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ON THE GENERALIZED ϑ-NUMBER AND RELATED PROBLEMS FOR HIGHLY SYMMETRIC GRAPHS[*]

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Abstract. This paper is an in-depth analysis of the generalized ϑ-number of a graph. The generalized ϑ-number, $\vartheta_k(G)$, serves as a bound for both the k-multichromatic number of a graph and the maximum k-colorable subgraph problem. We present various properties of $\vartheta_k(G)$, such as that the sequence $(\vartheta_k(G))_k$ is increasing and bounded from above by the order of the graph G. We study $\vartheta_k(G)$ when G is the strong, disjunction, or Cartesian product of two graphs. We provide closed form expressions for the generalized ϑ-number on several classes of graphs including the Kneser graphs, cycle graphs, strongly regular graphs, and orthogonality graphs. Our paper provides bounds on the product and sum of the k-multichromatic number of a graph and its complement graph, as well as lower bounds for the k-multichromatic number on several graph classes including the Hamming and Johnson graphs.

1. Introduction. A k-multicoloring of a graph is an assignment of k distinct colors to each vertex in the graph such that two adjacent vertices are assigned disjoint sets of colors. The k-multicoloring is also known as k-fold coloring, k-tuple coloring, or simply multicoloring. We denote by $\chi_k(G)$ the minimum number of colors needed for a valid k-multicoloring of a graph G and refer to it as the kth chromatic number of G or the multichromatic number of G. Multicoloring seems to have been independently introduced by Hilton, Rado, and Scott [45] and Stahl [80]. The k-multicoloring is a generalization of the well-known standard graph coloring. Namely, $\chi(G) := \chi_1(G)$ is known as the chromatic number of a graph G. Not surprisingly, multicoloring finds applications in comparable areas, such as job scheduling [32, 43], channel assignment in cellular networks [68] and register allocation in computers [16]. There exist several results on $\chi_k(G)$ for specific classes of graphs. In particular, Lin [55] and Lin, Liu, and Zhu [56] consider multicoloring the Mycielskian of graphs, Ren and Bu [73] study multicoloring of planar graphs, while Marx [63] proves that the multicoloring problem is strongly NP-hard in binary trees. Cranston and Rabern [21] show that, for any planar graph G, $\chi_2(G) \leq 9$. This result is implied by the famous four-color theorem by Appel and Haken [5], but it has a much simpler proof.

The maximum k-colorable subgraph (MkCS) problem is to find the largest induced subgraph in a given graph that can be colored with k colors so that no two adjacent vertices have the same color. When $k = 1$, the MkCS problem reduces to the well-known maximum stable set problem. The MkCS problem is one of the NP-complete problems considered by Lewis and Yannakakis [54]. We denote by $\alpha_k(G)$ the number of vertices in a maximum k-colorable subgraph of G and by $\omega_k(G)$ the size of the largest induced subgraph that can be partitioned into k cliques. When $k = 1$,

the graph parameter $\omega(G) := \omega_1(G)$ is known as the clique number of a graph and $\alpha(G) := \alpha_1(G)$ as the independence number of a graph. We note that $\alpha_k(G) = \omega_k(\overline{G})$, where $\overline{G}$ denotes the complement of G. The MkCS problem has a number of applications such as channel assignment in spectrum sharing networks [52, 81], VLSI design [62], and human genetic research [25, 57]. There exist several results on $\alpha_k(G)$ for specific classes of graphs. The size of the maximum k-colorable subgraph for the Kneser graph $K(v, 2)$ is provided by Füredi and Frankl [29]. Yannakakis and Gavril [84] consider the MkCS problem for chordal graphs, Addario-Berry et al. [2] study the problem for an i-triangulated graph, and Narasimhan [66] computes $\alpha_k(G)$ for circular-arc graphs and tolerance graphs.

Narasimhan and Manber [67] introduce a graph parameter $\vartheta_k(G)$ that serves as a bound for both the minimum number of colors needed for a k-multicoloring of a graph G and the number of vertices in a maximum k-colorable subgraph of G. The parameter $\vartheta_k(G)$ generalizes the concept of the famous ϑ-number that was introduced by Lovász [59] for bounding the Shannon capacity of a graph [76]. The Lovász theta number is a widely studied graph parameter; see, e.g., [17, 38, 40, 51, 60, 64]. The Lovász theta number provides bounds for both the clique number and the chromatic number of a graph, both of which are NP-hard to compute. The well-known result that establishes the relation $\alpha_1(G) \leq \vartheta_1(G) \leq \chi_1(\overline{G})$ or equivalently $\omega_1(G) \leq \vartheta_1(\overline{G}) \leq \chi_1(G)$ is known as the sandwich theorem [60]. The Lovász theta number can be computed in polynomial time as a semidefinite programming (SDP) problem by using interior point methods. Thus, when the clique number and chromatic number of a graph coincide, i.e., when the graph is weakly perfect, the Lovász theta number provides those quantities in polynomial time.

Despite the popularity of the Lovász theta number, the function $\vartheta_k(G)$ has received little attention in the literature. Narasimhan and Manber [67] show that $\alpha_k(G) \leq \vartheta_k(G) \leq \chi_k(\overline{G})$ or equivalently $\omega_k(G) \leq \vartheta_k(\overline{G}) \leq \chi_k(G)$. These inequalities can be seen as a generalization of the Lovász sandwich theorem. Alizadeh [3] formulates the generalized ϑ-number using SDP. Kuryatnikova, Sotirov, and Vera [53] introduce the generalized ϑ'-number that is obtained by adding nonnegativity constraints to the SDP formulation of the ϑ_k-number. The generalized ϑ-number and ϑ'-number are evaluated numerically as upper bounds for the MkCS problem in [53]. The authors of [53] characterize a family of graphs for which $\vartheta_k(G)$ and $\vartheta'_k(G)$ provide tight bounds for $\alpha_k(G)$. Here, we study also a relation between $\vartheta_k(G)$ and $\chi_k(G)$, and extend many known results for the Lovász ϑ-number to the generalized ϑ-number. This paper is based on the thesis of Sinjorgo [79].

Main results and outline. This paper provides various theoretical results for $\alpha_k(G)$, $\vartheta_k(G)$, and $\chi_k(G)$. We show numerous properties of $\vartheta_k(G)$ including results on different graph products of two graphs such as the Cartesian product, strong product, and disjunction product. We show that the sequence $(\vartheta_k(G))_k$ is increasing toward the number of vertices in G and that the increments of the sequence can be arbitrarily small. The latter result is proven by constructing a particular graph that satisfies the desired property. We also provide a closed form expression on the generalized ϑ-number for several graph classes including complete graphs, cycle graphs, complete multipartite graphs, strongly regular graphs, orthogonality graphs, the Kneser graphs, and some Johnson graphs. We compute $\vartheta_k(G)$ for circulant graphs and the Johnson graphs. Our results show that $\vartheta_k(G) = k\vartheta(G)$ for the Kneser graphs and more general Johnson graphs, strongly regular graphs, cycle graphs, and circulant graphs. Our paper presents lower bounds on the kth chromatic number for all regular graphs,

but also specialized bounds for the Hamming, Johnson, and orthogonality graphs. We also provide bounds on the product and sum of $\chi_k(G)$ and $\chi_k(\overline{G})$ and present graphs for which those bounds are attained. Those results generalize well-known results of Nordhaus and Gaddum [70] for $\chi(G)$ and $\chi(\overline{G})$.

This paper is organized as follows. Notation and definitions of several graphs and graph products are given in subsection 1.1. In section 2 we formally introduce $\vartheta_k(G)$ and $\chi_k(G)$ and show how those graph parameters relate. In section 3 we study the sequence $(\vartheta_k(G))_k$. Section 4 provides bounds for $\vartheta_k(G)$ when G is the strong graph product of two graphs and the disjunction product of two graphs. In section 5 one can find values of the generalized ϑ-number for complete graphs, cycle graphs, circulant graphs, and complete multipartite graphs. In subsection 5.1 we provide a closed form expression for the generalized ϑ-function on the Kneser graphs, as well as for the Johnson graphs. Subsection 5.2 relates $\vartheta(K_k \square G)$ and $\vartheta_k(G)$. We provide a closed form expression for the generalized ϑ-function for strongly regular graphs in section 6. In the same section we also relate the Schrijver's number $\vartheta'(K_k \square G)$ with $\vartheta_k(G)$ when G is a strongly regular graph. In section 7 we study a relation between the orthogonality graphs and the graph parameters considered here. Section 8 provides new lower bounds on the kth chromatic number for regular graphs and triangular graphs. We present several results for the multichromatic number of the Hamming graphs in subsection 8.1.

1.1. Notation and definitions. Let $\mathbb{S}^n$ be the space of symmetric n by n matrices. For matrix $X \in \mathbb{S}^n$, we write $X \succeq 0$ when X is positive semidefinite. Entries of matrix X are given by X_{ij}. The trace inner product for symmetric matrices is denoted $\langle X, Y \rangle = \text{Tr}(XY)$. The Kronecker product of matrices is denoted by $X \otimes Y$. By abuse of notation, we use the same symbol for the tensor product of graphs. The matrix of all ones is denoted by J, while the identity matrix is denoted by I. We sometimes use subscripts to indicate the size of a matrix. Denote by $\mathbf{0}$ and $\mathbf{1}$ the vector of all zeroes and ones, respectively.

For any graph $G = (V(G), E(G))$, we denote its adjacency matrix by A_G, or simply A when the context is clear. Similarly, we use V and E to denote the vertex and edge set of G when it is clear from the context. We assume that $|V| = n$, unless stated differently. The Laplacian matrix of a graph G is denoted by L_G. The complement graph of G, denoted by $\overline{G}$, is defined as the graph such that $A_{\overline{G}} + A_G = J - I$.

For the eigenvalues of $X \in \mathbb{S}^n$, we follow $\lambda_1(X) \geq \lambda_2(X) \geq \cdots \geq \lambda_n(X)$ and denote by $\sigma(A)$ the spectrum of matrix A. That is, $\sigma(A) = \{\lambda_1(A), \ldots, \lambda_n(A)\}$. We denote the set $\{1, \ldots, n\}$ by $[n]$. The "diag" operator maps an $n \times n$ matrix to the n-vector given by its diagonal. The adjoint operator of "diag" is denoted by "Diag."

In the rest of this section we provide several definitions. The first definition introduces several graph products, while the remaining definitions introduce different classes of graphs.

DEFINITION 1.1 (graph products). *An arbitrary graph product of graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is denoted by $G_1 * G_2$, having as vertex set the Cartesian product $V_1 \times V_2$. Table 1 shows when vertices (v_1, v_2) and (u_1, u_2) are adjacent in $G_1 * G_2$ for the lexicographic, tensor, Cartesian, strong, and disjunction (Abdo and Dimitrov [1]) graph products.*

In order to define the Hamming graphs, we first state the definition of the Hamming distance.

TABLE 1
Graph products.

Graph product	$G_1 * G_2$	Condition for $((v_1, v_2), (u_1, u_2)) \in E(G_1 * G_2)$
Lexicographic	$G_1 \circ G_2$	$(v_1, u_1) \in E_1$ or $[v_1 = u_1$ and $(v_2, u_2) \in E_2]$
Tensor	$G_1 \otimes G_2$	$(v_1, u_1) \in E_1$ and $(v_2, u_2) \in E_2$
Cartesian	$G_1 \square G_2$	$[v_1 = u_1$ and $(v_2, u_2) \in E_2]$
		or $[v_2 = u_2$ and $(v_1, u_1) \in E_1]$
Strong	$G_1 \boxtimes G_2$	$((v_1, v_2), (u_1, u_2)) \in E(G_1 \square G_2) \cup E(G_1 \otimes G_2)$
Disjunction	$G_1 \vee G_2$	$(v_1, u_1) \in E_1$ or $(v_2, u_2) \in E_2$

DEFINITION 1.2 (Hamming distance). *For two integer valued vectors* $\mathbf{u}$ *and* $\mathbf{v}$, *the Hamming distance between them, denoted by* $d(\mathbf{u}, \mathbf{v})$, *is the number of positions in which their entries differ.*

DEFINITION 1.3 (Hamming graph). *The Hamming graph* $H(n, q, F)$ *for* $n, q \in \mathbb{N}$ *and* $F \subset \mathbb{N}$ *has as vertices all the unique elements in* $(\mathbb{Z}/q\mathbb{Z})^n$. *In the Hamming graph, vertices* u *and* v *are adjacent if their Hamming distance* $d(u, v) \in F$.

Many authors define the Hamming graphs only for $F = \{1\}$.

DEFINITION 1.4 (Johnson graph). *Let* $n, m \in \mathbb{N}$, $1 \leq m \leq n/2$, $f \in \{0, 1, \ldots, m\}$, *and* $N = [n]$. *The Johnson graph* $J(n, m, f)$ *has as vertices all the possible* m-*sized subsets of* N. *Denote the subset corresponding to a vertex* u *by* $s(u)$. *Then* $|s(u)| = m$ *and vertices* u *and* v *are adjacent if and only if* $|s(u) \cap s(v)| = f$.

Many authors define the Johnson graph only for $f = m - 1$. When $f = 0$, the Johnson graph is better known as the Kneser graph.

DEFINITION 1.5 (Kneser graph). *Let* $n, m \in \mathbb{N}$ *and* $1 \leq m \leq n/2$. *Then the Kneser graph* $K(n, m)$ *is the Johnson graph* $J(n, m, 0)$.

DEFINITION 1.6 (strongly regular graph). *A* d-*regular graph* G *of order* n *is called strongly regular with parameters* (n, d, λ, μ) *if any two adjacent vertices share* λ *common neighbors and any two nonadjacent vertices share* μ *common neighbors.*

2. $\vartheta_k(G)$ and $\chi_k(G)$ formulations and their relation. In this section, we formally introduce the multichromatic number and the generalized ϑ-number of a graph. We also show a relationship between these two graph parameters.

Let $G = (V, E)$ be a simple undirected graph with n vertices. A valid k-multicoloring of G that uses R colors is a mapping $f : V \to 2^R$ such that $|f(i)| = k$ for all vertices $i \in V$ and $|f(i) \cap f(j)| = 0$ for all edges $(i, j) \in E$. The multichromatic number $\chi_k(G)$ is defined to be the size of a smallest R such that a valid k-multicoloring of G exists. Here we consider only valid k-multicoloring and refer to it as k-multicoloring.

