\mathcal{DNN}}(G) = \vartheta^+(\overline{G})$ (from (2.7)) with the inclusion $\mathcal{CS}_+ \subseteq \mathcal{DNN}$, we obtain $\lceil \vartheta^+(\overline{G}) \rceil \leq \lceil \Theta^{\mathcal{CS}_+}(G) \rceil$.

We now show the inequality $\lceil \Theta^{\mathcal{CS}_+}(G) \rceil \leq \chi^\star(G)$. For this, we use the fact that $\lceil \Theta^{\mathcal{CS}_+}(G) \rceil$ is the minimum integer t for which Proposition 4.10 (i) holds when selecting $\mathcal{K} = \mathcal{CS}_+$, and that $\chi^\star(G)$ is by definition the minimum integer t for which Proposition 4.10 (iii) holds with $\mathcal{K} = \mathcal{CS}_+$. Therefore, in order to prove that $\lceil \Theta^{\mathcal{CS}_+}(G) \rceil \leq \chi^\star(G)$ holds, it suffices to show that Proposition 4.10 (iii) implies Proposition 4.10 (i) also in the case $\mathcal{K} = \mathcal{CS}_+$. This is what we do next.

Let $Y \in \mathcal{CS}_+$ satisfy Proposition 4.10 (*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 $\mathsf{Tr}(A + (t-1)B - \frac{1}{t}J) = 0$. Next, following the proof of (*ii*) $\Rightarrow$ (*i*), we consider the matrix $X = t^2 A$. 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. ◻

4.3 Approximating the quantum graph parameters

In this section we show how one can use the convex sets $\mathcal{K}_{\mathrm{nc},\epsilon}$ introduced earlier in Section 3.4 to define parameters that approximate the quantum graph parameters. We give the details only for the quantum chromatic number $\chi_q(G)$, but the same reasoning can be extended to the other parameters $\chi^*(G)$, $\alpha_q(G)$ and $\alpha^*(G)$.

The construction will go as follows. In a first step we reformulate $\chi_q(G)$ as a single 'aggregated' minimization program over an affine section of the cone $\mathcal{CS}_+$. When replacing the cone $\mathcal{CS}_+$ by its closure $\mathrm{cl}(\mathcal{CS}_+)$ we get the parameter $\widetilde{\chi}_q(G)$, satisfying $\chi(G) \geq \widetilde{\chi}_q(G)$. The second step will consist of writing the dual of this aggregated conic program over the cone $\mathrm{cl}(\mathcal{CS}_+)$, which is thus a maximization program over the dual cone $\mathcal{CS}_+^*$, and show that strong duality holds. Finally we define the new graph parameters $\Psi_\epsilon(G)$ by replacing in this dual conic program the cone $\mathcal{CS}_+^*$ by the convex sets $\mathcal{K}_{\mathrm{nc},\epsilon}$.

We start with the formulation of $\chi_q(G)$ from Proposition 4.9. 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 $\chi_q(G)$. Indeed, observe that if the condition (O4) from Proposition 4.9 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, by Proposition 4.9, $\chi_q(G)$ 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 $\langle A^t, X \rangle = 0$. We can now reformulate $\chi_q(G)$ as the optimal value of a single conic optimization program over the cone $\mathcal{CS}_+$.

Proposition 4.15. *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:*

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

Proof. Set $t = \chi_q(G)$ and let μ denote the optimal value of the program (4.3).

Let (t, X) be a solution for the program from Proposition 4.9 defining $\chi_q(G)$. We obtain a solution $X^1, \ldots, X^n$ to the program (4.3) by setting $X^t = X$ and $X^i = 0$ if $i \in [n] \setminus \{t\}$. This shows that $\mu \leq t$.

Conversely, let $X^1, \ldots, X^n$ be a feasible 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 4.9. Then we have: $t \leq s = s \sum_{i \geq s} X_{0,0}^i \leq \sum_{i \geq s} iX_{0,0}^s = \sum_i iX_{0,0}^s$. This shows that $t \leq \mu$ and thus equality $\chi_q(G) = \mu$ holds. This also shows that program (4.3) indeed has an optimal solution, thus justifying writing 'min' rather than 'inf' in (4.3). ◻

As the problem of deciding whether $\chi_q(G) \leq 3$ is NP-hard [27], it follows that linear optimization over affine sections of the completely positive semidefinite cone is an NP-hard problem.

