Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 41, pp. 602-615, November 2025.

EIGENVALUE BOUNDS FOR THE QUANTUM CHROMATIC NUMBER OF GRAPH POWERS*

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Abstract. The quantum chromatic number, a generalization of the chromatic number, was first defined in relation to the nonlocal quantum coloring game. We generalize the former by defining the quantum k-distance chromatic number $\chi_{kq}(G)$ of a graph G, which can be seen as the quantum chromatic number of the k-th power graph, G^k, and as generalization of the classical k-distance chromatic number $\chi_k(G)$ of a graph. In this paper, we strengthen three classical eigenvalue bounds for the k-distance chromatic number by showing they also hold for the quantum counterpart of this parameter. This shows that several bounds by Elphick et al. [*J. Combinatorial Theory Ser. A* 168, 2019, *Electron. J. Comb.* 27(4), 2020] hold in the more general setting of distance-k colorings. As a consequence, we obtain several graph classes for which $\chi_{kq}(G) = \chi_k(G)$, thus increasing the number of graphs for which the quantum parameter (which is not known to be computable) is known.

Key words. Graph coloring, Distance chromatic number, Spectral bounds, Quantum information.

AMS subject classifications. 15A15, 15F10.

1. Introduction.

Quantum graph parameters originated in the context of nonlocal games. The latter are game-like models involving two or more cooperative players, whose objective is to win the game without being able to communicate with each other throughout the duration of the game. The players are only allowed to build a common strategy before the game starts. It turns out that by sharing an entangled quantum state, players can increase their probability of winning such nonlocal games. In this paper, we focus on the quantum chromatic number, a graph parameter related to a specific nonlocal game: the graph coloring game.

The graph coloring game is as follows. Given a graph G, two players, Alice and Bob, are each given a vertex of the graph, and each must respond with a integer in $[c] := \{1, \dots, c\}$. To win the game, the players must answer differently if their given vertices were adjacent, or answer identically if their vertices were equal. In a classical setting (i.e., no quantum states involved), Alice and Bob can win with certainty if $c \geq \chi(G)$, where $\chi(G)$ is the chromatic number of the graph. However, if the players were to share an entangled quantum state, they can, depending on the graph chosen, win the game with certainty even if $c < \chi(G)$. The quantum chromatic number is precisely the smallest integer c, for which Alice and Bob can win the graph coloring game with certainty, when allowed to share an entangled quantum state. This parameter appeared first in [5] building on [7, 13]. It has since received quite some attention, see e.g. [12, 15, 18, 20, 21, 24, 23].

For a positive integer k, the k^{th} *power of a graph* $G = (V, E)$, denoted by G^k, is a graph with vertex set V in which two distinct elements of V are joined by an edge if there is a path in G of length at most k between them. Problems related to the chromatic number $\chi(G^k)$ of power graphs G^k were first considered by Kramer and Kramer in [16, 17] in 1969 and have enjoyed significant attention ever since then.

*Received by the editors on March 3, 2025. Accepted for publication on October 21, 2025. Handling Editor: Joshua Cooper. Corresponding Author: Aida Abiad.

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We investigate a quantum analogue of the distance chromatic number $\chi_k(G)$. A natural extension of the combinatorial definition of the quantum chromatic number (see [21, Definition 1]) to the quantum k-distance chromatic number is as follows.

Definition 1.1. *A* quantum k-distance c-coloring *of a graph $G=(V,E)$, denoted by χ_{kq}, is a collection of orthogonal projectors $\{P_{v,h} : v \in V, h \in [c]\}$ in $\mathbb{C}^{d\times d}$ such that*

- *for all vertices $v \in V$*

$$\sum_{h\in[c]} P_{v,h} = I_d \quad \textit{(completeness)}, \tag{1.1}$$

- *for all distinct vertices $v, w \in V$ with $dist(v,w) \leq k$ and for all $h \in [c]$*

$$P_{v,h}P_{w,h} = 0_d \quad \textit{(orthogonality)}. \tag{1.2}$$

The quantum k-distance chromatic number $\chi_{kq}(G)$ *is the smallest c for which the graph G admits a quantum k-distance c-coloring for some dimension $d > 0$.*

Note that it is clear by definition that a quantum k-distance c-coloring is also a quantum ℓ-distance coloring for $\ell \leq k$. Thus $\chi_{\ell q}(G) \leq \chi_{kq}(G)$ for all $k \in [|V|]$ and $\ell \leq k$. Furthermore, for $k=1$ we obtain the definition of quantum c-coloring from [21, Definition 1]. Observe also that any classical c-coloring can be viewed as a 1-dimensional quantum coloring (i.e. letting $d=1$), where we set $P_{v,h}=1$ if vertex v has color h and we set $P_{v,h}=0$, otherwise. Thus, a quantum coloring is a relaxation of the classical coloring. Also, observe that

$$\chi_{kq}(G) = \chi_q(G^k). \tag{1.3}$$

Despite the above, even the simplest algebraic or combinatorial parameters (including the eigenvalues) of the power graph G^k cannot be easily deduced from the corresponding parameters of the graph G, see e.g.[2, 6, 8, 10]. In this regard, several eigenvalue bounds on $\chi_k(G)$ that depend only on the spectrum of G have been proposed in the literature. Notably, two inertial-type bounds were shown by Abiad et al. in [2] (see Theorems 2.1 and 2.3). The same authors also prove a Hoffman ratio-type bound on $\chi_k(G)$ (see Theorem 2.2). These three eigenvalue bounds are shown to be sharp for several graph classes. The quality of these bounds depends on the choice of a degree-k polynomial, so finding the best possible lower bound for a given graph is, in fact, an optimization problem which is investigated in [2, 3].