Multicoloring can be reduced to standard graph coloring by use of the lexicographic product of graphs; see Definition 1.1. Namely, Stahl [80] showed that for any graph H such that $\chi(H) = k$, we have $\chi_k(G) = \chi(G \circ H)$. For clarity purposes, the simplest choice for H is K_k, the complete graph of order k. This results in

$$(1) \qquad\qquad \chi_k(G) = \chi(G \circ K_k).$$

For bounds on the chromatic number of (lexicographic) graph products, we refer readers to Geller and Stahl [34] and Klavžar [49]. By the lexicographic product, any

bound on $\chi(G)$ can also be transformed to a bound on $\chi_k(G)$. In particular,

$$(2) \qquad \chi_k(G) = \chi(G \circ K_k) \geq \omega(G \circ K_k) = \omega(G)\omega(K_k) = k\omega(G).$$

Here we use that $\omega(G \circ H) = \omega(G)\omega(H)$ for general graphs G and H. We also mention the following result:

$$(3) \qquad \alpha(G \circ H) = \alpha(G)\alpha(H).$$

Both results are proven by Geller and Stahl [34]. Let us also state the following known result:

$$(4) \qquad \chi(G \circ H) \leq \chi(G)\chi(H).$$

This result can be explained as follows. Denote the vertex sets of G and H by $V(G)$ and $V(H)$, respectively. For an optimal coloring of G and H, define $c(u)$ as the color of some vertex u. Graph $G \circ H$ has vertices (g_i, h_i). Every vertex in $G \circ H$ can then be assigned a 2-color combination $(c(g_i), c(h_i))$. Note that, by interpreting these 2-color combinations as simply colors, this constitutes a valid coloring of $G \circ H$ by using $\chi(G)\chi(H)$ colors. Combining inequalities (2) and (4) results in

$$(5) \qquad k\omega(G) \leq \chi_k(G) = \chi(G \circ K_k) \leq k\chi(G).$$

The above inequalities may be strict. An example is the cycle graph with five vertices and $k = 2$, as $\chi_2(C_5) = 5$ [80]. Note that, by (5), any upper bound on $\chi(G)$ can be transformed into an upper bound on $\chi_k(G)$. To compute (or approximate) $\chi_k(G)$ one can consult the wide range of existing literature on standard graph coloring by using $\chi_k(G) = \chi(G \circ K_k)$. Next to that, more specific literature on multicoloring can also be examined. Campêlo, Mara, and Santos [15] present an integer linear programming formulation for the k-multicoloring of a graph and study the facial structure of the corresponding polytope. Malaguti and Toth [61] use a combination of tabu search and population management procedures as a metaheuristic to solve (slightly generalized) multicoloring problems. Mehrotra and Trick [65] apply branch and price to generate independent sets for solving the multicoloring problem.

Narasimhan and Manber [67] generalize $\vartheta(G)$ by introducing $\vartheta_k(G)$ as follows:

$$(6) \qquad \vartheta_k(G) = \underset{A \in \mathcal{A}(G)}{\text{Minimize}} \ \sum_{i=1}^{k} \lambda_i(A),$$

where

$$(7) \qquad \mathcal{A}(G) := \{A \in \mathbb{S}^n \mid A_{ij} = 1 \ \forall (i,j) \notin E(G)\}.$$

Narasimhan and Manber prove that $\vartheta_k(G)$ satisfies the inequality

$$(8) \qquad \alpha_k(\overline{G}) \leq \vartheta_k(\overline{G}) \leq \chi_k(G)$$

and thus also $\omega_k(G) \leq \vartheta_k(\overline{G}) \leq \chi_k(G)$. Recall that $\alpha_k(G)$ is the cardinality of the largest subset $C \subseteq V$ such that the subgraph induced in G by C, denoted $G[C]$, satisfies $\chi(G[C]) \leq k$. Inequality (8) generalizes the Lovász's sandwich theorem [60].

Alizadeh [3] derived the following SDP formulation of $\vartheta_k(G)$ (see also [53]):

$$\vartheta_k(G) = \underset{\mu \in \mathbb{R}, \ X, Y \in \mathbb{S}^n}{\text{Minimize}} \quad \langle I, Y \rangle + \mu k$$

$(\vartheta_k\text{-SDP})$
$$\text{subject to} \quad X_{ij} = 0 \quad \forall (i,j) \notin E(G),$$
$$\mu I + X - J + Y \succeq 0, \ Y \succeq 0.$$

The dual problem for ϑ_k-SDP is

$$\vartheta_k(G) = \underset{Y \in \mathbb{S}^n}{\text{Maximize}} \quad \langle J, Y \rangle$$

(ϑ_k-SDP2)   subject to $Y_{ij} = 0 \quad \forall (i,j) \in E(G),$

$$\langle I, Y \rangle = k, \ 0 \preceq Y \preceq I.$$

Note that for $k = 1$ constraint $Y \preceq I$ is redundant. We show below that $\vartheta_k(\overline{G}) \leq \chi_k(G)$. To prove the result we use different arguments from the arguments used in [67]. In an optimal k-multicoloring of G, define for each of the $\chi_k(G)$ colors used a vector $\mathbf{y}^j \in \{0, 1, k\}^{n+1}$, $1 \leq j \leq \chi_k(G)$. For the entries of $\mathbf{y}^j$, we have $\mathbf{y}_0^j = k$ and $\mathbf{y}_i^j = 1$ if vertex i has color j, 0 otherwise. Then

$$\frac{1}{k^2} \sum_{j=1}^{\chi_k(G)} \mathbf{y}^j (\mathbf{y}^j)^\top = \begin{bmatrix} \chi_k(G) & \mathbf{1}^\top \\ \mathbf{1} & \frac{1}{k}I + \frac{1}{\chi_k(G)}X \end{bmatrix}$$

for some $X \in \mathbb{S}^n$ satisfying $X_{ij} = 0$ for all $(i,j) \in E(G)$. By the Schur complement we find $\frac{\chi_k(G)}{k}I + X - J \succeq 0$. Simply set $Y = 0 \in \mathbb{S}^n$. Then the triple $(\frac{\chi_k(G)}{k}, X, Y)$ is feasible for ϑ_k-SDP (for $\overline{G}$) with objective value $\chi_k(G)$.

To conclude this section we state the following result:

(9) $\vartheta_k(\overline{G}) \leq k\vartheta(\overline{G}) \leq \chi_k(G).$

Narasimhan and Manber [67] prove the first inequality in (9). To show this, let $\widetilde{A} \in \mathcal{A}(\overline{G})$ such that $\lambda_1(\widetilde{A}) = \vartheta(\overline{G})$. Then $\vartheta_k(\overline{G}) \leq \sum_{i=1}^k \lambda_i(\widetilde{A}) \leq k\lambda_1(\widetilde{A})$ and the proof follows. The second inequality follows from $\vartheta(\overline{G \circ K_k}) = k\vartheta(\overline{G})$ and $\vartheta(\overline{G \circ K_k}) \leq \chi(G \circ K_k) = \chi_k(G)$. The second inequality in (9) also follows from the following known results $\vartheta(\overline{G}) \leq \chi_f(G)$ and $k\chi_f(G) \leq \chi_k(G)$ where $\chi_f(G)$ is the fractional chromatic number of a graph; see, e.g., [14]. In this paper we show that $\vartheta_k(G) = k\vartheta(G)$ for many highly symmetric graphs.

3. The sequence $(\vartheta_k(G))_k$. In this section we consider the sequence $\vartheta_1(G)$, $\vartheta_2(G)$, ..., $\vartheta_n(G)$ where G is a graph of order n. We first prove that this sequence is bounded from above (Proposition 3.1) and increasing (Proposition 3.2). Then, we prove that the increments of the sequence, i.e., $\vartheta_k(G) - \vartheta_{k-1}(G)$ are decreasing in k; see Theorem 3.4. We also show that this increment can be arbitrarily small for a particular graph; see Theorem 3.5.

Let us first establish a relation between $\vartheta_k(G)$ and $\chi(G)$.

PROPOSITION 3.1. *For $k \geq \chi(G)$, $G = (V, E)$, we have $\vartheta_k(G) = |V|$. Furthermore, $\vartheta_k(G) \leq \min\{k\vartheta(G), |V|\}$ for all $k \leq n$.*

Proof. Let $k \geq \chi(G)$. Then $\alpha_k(G) = |V|$, where we take the k independent sets to be the color classes in an optimal coloring of G. Thus, it follows from (8) that $|V| \leq \vartheta_k(G)$.

Furthermore, note that for any graph G, matrix $J \in \mathcal{A}(G)$ is feasible for (6). Since matrix J has eigenvalue $|V|$ with multiplicity one and the other eigenvalues equal to 0, we have $\vartheta_k(G) \leq |V|$ for any graph G. Therefore, when $k \geq \chi(G)$ we have $\vartheta_k(G) = |V|$. Besides, $\vartheta_k(G) \leq k\vartheta(G)$ by (9). $\square$

Part of Proposition 3.1 can be more succinctly stated as $\vartheta_{\chi(G)}(G) = |V|$. The parameter $\vartheta_k(G)$ induces a sequence of parameters for a graph, given by $\vartheta_1(G), \vartheta_2(G), \ldots, \vartheta_n(G) = |V|$. Proposition 3.1 shows that this sequence is bounded from above by $|V|$. The next proposition shows that this sequence is nondecreasing in k.

PROPOSITION 3.2. *For any graph G, $\vartheta_k(G) \leq \vartheta_{k+1}(G)$, with equality if and only if $\vartheta_k(G) = |V|$.*

Proof. By Proposition 3.1, it is enough to consider $k < n$. Consider graph G of order n and let Y be optimal for ϑ_k-SDP2. We have $\text{Tr}(Y) = k$ and $0 \preceq Y \preceq I$. Define matrix Z as follows: $Z := (1 - \frac{1}{n-k})Y + \frac{1}{n-k}I$. It follows that matrix Z is feasible for ϑ_{k+1}-SDP2 and thus

$$\vartheta_{k+1}(G) \geq \langle J, Z \rangle = \vartheta_k(G) + \frac{n - \vartheta_k(G)}{n - k} \geq \vartheta_k(G).$$

$\square$

Proposition 3.2 allows us to further restrict ϑ_k-SDP.

PROPOSITION 3.3. *Let (X^*, Y^*, μ^*) be an optimal solution to ϑ_k-SDP for an arbitrary graph G. Then $\mu^* \geq 0$.*

Proof. We prove the statement by contradiction. Assume that the triple (X^*, Y^*, μ^*) is optimal for ϑ_k-SDP and $\mu^* < 0$. Note that the triple (X^*, Y^*, μ^*) is then also feasible for ϑ_{k+1}-SDP. Since $\mu^* < 0$, this would imply that $\vartheta_k(G) > \vartheta_{k+1}(G)$, which contradicts Proposition 3.2. Thus $\mu^* \geq 0$. $\square$

Next, we investigate the increments of the sequence $(\vartheta_k(G))_k$. For that purpose, we define for any graph G and $k \geq 2$ the increment of $(\vartheta_k(G))_k$,

$$\Delta_k(G) := \vartheta_k(G) - \vartheta_{k-1}(G), \tag{10}$$

and set $\Delta_1(G) = \vartheta_1(G)$.

THEOREM 3.4. *For any graph G and $k \geq 1$, $\Delta_k(G) \geq \Delta_{k+1}(G)$.*

Proof. Let $k \geq 1$ and matrix $A_k \in \mathcal{A}(G)$, where $\mathcal{A}(G)$ is defined in (7), satisfy

$$\sum_{i=1}^{k} \lambda_i(A_k) = \vartheta_k(G). \tag{11}$$

Stated differently, matrix A_k is an optimal solution to (6) for computing $\vartheta_k(G)$. Since (6) is a minimization problem,

$$\vartheta_k(G) \leq \sum_{i=1}^{k} \lambda_i(A_{k'}), \ k' \neq k. \tag{12}$$

By substituting (11) and (12) in the definition of $\Delta_k(G)$ for $k \geq 2$ (see (10)), we obtain

$$\Delta_k(G) \leq \sum_{i=1}^{k} \lambda_i(A_{k-1}) - \sum_{i=1}^{k-1} \lambda_i(A_{k-1}) = \lambda_k(A_{k-1}). \tag{13}$$

Similarly,

$$\Delta_k(G) \geq \sum_{i=1}^{k} \lambda_i(A_k) - \sum_{i=1}^{k-1} \lambda_i(A_k) = \lambda_k(A_k). \tag{14}$$

Combining (13) and (14) yields $\Delta_k(G) \geq \lambda_k(A_k) \geq \lambda_{k+1}(A_k) \geq \Delta_{k+1}(G)$, $k \geq 2$. The inequality $\Delta_1(G) \geq \Delta_2(G)$ follows from (9). $\square$

Let us summarize the implications of Proposition 3.2 and Theorem 3.4. Proposition 3.2 proves that

$$\Delta_k(G) = 0 \iff \vartheta_{k-1}(G) = |V|. \tag{15}$$

For complete graphs we have $\Delta_k(K_n) = 1$; see Theorem 5.1. There exist, however, graphs for which $\Delta_k(G) < 1$. We investigate the limiting behavior of $\Delta_k(G)$ in subsection 3.1.

When we consider the sequence induced by $\vartheta_k(G)$ as a function of k, we know that this sequence is increasing toward $|V(G)|$. Theorem 3.4 shows that the increments in this sequence decrease in k. Loosely speaking, one might say the second derivative of $f(k) = \vartheta_k(G)$ is negative.

3.1. Limiting behavior of $\Delta_k(G)$. In this section we show that, for any real number $\varepsilon > 0$, there exists a graph G and a number $k \geq 1$ such that $0 < \Delta_k(G) < \varepsilon$. For this purpose, define graph $\mathcal{G}_n = (V(\mathcal{G}_n), E(\mathcal{G}_n))$ as follows:

$$V(\mathcal{G}_n) := [n] \text{ and } E(\mathcal{G}_n) := \{(i,j) \mid i < j \leq n-1\} \cup \{(n-1,n)\}. \tag{16}$$

Graph $\mathcal{G}_n$ is thus a complete graph on $n-1$ vertices plus one additional vertex. This additional vertex is connected to the complete graph K_{n-1} by a single edge.