It is convenient to rewrite program (4.3) in a more compact way. For this set $N = \sum_{t=1}^n (nt+1)$, where $n = |V(G)|$, and define the matrix $A = \oplus_{t=1}^n A^t \in \mathcal{S}^N$. Let $E_{0,ui}^t$, $E_{ui,vj}^t$ denote the elementary matrices in $\mathcal{S}^{nt+1}$ and let $\widetilde{E}^t_{0,ui}, \widetilde{E}^t_{ui,vj}$ denote their extensions to $\mathcal{S}^N$ obtained by adding zero entries. Moreover, set $C = \oplus_{t=1}^n tE^t_{0,0}$ and $B = \oplus_{t=1}^n E^t_{0,0} \in \mathcal{S}^N$. Then we can rewrite the program (4.3) as follows:

$$\chi_q(G) = \min \langle C, X\rangle \text{ s.t. } \begin{array}{l} X \in \mathcal{CS}_+^N, \ \langle B, X\rangle = 1, \ \langle A, X\rangle = 0, \\ \langle \widetilde{E}^t_{ui,vi}, X\rangle = 0 \quad \forall i \in [t], \ \forall \{u,v\} \in E(G), \ \forall t \in [n], \\ \langle \widetilde{E}^t_{ui,uj}, X\rangle = 0 \quad \forall i \neq j \in [t], \ \forall u \in V(G), \ \forall t \in [n]. \end{array} \tag{4.4}$$

If we replace the cone $\mathcal{CS}_+$ by its closure $\mathrm{cl}(\mathcal{CS}_+)$ in the program (4.4), then its optimal value is equal to $\widetilde{\chi}_q(G)$ and we have: $\widetilde{\chi}_q(G) \leq \chi_q(G)$. Note that it is not clear whether these two parameters coincide. Indeed the argument we used to show equality $\vartheta^{\mathcal{CS}_+}(G) = \vartheta^{\mathrm{cl}(\mathcal{CS}_+)}(G)$ in Lemma 2.4 does not extend to show $\widetilde{\chi}_q(G) = \chi_q(G)$. This is because the matrix A is psd so that it belongs to the dual cone $\mathcal{CS}_+^*$, and thus the constraint $\langle A, X\rangle = 0$ implies that any feasible solution X of (4.4) lies on the border of the cone $\mathcal{CS}_+$. On the other hand, it is easy to verify that the result of Proposition 4.15 (and its proof) extend to the case when the cone $\mathcal{CS}_+$ is replaced by its closure $\mathrm{cl}(\mathcal{CS}_+)$. Hence, $\widetilde{\chi}_q(G)$ can be equivalently defined by using the program from Proposition 4.9 after replacing the cone $\mathcal{CS}_+$ by its closure $\mathrm{cl}(\mathcal{CS}_+)$. Using this, Corollary 4.11 and the fact that $\mathcal{CS}_+ \subseteq \mathrm{cl}(\mathcal{CS}_+) \subseteq \mathcal{DNN}$, we have the following inequalities:

$$\lceil \vartheta^+(\overline{G})\rceil \leq \widetilde{\chi}_q(G) \leq \chi_q(G). \tag{4.5}$$

The dual program of (4.4) reads:

$$\lambda_q(G) := \sup \ \lambda \ \text{ s.t. } M = C - \lambda B - \mu A - \sum y^t_{u,v,i}\widetilde{E}^t_{ui,vi} - \sum z^t_{u,i,j}\widetilde{E}^t_{ui,uj} \in \mathcal{CS}_+^{N*}, \tag{4.6}$$

where the variables are $\lambda, \mu, y^t_{u,v,i}$ and $z^t_{u,i,j}$, the first summation is over $t \in [n]$, $i \in [t]$ and $\{u,v\} \in E(G)$, and the second summation is over $t \in [n]$, $i \neq j \in [t]$ and $u \in V(G)$. By weak duality, we obtain the inequality: $\lambda_q(G) \leq \widetilde{\chi}_q(G) \leq \chi_q(G)$.