In this work, we show that the three eigenvalue bounds on the classical parameter $\chi_k(G)$ also hold in the quantum setting. It is not known whether the quantum counterpart of $\chi_k(G)$ is a computable function. As a consequence of our results, we can use the bounds optimization shown in the classical setting to obtain several graph classes for which $\chi_k(G) = \chi_{kq}(G)$, thus increasing the number of graphs for which the quantum parameter is known. Our work extends several known results from [2, 11, 12, 24]. While an application of the Hoffman ratio-type bound on $\chi_k(G)$ to coding theory has been recently presented [3], our results show the first quantum application of the three aforementioned eigenvalue bounds.

2. Three eigenvalue bounds in the classical setting.

In this section, we recall several bounds on the classical k-distance chromatic number of a graph which use the eigenvalues of the adjacency matrix. In Sections 4 and 5, we will show that all these bounds hold for the quantum k-distance chromatic number as well.

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Recall that the *inertia* of a graph G is the ordered triple (n^+, n^0, n^-), where n^+, n^0, and n^- are the numbers of positive, zero, and negative eigenvalues of the adjacency matrix A, respectively, including multiplicities. Furthermore, we denote by $\mathbb{R}_k[x]$ the collection of polynomials in x over $\mathbb{R}$ of degree at most $k \in \mathbb{N}_{\geq 0}$.

The first bound is derived by Abiad, Coutinho, and Fiol, from the inertial-type bound in [1, Theorem 3.1] using the fact that upper bounds on $\alpha_k(G)$ directly yield lower bounds on $\chi_k(G)$ using the fact that $\chi_k(G) \geq \frac{n}{\alpha_k(G)}$.

THEOREM 2.1 (First inertial-type bound). *[1, Theorem 3.1] Let G be a graph with adjacency matrix A having eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p) := \max_{u\in V}\{(p(A))_{uu}\}$ and $w(p) := \min_{u\in V}\{(p(A))_{uu}\}$. Then,*

$$\chi_k(G) \geq \frac{n}{\min\{|\{i : p(\lambda_i) \geq w(p)\}|, |\{i : p(\lambda_i) \leq W(p)\}|\}}. \tag{2.4}$$

Similarly, one can use the ratio-type bound for $\alpha_k(G)$ which appears in [1, Theorem 3.2] and obtain:

THEOREM 2.2 (Hoffman ratio-type bound). *[2, Theorem 4.3] Let G be a graph with n vertices and adjacency matrix A having eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p) := \max_{u\in V} \ \{(p(A))_{uu}\}$ and $\lambda(p) := \min_{i\in[2,n]}\{p(\lambda_i)\}$, and assume $p(\lambda_1) > \lambda(p)$. Then,*

$$\chi_k(G) \geq \frac{p(\lambda_1) - \lambda(p)}{W(p) - \lambda(p)}. \tag{2.5}$$

For $k = 1$, the above gives the celebrated Hoffman bound on the chromatic number, $\chi(G) \geq 1 - \frac{\lambda_1}{\lambda_n}$.

In [2], yet another stronger inertial-type bound for χ_k is shown by assuming k-partially walk-regularity. Recall that a graph G is *k-partially walk-regular* for some integer $k \geq 0$ if the number of closed walks rooted at some vertex v of any given length $\ell \leq k$ is independent of the choice of v.

THEOREM 2.3 (Second inertial-type bound). *[2, Theorem 4.2] Let G be a k-partially walk-regular graph with adjacency eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Then,*

$$\chi_k(G) \geq 1 + \max\left\{\frac{|\{j : p(\lambda_j) < 0\}|}{|\{j : p(\lambda_j) > 0\}|}\right\}, \tag{2.6}$$

where the maximum is taken over all $p \in \mathbb{R}_k[x]$ such that $\sum_{i=1}^n p(\lambda_i) = 0$.

Theorem 2.3 is an extension of [12, Theorem 1]. Note for the $k = 1$ case, the assumption of partially walk-regularity is not needed.

THEOREM 2.4. *[12, Theorem 1] Let G be a graph with inertia (n^+, n^0, n^-). Then,*

$$\chi(G) \geq 1 + \max\left\{\frac{n^+}{n^-}, \frac{n^-}{n^+}\right\}. \tag{2.7}$$

In [12], Elphick and Wocjan also show that the inertial-type bound (2.7) for χ is in fact also a lower bound for the corresponding quantum chromatic parameter χ_q.

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3. Pinching and the quantum k-distance coloring. In [12], the authors establish the existence of a quantum coloring using the pinching operation of a suitable set of orthogonal projectors. We mimic this proof in order to determine whether a set of orthogonal projector forms a quantum k-distance coloring.

First we recall the pinching operation.

DEFINITION 3.1 (Pinching). *Let $\mathcal{P} := \{P_s \in \mathbb{C}^{d\times d} : s \in [c]\}$ be a collection of orthogonal projectors that form a resolution of the identity matrix. For all $X \in \mathbb{C}^{d\times d}$, we define the* pinching of X by $\mathcal{P}$ *to be*

$$\mathcal{C}_{\mathcal{P}}(X) := \sum_{s\in[c]} P_s X P_s.$$

We say the pinching $\mathcal{C}_{\mathcal{P}}$ annihilates X if $\mathcal{C}_{\mathcal{P}}(X) = 0$.

We now focus on the desired result.

THEOREM 3.2. *Let $\{P_{v,s} : v \in V, s \in [c]\}$ be a quantum k-distance coloring of G in $\mathbb{C}^{d\times d}$. Then, the following block-diagonal orthogonal projectors*

$$P_s := \sum_{v\in V} e_v e_v^\dagger \otimes P_{v,s} \in \mathbb{C}^{n\times n} \otimes \mathbb{C}^{d\times d},$$

whose collection we denote by $\mathcal{P}$, form a resolution of the identity matrix and the corresponding pitching operation $\mathcal{C}_{\mathcal{P}}$ satisfies:

(1) $\mathcal{C}_{\mathcal{P}}(A^\ell \otimes I_d) = \sum_{v\in V} A^\ell_{vv} \cdot e_v e_v^\dagger \otimes I_d$ for all $\ell \le k$,
(2) $\mathcal{C}_{\mathcal{P}}(E \otimes I_d) = E \otimes I_d$ for all diagonal matrices $E \in \mathbb{C}^{n\times n}$.