THEOREM 3.5. *For $n \geq 5$, we have $\vartheta_{n-2}(\mathcal{G}_n) = n - 2 + \frac{2}{n-3}\sqrt{(n-2)(n-4)}$.*

Proof. We prove the theorem by finding a lower and upper bound on $\vartheta_{n-2}(\mathcal{G}_n)$, both of which equal the expression stated in Theorem 3.5. Let $p = \sqrt{\frac{n-4}{(n-2)(n-3)^2}}$. Define matrix $Y \in \mathbb{S}^n$ as follows:

$$Y = \begin{bmatrix} \frac{n-4}{n-3}I_{n-2} & \mathbf{0}_{n-2} & p\mathbf{1}_{n-2} \\ \mathbf{0}_{n-2}^\top & 1 & 0 \\ p\mathbf{1}_{n-2}^\top & 0 & \frac{1}{n-3} \end{bmatrix}.$$

Matrix Y is feasible for ϑ_{n-2}-SDP2 if $0 \preceq Y \preceq I$. Therefore we derive

$$I - Y = \begin{bmatrix} \frac{1}{n-3}I_{n-2} & \mathbf{0}_{n-2} & -p\mathbf{1}_{n-2} \\ \mathbf{0}_{n-2}^\top & 0 & 0 \\ -p\mathbf{1}_{n-2}^\top & 0 & \frac{n-4}{n-3} \end{bmatrix},$$

and take the Schur complement of the block $\frac{1}{n-3}I_{n-2}$ of $I - Y$:

$$\begin{bmatrix} 0 & 0 \\ 0 & \frac{n-4}{n-3} \end{bmatrix} - \begin{bmatrix} \mathbf{0}_{n-2}^\top \\ p\mathbf{1}_{n-2}^\top \end{bmatrix} (n-3)I_{n-2} \begin{bmatrix} \mathbf{0}_{n-2} & p\mathbf{1}_{n-2} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \succeq 0.$$

Thus $Y \preceq I$. Similarly, by taking the Schur complement of the upper left $(n-1) \times (n-1)$ block matrix of Y, we find that $Y \succeq 0$. We omit the details of this computation. This implies that Y is feasible for ϑ_{n-2}-SDP2 and

$$\vartheta_{n-2}(\mathcal{G}_n) \geq \langle J, Y \rangle = n - 2 + \frac{2}{n-3}\sqrt{(n-2)(n-4)}. \tag{17}$$

Finding the (equal) upper bound on $\vartheta_{n-2}(\mathcal{G}_n)$ is a bit more involved. Let $\alpha =$

$\frac{n-5}{n-3}\sqrt{\frac{n-2}{n-4}}$ and set

$$A = \begin{bmatrix} \alpha J_{n-2} + (1-\alpha)I_{n-2} & \mathbf{0}_{n-2} & \mathbf{1}_{n-2} \\ \mathbf{0}_{n-2}^\top & 1 & 0 \\ \mathbf{1}_{n-2}^\top & 0 & 1 \end{bmatrix}.$$

Note that $A \in \mathcal{A}(\mathcal{G}_n)$; see (7). We show that for

(18) $$\beta_{1,2} = \frac{-\alpha(n-3) \pm \sqrt{\alpha^2(n-3)^2 - 4(2-n)}}{2},$$

the vectors $v_i = [\mathbf{1}_{n-2}^\top, 0, \beta_i]^\top$, $i \in \{1, 2\}$, are two eigenvectors of matrix A. Consider

(19) $$Av_i = \begin{bmatrix} (\alpha(n-3) + 1 + \beta_i)\mathbf{1}_{n-2} \\ 0 \\ \left(\frac{n-2}{\beta_i} + 1\right)\beta_i \end{bmatrix}.$$

By (18) we have that β_i, $i \in \{1, 2\}$, are the roots of the equation $\beta^2 + \alpha(n-3)\beta + (2 - n) = 0$, and so $\beta_i + \alpha(n-3) = (n-2)/\beta_i$. Then, the right-hand side of (19) equals v_i scaled by the corresponding eigenvalue, which is given by the following equation:

(20) $$\alpha(n-3) + 1 + \beta_i = \frac{n-2}{\beta_i} + 1.$$

Also $u = [\mathbf{0}_{n-2}^\top, 1, 0]^\top$ is an eigenvector of A with corresponding eigenvalue one (and multiplicity one). Since A is a real symmetric matrix, its eigenvectors are orthogonal. The remaining eigenvectors are thus $w_i = [c_i^\top, 0, 0]^\top$ where $c_i \in \mathbb{R}^{n-2}$ is a vector whose entries sum to 0. The eigenvectors w_i correspond to eigenvalues of $1 - \alpha$. We have described all eigenvectors of A. By substituting (18) in (20) one can verify that the four unique eigenvalues of A are ordered as follows:

$$\sqrt{(n-2)(n-4)} + 1 > 1 > 1 - \alpha > 1 - \sqrt{\frac{n-2}{n-4}},$$

with corresponding multiplicities 1, 1, $n-3$, 1, respectively. The sum of the largest $n-2$ eigenvalues of A serves as upper bound on $\vartheta_{n-2}(\mathcal{G}_n)$; see (6). That is,

$$\vartheta_{n-2}(\mathcal{G}_n) \leq \sum_{i=1}^{n-2} \lambda_i(A) = n - 2 + \frac{2}{n-3}\sqrt{(n-2)(n-4)}.$$

This upper bound on $\vartheta_{n-2}(\mathcal{G}_n)$ coincides with the lower bound (17), which proves the theorem. □

Using Theorem 3.5 we can show that $\Delta_{n-1}(\mathcal{G}_n)$ ($n \geq 5$) converges to zero. Namely,

$$\Delta_{n-1}(\mathcal{G}_n) = \vartheta_{n-1}(\mathcal{G}_n) - \vartheta_{n-2}(\mathcal{G}_n) \leq 2\left(1 - \sqrt{\frac{(n-2)(n-4)}{(n-3)^2}}\right),$$

from where it follows that $\Delta_{n-1}(\mathcal{G}_n)$ ($n \geq 5$) converges to zero. To conclude, strictly positive values of $\Delta_k(G)$ can be arbitrarily small. It is unclear whether lower bounds exist on $\Delta_k(G)$ for fixed k. One example of such a bound is simple for $k = 1$, i.e., $\Delta_1(G) = \vartheta_1(G) \geq \alpha(G) \geq 1$.

4. Graph products and the generalized ϑ-number. In this section we present bounds for $\vartheta_k(G)$ when G is the strong product of two graphs (Theorem 4.2) and the disjunction product of two graphs (Theorem 4.3).

In [59], Lovász proved the following result:

$$\vartheta(G_1 \boxtimes G_2) = \vartheta(G_1)\vartheta(G_2), \tag{21}$$

where $G_1 \boxtimes G_2$ is the strong product of G_1 and G_2; see Definition 1.1. Since $G_1 \boxtimes K_k$ is isomorphic to $G_1 \circ K_k$ and $\vartheta(K_k) = 1$ we have that

$$\vartheta(G \circ K_k) = \vartheta(G \boxtimes K_k) = \vartheta(G) \leq \vartheta_k(G);$$

see also Proposition 3.2. Below, we generalize the result for $\vartheta(G_1 \boxtimes G_2)$ to $\vartheta_k(G_1 \boxtimes G_2)$. For that purpose we need the following well-known result.

LEMMA 4.1. *For square matrices A and B with eigenvalues λ_i and μ_j, respectively, the eigenvalues of $A \otimes B$ equal $\lambda_i \mu_j$, and so $\mathrm{Tr}(A \otimes B) = \mathrm{Tr}(A)\mathrm{Tr}(B)$.*

For a reference for Lemma 4.1 one can see Horn and Johnson [47], for example.

THEOREM 4.2. *For any graphs G_1 and G_2*

$$\frac{1}{k}\vartheta_k(G_1)\vartheta_k(G_2) \leq \vartheta_k(G_1 \boxtimes G_2) \leq k\vartheta(G_1)\vartheta(G_2).$$

Proof. Let X_1^* and X_2^* be optimal to ϑ_k-$SDP2$ for G_1, and G_2, respectively. The adjacency matrix of $G_1 \boxtimes G_2$ is given by

$$A_{G_1 \boxtimes G_2} = (A_{G_1} + I) \otimes (A_{G_2} + I) - I;$$

see, e.g., [75]. Here $\otimes$ denotes the Kronecker product. Consider $Y = \frac{1}{k}X_1^* \otimes X_2^*$. From the adjacency matrix of $G_1 \boxtimes G_2$ it can be verified that $Y_{ij} = 0$ for all $(i,j) \in E(G_1 \boxtimes G_2)$. By Lemma 4.1, the eigenvalues of Y lie between 0 and 1 and thus $0 \preceq Y \preceq I$. More specifically, the eigenvalues of Y lie between 0 and $\frac{1}{k}$, since the sum of the (nonnegative) eigenvalues of X_i^* is $\mathrm{Tr}(X_i^*) = k$ for $i = 1, 2$. Besides $\mathrm{Tr}(Y) = (1/k)\mathrm{Tr}(X_1^*)\mathrm{Tr}(X_2^*) = k$. It follows that matrix Y is feasible to ϑ_k-$SDP2$ for $G_1 \boxtimes G_2$ and attains the following objective value:

$$\langle J, Y \rangle = \frac{1}{k}\langle J, X_1^* \otimes X_2^* \rangle = \frac{1}{k}\vartheta_k(G_1)\vartheta_k(G_2).$$

This proves the lower bound. The upper bound follows from (9) and (21).   □

The bounds from Theorem 4.2 are attained, for example, when both G_1 and G_2 are complete graphs (see Theorem 5.1). In general, the bounds for $\vartheta_k(G_1 \boxtimes G_2)$ from Theorem 4.2 are looser for larger values of k. We now focus on the disjunction graph product (see Definition 1.1). For graphs G_1 and G_2 of order n_1 and n_2, respectively, we have

$$A_{G_1 \vee G_2} = J_{n_1} \otimes A_{G_2} + A_{G_1} \otimes (A_{\overline{G}_2} + I_{n_2}).$$

Equivalently, by noting that $A_{\overline{G}_2} + I_{n_2} = J_{n_2} - A_{G_2}$, we have $A_{G_1 \vee G_2} = \min(J_{n_1} \otimes A_{G_2} + A_{G_1} \otimes J_{n_2}, 1)$. Our next result provides an upper bound on the generalized ϑ-number for the disjunction product of two graphs.

THEOREM 4.3. *For graphs G_1 and G_2 of orders n_1 and n_2, respectively, we have*

$$\vartheta_k(G_1 \vee G_2) \leq \min\left\{n_1\vartheta_k(G_2), n_2\vartheta_k(G_1)\right\}.$$

Proof. Consider the SDP problem ϑ_k-*SDP2* for $G_1 \vee G_2$. This maximization problem is least constrained when $G_1 = \overline{K}_{n_1}$. Thus

$$(22) \qquad \vartheta_k(G_1 \vee G_2) \leq \vartheta_k(\overline{K}_{n_1} \vee G_2).$$

We will show that $\vartheta_k(\overline{K}_{n_1} \vee G_2) = n_1\vartheta_k(G_2)$. Let X^* be an optimal solution to ϑ_k-*SDP2* for G_2. Matrix $J_{n_1} \otimes \frac{1}{n_1}X^*$ is a feasible solution to ϑ_k-*SDP2* for $\overline{K}_{n_1} \vee G_2$. The objective value of this solution equals

$$(23) \qquad \left\langle J, J_{n_1} \otimes \frac{1}{n_1}X^* \right\rangle = n_1\langle J, X^*\rangle = n_1\vartheta_k(G_2) \Longrightarrow \vartheta_k(\overline{K}_{n_1} \vee G_2) \geq n_1\vartheta_k(G_2).$$

Let (Y^*, X^*, μ^*) be an optimal solution to ϑ_k-*SDP* for G_2. Then $J_{n_1} \otimes Y^*$, $J_{n_1} \otimes X^*$, and $n_1\mu^*$ form a feasible solution to ϑ_k-*SDP* for $\overline{K}_{n_1} \vee G_2$. Namely, by Lemma 4.1 we have that $J_{n_1} \otimes Y^* \succeq 0$. Also

$$n_1\mu^* I + J_{n_1} \otimes X^* - J + J_{n_1} \otimes Y^*$$
$$= \mu^*(n_1 I_{n_1} - J_{n_1}) \otimes I_{n_2} + J_{n_1} \otimes (\mu^* I_{n_2} + X^* - J_{n_2} + Y^*) \succeq 0,$$

where we use that $\mu^* \geq 0$; see Proposition 3.3. Last, this feasible solution to the minimization problem obtains an objective value of

$$(24) \qquad \langle I, J_{n_1} \otimes Y^*\rangle + n_1\mu^* k = n_1\left(\langle I, Y^*\rangle + \mu^* k\right) = n_1\vartheta_k(G_2)$$
$$\Longrightarrow \vartheta_k(\overline{K}_{n_1} \vee G_2) \leq n_1\vartheta_k(G_2).$$

Now (23) and (24) imply that $\vartheta_k(\overline{K}_{n_1} \vee G_2) = n_1\vartheta_k(G_2)$. This result combined with (22) proves that

$$(25) \qquad \vartheta_k(G_1 \vee G_2) \leq n_1\vartheta_k(G_2).$$

From the definition of the disjunction graph product (see Definition 1.1), it follows that the disjunction graph product is commutative and thus

$$(26) \qquad \vartheta_k(G_1 \vee G_2) = \vartheta_k(G_2 \vee G_1) \leq n_2\vartheta_k(G_1).$$

Combining (25) and (26) proves the theorem. □

The proof shows that when either G_1 or G_2 is the complement of a complete graph, graph $G_1 \vee G_2$ attains the bound of Theorem 4.3.

5. Value of ϑ_k for some graphs. In [59], Lovász derived an explicit expression for the ϑ-number of cycle graphs and the Kneser graphs. In this section, we derive the generalized ϑ-number for those graphs, as well as for circulant, complete, and complete multipartite graphs, and the Johnson graphs. In subsection 5.1 we present bounds for $\vartheta_k(G)$ when G is a regular graph and show that the bound is tight for edge-transitive graphs. Subsection 5.2 provides an analysis of $\vartheta(K_k\square G)$, which is an upper bound on the number of vertices in the maximum k-colorable subgraph of G.

We denote cycle graphs of order n by C_n, complete graphs of order n by K_n, and complete multipartite graphs by $K_{m_1,\dots,m_p}$. Note that $K_{m_1,\dots,m_p}$ is a graph on $n = \sum_{i=1}^{p} m_i$ vertices.

THEOREM 5.1. *For $k \leq n$, $\vartheta_k(K_n) = k$.*

Proof. Consider the SDP problem ϑ_k-*SDP2*. For the complete graph, the only matrices feasible for ϑ_k-*SDP2* are diagonal matrices with trace equal to k. Set for example $Y = \frac{k}{n}I$. Then Y is feasible for ϑ_k-*SDP2* and has objective value k. $\quad\square$

Stahl [80] determined $\chi_k(C_n)$. For odd cycles, he showed that $\chi_k(C_{2n+1}) = 2k + 1 + \lfloor \frac{k-1}{n} \rfloor$, and for even cycles that $\chi_k(C_{2n}) = 2k$. The latter result follows trivially from (66).

Since C_n is bipartite when n is even, it follows from Proposition 3.1 that $\vartheta_k(C_n) = n$ for all $k \geq 2$. To compute $\vartheta_2(C_n)$ for odd cycle graphs, we require the following lemma.

LEMMA 5.2. *For n odd, $n \geq 5$, we have $0.447 \approx \frac{\sqrt{5}}{5} \leq \frac{\vartheta(C_n)}{n} < \frac{\vartheta(C_{n+2})}{n+2} < \frac{1}{2}$.*

Proof. By Lovász [59], we have

$$(27) \qquad \vartheta(C_n) = \frac{n\cos(\pi/n)}{1 + \cos(\pi/n)}, \quad n \text{ odd}.$$

Define $f(n) := \vartheta(C_n)/n$. Then $f'(n) = \dfrac{\pi\sin(\frac{\pi}{n})}{(1 + \cos(\frac{\pi}{n}))^2 n^2}$. For $n \geq 5$, $f'(n) > 0$. Moreover, for $n \geq 5$, we have $\cos(\pi/n) < 1$. This results in $f(n) < 1/2$ and since $f(5) = \sqrt{5}/5$, this proves the lemma. $\quad\square$

Let us introduce a circulant matrix and an edge-transitive graph. We need both terms in the proof of the following theorem. Each row of a circulant matrix equals the preceding row in the matrix rotated one element to the right. Circulant matrices thus have a constant row sum. This constant row sum is also one of the eigenvalues with $\mathbf{1}$ as its corresponding eigenvector. A graph is edge-transitive if its automorphism group acts transitively on edges, i.e., if for every two edges there is an automorphism that maps one to the other.