Moreover, the program (4.6) is strictly feasible, hence there is no duality gap and the optimal value of (4.6) is equal to $\widetilde{\chi}_q(G)$; that is, $\lambda_q(G) = \widetilde{\chi}_q(G) \leq \chi_q(G)$. To see that (4.6) is strictly feasible, define the matrix $M^t = (t+n^2)E^t_{0,0} + A^t - \sum_{u\in V(G)}\sum_{i\neq j\in[t]} E^t_{ui,uj}$ and set $M = \oplus_{t=1}^n M^t$. Then, M is feasible for the program (4.6). Moreover, M lies in the interior of $\mathcal{CS}_+^*$ since $M \succ 0$, as $M^t \succ 0$ for all t. (Indeed note that the 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 $M^t \succ 0$).

We now introduce the new parameter $\Psi_\epsilon(G)$, which is obtained by replacing in the program (4.6) the cone $\mathcal{CS}_+^*$ by the convex set $\mathcal{K}_{\mathrm{nc},\epsilon}$.

Definition 4.16. *For $\epsilon \geq 0$, let $\Psi_\epsilon(G)$ denote the optimal value of the program:*

$$\sup \ \lambda \text{ s.t. } M = C - \lambda B - \mu A - \sum y^t_{u,v,i}\widetilde{E}^t_{ui,vi} - \sum z^t_{u,i,j}\widetilde{E}^t_{ui,uj} \in \mathcal{K}_{\mathrm{nc},\epsilon}. \tag{4.7}$$

First we relate the parameter $\Psi_\epsilon(G)$ to the classical theta number.

Lemma 4.17. *For $\epsilon \geq 0$, we have: $\lceil \vartheta^+(\overline{G})\rceil \leq \Psi_\epsilon(G)$, with equality if $\epsilon = 0$.*

Proof. By Lemma 3.14, we have the inclusion $\mathcal{DNN}^* \subseteq \mathcal{K}_{\mathrm{nc},\epsilon}$, with equality if $\epsilon = 0$. Hence the lemma will follow if we can show that the optimal value of the program (4.7) is equal to $\lceil \vartheta^+(\overline{G})\rceil$ when we replace the set $\mathcal{K}_{\mathrm{nc},\epsilon}$ by its subset $\mathcal{DNN}^*$.

In other words, let us consider the program (4.6) where we replace the cone $\mathcal{CS}_+^*$ by the cone $\mathcal{DNN}^*$. Using the same argument as above, we can conclude that its optimal value is equal to the optimal value of the program (4.4) where we replace the cone $\mathcal{CS}_+$ by the cone $\mathcal{DNN}$ (strong duality holds and use the fact that the cone $\mathcal{DNN}$ is closed). Next, it is not difficult to see that the result of Proposition 4.15 (and its proof) extend to the case when we replace the cone $\mathcal{CS}_+$ by the cone $\mathcal{DNN}$. Now we can conclude the proof by using the result of Corollary 4.12. ☐

As the sets $\mathcal{K}_{\mathrm{nc},\epsilon}$ aim to approximate the dual cone $\mathcal{CS}_+^*$, the parameters $\Psi_\epsilon(G)$ aim to approximate the quantum coloring number $\chi_q(G)$. However, as there is no apparent inclusion relationship between $\mathcal{CS}_+^*$ and $\mathcal{K}_{\mathrm{nc},\epsilon}$, we do not know the exact relationship between $\Psi_\epsilon(G)$ and $\chi_q(G)$. Moreover, as the cone $\mathcal{CS}_+$ is not known to be closed, there is a possible gap between the two parameters $\chi_q(G)$ and $\widetilde{\chi}_q(G)$. Nevertheless, what we can claim is the following relationship under Connes' embedding conjecture.

Lemma 4.18. *Assume that Connes' embedding conjecture holds. Then,* $\widetilde{\chi}_q(G) \le \inf_{\epsilon>0} \Psi_\epsilon(G)$.