Proof. Since $\{P_{v,s} : v \in V, s \in [c]\}$ is a quantum k-distance coloring, it is also a quantum coloring. Therefore, by [12, Theorem 1], the collection $\mathcal{P}$ forms a resolution of the identity and (2) holds as well. Hence, we are left to show that (1) holds for all $1 \le \ell \le k$. Fix such an ℓ.

$$\begin{aligned}
&\mathcal{C}_{\mathcal{P}}(A^\ell \otimes I_d)\\
&= \sum_{s\in[c]} P_s (A^\ell \otimes I_d) P_s\\
&= \sum_{s\in[c]} \left(\sum_{v\in V} e_v e_v^\dagger \otimes P_{v,s}\right)(A^\ell \otimes I_d)\left(\sum_{w\in V} e_w e_w^\dagger \otimes P_{v,s}\right)\\
&= \sum_{s\in[c]} \sum_{v,w\in V} A^\ell_{vw} \cdot e_v e_w^\dagger \otimes P_{v,s}P_{w,s}\\
&= \sum_{s\in[c]} \left(\sum_{\substack{v,w\in V\\ 0=d(v,w)}} A^\ell_{vw} \cdot e_v e_w^\dagger \otimes P_{v,s}P_{w,s} + \sum_{\substack{v,w\in V\\ 0<d(v,w)\le k}} A^\ell_{vw} \cdot e_v e_w^\dagger \otimes 0_d + \sum_{\substack{v,w\in V\\ d(v,w)>k}} 0 \cdot e_v e_w^\dagger \otimes P_{v,s}P_{w,s} \right)\\
&= \sum_{s\in[c]} \sum_{v\in V} A^\ell_{vv} \cdot e_v e_v^\dagger \otimes P_{v,s}\\
&= \sum_{v\in V} A^\ell_{vv} \cdot e_v e_v^\dagger \otimes I_d.
\end{aligned}$$

The third to last equality follows from the fact that $A^\ell_{v,w}$ counts the number of walks of length ℓ between v and w. Hence, if $d(v,w) > k$, then $A^\ell_{v,w} = 0$ for all $\ell \le k$. If $d(v,w) \le \ell$ then $P_{v,s}P_{w,s} = 0$ for all

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$s \in [c]$ by definition of quantum k-distance coloring. Furthermore, the last equality follows from the fact that $\sum_{s\in[c]} P_{v,s} = I_d$. ◻

We now establish a converse statement similar to that of [12, Theorem 2].

THEOREM 3.3. *Assume that there exists a pinching $\mathcal{C}_{\mathcal{P}}$ where $\mathcal{P} := \{P_s \in \mathbb{C}^{nd\times nd} : 1 \le s \le c\}$ is a collection of orthogonal projectors such that $\mathcal{P}$ forms a resolution of the identity, $\mathcal{C}_{\mathcal{P}}(A^\ell \otimes I_d) = \sum_{v\in V} A^\ell_{vv} \cdot e_v e_v^\dagger \otimes I_d$ for all $1 \le \ell \le k$ and $\mathcal{C}_{\mathcal{P}}(E \otimes I_d) = E \otimes I_d$ for all diagonal matrices $E \in \mathbb{C}^{n\times n}$. Then there exists a quantum k-distance coloring of G.*

Proof. Using the same argument as the proof of [12, Theorem 2], we must have that P_s are block diagonal for all $s \in [c]$, and the block are indexed by the vertices v of G. We refer to each of those block as $P_{v,s}$ for $v \in V$ and $s \in [c]$, in other words, $P_s = \sum_{v\in V} e_v e_v^\dagger \otimes P_{v,s}$. Because P_s is an orthogonal projector, it can easily be seen that each $P_{v,s}$ for $v \in V$ are also orthogonal projectors. Moreover, since $\mathcal{P}$ forms a resolution of the identity, then for each $v \in V$, we must have $\sum_{s\in[c]} P_{v,s} = I_d$.

Because $\mathcal{C}_{\mathcal{P}}(A^\ell \otimes I_d) = \sum_{v\in V} A^\ell_{vv} \cdot e_v e_v^\dagger \otimes I_d$ for all $\ell \le k$ then following the operations of pinching we get

$$\sum_{\substack{v,w\in V\\ 0<d(v,w)\le k}} A^\ell_{vw} \cdot e_v e_w^\dagger \otimes \left(\sum_{s\in[c]} P_{v,s} P_{w,s}\right) = 0.$$

However, if $0 < d(v,w) \le k$, then for some $1 \le \ell \le k$ we must have $A^\ell_{v,w} > 0$. Thus, it must be that $\sum_{s\in[c]} P_{v,s} P_{w,s} = 0$. Finally, multiplying on the left by $P_{v,t}$ and on the right by $P_{w,t}$ for an arbitrary $t \in [c]$, we get that $P_{v,t} P_{w,t} = 0$. Thus, we have an k-distance coloring $\{P_{v,s} : s \in [c], v \in V\}$. ◻

4. Inertial-type bounds for the quantum distance-k chromatic number.

4.1. First inertial-type bound. The following bound on χ_{kq} extends Theorem 2.1 to its quantum counterpart:

THEOREM 4.1 (First inertial-type bound). *Let G be a graph of order n with adjacency matrix A having eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$. Let $p \in \mathbb{R}_k[x]$ with corresponding parameters $W(p) := \max_{u\in V}\{(p(A))_{uu}\}$ and $w(p) := \min_{u\in V}\{(p(A))_{uu}\}$. If $\chi_{kq}(G)\alpha_{kq}(G) \ge n$, then*

$$\chi_{kq}(G) \ge \frac{n}{\min\{|\{i : p(\lambda_i) \ge w(p)\}|, |\{i : p(\lambda_i) \le W(p)\}|\}}.$$

Proof. The result follows immediately from the assumption $\chi_{kq}(G) \ge \frac{n}{\alpha_{kq}(G)}$ and [25, Theorem 3.3]. ◻

Details on the optimization of this bound can be found in [2].