THEOREM 5.3. *Let n be odd and $n > 1$. Then $\vartheta_2(C_n) = 2\vartheta(C_n)$ and $\vartheta_k(C_n) = n$ for all $k \geq 3$.*

Proof. For $n = 3$, $C_3 = K_3$ and the result follows from Theorem 5.1. Thus let $n \geq 5$. Let $\Gamma \subset \mathbb{S}^n$ be the set of optimal feasible solutions to ϑ_1-*SDP2* for C_n and let $Y \in \Gamma$. Note Γ is convex. Let $p(Y)$ denote an optimal solution to ϑ_1-*SDP2* obtained by permuting the vertices of C_n by automorphism p. Note that matrix $p(Y)$ is an element of Γ. Denote the average over all automorphisms p by $\bar{Y}$. Then $\bar{Y} \in \Gamma$ by convexity of Γ and since C_n is edge-transitive, $\bar{Y}$ is a circulant matrix, like the adjacency matrix of C_n.

As $\bar{Y} \in \Gamma$, we find

$$(28) \qquad \langle J, \bar{Y} \rangle = \mathrm{Tr}(\mathbf{1}\mathbf{1}^\top \bar{Y}) = \mathrm{Tr}(\mathbf{1}^\top \bar{Y}\mathbf{1}) = \mathbf{1}^\top \bar{Y}\mathbf{1} = \vartheta_1(C_n).$$

As $\bar{Y}$ is also circulant, it has eigenvector $\mathbf{1}$. By (28), its corresponding eigenvalue equals $\bar{\lambda} = \vartheta(C_n)/n$.

We will prove that the largest eigenvalue of $\bar{Y}$ equals $\bar{\lambda}$. Assume that the largest eigenvalue of $\bar{Y}$ does not equal $\bar{\lambda}$. Then $\bar{Y}$ has eigenvalue Λ for some $\Lambda > \bar{\lambda}$. Since $\bar{Y}$ is a symmetric circulant matrix of odd dimension, $\bar{Y}$ has only one eigenvalue with odd multiplicity (Tee [82]). Thus Λ or $\bar{\lambda}$ has multiplicity greater than one. Note that since $\bar{Y}$ is feasible for ϑ_1-*SDP2*, it has nonnegative eigenvalues that sum to one. However, both terms $\Lambda + 2\bar{\lambda}$ and $2\Lambda + \bar{\lambda}$ are strictly greater than one by Lemma 5.2, and hence, the assumption that $\bar{\lambda}$ is not the largest eigenvalue of $\bar{Y}$ leads to a contradiction.

The largest eigenvalue of $\bar{Y}$ is thus smaller than $1/2$. Then $2\bar{Y} \preceq I$. Clearly, $2\bar{Y}$ satisfies the other feasibility conditions of ϑ_2-$SDP2$. Thus $2\bar{Y}$ is feasible for ϑ_2-$SDP2$ and $\vartheta_2(C_n) \geq 2\vartheta(C_n)$. Combined with (9), the theorem follows.

Since $\chi(C_n) = 3$ for odd cycles, $\vartheta_3(C_n) = n$ follows trivially from Proposition 3.1. □

Graphs for which the adjacency matrix is a circulant matrix are called *circulant graphs*, like the cycle graphs and some Paley graphs. There has been research done on computing $\vartheta(G)$ for circulant graphs [6, 10, 11, 22]. In particular, Crespi [22] computes the Lovász theta function for the circulant graphs of degree four having even displacement, while Brimkov et al. [11] consider $\vartheta(C_{n,j})$, where $V(C_{n,j}) = \{0, 1, \ldots, n-1\}$ and $E(C_{n,j}) = E(C_n) \cup \{(i, i') \mid i - i' = j \mod n\}$.

Let H_n be a connected circulant graph on n vertices. Then H_n contains a Hamiltonian cycle (Boesch and Tindell [8]). Equivalently, the cycle graph C_n is a minor of H_n. Maximization problem ϑ_k-$SDP2$ is then more restricted for H_n than it is for C_n. Thus

$$\vartheta_1(H_n) \leq \vartheta_1(C_n) \leq \frac{n}{2}.$$

Consider ϑ_1-$SDP2$ for H_n. Graph H_n has a circulant adjacency matrix, meaning we can restrict optimization of ϑ_1-$SDP2$ over the Lee scheme, the association scheme of symmetric circulant matrices, without loss of generality [33]. As (28) shows, ϑ_1-$SDP2$ is now equivalent to maximizing the largest (scaled) eigenvalue over feasible matrices. Let M be a matrix optimal for ϑ_1-$SDP2$ for graph H_n. Then $\lambda_1(M) = \vartheta(H_n)/n \leq 1/2$. Then $2M$ is also optimal for ϑ_2-$SDP2$ for graph H_n. More generally, if $k \leq n/\vartheta(H_n)$, then $\lambda_1(kM) \leq 1$ and kM is then feasible for ϑ_k-$SDP2$, attaining the objective value $\min\{k\vartheta(H_n), n\}$. In case $k > n/\vartheta(H_n)$, we have $\vartheta_k(H_n) = n$. Thus, in general

$$(29) \qquad \vartheta_k(H_n) = \min\{k\vartheta(H_n), n\}.$$

For any k, there exists a circulant graph P on n vertices such that $\vartheta_k(P) < n$. Specifically, if P is the Paley graph of order n, then $\vartheta(P) = \sqrt{n}$ (cf. [39]). For fixed k and n large enough, $k\sqrt{n} < n$.

THEOREM 5.4. *For $m_1 \geq m_2 \geq \cdots \geq m_p$ and $k \leq p$, $\vartheta_k(K_{m_1,\ldots,m_p}) = \sum_{i=1}^k m_i$.*

Proof. Let $n = \sum_{i=1}^p m_i$. For notational convenience, we write $K = K_{m_1,\ldots,m_p}$, with corresponding adjacency matrix A_K. Since K is a graph on n vertices, A_K can be written as $A_K = J_n - \text{Diag}(J_{m_1}, \ldots, J_{m_p})$. Note that $X := \text{Diag}(J_{m_1}, \ldots, J_{m_p}) \in \mathcal{A}(K)$; see (7). Therefore X is feasible for (6). The eigenvalues of X are the eigenvalues of the block matrices J. Then, $\lambda_i(X) = m_i$ for $i \in [p]$. Thus, we have $\vartheta_k(K) \leq \sum_{i=1}^k \lambda_i(X) = \sum_{i=1}^k m_i$. Note that $\alpha_k(K) = \sum_{i=1}^k m_i$, and the proof follows from (8) and the above inequality. □

Recall again the definition of $\Delta_k(G)$, given in (10). In subsection 3.1, we show that strictly positive values $\Delta_k(G)$ can be arbitrarily small. We show now, by use of Theorem 5.4, that the ratio between strictly positive successive values of $\Delta_k(G)$ can be arbitrarily small. More formally, for any $\varepsilon > 0$ and any $k \geq 1$, there exists a graph G such that

$$(30) \qquad 0 < \frac{\Delta_{k+1}(G)}{\Delta_k(G)} < \varepsilon.$$

We again ignore the case $\Delta_k(G) = 0$; see (15). In view of Theorem 5.4, we have

$$\frac{\Delta_2(K_{n,1})}{\Delta_1(K_{n,1})} = \frac{1}{n} < \varepsilon$$

for some integer n sufficiently large. Thus for sufficiently large n, graph $K_{n,1}$ satisfies (30) for $k = 1$. Graph $K_{n,n,1}$ satisfies (30) for $k = 2$. Graph $K_{n,n,n,1}$ satisfies (30) for $k = 3$, and so on.

5.1. Regular graphs. In this section we present an upper bound on the ϑ_k-function for regular graphs; see Theorem 5.6. This result can be seen as a generalization of the Lovász upper bound on the ϑ-function for regular graphs. We exploit the result of Theorem 5.6 to derive an explicit expression for the generalized theta function for the Kneser graph; see Theorem 5.7. Moreover, we prove that $\vartheta_k(G) = k\vartheta(G)$ when G is the Johnson graph; see Theorem 5.8.

Let us first state the following well-known result.

THEOREM 5.5 (Lovász [59]). *For a regular graph G of order n, having adjacency matrix A_G and $\lambda_1(A_G) \geq \lambda_2(A_G) \geq \cdots \geq \lambda_n(A_G)$, we have*

$$\vartheta(G) \leq \frac{n\lambda_n(A_G)}{\lambda_n(A_G) - \lambda_1(A_G)}.$$

If G is an edge-transitive graph, this inequality holds with equality.

For a finite set of real numbers P, we denote by $\mathbf{S}_k(P)$ the sum of the largest k elements in P. Now, we state our result.

THEOREM 5.6. *For any regular graph G of order n, we have*
(31)

$$\vartheta_k(G) \leq \min_x \mathbf{S}_k(\sigma(J + xA_G)) \leq n + \frac{n}{\lambda_n(A_G) - \lambda_1(A_G)}\Big(\lambda_1(A_G) + \sum_{i=0}^{k-2} \lambda_{n-i}(A_G)\Big),$$

where we set the summation equal to 0 when $k = 1$ and $\sigma(\cdot)$ denotes the spectrum of a matrix. The first inequality holds with equality if G is also edge-transitive.

Proof. The proof is an extension of Lovász's [59] proof of Theorem 5.5. Let G be a regular graph of order n. For notational convenience, we write $A_G = A$ and $\lambda_i(A_G) = \lambda_i$. Since G is a regular graph, vector $\mathbf{1}$ is an eigenvector of A. Let $v \neq \mathbf{1}$ be an eigenvector of A. As A is symmetric, its eigenvectors are orthogonal. Thus $\mathbf{1}^\top v = 0$, which implies that $Jv = 0$. Thus the eigenvectors of A are also eigenvectors of $J + xA$. In particular, we have

(32) $$\sigma(J + xA) = \{n + x\lambda_1, \, x\lambda_2, \, \ldots, \, x\lambda_n\}$$

for any $x \in \mathbb{R}$. Note that $J + xA \in \mathcal{A}(G)$; see (7). Therefore, it follows from (6) that

$$\vartheta_k(G) \leq \min_x \mathbf{S}_k(\sigma(J + xA)).$$

Minimizing $\mathbf{S}_k(\sigma(J + xA))$ can be done analytically when $k = 1$. Lovász [59] showed that setting $x = \frac{n}{\lambda_n - \lambda_1}$ minimizes $\mathbf{S}_k(\cdot)$ when $k = 1$. Setting x to this negative value provides the second upper bound in the theorem. Note that $x = \frac{n}{\lambda_n - \lambda_1}$ implies that $n + x\lambda_1 = x\lambda_n$.

We now prove that $\vartheta_k(G) = \min_x \mathbf{S}_k(\sigma(J + xA))$ when G is edge-transitive. Assume that G is edge-transitive. It is known that the sum of the k largest eigenvalues of a matrix is a convex function (Overton and Womersley [72]). Thus the average over all optimal solutions to (6) of all automorphisms of G is also optimal. Since G is edge-transitive, this average is of the form $J + xA$, which proves the equality claim. $\square$

We remark that Theorem 5.3 can also be proven by applying Theorem 5.6.

To obtain sharper bounds for $\vartheta_k(G)$, one can minimize $\mathbf{S}_k(\sigma(J+xA))$, or compute $\vartheta_k(G)$ directly. Note that computing $\vartheta_k(G)$ by interior point methods is computationally demanding for some graphs with 200 vertices; see [53]. In general, $\mathbf{S}_k(\sigma(J+xA))$ is the sum of the k largest linear functions given by $\sigma(J + xA)$. Ogryczak and Tamir [71] consider this problem, which they show is solvable in linear time, but unfortunately, obtaining a general solution is not possible. When we consider specific graphs, and $\sigma(J + xA)$ is thus explicit, minimizing $\mathbf{S}_k(\cdot)$ can be done analytically, as we show for the Kneser graph.

Lovász [59] proved that $\vartheta(K(n,m)) = \binom{n-1}{m-1}$, where $K(n,m)$ is the Kneser graph; see Definition 1.5. The Kneser graph $K(n,m)$ is regular of valency $\binom{n-m}{m}$. We provide an explicit expression for $\vartheta_k(K(n,m))$.

THEOREM 5.7. *For $k \leq \lfloor \frac{n}{m} \rfloor$ and $1 \leq k \leq n - 2m + 1$, we have*

$$\vartheta_k(K(n,m)) = k\vartheta(K(n,m)) = k\binom{n-1}{m-1}.$$

When $k > \frac{n}{m}$ or $k > n - 2m + 1$

$$\vartheta_k(K(n,m)) = \binom{n}{m}.$$

Proof. Note that n does not refer to the number of vertices but to a parameter of the Kneser graph $K(n,m)$. We will use v to denote the number of vertices of $K(n,m)$, i.e., $v = \binom{n}{m}$. Let A be the adjacency matrix of $K(n,m)$, having eigenvalues $\lambda_1 \geq \cdots \geq \lambda_v$. We compute the minimum of $\mathbf{S}_k(\sigma(J + xA))$; see Theorem 5.6. Recall that $\sigma(\cdot)$ denotes the spectrum of a matrix, and $\mathbf{S}_k(\sigma(\cdot))$ the sum of k largest eigenvalues in a matrix. Define $f_k(x) := \mathbf{S}_k(\sigma(J + xA))$. For $x^* = \frac{v}{\lambda_v - \lambda_1} < 0$ and $k \leq v$, we have

$$(33) \qquad f_k(x^*) = v + x^* \left(\lambda_1 + \sum_{i=0}^{k-2} \lambda_{v-i} \right).$$

The greatest and smallest eigenvalues of A equal $\lambda_1 = \binom{n-m}{m}$ and $\lambda_v = -\binom{n-m-1}{m-1}$, with corresponding multiplicities 1 and $n-1$; see [59]. Thus, in the case that $k \leq \lfloor n/m \rfloor \leq n$, function f_k is determined only by λ_1 and λ_v. More precisely,

$$(34) \quad f_k(x^*) = v + x^* \left[\binom{n-m}{m} - (k-1)\binom{n-m-1}{m-1} \right] = v + x^*(\lambda_1 + (k-1)\lambda_v).$$

Since $\vartheta(K(n,m)) = \mathbf{S}_1(\sigma(J + x^*A)) = x^*\lambda_v = v + x^*\lambda_1$ (see [59]), we can rewrite (34) as

$$(35) \qquad f_k(x^*) = kx^*\lambda_v = k\vartheta(K(n,m)).$$

We show now that x^* minimizes f_k when $k < \frac{n}{m}$, $1 \leq k \leq n - 2m + 1$. For any $\varepsilon > 0$ we have

$$f_k(x^* + \varepsilon) = f_k(x^*) + \varepsilon\left[\binom{n-m}{m} - (k-1)\binom{n-m-1}{m-1}\right],$$

and thus $k < \frac{n}{m} \implies \binom{n-m}{m} - (k-1)\binom{n-m-1}{m-1} > 0 \implies f_k(x^*+\varepsilon) > f_k(x^*)$. Similarly, for any sufficiently small $\varepsilon > 0$, we have

$$(36) \qquad f_k(x^* - \varepsilon) = k(x^* - \varepsilon)\lambda_v = kx^*\lambda_v - k\varepsilon\lambda_v > x^*\lambda_v + (k-1)x^*\lambda_v = f_k(x^*).$$

Here we used the fact that $x^*\lambda_v = v + x^*\lambda_1$. From the previous discussion it follows that for any sufficiently small positive ε we have

$$f_k(x^*) < f_k(x^* \pm \varepsilon).$$

By convexity of f_k, x^* is the global minimizer of f_k. From (35), the theorem follows for the case $k < \frac{n}{m}$.