Proof. If Connes' conjecture holds then $\mathcal{CS}_+^* \subseteq \mathcal{K}_{\mathrm{nc},\epsilon}$ for any $\epsilon > 0$ (Lemma 3.16). The result now follows using the definition of $\Psi_\epsilon(G)$ and the definition of $\widetilde{\chi}_q(G)$ as the optimal value of (4.6). □

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. [34, 43]).

If in the definition of the quantum chromatic number $\chi_q(G)$ from Definition 2.7, instead of requiring that ρ, ρ_u^i lie in $\mathcal{S}_+^d$ (for some $d \ge 1$), we require that ρ, ρ_u^i lie in $\mathcal{S}_+^{\mathbb{N}}$, we obtain a (possibly different) parameter that we denote by $\chi_q^\infty(G)$. Equivalently, $\chi_q^\infty(G)$ 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, $\chi_q^\infty(G) \le \chi_q(G)$, with equality if $\mathcal{CS}_+ = \mathcal{CS}_{\infty+}$. Moreover, as $\mathcal{CS}_{\infty+} \subseteq \mathrm{cl}(\mathcal{CS}_+)$ (by Theorem 3.3), we also have that $\widetilde{\chi}_q(G) \le \chi_q^\infty(G)$. Hence we have the possible variations of the quantum chromatic number:

$$\widetilde{\chi}_q(G) \le \chi_q^\infty(G) \le \chi_q(G), \tag{5.1}$$

with equality throughout if the cone $\mathcal{CS}_+$ is closed.

Moreover, observe that if in the definition of $\chi_q(G)$ we would require that ρ, ρ_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 $i \ne j \in [t]$, $u \in V(G)$), then we would get again the parameter $\chi_q^\infty(G)$. Indeed, by the first Hilbert-Schmidt theorem (see e.g. [20, 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 ρ and admits an orthonormal base $\{f_k : k \in \mathbb{N}\}$ consisting of the eigenvectors of ρ. Let $\rho', \rho_u'^i$ denote the restrictions of ρ, ρ_u^i to H'. Then, $\rho' \ne 0$ and $\rho', \rho_u'^i$ are positive operators on H'. Moreover, the operators $\rho_u'^i$ satisfy the same orthogonality conditions as the operators ρ_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 $\{f_k : k \in \mathbb{N}\}$ 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 Proposition 2.4). In contrast, as we already observed in the preceding section, we point out again that we do not know whether we can replace the cone $\mathcal{CS}_+$ by its closure, for instance in Lemma 4.15. 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, $\mathrm{cl}(\mathcal{CS}_+ \cap \mathcal{A}) \subseteq \mathcal{A} \cap \mathrm{cl}(\mathcal{CS}_+)$. However we cannot prove that equality holds. If we could prove equality then this would imply that equality holds throughout in (5.1).

We have studied quantum analogues of several classical graph parameters. In particular, we have extended the known lower bound $\chi(G) \ge \vartheta^+(\overline{G})$ to the quantum setting. We showed that $\chi_q(G) \ge \Theta^{\mathcal{CS}_+}(G)$ and studied analogous relationships between the other quantum graph parameters and the various theta numbers. As a step towards further approximations for the quantum chromatic number, we have introduced parameters $\Psi_\epsilon(G)$ defined by replacing the dual cone $\mathcal{CS}_+^*$ with the convex sets $\mathcal{K}_{\text{nc},\epsilon}$ in the dual program of $\widetilde{\chi}_q(G)$, where $\widetilde{\chi}_q(G) \leq \chi_q(G)$. However, the exact relationship between $\Psi_\epsilon(G)$ and $\widetilde{\chi}_q(G)$ is unknown and only if Connes' embedding conjecture holds we can claim that $\widetilde{\chi}_q(G) \leq \inf_{\epsilon>0} \Psi_\epsilon(G)$. We hope that these first results will stimulate further research leading to a better understanding of the quantum graph parameters.

We believe that the cone $\mathcal{CS}_+$ is an intrinsically very interesting cone, whose structure deserves to be better understood. To conclude we mention another interesting problem about this cone: given a matrix $A \in \mathcal{CS}_+$, 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 [11] and to finding low dimensional factorizations of nonnegative matrices [22, 24], which are currently attracting much attention.

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