REMARK 4.2. *Note that Theorem 4.1 uses the assumption that $\chi_{kq}(G)\alpha_{kq}(G) \ge n$. In the case of the classical graph parameters, it is well known that $\chi(G)\alpha(G) \ge n$ for any graph G, which then makes the proof of the classical first inertial bound (Theorem 2.1) straight forward. However, it was shown in [20, Section 4] that there exist graphs for which $\chi_q(G)\alpha_q(G) < n$. Although we are unable to prove the first inertial-type bound without using this fact, the next example suggests that it may still be that the first inertial-type bound for the quantum k-distance chromatic number still holds for all graphs, regardless of this assumption.*

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EXAMPLE 4.3. *Let Ω_n be the orthogonality graph where $4|n$, and n is not a power of 2. It was shown in [20] that $\chi_q(\Omega_n) = n$ and $\alpha_q(\Omega_n) \leq \lfloor \frac{2^n}{n} \rfloor < \frac{2^n}{n}$. However, since $|V(\Omega_n)| = 2^n$, we have that*

$$\frac{|V(\Omega_n)|}{\alpha_q(\Omega_n)} > \frac{2^n}{2^n/n} = n = \chi_q(\Omega_n).$$

However, the first inertial-type bound still holds for the orthogonality graph. In fact it is known that 0 is an eigenvalue of Ω_n with multiplicity 2^{n-1}. Hence,

$$\min\{|\{i : \lambda_i \geq 0\}|, |\{i : \lambda_i \leq 0\}|\} \geq 2^{n-1}.$$

This implies that

$$\chi_q(\Omega_n) = n \geq \frac{2^n}{2^{n-1}} \geq \frac{2^n}{\min\{|\{i : \lambda_i \geq 0\}|, |\{i : \lambda_i \leq 0\}|\}}.$$

4.2. Second inertial-type bound. Next, we show that the inertial bound from Theorem 2.3 is also a lower bound for quantum k-distance chromatic number $\chi_{kq}(G)$ in the case when G is k-partially walk-regular. This, in turn, extends the bound for χ_k from [2, Theorem 4.2] to its quantum counterpart.

Before stating the following results, note that for all $p \in \mathbb{R}[x]$, we have that $p(A \otimes I) = p(A) \otimes I$. This follows directly from the properties of the Kronecker product.

THEOREM 4.4 (Second inertial-type bound). *Let G be a k-partially walk-regular graph with adjacency eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Then,*

$$\chi_{kq}(G) \geq 1 + \max\left\{\frac{|\{j : p(\lambda_j) < 0\}|}{|\{j : p(\lambda_j) > 0\}|}\right\}, \tag{4.8}$$

where the maximum is taken over all $p \in \mathbb{R}_k[x]$ such that $\sum_{i=1}^n p(\lambda_i) = 0$.

Proof. Let $\{P_{v,s} : v \in V, s \in [c]\}$ be a quantum k-distance coloring of G and $\mathcal{P} = \{P_1, \ldots, P_c\}$ be the orthogonal projection as defined in Theorem 3.2. Let $\omega = e^{2\pi i/c}$ and define

$$U := \sum_{s \in [c]} \omega^s P_s.$$

It is easy to show that U is a unitary matrix, and hence U^ℓ is unitary for all $\ell \in \mathbb{N}$. It was shown in [12, Lemma 1] that for any $X \in \mathbb{C}^{nd \times nd}$,

$$\mathcal{C}_{\mathcal{P}}(X) = \frac{1}{c} \sum_{\ell \in [c]} U^\ell X (U^\dagger)^\ell.$$

Hence, by Theorem 3.2, for all $p \in \mathbb{R}_k[x]$ such that $\sum_{i=1}^n p(\lambda_i) = 0$, we have

$$\frac{1}{c} \sum_{\ell \in [c]} U^\ell p(A) \otimes I_d (U^\dagger)^\ell = \frac{1}{c} \sum_{v \in V} p(A)_{vv} \cdot e_v e_v^\dagger \otimes I_d = 0.$$

where the last equality follows from the fact that $\sum_{i=1}^n p(\lambda_i) = 0$ if and only if $p(A)$ has constant zero diagonal. Therefore, we get

$$-p(A) \otimes I = \sum_{\ell=1}^{c-1} U^\ell (p(A) \otimes I)(U^\dagger)^\ell.$$

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Let $v_1, \dots, v_n$ be the eigenvectors of unit length corresponding to the eigenvalues $p(\lambda_{i_1}) \geq \cdots \geq p(\lambda_{i_n})$ of $p(A)$ for some ordering $(i_1, \dots, i_n)$ of $[n]$. W.l.o.g. we can assume $i_j = j$ for $1 \leq j \leq n$. Note that $p(A) \otimes I_d$ has for eigenvalue $p(\lambda_i)$ with multiplicity d and this for all $1 \leq i \leq n$. Furthermore, $\{v_i \otimes e_j \ :, 1 \leq j \leq d\}$, for $1 \leq i \leq n$ are eigenvectors with eigenvalue $p(\lambda_i)$. Let $p(A) \otimes I_d = p(B) - p(C)$, where

$$p(B) = \sum_{i=1}^{|\{j\,:\,p(\lambda_j)>0\}|} \sum_{\ell=1}^{d} p(\lambda_i)(v_i \otimes e_\ell)(v_i \otimes e_\ell)^*$$

$$p(C) = \sum_{i=n-|\{j\,:\,p(\lambda_j)>0\}|+1}^{n} \sum_{\ell=1}^{d} -p(\lambda_i)(v_i \otimes e_\ell)(v_i \otimes e_\ell)^*.$$

Note $p(B)$ and $p(C)$ are positive semidefinite matrices, hence and we know $\operatorname{rank}(p(B)) = d|\{j \,:\, p(\lambda_j) > 0\}|$ and $\operatorname{rank}(p(C)) = d|\{j \,:\, p(\lambda_j) < 0\}|$.