Now we consider the case $k = \frac{n}{m}$, $1 \leq k \leq n - 2m + 1$. From (34) it follows that $f_k(x^*) = v$. In fact, for any β satisfying $x^* \leq \beta \leq 0$, $f_k(\beta) = v$. For any $\varepsilon > 0$,

$$(37) \qquad\qquad f_k(\varepsilon) = v + \varepsilon\Big(\sum_{i=1}^{k} \lambda_i\Big).$$

As the λ_i sum to zero, the sum of the k largest λ_i must be strictly positive. Thus $f_k(\varepsilon) > v$. The derivation from (36) is also valid for the case $k = \frac{n}{m}$. Invoking again the convexity of f_k proves that v is the minimum value of f_k. Thus

$$\vartheta_{n/m}(K(n,m)) = \frac{n}{m}\binom{n-1}{m-1} = \binom{n}{m} = v.$$

It follows from Proposition 3.2 that $\vartheta_k(K(n,m)) = v$ for $k > n/m$. Last, Kneser's conjecture (Kneser [50]), which was proved by Lovász [58], states that $\chi(K(n,m)) = n - 2m + 2$. The inequality $k > n - 2m + 1$ is thus equivalent to $k \geq \chi(K(n,m))$. Therefore, we can apply Proposition 3.1 to prove the last claim. $\qquad\square$

Since the Johnson graphs (Definition 1.4) are edge-transitive (see, e.g., Chen and Lih [19]), we can apply Theorem 5.6 to compute the corresponding generalized ϑ-number. The next theorem generalizes Theorem 5.7.

THEOREM 5.8. *For $0 \leq f < m$, $k \leq n$, and the Johnson graph $J(n,m,f)$, it follows that*

$$\vartheta_k(J(n,m,f)) = \min\left\{k\vartheta\left(J(n,m,f)\right), \binom{n}{m}\right\}.$$

Proof. Let v denote the order of $J(n,m,f)$, i.e., $v = \binom{n}{m}$. The multiplicities μ_i of the (not necessarily distinct) $m + 1$ eigenvalues λ_i of the adjacency matrix A of $J(n,m,f)$ are

$$\mu_i = \binom{n}{i} - \binom{n}{i-1}, \quad 0 \leq i \leq m;$$

see, e.g., Brouwer, Cohen, and Neumaier [12]. We set $\mu_0 = 1$, corresponding to the multiplicity of λ_1. The multiplicities are unordered, that is, the multiplicity of λ_i does not necessarily equal μ_i. When $n \leq 4$, the theorem can be verified numerically. We will now assume that $n > 4$. Then $\mu_i \geq n - 1$, and in particular, the multiplicity of λ_v is at least $n - 1$. From Theorem 5.6 it follows that

$$\vartheta_k(J(n, m, f)) = \min \mathbf{S}_k(\sigma(J + xA)).$$

Define $f(x) := \mathbf{S}_k(\sigma(J+xA))$. Because the multiplicity of λ_v is at least $n-1$, for $k \leq n$, we have that $x^* = n/(\lambda_v - \lambda_1)$ minimizes $f(x)$, and $f(x^*) = v + x^*(\lambda_1 + (k-1)\lambda_v)$. If $f(x^*) > n$, the minimum will occur at $f(0) = n$. $\qquad\square$

We can explicitly compute $\vartheta_k(J(n, m, m - 1))$. Taking the eigenvalues of this graph from [12, Chapter 9], we find

$$\vartheta_k(J(n, m, m - 1)) = \frac{k}{n+1}\binom{n+1}{m}, \quad k \leq n - m + 1.$$

For $k^* = n - m + 1$, we see that $\vartheta_{k^*}(J(n, m, m - 1))$ equals the number of vertices in $J(n, m, m - 1)$.

5.2. Relation between $\vartheta(K_k \square G)$ and $\vartheta_k(G)$. Gvozdenović and Laurent [40] show how to exploit an upper bound on the independence number of a graph to obtain a lower bound for the chromatic number of its complement graph. They do not consider the generalized ϑ-number in the bounding procedure. Kuryatnikova, Sotirov, and Vera [53] exploit the generalized ϑ-number to compute bounds on the chromatic number of a graph. For some graphs, the lower bounds on $\chi(G)$ from [53] coincide with the bounds obtained by using the theta function as suggested by [40]. Here we explain that finding by analyzing $\vartheta(K_k \square G)$ for symmetric graphs. We also show that the gap between $\vartheta_k(G)$ and $\vartheta(K_k \square G)$ can be arbitrarily large.

Chvátal [20] noted that

$$\alpha_k(G) = |V(G)| \iff \chi(G) \leq k.$$

Stated differently, $\chi(G) = \min\{k \mid k \in \mathbb{N}, \alpha_k(G) = |V(G)|\}$, or in plain words, the k independent sets giving $\alpha_k(G)$ correspond to the color classes of G in an optimal coloring. Analogous to $\chi_k(G) = \chi(G \circ K_k)$, it is known (cf. [53]) that

$$(38) \qquad \alpha_k(G) = \alpha(K_k \square G),$$

where $K_k \square G$ is the graph Cartesian product; see Definition 1.1. For a graph parameter $\beta(G)$ that satisfies

$$\alpha(G) \leq \beta(G) \leq \chi(\overline{G}),$$

Gvozdenović and Laurent [40] define $\Psi_\beta(G)$ as follows:

$$\Psi_\beta(G) := \min\{k \mid k \in \mathbb{N}, \beta(K_k \square G) = |V(G)|\}.$$

Then $\Psi_\alpha(G) = \chi(G)$. The operator $\Psi_\beta(\cdot)$ can be applied to a variety of graph parameters $\beta(G)$ and enables obtaining a hierarchy of bounds for $\chi(G)$ from a hierarchy of bounds for $\alpha(G)$. For example, when $\beta(G) = \vartheta(G)$, Gvozdenović and Laurent [40]

show that $\Psi_\vartheta(G) = \lceil \vartheta(\overline{G}) \rceil$. It follows from (38) that parameters $\vartheta_k(G)$ and $\vartheta(K_k \square G)$ both provide upper bounds on $\alpha_k(G)$. Therefore, it is natural to compare $\Psi_\vartheta(G)$ with

$$(39) \qquad \Psi_{\vartheta_k}(G) = \min\{k \mid k \in \mathbb{N}, \, \vartheta_k(G) = |V(G)|\}.$$

This comparison boils down to the comparison of $\vartheta(K_k \square G)$ and $\vartheta_k(G)$. Numerical results in [53] suggest the following conjecture.

CONJECTURE 1. *For any graph G and any natural number k, $\vartheta(K_k \square G) \leq \vartheta_k(G)$. Equality holds when $\vartheta_k(G) = k\vartheta(G)$.*

We show below that the gap between $\vartheta_k(G)$ and $\vartheta(K_k \square G)$ can be made arbitrarily large. We first state the following lemma that is needed in the rest of this section.

LEMMA 5.9 (Gvozdenović and Laurent [40]). *Given $A, B \in \mathbb{S}^n$ and $Y = I_k \otimes A + (J_k - I_k) \otimes B$, then $Y \succeq 0$ if and only if $A - B \succeq 0$ and $A + (k-1)B \succeq 0$. Furthermore, $\sigma(Y) = \sigma(A + (k-1)B) \cup \sigma(A - B)^{\{k-1\}}$.*

Now, we are ready to present our result.

PROPOSITION 5.10. *For any number $M \geq 0$, there exists a graph G and integer k such that*

$$\vartheta_k(G) - \vartheta(K_k \square G) \geq M.$$

Proof. Consider again graph $\mathcal{G}_n$, as defined in (16) for even n and set $k = n/2$. We will show that $\vartheta_{n/2}(\mathcal{G}_n) - \vartheta(K_{n/2} \square \mathcal{G}_n)$ is increasing in n. Let $p = 1/(2\sqrt{n-2})$ and consider first

$$X = \begin{bmatrix} \frac{1}{2} I_{n-2} & \mathbf{0}_{n-2} & p\mathbf{1}_{n-2} \\ \mathbf{0}_{n-2}^\top & \frac{1}{2} & 0 \\ p\mathbf{1}_{n-2}^\top & 0 & \frac{1}{2} \end{bmatrix}.$$

Taking the Schur complement of the bottom right 2×2 block of X shows that $0 \preceq X \preceq I$ (see the proof of Theorem 3.5 for more details). Combined with the fact that $\langle I, X \rangle = k$, it follows that X is feasible for ϑ_k-SDP2. Hence,

$$(40) \qquad \vartheta_{n/2}(\mathcal{G}_n) \geq \langle J, X \rangle = n/2 + \sqrt{n-2}.$$

As for $\vartheta(K_{n/2} \square G)$, let

$$A = \begin{bmatrix} -kJ_{n-1} + (k+1)I_{n-1} & \mathbf{1}_{n-1} \\ \mathbf{1}_{n-1}^\top & 1 \end{bmatrix}, \quad B = \begin{bmatrix} J_{n-1} & \mathbf{1}_{n-1} \\ \mathbf{1}_{n-1}^\top & -k \end{bmatrix},$$

and set $Y := I \otimes A + (J - I) \otimes B$. Then matrix $Y \in \mathcal{A}(K_{n/2} \square G)$; see (7). Furthermore, matrix Y is of the form described in Lemma 5.9. Then the largest eigenvalue of Y satisfies $\lambda_1(Y) = \max\{\lambda_1(A - B), \lambda_1(A + (k-1)B)\}$. Similar to the methods used in the proof of Theorem 3.5, it can be shown that $\lambda_1(Y) = k + 1$. Thus,

$$(41) \qquad \vartheta(K_{n/2} \square \mathcal{G}_n) \leq \lambda_1(Y) = n/2 + 1.$$

Combining (40) and (41) for fixed M and large enough (even) n, gives $\vartheta_{n/2}(\mathcal{G}_n) - \vartheta(K_{n/2} \square \mathcal{G}_n) \geq \sqrt{n-2} - 1 \geq M$. $\qquad\square$

We prove Conjecture 1 only for a particular class of graphs. Let us first show the following result.

THEOREM 5.11. *Let G be graph of order n that is both edge-transitive and vertex-transitive. Then*

$$\vartheta(K_k \square G) = \min\{k\vartheta(G), n\} = \vartheta_k(G).$$

Proof. For notational convenience we denote $A = A_G$. Because G is regular, edge-transitive, and vertex-transitive, we may assume without loss of generality that $\mathcal{A}(K_k \square G)$ (see (7)) contains only matrices of the form $X = I_k \otimes (J_n + xA) + (J_k - I_k) \otimes (J_n + yI_n)$. In order to minimize the largest eigenvalue of X we apply Lemma 5.9 and find

$$\lambda_1(X) = f(x,y) = \max\left\{\lambda_1(xA - yI_n), \lambda_1(kJ_n + xA + (k-1)yI_n)\right\}$$

$$= \max \begin{cases} f_1 = x\lambda_1 - y, \\ f_2 = x\lambda_n - y, \\ f_3 = kn + x\lambda_1 + (k-1)y, \\ f_4 = x\lambda_n + (k-1)y, \end{cases}$$

where λ_1 and λ_n are the greatest and smallest eigenvalues of A, respectively. We have used that $\sigma(kJ_n + xA + (k-1)yI_n)$ can be expressed similarly to (32). We minimize $\lambda_1(X)$ by considering different intervals of x. In case $x \geq 0$, we have $f(x,y) = \max\{f_1, f_3\}$, which is minimized when $x = 0$ and $f_1 = f_3$. Solving $f_1 = f_3$ for y, when $x = 0$, yields $y = -n$. Thus, when $x \geq 0$, we find that $f(0, -n) = n$ is the minimum. Furthermore,

$$\frac{kn}{\lambda_n - \lambda_1} \leq x \leq 0 \Longrightarrow f(x,y) = \max\{f_2, f_3\}.$$

The minimum here is attained when

$$f_2 = f_3 \implies y = x\left(\frac{\lambda_n - \lambda_1}{k}\right) - n \implies f_2 = n + \frac{1}{k}\left((k-1)\lambda_n + \lambda_1\right)x.$$

Depending on the sign of $(k-1)\lambda_n + \lambda_1$ we find either $f(0, -n) = n$ or $f(\frac{kn}{\lambda_n - \lambda_1}, 0) = k\frac{n\lambda_n}{\lambda_n - \lambda_1} = k\vartheta(G)$ by Theorem 5.5. For the case $x \leq \frac{kn}{\lambda_n - \lambda_1}$, note that

$$x \leq \frac{kn}{\lambda_n - \lambda_1} \Longrightarrow f(x,y) = \max\{f_2, f_4\},$$

which is minimized when $x = kn/(\lambda_n - \lambda_1)$ and $f_2 = f_4$. Solving $f_2 = f_4$ for y, when $x = kn/(\lambda_n - \lambda_1)$, yields $y = 0$ and thus $f(\frac{kn}{\lambda_n - \lambda_1}, 0) = k\vartheta(G)$. The minimum value of $\lambda_1(X)$, equivalently, the value $\vartheta(K_k \square G)$, thus equals $\min\{k\vartheta(G), n\}$.

Last, by edge-transitivity and vertex-transitivity of G, matrices optimal to ϑ_k-SDP2 for G have a constant row sum. Thus, as (28) shows, ϑ_k-SDP2 is then equivalent to maximizing the largest (scaled) eigenvalue over feasible matrices. Hence, $\vartheta_k(G) = \min\{k\vartheta(G), n\}$, as can be shown by derivations similar to those used for (29). $\square$

A graph that is both edge-transitive and vertex-transitive is also known as a symmetric graph. Many Johnson graphs (Definition 1.4) satisfy these properties.

Kuryatnikova, Sotirov, and Vera [53] compute $\vartheta_k(G)$ for several highly symmetric graphs (Table 13 in the online supplement to [53]). They remark that for those graphs, $\Psi_{\vartheta_k}(G) = \lceil \vartheta(\overline{G}) \rceil$. We explain this result for all the graphs present in Table 13 except

for the graph $H(12, 2, \{i \mid 1 \le i \le 7\})$ (see subsection 8.1 for the notation). All the other graphs evaluated by Kuryatnikova, Sotirov, and Vera in Table 13 satisfy the assumptions of Theorem 5.11, hence, $\vartheta_k(G) = \vartheta(K_k \square G)$ for those graphs. Therefore,

$$\Psi_{\vartheta_k}(G) = \Psi_\vartheta(G) = \lceil \vartheta(\overline{G}) \rceil. \tag{42}$$

Note that the Johnson graph $J(n, m, m - 1)$ is regular, vertex-transitive, and edge-transitive. Therefore, (42) holds and $\lceil \vartheta(\overline{J(n, m, m - 1)}) \rceil = n - m + 1$.

6. Strongly regular graphs. In the previous section we showed that certain classes of graphs allow an analytical computation of $\vartheta_k(G)$. This section expands on the considered classes with strongly regular graphs; see Definition 1.6. We also derive analogous of Theorem 5.11 for strongly regular graphs and the generalized ϑ'-number; see Theorem 6.4.

Let G be a strongly regular graph with parameters (n, d, λ, μ) and A_G its adjacency matrix. Since G is regular with valency d, we have that d is an eigenvalue of A_G with eigenvector $\mathbf{1}$. The matrix A_G has exactly two distinct eigenvalues associated with eigenvectors orthogonal to $\mathbf{1}$. These two eigenvalues are known as restricted eigenvalues and are usually denoted by r and s, where $r \ge 0$ and $s \le -1$. We consider here connected, noncomplete, strongly regular graphs. For those graphs we have that $s < -1$. Thus, we exclude trivial cases.

Strongly regular graphs attain Lovász bound of Theorem 5.5, see e.g., Haemers [42]. In particular, for a strongly regular graph G we have

$$\vartheta(G) = \frac{n\lambda_n(A_G)}{\lambda_n(A_G) - \lambda_1(A_G)}.$$

In the following theorem we derive an explicit expression for $\vartheta_k(G)$ for strongly regular graphs.

THEOREM 6.1. *For any strongly regular graph G with parameters (n, d, λ, μ) and restricted eigenvalues $r \ge 0$ and $s < -1$, we have*

$$\vartheta_k(G) = \min\{k\vartheta(G), n\} = \min \left\{ k\frac{n\lambda_n(A_G)}{\lambda_n(A_G) - \lambda_1(A_G)}, n \right\}.$$

Proof. We prove the result by showing that the lower and upper bounds on $\vartheta_k(G)$ coincide. Consider ϑ_k-*SDP*2, and set $Y = \frac{k}{n}I + xA_{\overline{G}}$. When $0 \preceq Y \preceq I$, Y is feasible for ϑ_k-*SDP*2. These SDP constraints on Y can be rewritten in terms of x. As ϑ_k-*SDP*2 is a maximization problem we may assume without loss of generality $x \ge 0$. Thus, for all $i \le n$,

$$\lambda_i(Y) = k/n + x\lambda_i(A_{\overline{G}}). \tag{43}$$

Since three eigenvalues of A_G satisfy $d \ge r > s$, we have

$$\sigma(A_{\overline{G}}) = (n - d - 1, -1 - s, -1 - r). \tag{44}$$

Substituting (44) in (43) and exploiting the fact that $n - d - 1 > -(s+1) > -(1+r)$ we have

$$0 \preceq Y \preceq I \iff 0 \le \lambda_i(Y) \le 1 \iff \begin{cases} k/n + x(-1 - r) \ge 0, \\ k/n + x(n - d - 1) \le 1. \end{cases}$$

The last two inequalities provide upper bounds on x, i.e.,

$$(45) \qquad x \leq \min\left\{\frac{k}{n(1+r)}, \frac{n-k}{n(n-d-1)}\right\}.$$

When x satisfies (45), Y is thus feasible for ϑ_k-SDP2 and $\langle J, Y \rangle$ will provide a lower bound for $\vartheta_k(G)$. In particular, with (45) at equality,

$$(46) \qquad \langle J, Y \rangle = k + n(n-d-1)x = \min\left\{k\left(\frac{r+n-d}{1+r}\right), n\right\}.$$

Equation (46) implies

$$(47) \qquad \vartheta_k(G) \geq \min\left\{k\left(\frac{r+n-d}{1+r}\right), n\right\}.$$

By (9) and Proposition 3.1, we have $\vartheta_k(G) \leq \min\{k\vartheta(G), n\}$. It remains only to show that

$$(48) \qquad k\left(\frac{r+n-d}{1+r}\right) = k\vartheta(G).$$

The eigenvalues of A_G can be written in terms of the parameters of G, i.e.,

$$(49) \qquad rs = \mu - d, \quad r + s = \lambda - \mu.$$

Furthermore, the parameters of any strongly regular graph satisfy

$$(50) \qquad (n-d-1)\mu = d(d-\lambda-1);$$

see, e.g., Theorem 9.1.3 in [13]. Let us now rewrite the term

$$(51) \qquad \frac{r+n-d}{1+r} = \frac{ns}{s-d}\frac{(r+n-d)(s-d)}{ns(1+r)}$$
$$= \frac{ns}{s-d}\frac{ns+nrs+[d^2-nd-(n-1)sr-d(r+s)]}{ns+nrs}$$

and evaluate the expression between the square brackets by using (49) and (50), i.e.,

$$d^2 - nd - (n-1)rs - d(r+s)$$
$$= d\lambda + d + (n-d-1)\mu - nd - (n-1)(\mu-d) - d(\lambda-\mu) = 0.$$

Thus (51) equals $ns/(s-d)$ and $ns/(s-d) = \vartheta(G)$, which proves the theorem. $\qquad\square$

Recall that in subsection 5.2 we consider symmetric graphs (graphs that are both edge-transitive and vertex-transitive). Although many graphs belong to both symmetric and strongly regular classes, note that neither one is a subset of the other. The graph C_6 is an example of a graph that is symmetric, but not strongly regular. The strongly regular Chang graphs (Chang [18]) provide an example of a strongly regular graph which is not symmetric.

In subsection 5.2 we have proved that $\vartheta(K_k \square G) = \min\{k\vartheta(G), n\} = \vartheta_k(G)$ holds for symmetric graphs; see Theorem 5.11. We show below that a similar relation

holds also for strongly regular graphs. In fact we prove a result for the generalized ϑ'-number, denoted by $\vartheta'_k(G)$, that is the optimal value of the SDP relaxation ϑ_k-$SDP2$ strengthened by adding nonnegativity constraints on the matrix variable. The generalized ϑ'-number for $k = 1$ is also known as the Schrijver's number.

To prove our result, we first present an SDP relaxation that relates $\vartheta'(K_k \square G)$ and $\vartheta_k(G)$. Kuryatnikova, Sotirov, and Vera [53] introduce the SDP relaxation

$$
\begin{aligned}
\theta^3_k(G) = \underset{Z \in \mathbb{S}^n}{\text{Maximize}} \quad & \langle I, Y \rangle \\
\text{subject to} \quad & Y_{ij} = 0 \quad \forall (i,j) \in E(G), \\
& Y_{ii} \leq 1 \quad \forall i \in [n], \\
& \begin{bmatrix} k & \text{diag}(Y)^\top \\ \text{diag}(Y) & Y \end{bmatrix} \succeq 0, \ Y \geq 0,
\end{aligned}
$$

which provides an upper bound for $\alpha_k(G)$, the optimal value for the MkCS problem. The above relaxation can be simplified when G is a highly symmetric graph. In particular, if G is a strongly regular graph one can restrict optimization of the above SDP relaxation to feasible points in the coherent algebra spanned by $\{I, A, J - I - A\}$. By applying symmetry reduction, the above SDP relaxation reduces to the following convex optimization problem:

$$
(52a) \qquad \theta^3_k(G) := \text{Maximize} \quad ny_1,
$$

$$
(52b) \qquad \text{subject to} \quad y_1 + (n - d - 1)y_2 - \frac{n}{k}y_1^2 \geq 0,
$$

$$
(52c) \qquad \qquad y_1 - (r + 1)y_2 \geq 0,
$$

$$
(52d) \qquad \qquad y_1 - (s + 1)y_2 \geq 0,
$$

$$
(52e) \qquad \qquad y_1 \leq 1,
$$

$$
(52f) \qquad \qquad y_1, y_2 \geq 0.
$$

For details on symmetry reduction see, e.g., [33, 53] and references therein.

In [53] the authors conjecture that $\theta^3_k(G) \leq \vartheta'_k(G)$ for any graph G. Here we show that $\theta^3_k(G) = \vartheta'_k(G)$ for any (nontrivial) strongly regular graph G.

LEMMA 6.2. *Let G be a strongly regular graph with parameters (n, d, λ, μ) and restricted eigenvalues $r \geq 0$ and $s < -1$. Then*

$$
\theta^3_k(G) = \min \left\{ k \left(\frac{r + n - d}{r + 1} \right), n \right\} = \vartheta_k(G) = \vartheta'_k(G).
$$

Proof. Note that for $s < -1$ constraint (52d) is trivially satisfied. Points in which constraints (52b) and (52c) intersect are $(0, 0)$ and $\left(\frac{k(r+n-d)}{n(r+1)}, \frac{k(n+r-d)}{n(r+1)^2} \right)$. The first equality follows by combining the latter point and constraint (52e). The second equality follows from $\vartheta(G) = (r + n - d)/(1 + r)$ (see (48)) and Theorem 6.1. The third equality follows from (45) and the fact that $\frac{k}{n(1+r)} \geq 0$ and $\frac{n-k}{n(n-d-1)} \geq 0$. $\square$

It is known that $\vartheta'(K_k \square G) \leq \theta^3_k(G)$; see section 5.1 in [53]. We show below that equality holds when $k < n(r + 1)/(r + n - d)$ and G is a (nontrivial) strongly regular graph by proving an equivalence between the SDP relaxations that give $\vartheta'(K_k \square G)$ and $\theta^3_k(G)$. The SDP relaxation for $\vartheta'(K_k \square G)$ (see also ϑ_k-$SDP2$) is invariant under permutations of k colors when the graph under the consideration is $K_k \square G$. This was

exploited in [53] to derive the following symmetry reduced relaxation:

$$\vartheta'(K_k \square G) = \underset{X,Z \in \mathbb{S}^n}{\text{Maximize}} \quad \langle I, X \rangle$$

$$\text{subject to} \quad X_{ij} = 0 \quad \forall (i,j) \in E(G),$$
$$Z_{ii} = 0 \quad \forall i \in [n],$$
$$X \geq 0, \ Z \geq 0, \ X - Z \succeq 0,$$
$$\begin{bmatrix} 1 & \text{diag}(X)^\top \\ \text{diag}(X) & X + (k-1)Z \end{bmatrix} \succeq 0.$$

The above relaxation can be further simplified when G is a strongly regular graph. One can restrict optimization to the corresponding coherent algebra. By applying symmetry reduction, the above SDP relaxation reduces to the following optimization problem:

$$(53a) \qquad \vartheta'(K_k \square G) := \text{Maximize} \quad nx_1$$
$$(53b) \qquad \qquad \text{subject to} \quad x_1 + (n-d-1)x_2 - (dz_1 + (n-d-1)z_2) \geq 0,$$
$$(53c) \qquad \qquad \qquad x_1 - (r+1)x_2 - (rz_1 - (r+1)z_2) \geq 0,$$
$$(53d) \qquad \qquad \qquad x_1 - (s+1)x_2 - (sz_1 - (s+1)z_2) \geq 0,$$
$$(53e) \qquad \qquad \qquad x_1 + (n-d-1)x_2$$
$$(53f) \qquad \qquad \qquad \qquad + (k-1)(dz_1 + (n-d-1)z_2) - nx_1^2 \geq 0,$$
$$(53g) \qquad \qquad \qquad x_1 - (r+1)x_2 + (k-1)(rz_1 - (r+1)z_2) \geq 0,$$
$$(53h) \qquad \qquad \qquad x_1 - (s+1)x_2 + (k-1)(sz_1 - (s+1)z_2) \geq 0,$$
$$(53i) \qquad \qquad \qquad x_1 \leq 1,$$
$$(53j) \qquad \qquad \qquad x_1, x_2, z_1, z_2 \geq 0.$$

Our next result relates optimization problems (52) and (53).

PROPOSITION 6.3. *Let G be a strongly regular graph with parameters (n, d, λ, μ) and restricted eigenvalues $r \geq 0$ and $s < -1$, and $k < \frac{n(r+1)}{r+n-d}$. Then the optimization problems* (52) *and* (53) *are equivalent.*

Proof. Let (x_1, x_2, z_1, z_2) be feasible for (53). We show that (y_1, y_2) where $y_1 := x_1$ and $y_2 := x_2$ is feasible for (52).

From (53b) and (53f) we have

$$\begin{cases} x_1 + (n-d-1)x_2 \geq (dz_1 + (n-d-1)z_2), \\ x_1 + (n-d-1)x_2 \geq nx_1^2 - (k-1)(dz_1 + (n-d-1)z_2), \end{cases}$$

from where it follows that

$$x_1 + (n-d-1)x_2 - \frac{n}{k}x_1^2$$
$$\geq \max\left\{ (dz_1 + (n-d-1)z_2) - \frac{n}{k}x_1^2, (k-1)\left(\frac{n}{k}x_1^2 - (dz_1 + (n-d-1)z_2)\right) \right\}.$$

To verify that the right-hand side above is nonnegative, note that either $dz_1 + (n-d-1)z_2 \geq \frac{n}{k}x_1^2$ or $dz_1 + (n-d-1)z_2 < \frac{n}{k}x_1^2$. Therefore $x_1 + (n-d-1)x_2 - \frac{n}{k}x_1^2 \geq 0$ and constraint (52b) is satisfied.

Similarly, from (53c) and (53g) it follows that constraint (52c) is satisfied. Constraint (52d) is trivially satisfied by (53d) and (53h).