Let P^+ and P^- be the orthogonal projections onto the subspaces spanned by the eigenvectors corresponding to the positive and negative eigenvalues of $p(A) \otimes I_d$, that is,

$$P^+ = \sum_{i=1}^{|\{j\,:\,p(\lambda_j)>0\}|} \sum_{\ell=1}^{d} (v_i \otimes e_\ell)(v_i \otimes e_\ell)^*$$

$$P^- = \sum_{i=n-|\{j\,:\,p(\lambda_j)>0\}|+1}^{n} \sum_{\ell=1}^{d} (v_i \otimes e_\ell)(v_i \otimes e_\ell)^*.$$

Then,

$$p(B) = P^+(p(A) \otimes I_d)P^+ \quad \text{and} \quad p(C) = -P^-(p(A) \otimes I_d)P^-,$$

and therefore, we get

$$\sum_{i=1}^{c} U_i p(B) U_i^\dagger - \sum_{i=1}^{c} U_i p(C) U_i^\dagger = p(C) - p(B).$$

Multiplying both sides by P^- we get

$$P^- \sum_{i=1}^{c} U_i p(B) U_i^\dagger P^- - P^- \sum_{i=1}^{c} U_i p(C) U_i^\dagger P^- = p(C).$$

Since $P^- \sum_{i=1}^{c} U_i p(C) U_i^\dagger P^-$ is positive semi-definite, we obtain

$$P^- \sum_{i=1}^{c} U_i p(B) U_i^\dagger P^- \geq p(C).$$

Playing with ranks of sums and rank of products together with [11, Lemma 2], we get that

$$(c-1)d|\{j \,:\, p(\lambda_j) > 0\}| \geq d|\{j \,:\, p(\lambda_j) < 0\}|.$$ □

Note that the above bound can be optimized by finding a suitable polynomial p. Although a closed formula for optimal polynomials is unknown in most cases, in [3], a linear program that optimizes (4.8) was

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A publication of the International Linear Algebra Society
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proposed. Furthermore, as an immediate corollary of Theorem 4.4, for $k = 1$, we get that [2, Theorem 4.2]. Finally, the second inertia bound for the classical k-distance chromatic number is known to be tight for certain classes of graph such as the (generalized) Petersen graphs with $(n, k) \in \{(5, 2), (8, 3), (10, 2)\}$ (see [2, Section 3]). Hence for those graphs and specified values of k, the quantum k-distance chromatic is equal to the k-distance chromatic number.

5. Hoffman ratio-type bound for the quantum distance-k chromatic number.

The authors from [12] prove several Hoffman ratio-type bounds (see [12, Eq. (3)]), like the well-known Hoffman bound on the chromatic number of a graph, $\chi(G) \geq 1 - \frac{\lambda_1}{\lambda_n}$, hold for the quantum chromatic number of a graph as well.

In this section, we show that Hoffman ratio-type bounds for the k-distance chromatic number also hold for its quantum counterpart. We will do so through the intermediate of quantum homomorhpisms and the Lovász theta number of a graph. As we will only need a few properties of the latter concepts to prove our bound, we refer the reader to the work of Mančinska and Roberson [19], for precise definitions. We write $G \xrightarrow{q} H$ if there exists a quantum homomorphism from G to H. Furthermore, we denote by $\overline{\vartheta}(G)$ the Lovász theta number of the complement of G.

We will need the following theorem.

THEOREM 5.1. *[19, Theorem 3.2] If $G \xrightarrow{q} H$ then $\overline{\vartheta}(G) \leq \overline{\vartheta}(H)$.*

The quantum chromatic number can be determined using quantum homomorphism in the following way (see [19, Section 4] for more details):

$$\chi_q(G) = \min\{n \in \mathbb{N} : G \xrightarrow{q} K_n\},$$

where K_n is the complete graph on n vertices. Furthermore, recall that $\overline{\vartheta}(K_n) = n$.

We are now ready to prove the Hoffman ratio-type bound for quantum k-distance chromatic number.

THEOREM 5.2 (Hoffman ratio-type bound). *Let G be a graph on n vertices with adjacency matrix A having eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let $p \in \mathbb{R}_k[x]$ such that $p(\lambda_1) > p(\lambda_i)$ for all $i \in [2, n]$. Then,*

$$\chi_{kq}(G) \geq \frac{p(\lambda_1) - \lambda(p)}{W(p) - \lambda(p)}, \tag{5.9}$$

where $W(p) := \max_{u \in V}\{(p(A))_{uu}\}$ and $\lambda(p) := \min_{i\in[2,n]}\{p(\lambda_i)\}$.

Proof. Let $c := \chi_{kq}(G)$. By (1.3), we also have $c = \chi_q(G^k)$. By definition of the quantum chromatic number (see Definition 1.1 for $k = 1$), this implies $G^k \xrightarrow{q} K_c$, and hence by Theorem 5.1, $\overline{\vartheta}(G^k) \leq \overline{\vartheta}(K_c) = c = \chi_{kq}(G)$.