Conversely, let (y_1, y_2) be feasible for (52). Define $x_1 := y_1$ and $x_2 := y_2$. Let z_1 and z_2 be the solutions of the following system of equations:

$$rz_1 = (r+1)z_2, \quad dz_1 + (n-d-1)z_2 = \frac{n}{k}x_1^2.$$

Thus, $z_1 = \frac{n(r+1)}{k(d+r(n-1))}x_1^2$, $z_2 = z_1 \frac{r}{r+1}$. Therefore, constraint (53b) follows from (52b) and the construction of z_1 and z_2. Similar arguments applied to (52c) can be used to verify that (53c) and (53g) are satisfied. To verify (53f) we rewrite the constraint as follows:

$$x_1 + (n-d-1)x_2 + (k-1)(dz_1 + (n-d-1)z_2) - nx_1^2$$
$$= x_1 + (n-d-1)x_2 - \frac{n}{k}x_1^2 + (k-1)\left(dz_1 + (n-d-1)z_2 - \frac{n}{k}x_1^2\right) \geq 0.$$

To verify constraint (53d) we exploit the construction of z_1 and z_2 as well as $r \geq 0$ and $s < -1$ to obtain $-(sz_1 - (s+1)z_2) = \frac{r-s}{r+1}z_1 \geq 0$. It remains to show that constraint (53h) is redundant for $k < \frac{n(r+1)}{r+n-d}$. Let us rewrite the constraint as follows:

(54)

$$x_1 - (s+1)x_2 + (k-1)(sz_1 - (s+1)z_2) = x_1 - (s+1)x_2 - \frac{n(k-1)(r-s)}{k(d+r(n-1))}x_1^2 \geq 0.$$

A point of intersection of $x_1 - (s+1)x_2 - \frac{n(k-1)(r-s)}{k(d+r(n-1))}x_1^2 = 0$ and $x_1 = (r+1)x_2$ is $\left(\frac{k(d+r(n-1))}{n(k-1)(r+1)}, \frac{k(d+r(n-1))}{n(k-1)(r+1)^2}\right)$, and a point of intersection of $x_1 + (n-d-1)x_2 - \frac{n}{k}x_1^2 = 0$ and $x_1 = (r+1)x_2$ is $\left(\frac{k(r+n-d)}{n(r+1)}, \frac{k(r+n-d)}{n(r+1)^2}\right)$. Furthermore, an intersection point of $x_1 + (n-d-1)x_2 - \frac{n}{k}x_1^2 = 0$ and the x_1-axis is $\left(\frac{k}{n}, 0\right)$, and a point of intersection of $x_1 - (s+1)x_2 - \frac{n(k-1)(r-s)}{k(d+r(n-1))}x_1^2 = 0$ and the x_1-axis is $\left(\frac{k(d+r(n-1))}{n(k-1)(r-s)}, 0\right)$. Note that the common intersection point of both parabolas, $x_1 = (r+1)x_2$, and the x_1-axis equals $(0,0)$. Let us find k for which

$$\frac{k(r+n-d)}{n(r+1)} < \frac{k(d+r(n-1))}{n(k-1)(r+1)} \quad \Leftrightarrow \quad k < \frac{n(r+1)}{r+n-d}$$

and

$$\frac{k}{n} < \frac{k(d+r(n-1))}{n(k-1)(r-s)} \quad \Leftrightarrow \quad k < \frac{d+rn-s}{r-s}.$$

By using (51), one can verify that $\frac{n(r+1)}{r+n-d} < \frac{d+rn-s}{r-s}$, from where it follows that the constraint (54) is redundant when $\frac{k(r+n-d)}{n(r+1)} < 1$.

It follows trivially that the objective values coincide for feasible solutions of two models that are related as described. □

Now, from the previous discussion the next result follows.

THEOREM 6.4. *Let G be a strongly regular graph with parameters (n, d, λ, μ) and restricted eigenvalues $r \geq 0$ and $s < -1$, and $k < \frac{n(r+1)}{r+n-d}$. Then $\vartheta'(K_k \square G) = \vartheta'_k(G)$.*

Proof. The proof follows from Lemma 6.2 and Proposition 6.3. □

7. Orthogonality graphs. In this section we compute the generalized ϑ-number for the orthogonality graphs.

We motivate the study of orthogonality graphs by a scenario, taken from Galliard, Tapp, and Wolf [31]. Let $n = 2^r$ for some $r \geq 1$. Consider a game where two players, Alice and Bob, each receive an n-dimensional binary vector as input. Either these vectors are equal or their Hamming distance (see Definition 1.2) equals $n/2$, that is, they differ in exactly 2^{r-1} positions. Given these inputs, Alice and Bob must each return an r-dimensional binary vector as output. To win the game, Alice and Bob must return equal outputs if and only if their inputs were equal. Alice and Bob are not permitted to communicate once they receive their inputs. The players are, however, allowed to coordinate a strategy beforehand. One such strategy results in the definition of an orthogonality graph.

Vertices of the orthogonality graph Ω_n are represented by all the unique n-dimensional binary vectors. Vertices (equivalently vectors) are adjacent if their Hamming distance equals $n/2$ and thus, $\Omega_n = H(n, 2, \{n/2\})$. Here $H(n, 2, \{n/2\})$ denotes the Hamming graph; see Definition 1.3.

The strategy of Alice and Bob then comprises graph coloring for Ω_n before the game starts. After being given their input vector, Alice and Bob should return as output the, earlier agreed upon, color of their vector, encoded as an r-dimensional binary vector. With this r-dimensional vector, Alice and Bob can indicate $2^r = n$ distinct colors. Disregarding any luck in guessing, the game can always be won if and only if $\chi(\Omega_n) \leq n$.

The orthogonality graph gets its name from another description of the graph, that is, when the vectors have $\{\pm 1\}$ entries. The Hamming distance between two binary vectors of $n/2$ then corresponds to those $\{\pm 1\}$ vectors being orthogonal to each other.

Godsil and Newman [35] prove that $\chi(\Omega_{2^r}) = 2^r$ for $r \in \{1, 2, 3\}$ and $\chi(\Omega_{2^r}) > 2^r$ otherwise. This means that the game can only be won for $r \leq 3$.

Clearly, for odd n, Ω_n is edgeless. We therefore restrict the analysis of Ω_n to the case when n is a multiple of 4. When that is the case, Ω_n consists of two isomorphic components, for vectors of even and odd Hamming weights, respectively.

Next to $\chi(\Omega_n)$, the independence number $\alpha(\Omega_n)$ has been studied in multiple papers. The two graph parameters are related by $|V| \leq \chi(G)\alpha(G)$ for any graph $G = (V, E)$; see (62). Frankl [26] and Galliard [30] constructed a stable set of Ω_n of size $\underline{\alpha}(n)$ for $n \equiv 0 \mod 4$. In particular,

$$(55) \qquad \alpha(\Omega_n) \geq \underline{\alpha}(n) = 4 \sum_{i=0}^{n/4-1} \binom{n-1}{i}.$$

On the other hand, de Klerk and Pasechnik [23] used an SDP relaxation to find $\alpha(\Omega_{16}) = \underline{\alpha}(16) = 2306$. It is also known that $\alpha(\Omega_{24}) = \underline{\alpha}(24) = 178208$; see [48]. More recently, Ihringer and Tanaka [48] have proven $\alpha(\Omega_{2^r}) = \underline{\alpha}(2^r)$ for $r \geq 2$. The *conjecture* by Godsil and Newman [35] (see also Frankl and Rödl [27]) whether

$$(56) \qquad \alpha(\Omega_{4m}) = \underline{\alpha}(4m) \text{ for } m \geq 1$$

remains an open problem.

We proceed by computing $\vartheta_k(\Omega_n)$ when n is a multiple of four. From Newman [69], the (unordered) eigenvalues of Ω_n are then given by

$$\lambda_r = \frac{2^{n/2}}{(n/2)!} \prod_{i=1}^{n/2} (2i - 1 - r), \quad 1 \leq r \leq n,$$

and $\lambda_0 = \binom{n}{n/2}$ (since Ω_n is regular with degree λ_0). The smallest eigenvalue is obtained for $r = 2$ and thus

$$\lambda_2 = \frac{1}{1-n}\binom{n}{n/2}.$$

Since Ω_n is isomorphic to a binary Hamming graph, Ω_n is a symmetric graph. The bound of Theorem 5.6 thus holds with equality. Newman [69] also shows that the multiplicity of λ_2 equals $n^2 - n$. This multiplicity exceeds n since n is a multiple of 4. Then it is not hard to show (by a method comparable to the one used in the proof of Theorem 5.7) that

$$\vartheta_k(\Omega_n) = k\frac{2^n}{n}, \quad k \leq n.$$

When $k = 1$, $\vartheta_k(\Omega_n)$ coincides here with the so-called ratio bound. This bound refers to (65) for regular graphs and was also computed for Ω_n in [69].

Let S be a stable set of size $\underline{\alpha}(n)$ that contains no vectors that have their Hamming weight contained in $W = \{n/4+1, n/4+3, \ldots, 3n/4-1\}$. Furthermore, note that the Johnson graphs (see Definition 1.4) appear as induced subgraphs of Ω_n. Let $w \in W$ and consider the subgraph of Ω_n induced by $J(n, w, w-n/4)$. This subgraph contains no vertices in S and thus

$$(57) \qquad \alpha_2(\Omega_n) \geq \underline{\alpha}(n) + 4\max_{w \in W}\{\alpha(J(n, w, w - n/4))\}.$$

We may multiply the independence number of $J(n, w, w - n/4)$ by 4 since we can take bitwise complements and find an isomorphic stable set in the isomorphic second component of Ω_n.

In subsection 8.1 we prove that $\chi_k(\Omega_{4n+2}) = 2k$.

8. New bounds on $\chi_k(G)$. In this section we first derive bounds on the product and sum of $\chi_k(G)$ and $\chi_k(\overline{G})$. Then, we provide graphs for which the bounds are sharp. Last, we derive spectral lower bounds on the multichromatic number of a graph.

A famous result by Nordhaus and Gaddum [70] states that

$$(58) \qquad n \leq \chi(G)\chi(\overline{G}) \leq \left(\frac{n+1}{2}\right)^2,$$

$$(59) \qquad 2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n+1.$$

Various papers have been published on determining Nordhaus-Gaddum inequalities for other graph parameters, such as the independence and edge-independence number (see [4] for a survey). We provide Nordhaus-Gaddum inequalities for k-multicoloring.

THEOREM 8.1. *For any graph $G = (V, E)$, $|V| = n$, we have*

$$k^2 n \leq \chi_k(G)\chi_k(\overline{G}) \leq k^2\left(\frac{n+1}{2}\right)^2,$$
$$2k\sqrt{n} \leq \chi_k(G) + \chi_k(\overline{G}) \leq k(n+1).$$

Proof. We follow the original proof as given by Nordhaus and Gaddum [70], extended to the k-multicoloring case. Consider an optimal k-multicoloring of G, using

$\chi_k(G)$ colors. Then for $i = 1, 2, \ldots, \chi_k(G)$, define n_i as the set of vertices that are colored with color i. We have $\sum_{i=1}^{\chi_k(G)} |n_i| = nk$. Furthermore,

$$(60) \qquad \max |n_i| \geq \frac{nk}{\chi_k(G)}.$$

Consider the largest set n_i. Since the vertices in this set share a color, they form a stable set in G. Thus they form a clique in $\overline{G}$. Accordingly,

$$(61) \qquad \chi_k(\overline{G}) \geq k\omega(\overline{G}) \geq k \max |n_i|.$$

Combining (60) and (61) proves the lower bound on the product of $\chi_k(G)$ and $\chi_k(\overline{G})$.

The lower bound on the sum of $\chi_k(G)$ and $\chi_k(\overline{G})$ can be proven by algebraic manipulation:

$$(\chi_k(G) - \chi_k(\overline{G}))^2 \geq 0 \implies \chi_k(G)^2 + \chi_k(\overline{G})^2 + 2\chi_k(G)\chi_k(\overline{G}) \geq 4\chi_k(G)\chi_k(\overline{G})$$
$$\implies \chi_k(G) + \chi_k(\overline{G}) \geq 2\sqrt{\chi_k(G)\chi_k(\overline{G})} \geq 2k\sqrt{n}.$$

The two upper bounds can be proven by combining (5), (58), and (59) as follows:

$$\chi_k(G)\chi_k(\overline{G}) \leq k^2\chi(G)\chi(\overline{G}) \leq k^2\left(\frac{n+1}{2}\right)^2,$$
$$\chi_k(G) + \chi_k(\overline{G}) \leq k(\chi(G) + \chi(\overline{G})) \leq k(n+1). \qquad \square$$

The second upper bound in Theorem 8.1 can also be found in [9] (in a slightly generalized form). We present below graphs for which the bounds in Theorem 8.1 are attained. For that purpose we define the graph sum of two graphs. The graph sum of graphs G_1 and G_2 is the graph, denoted by $G_1 + G_2$, whose vertices and edges are defined as follows:

$$V(G_1 + G_2) := V(G_1) \cup V(G_2), \ \ E(G_1 + G_2) := E(G_1) \cup E(G_2).$$

Nordhaus and Gaddum [70] show that the upper bounds in their theorem are attained by graph $G = K_p + \overline{K}_{p-1}$. Graph G has $n = 2p - 1$ vertices. It is clear that $\chi(G) = \chi(\overline{G}) = p = \frac{n+1}{2}$. Thus G attains both upper bounds simultaneously. As both G and $\overline{G}$ are weakly perfect graphs, we can apply (66) to find $\chi_k(G) = \chi_k(\overline{G}) = kp = k\frac{n+1}{2}$. This implies that graph G also attains the upper bounds in Theorem 8.1. Nordhaus and Gaddum [70] also provide an example of a graph which attains the lower bounds in their theorem. This example extends to the multichromatic variant as well. Let $m_1 = m_2 = \cdots = m_p = p$ and consider the complete multipartite graph $G = K_{m_1,\ldots,m_p}$. Then $\chi_k(G) = \chi_k(\overline{G}) = kp = k\sqrt{n}$. Thus, this graph G attains the lower bounds in Theorem 8.1. In fact, for any graph G such that $\chi(G)\chi(\overline{G}) = |V(G)|$, we have $k^2|V(G)| \leq \chi_k(G)\chi_k(\overline{G})$ by Theorem 8.1, and $\chi_k(G)\chi_k(\overline{G}) \leq k^2\chi(G)\chi(\overline{G}) = k^2|V(G)|$ by (5). Since the upper and lower bounds coincide, we have $\chi_k(G)\chi_k(\overline{G}) = k^2|V(G)|$. The set of vertex-transitive graphs provides a number of examples for which this bound is attained, such as the Johnson graph $J(n, 2, 1)$ when n is even.

The chromatic number of a graph is bounded by the spectrum of matrices related to its adjacency matrix. This well-known result is given below.

THEOREM 8.2 (Hoffman [46]). *If G has at least one edge, then $\chi(G) \geq 1 - \frac{\lambda_1(A_G)}{\lambda_n(A_G)}$.*

Since each color class has size at most $\alpha(G)$, we have that

$$(62) \qquad \chi(G) \geq \frac{n}{\alpha(G)},$$

where n is the number of vertices in G. Therefore one can use upper bounds for $\alpha(G)$ to derive lower bounds for $\chi(G)$. From (3) it follows that $\alpha(G \circ K_k) = \alpha(G)$. Thus we can establish the multicoloring variant of (62):

$$(63) \qquad \chi_k(G) = \chi(G \circ K_k) \geq \frac{|V(G \circ K_k)|}{\alpha(G \circ K_k)} = k\frac{n}{\alpha(G)}.$$

Note that the above result also follows from (60). The bound (63) is also given in [14], where the authors show that the lower bound is tight for webs and antiwebs. Note that for a graph G such that $\alpha_k(G) = k\vartheta(G)$ we have that $\alpha_k(G) = k\alpha(G)$ (see Lemma 5 in [53]), and thus $\chi_k(G) \geq \frac{k^2 n}{\alpha_k(G)}$. The above inequality is satisfied, for example, for the Johnson graph $J(n, 2, 1)$ when n is even, and for $J(n, 3, 2)$ when $v \equiv$ 1 or 3 mod 6.

Let us now present known upper bounds for the independence number of a graph.

THEOREM 8.3 (Hoffman [46]). *For any d-regular graph G of order n, we have* $\alpha(G) \leq n\frac{\lambda_n(A_G)}{\lambda_n(A_G)-d}$.

The result of Theorem 8.3 applies only to regular graphs with no loops. Haemers [41] generalizes the Hoffman bound as follows.

THEOREM 8.4 (Haemers [41]). *Let G have minimum vertex degree δ. Then*

$$(64) \qquad \alpha(G) \leq n\frac{\lambda_1(A_G)\lambda_n(A_G)}{\lambda_1(A_G)\lambda_n(A_G) - \delta^2}.$$

If G is regular, then the result of Theorem 8.4 reduces to Hoffman's bound. Another extension of the bound of Hoffman is given by Godsil and Newman [36].

THEOREM 8.5 (Godsil and Newman [36]). *Let G be a loopless graph and L_G its Laplacian matrix. Then*

$$(65) \qquad \alpha(G) \leq n\frac{\lambda_1(L_G) - \overline{d}_G}{\lambda_1(L_G)},$$

where $\overline{d}_G$ denotes the average degree of the vertices of G.

Now we are ready to present our results.

LEMMA 8.6. *Let G have minimum vertex degree δ. Then*

$$\chi_k(G) \geq k\frac{\lambda_1(A_G)\lambda_n(A_G) - \delta^2}{\lambda_1(A_G)\lambda_n(A_G)}.$$

Proof. The result follows by combining (63) and (64). $\square$

LEMMA 8.7. *For any loopless graph G, we have*

$$\chi_k(G) \geq k\frac{\lambda_1(L_G)}{\lambda_1(L_G) - \overline{d}_G},$$

where $\overline{d}_G$ denotes the average degree of its vertices, and L_G the Laplacian matrix of G.

Proof. The result follows by combining (63) and (65). □

When G is a regular graph, (65) is equivalent to the result of Theorem 8.3, and therefore the result of Lemma 8.7 is equivalent to

$$\chi_k(G) \geq k\left(1 - \frac{\lambda_1(A_G)}{\lambda_n(A_G)}\right).$$

It is not difficult to verify that complete graphs attain the bounds of Lemmas 8.6 and 8.7.

We end this section by presenting bounds on the multichromatic number of Johnson graphs; see Definition 1.4. We study the simple case $J(n,2,1)$, $n \geq 4$. Graph $J(n,2,1)$ is sometimes referred to as the triangular graph. The graph $J(n,2,1)$ is the complement graph of the Kneser graph $K(n,2)$, and both are known to be strongly regular. Every vertex of $J(n,2,1)$ corresponds to a set of two elements. These two elements can be thought of as two vertices of the complete graph K_n, with the vertex in $J(n,2,1)$ representing the edge between these two vertices of K_n. Graph $J(n,2,1)$ is thus the line graph of the complete graph K_n. For any graph G, its line graph is denoted $L(G)$.

PROPOSITION 8.8. *For the triangular graph $J(n,2,1)$ and $n \geq 4$, we have*

$$k(n-1) \leq \chi_k\left(J(n,2,1)\right) \leq k\left(2\left\lfloor\frac{n-1}{2}\right\rfloor + 1\right).$$

Proof. As $J(n,2,1)$ is isomorphic to $L(K_n)$, a coloring of $J(n,2,1)$ is equivalent to an edge coloring of K_n. It is not hard to see that $\omega(L(G))$ equals the maximum degree of a vertex of G. Thus $\omega(L(K_n)) = n - 1$. For even n, $\chi(L(K_n)) = n - 1$; see Baranyai [7]. Therefore, for even n we have

$$\chi(L(K_n)) = \omega(L(K_n)) \implies \chi_k(L(K_n)) = k\chi(L(K_n)) = k(n-1),$$

where the implication follows from (5). For odd n, $\chi(L(K_n)) = n$, see Vizing [83]. By (5), the proposition follows. □

Note that in the proof of the previous proposition we could also exploit the following well-known result: $\alpha(K(n,2)) = n - 1$.

8.1. Hamming graphs. In this section we present results for the (multi)chromatic number of Hamming graphs (Definition 1.3). We also provide sufficient and necessary conditions for the Hamming graph to be perfect.

In the Hamming graph $H(n,q,F)$, the vertex set is the set of n-tuples of letters from an alphabet of size q, and vertices u and v are adjacent if their Hamming distance satisfies $d(u,v) \in F$. Note that $|V(H(n,q,F))| = q^n$. By slight abuse of notation, we will use the terms vectors and vertices interchangeably, as they permit a one-to-one correspondence in Hamming graphs. Many authors refer to $H(n,q,\{1\})$ as the Hamming graph. The graph $Q_n := H(n,2,\{1\})$ is also known as the binary Hamming graph or hypercube graph.

We first list several known results for $H(n,q,\{1\})$. Graph $H(n,q,\{1\})$ equals the Cartesian product of n copies of K_q. Thus $H(n,q,\{1\}) = \square^n K_q$; see Definition 1.1. Furthermore, it holds $\chi(G_1 \square G_2) = \max\{\chi(G_1), \chi(G_2)\}$; see Sabidussi [74]. Therefore, $\chi(H(n,q,\{1\})) = q$. To derive the independence number of $H(n,q,\{1\})$, we proceed

as follows. Let $S \subset V$ be a stable set of $H(n, q, \{1\})$. Then $\text{Min}_{u,v \in S,\, u \neq v} d(u, v) \geq 2$. From coding theory, the Singleton bound (Singleton [78]) is an upper bound on the maximum number of codes of length n, using an alphabet of size q, such that a Hamming distance between any two codes is at least two. In particular, from the Singleton bound we have $\alpha(H(n, q, \{1\})) \leq q^{n-1}$.

To show that $\alpha(H(n, q, \{1\})) \geq q^{n-1}$, we construct an independent set in the Hamming graph of size q^{n-1}, by a construction employed in [78]. Consider all the vectors in $(\mathbb{Z}/q\mathbb{Z})^n$ for which the coordinates sum to some $x \in \mathbb{Z}/q\mathbb{Z}$. By symmetry, there exist q^{n-1} vectors satisfying this condition. Note that any two different vectors satisfying this condition must differ in at least two positions, which implies they are not adjacent. Thus, $\alpha(H(n, q, \{1\})) \geq q^{n-1}$ and combined with the Singleton bound, this gives $\alpha(H(n, q, \{1\})) = q^{n-1}$.

To the best of our knowledge, the following results are not known in the literature.

LEMMA 8.9. *For $k \leq q^n$, $\chi_k(H(n, q, \{1\})) = kq$.*

Proof. Let us denote $H = H(n, q, \{1\})$. Consider the vectors in H for which the first entry ranges from 0 up to and including $q - 1$, while the other entries equal 0. This gives a clique of size q and since $\omega(H) \leq \chi(H) = q$, we have $\omega(H) = q$. From (5), it follows the result. $\quad\square$

The proof of Lemma 8.9 relies on the fact that $\omega(H) = \chi(H)$, or equivalently, that $H(n, q, \{1\})$ is a weakly perfect graph. In general, for any weakly perfect graph G

$$(66) \qquad \omega(G) = \chi(G) \implies \chi_k(G) = k\chi(G).$$

This gives rise to the question for which values of q and n the graph $H(n, q, \{1\})$ is perfect. The strong perfect graph theorem states that a graph is perfect if and only if it does not contain C_{2n+1} or $\overline{C}_{2n+1}$ as induced subgraphs, for all $n > 1$.

PROPOSITION 8.10. *The Hamming graph $H(n, q, \{1\})$ is a perfect graph if and only if $n \leq 2$ or $q \leq 2$.*

Proof. Denote $H(n, q) = H(n, q, \{1\})$. Graph $H(1, q)$ is K_q, which is clearly a perfect graph. Graph $H(2, q)$ is a lattice graph, or Rook's graph, which is also a perfect graph. Graph $H(n, 1)$ is a single vertex and thus also perfect. Last, graph $H(n, 2)$ is bipartite and thus perfect. For $q \geq 3$, the following vectors from $H(3, q)$ form C_7:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}.$$

Then by the strong perfect graph theorem, $H(3, q)$ is not perfect. An odd cycle in $H(n, q)$ for general $n, q \geq 3$, is obtained by simply adjoining zeros to the above vectors such that they become n-dimensional. $\quad\square$

As $H(n, q, \{f\})$ is edgeless for $f > n$, we consider the extremal case $H(n, q, \{n\})$ for $n > 1$. Note that $H(1, q, \{1\}) = K_q$. Graph $H(n, q, \{n\})$ can be described by use of the tensor product of graphs (see Definition 1.1). In particular, we have that $H(n, q, \{n\}) = \otimes^n K_q$.

Since all the edges of $G_1 \otimes G_2$ also appear in $G_1 \circ G_2$, it follows that $\chi(G_1 \otimes G_2) \leq \chi(G_1 \circ G_2)$. Moreover, by Hedetniemi [44], we have

$$(67) \qquad \chi(G_1 \otimes G_2) \leq \min\{\chi(G_1), \chi(G_2)\}.$$

Hedetniemi's conjecture states that (67) holds with equality. The conjecture was recently disproved by Shitov [77]. Inequality (67) implies that $\chi(\otimes^n K_q) \leq q$.

The vectors $i \cdot \mathbf{1}$ for $0 \leq i \leq q - 1$ form a clique of size q in graph $H(n, q, \{n\})$. Thus $q \leq \omega(H(n, q, \{n\}))$. Now, from this inequality and $\chi(\otimes^n K_q) \leq q$ it follows that $\chi(H(n, q, \{n\})) = q$. Using (5) or (66), we find $\chi_k(H(n, q, \{n\})) = kq$. The coloring of these tensor products of graphs has been previously considered by Greenwell and Lovász [37], where they also proved this result.

Let us now define $f^+ := \{i \in \mathbb{N} \mid f \leq i\}$. The Hamming graph $H(n, q, f^+)$ has been studied by El Rouayheb et al. [24] among others. They show that, under some condition on the parameters n, q, and f, $\chi(H(n, q, f^+)) = q^{n-f+1}$. We extend this result to multicoloring in the following proposition.

PROPOSITION 8.11. *For $q \geq n - f + 2$ and $1 \leq f \leq n$, we have $\chi_k(H(n, q, f^+)) = kq^{n-f+1}$.*

Proof. For parameters n, q, and f satisfying the conditions of the proposition, it is known (cf. [28]) that $\alpha(H(n, q, f^+)) = q^{f-1}$. By (5) and (63), the proposition follows. □

Binary Hamming graphs $H(n, 2, \{f\})$, $f \leq n$, form another interesting case. Recall that the Hamming weight of a vector is its Hamming distance to the zero vector, and that the Hamming graphs are vertex-transitive.

THEOREM 8.12. *For all $n \in \mathbb{N}$, f odd, and $f \leq n$, $\chi_k(H(n, 2, \{f\})) = 2k$.*

Proof. Let $n, f \in \mathbb{N}$, f odd, and $f \leq n$. Consider the zero vector in $H(n, 2, \{f\})$. Note that every vector adjacent (orthogonal) to the zero vector has an odd Hamming weight. By vertex transitivity, all vectors of even Hamming weight only have vectors of odd Hamming weight as neighbors. Similarly, vectors of odd Hamming weight only have vectors of even Hamming weight as neighbors. Graph $H(n, 2, \{f\})$ is thus bipartite, which, combined with (5), proves the theorem. □

It readily follows the following results for orthogonality graphs.

COROLLARY 8.13. *Let Ω_{4n+2} $(n \in \mathbb{N})$ be the orthogonality graph. Then,*

$$\chi_k(\Omega_{4n+2}) = 2k.$$

Proof. Graph Ω_{4n+2} is isomorphic to $H(4n + 2, 2, \{2n + 1\})$. This corollary is thus a special case of Theorem 8.12. □

9. Conclusion. In this paper, we study the generalized ϑ-number for highly symmetric graphs and beyond. The parameter $\vartheta_k(G)$ generalizes the concept of the famous ϑ-number that was introduced by Lovász [59]. Since $\vartheta_k(G)$ is sandwiched between the $\alpha_k(G)$ and $\chi_k(\overline{G})$ it serves as a bound for both graph parameters.

Several results in this paper are not restricted to highly symmetric graphs, in particular, the results in sections 2, 3, and 4. In section 2 we present in an elegant way a known result that $\vartheta_k(G)$ is a lower bound for $\chi_k(\overline{G})$. Another lower bound for $\chi_k(\overline{G})$ is $k\vartheta(G)$; see (9). The inequality (9) is rather counterintuitive since it is more difficult to compute $\vartheta_k(G)$ than $\vartheta(G)$, while $k\vartheta(G)$ provides a better bound for the kth chromatic number. However, the generalized ϑ-number can also be used to compute lower bounds for the (classical) chromatic number of a graph; see subsection 5.2.

In section 3 we show that the sequence $(\vartheta_k(G))_k$ is increasing and bounded above by the order of G (Proposition 3.2 and Theorem 3.4) and that the increments of the

sequence can be arbitrarily small (Theorem 3.5). Section 4 provides bounds for $\vartheta_k(G)$ where G is the strong graph product of two graphs (Theorem 4.2) and the disjunction product of two graphs (Theorem 4.3).

Sections 5, 6, and 7 consider highly symmetric graphs. We derive closed form expressions for the generalized ϑ-number on cycles (Theorem 5.3), Kneser graphs (Theorem 5.7), Johnson graphs (Theorem 5.8), and strongly regular graphs (Theorem 6.1), among other results. It is known that $\vartheta(K_k\square G)$ and $\vartheta_k(G)$ provide upper bounds on $\alpha_k(G)$. However, it is more computationally demanding to compute $\vartheta(K_k\square G)$ than $\vartheta_k(G)$. We show that for graphs that are both edge-transitive and vertex-transitive it suffices to solve $\vartheta_k(G)$, see Theorem 5.11. However, the gap between $\vartheta_k(G)$ and $\vartheta(K_k\square G)$ can be arbitrarily large (Proposition 5.10). We also prove that $\vartheta'(K_k\square G)$ equals $\vartheta'_k(G)$ for any (nontrivial) strongly regular graph G and $k < n(r+1)/(r+n-d)$; see Theorem 6.4. Section 7 presents results for $\vartheta_k(G)$ and $\chi_k(G)$ on orthogonality graphs.

Bounds on the kth chromatic number of various graphs are given in section 8. In particular, bounds on the product and sum of $\chi_k(G)$ and $\chi_k(\overline{G})$ are presented in Theorem 8.1. Lemma 8.9, Proposition 8.11, and Theorem 8.12 provide the multichromatic number for several Hamming graphs, while Proposition 8.8 provides bounds for the multichromatic number on triangular graphs.

Let us list several open problems. Prove Conjecture 1 for any graph. Recall that we prove Conjecture 1 only for symmetric graphs; see Theorem 5.11. It would be interesting to prove the conjecture by Godsil, Newman, and Frankl (56) for the first open case Ω_{40}. Another open problem is to generalize the well-known inequality $\vartheta(G)\vartheta(\overline{G}) \geq |V|$ (see [59]) for $\vartheta_k(G)$, $k \geq 2$.

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