Finally, it is known (see [1]) that

$$\frac{p(\lambda_1) - \lambda(p)}{W(p) - \lambda(p)} \leq \overline{\vartheta}(G^k).$$

Combined with the above this proves the desired inequality. ∎

Similarly to the second inertia bound, one needs to establish the polynomial $p \in \mathbb{R}_K[x]$ that optimizes (5.9). For $k = 2, 3$, closed formulas with the optimal polynomials are derived in [3, Section 2.2]. For all

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A publication of the International Linear Algebra Society
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other k, the optimal polynomials are still unknown. However, the authors of [3] establish a linear program that can be used to optimize (5.9).

Finally, as an immediate corollary we obtain for $k = 1$ [2, Theorem 4.3].

The bound (5.9) for the classical distance 2 chromatic number is tights for several classes of graphs, including but not limited to the Dodecahedron, the F26A, the Heawood graph, the Nauru graph (see Table 3.5 [26, Section 3.3 Table 3.5]), as well as for Lee-metric graphs $G(n, q)$, where $n = 3$ and $7|q$ (see [3, Proposition 31] for more details).

6. Concluding remarks. We showed that three classical eigenvalue lower bounds for the distance-k chromatic number are also lower bounds for the corresponding quantum parameter. The quality of our bounds depends on the choice of a polynomial, so finding the best possible upper bound for a given graph is in fact an optimization problem. Since such optimization has been studied for the classical case (see [2, 3]), as a consequence of our results, now we can use the mentioned existing optimization methods to compute the best eigenvalue bound for the quantum distance chromatic number. This allows us to obtain several graph classes for which $\chi_k(G) = \chi_{kq}(G)$, thus increasing the number of graphs for which the exact value of the quantum parameter is known.

Indeed, since we know that $\chi_{kq} \leq \chi_k$, an immediate consequence of Theorems (2.2), (4.4) and (5.2) is that

$$(2.5), (4.8), (5.9) \leq \chi_{kq} \leq \chi_k.$$

This implies that we can use the existing optimization methods for the bounds on the left which appeared in [2] (for the two inertial-type bounds) and in [3] (for the Hoffman ratio-type bound). See Appendix for more details. For instance, for $k > 1$ and for (4.8), we can use the MILP (27) from [2] to find χ_{kq} of graphs for which $\chi_k = \chi_{kq} = (4.8)$, such as the (generalized) Petersen graphs with $(n, k) \in \{(5, 2), (8, 3), (10, 2)\}$ (see [2, Section 3]) and the Kneser graphs, where $\chi_2(K(p, 2)) = n(n-1)/2$. See [2, Section 4.2.1] for further details on other graph classes for which now we can obtain the value of the quantum distance-k chromatic number. We should note that the mentioned optimization methods for the three eigenvalue bounds only plays a role when $k > 1$, since for $k = 1$ it corresponds with $p(x) = x$. Moreover, and as previously discussed (5.9) is known to be a tight bound for the distance 2 chromatic number of several graphs. Many of those graphs can be found in [26, Section 3.3, see e.g. Table 3.5]. The Lee-metric graphs $G(n, q)$, where $n = 3$ and $7|q$, which can be found in [3, Proposition 31] are also examples of such graphs.

Furthermore, several authors [20, 18, 15] have been looking at separation-type results for $\chi(G)$ and $\chi_q(G)$. In this regard, our eigenvalue bounds and their corresponding optimization methods can be used to obtain graphs that are not candidates to hold such separation.

We end up this paper with several intriguing directions and questions.

- If for $k = 1$, the quantum and the classical distance chromatic parameters coincide, does it imply anything for larger k?
- Several authors have looked at separation results between χ_q and χ (see e.g. [15, 18, 20, 22]). Using the fact that $\chi_{kq}(G) = \chi_q(G^k)$, and that a k-quantum coloring of G is a quantum coloring of G^k (and vice-versa), it is immediate that [22, Theorem 12] holds for $\chi_{kq}(G)$ as well. However, it is unclear whether a separation in the quantum k-distance chromatic number implies a separation in the quantum ℓ-distance chromatic number for all $\ell \leq k$.

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A publication of the International Linear Algebra Society
Volume 41, pp. 602-615, November 2025.

Acknowledgment. The authors would like to thank the reviewer as well as Jan Meeus for their careful reading and insightful comments that helped improve the quality of the paper. Aida Abiad is supported by the Dutch Research Council (NWO) through the grants VI.Vidi.213.085 and OCENW.KLEIN.475. Benjamin Jany is supported by the Eindhoven Hendrik Casimir Institute (EHCI) of the Eindhoven University of Technology.

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A publication of the International Linear Algebra Society
Volume 41, pp. 602-615, November 2025.

Appendix A. Since we showed that three eigenvalue bounds on the distance-k chromatic number also hold in the quantum setting, one can use the existing optimization methods for such eigenvalue bounds in the classical setting.

Indeed, the optimization of the first inertial-type bound (Theorem 4.1) and of the second inertial-type bound (Theorem 4.4) appeared in [2]. The optimization of the Hoffman ratio-type bound from Theorem 5.2 appeared in [3]. Nevertheless, we decided to add them here for completeness.

A.1. Optimization of the first inertial-type bound (Theorem 4.1). Here, we introduce a mixed-integer linear programming (MILP) formulation to compute the best polynomial for Theorem 4.1. Although solving an MILP is known to be NP-hard in general, we find that in practice our method effectively minimizes the bound in Theorem 4.1 for numerous interesting graphs.

Let $\mathcal{G}$ have spectrum $^{\mathcal{G}} = \{\theta_0^{[m_0]}, \dots, \theta_d^{[m_d]}\}$. Theorem 4.1 can be written in terms of these distinct eigenvalues and multiplicities as

$$\alpha_k(\mathcal{G}) \leq \min\left\{\sum_{j:p(\theta_j)\geq w(p)} m_j, \sum_{j:p(\theta_j)\leq W(p)} m_j\right\}. \tag{A.10}$$

Equation (A.10) only requires the computation of $p(\theta_j)$ for $j = 0, 1, \dots, d$, instead of $p(\lambda_j)$ for all $j \in [n]$. We will therefore base our MILP on this alternative formulation to reduce the number of variables and constraints. Note that Equation (A.10) is invariant under scaling and translation of polynomial p. Upon changing the sign of p, we can therefore always assume we are minimizing $\sum_{j:p(\theta_j)\geq w(p)} m_j$. Moreover, a constant can be added to $p(x)$ such that $w(p) = 0$.

Let $p(x) = a_k x^k + \cdots + a_0$, $\boldsymbol{b} = (b_0, \dots, b_d) \in \{0,1\}^{d+1}$ and $\boldsymbol{m} = (m_0, \dots, m_d)$. As $w(p) = 0$, there exist a vertex $u \in V(\mathcal{G})$ such that $p(A)_{uu} = 0$. Moreover, every other vertex v must satisfy $p(A)_{vv} \geq 0$. The following MILP, with variables $a_0, \dots, a_k$ and $b_1, \dots, b_d$, formulates the problem of finding the best polynomial for the bound in Equation (A.10) under the assumption that $w(p) = p(A)_{uu} = 0$. To obtain the best upper bound on α_k, we iterate over all vertices $u \in V(\mathcal{G})$, solve the corresponding MILP, and find the lowest objective value of all.

$$\begin{array}{lll} \texttt{minimize} & \boldsymbol{m}^\top \boldsymbol{b} & \\ \texttt{subject to} & \sum_{i=0}^k a_i \cdot (A^i)_{vv} \geq 0, & v \in V(\mathcal{G}) \setminus \{u\} \\ & \sum_{i=0}^k a_i \cdot (A^i)_{uu} = 0, & \\ & \sum_{i=0}^k a_i \theta_j^{\,i} - M b_j + \varepsilon \leq 0, & j = 0, \dots, d \quad (*) \\ & \boldsymbol{b} \in \{0,1\}^{d+1} & \end{array} \tag{A.11}$$

The constant M in MILP formulation (A.11) is a large number and $\varepsilon > 0$ small. The value of each variable b_j represents whether $p(\theta_j) \geq w(p) = 0$. Constraint $(*)$ ensures that $b_j = 1$ if $p(\theta_j) \geq 0$, and since $\boldsymbol{m}^\top \boldsymbol{b}$ is minimized in the objective function, $b_j = 1$ only if $p(\theta_j) \geq 0$. So, upon minimizing the weighted sum of b_j's, we are optimizing the corresponding bound $\alpha_k \leq \boldsymbol{m}^\top \boldsymbol{b}$. We will see a concrete example of this MILP formulation for a specific graph later on in this section, in Example A.1.

As mentioned earlier, Equation (A.10) is invariant under the scaling of p. This means that we can always set $\varepsilon = 1$ without loss of generality. If the chosen M is not large enough, the MILP will be infeasible and we can repeat with a larger M.

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A publication of the International Linear Algebra Society
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If $\mathcal{G}$ is a k-partially walk-regular graph, all powers A^i of the adjacency matrix have constant diagonal, where $i \le k$. This means that $w(p) = 0$ if and only if $p(A)_{uu} = 0$ for all $u \in V(\mathcal{G})$, and hence

$$\operatorname{tr} p(A) = \sum_{u \in V(\mathcal{G})} p(A)_{uu} = \sum_{j=0}^{d} m_j p(\theta_j) = 0.$$

For k-partially walk-regular graphs, MILP formulation (A.11) can therefore be simplified by replacing the first two constraints by $\sum_{j=0}^{d} m_j p(\theta_j) = 0$, which results in MILP (A.11). As the constraints of this new formulation no longer depend on a chosen vertex u, it suffices to solve a single MILP instance, whereas for general graphs, we needed to solve one for every vertex.

$$\text{(A.12)} \qquad \begin{array}{|rl|} \texttt{minimize} & \boldsymbol{m}^\top \boldsymbol{b} \\ \texttt{subject to} & \sum_{j=0}^{d} m_j \sum_{i=0}^{k} a_i \theta_j^{\,i} = 0 \\ & \sum_{i=0}^{k} a_i \theta_j^{\,i} - M b_j + \varepsilon \le 0, \quad j = 0, \ldots, d \\ & \boldsymbol{b} \in \{0,1\}^{d+1} \end{array}$$

Example A.1. *Let $G = C_6$ with $^{G} = \{2^{[1]}, 1^{[2]}, -1^{[2]}, -2^{[1]}\}$. This graph is 2-partially walk-regular (i.e., regular), hence we can apply MILP (A.12) to compute an upper bound on $\alpha_2(\mathcal{G})$. The objective function of MILP (A.12) is $b_0 + 2b_1 + 2b_2 + b_3$, which we want to minimize under the constraints*

$$\begin{aligned} 6a_0 + 0a_1 + 12a_2 &= 0 \\ a_0 + 2a_1 + 4a_2 - Mb_0 + \varepsilon &\le 0 \\ a_0 + a_1 + a_2 - Mb_1 + \varepsilon &\le 0 \\ a_0 - a_1 + a_2 - Mb_2 + \varepsilon &\le 0 \\ a_0 - 2a_1 + 4a_2 - Mb_3 + \varepsilon &\le 0. \end{aligned}$$

The first constraint simplifies to $a_0 + 2a_2 = 0$. By substituting this into the other constraints, we find

$$\begin{aligned} 2a_1 + 2a_2 - Mb_0 + \varepsilon &\le 0 & \qquad -a_1 - a_2 - Mb_2 + \varepsilon &\le 0 \\ a_1 - a_2 - Mb_1 + \varepsilon &\le 0 & \qquad -2a_1 + 2a_2 - Mb_3 + \varepsilon &\le 0, \end{aligned}$$

which can be rewritten as

$$\frac{1}{2}(Mb_0 - \varepsilon) \ge a_2 + a_1 \ge -Mb_2 + \varepsilon, \qquad Mb_1 - \varepsilon \ge -a_2 + a_1 \ge -\frac{1}{2}(Mb_3 + \varepsilon).$$

These two sandwiching inequalities imply that b_0 and b_2 cannot be zero simultaneously and neither can b_1 and b_3. Since m_0 and m_3 have lowest multiplicity, the best objective value is obtained by setting $b_0 = b_3 = 1$, $b_1 = b_2 = 0$. The resulting upper bound is for $\alpha_2(\mathcal{G})$ equals two, which is tight, since $\mathcal{G}$ admits a 2-independent set of size two. Vector $\boldsymbol{a} = (0, \frac{1}{2}(M - \varepsilon), 0)$ complies with this choice of $\boldsymbol{b}$ and satisfies the constraints, hence $p_2(x) = \frac{1}{2}(M - \varepsilon)x$ is a corresponding optimal polynomial.

A.2. Optimization of the second inertial-type bound (Theorem 4.4). We can use MILPs to optimize the polynomial p in Theorem 4.4. However, in this case, we must solve $n - 1$ MILPs to obtain the best possible bound, whereas the first inertial-type bound only required one in case of k-partial walk-regularity. Let G have spectrum $^{G} = \{\theta_0^{[m_0]}, \ldots, \theta_d^{[m_d]}\}$ and let $\boldsymbol{m} = (m_0, \ldots, m_d) \in \{0,1\}^{d+1}$. For

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each $\ell \in \{1, \ldots, n-1\}$, we solve the following MILP. Note, however, that it may be infeasible for certain values of ℓ if there is no subset of multiplicities adding up to ℓ.

$$
\text{(A.13)}\qquad
\begin{array}{|rll|}
\hline
\texttt{maximize} & 1 + \frac{n - \boldsymbol{m}^\top \boldsymbol{b}}{\ell} & \\
\texttt{subject to} & \sum_{j=0}^{d} \sum_{i=0}^{k} a_i m_j \theta_j^i = 0 & \\
 & \sum_{i=0}^{k} a_i \theta_j^i - M b_j + \varepsilon \leq 0, & j = 0, \ldots, d \\
 & \sum_{i=0}^{k} a_i \theta_j^i - M c_j \leq 0, & j = 0, \ldots, d \\
 & \sum_{i=0}^{k} a_i \theta_j^i + M(1 - c_j) - \epsilon \geq 0, & j = 0, \ldots, d \\
 & \boldsymbol{m}^\top \boldsymbol{c} = \ell & \\
 & \boldsymbol{b} \in \{0,1\}^{d+1}, \quad \boldsymbol{c} \in \{0,1\}^n & \\
\hline
\end{array}
$$

As before, the variables a_i are the coefficients of the polynomial of degree at most k, $p(x) = a_k x^k + \cdots + a_0$, and the first constraint is the hypothesis of Theorem 4.4, $\operatorname{tr} p(A) = 0$. The second set of constraints implies that $b_j = 1$ if $p(\lambda_j) \geq 0$. Moreover, as the objective function minimizes $\boldsymbol{m}^\top \boldsymbol{b}$, we do not have $b_j = 1$ unless it is forced by the constraints. Therefore, $p(\lambda_j) \geq 0$ if and only if $b_j = 1$. Similarly, the third set of constraints implies that $c_j = 1$ if $p(\lambda_j) > 0$. Since, contrary to $\boldsymbol{m}^\top \boldsymbol{b}$, the value of $\boldsymbol{m}^\top \boldsymbol{c}$ is not minimized by the MILP (in fact, we assume it to be constant), we need to explicitly add the fourth set of constraints to ensure that also $p(\lambda_j) > 0$ whenever $c_j = 1$. Note that this is a correction to MILP (27) in [2], where these constraints are missing.

Summarizing the above, we have

- $|j : p(\lambda_j) > 0| = \boldsymbol{m}^\top \boldsymbol{c} = \ell$ (fifth constraint),
- $|j : p(\lambda_j) = 0| = \boldsymbol{m}^\top (\boldsymbol{b} - \boldsymbol{c})$,
- $|j : p(\lambda_j) < 0| = n - \boldsymbol{m}^\top \boldsymbol{b}$.

This means that an optimal solution of MILP (A.13) indeed corresponds to the maximum value for the bound in Theorem 4.4.

Example A.2. *Consider again the 2-partially walk-regular graph $G = C_6$ with ${}^G = \{2^{[1]}, 1^{[2]}, -1^{[2]}, -2^{[1]}\}$. Let $\ell = 3$. The first two sets of constraints of MILP (A.13) are the same as in MILP (A.12), hence we know from Example A.1 that they simplify to $2a_2 + a_0 = 0$, $b_0 + b_2 \geq 1$ and $b_1 + b_3 \geq 1$. The third, fourth, and fifth set of constraints are*

$$
\begin{aligned}
&a_0 + 2a_1 + 4a_2 - Mc_0 \leq 0 && a_0 + 2a_1 + 4a_2 + M(1 - c_0) - \varepsilon \leq 0 \\
&a_0 + a_1 + a_2 - Mc_1 \leq 0 && a_0 + a_1 + a_2 + M(1 - c_1) - \varepsilon \leq 0 \\
&a_0 - a_1 + a_2 - Mc_2 \leq 0 && a_0 - a_1 + a_2 + M(1 - c_2) - \varepsilon \leq 0 \\
&a_0 - 2a_1 + 4a_2 - Mc_3 \leq 0 && a_0 - 2a_1 + 4a_2 + M(1 - c_3) - \varepsilon \leq 0 \\
& && c_0 + 2c_1 + 2c_2 + c_3 = \ell.
\end{aligned}
$$

The fourth set of constraints combines to

$$M(1 - c_2) - \varepsilon \geq a_2 + a_1 \geq -\frac{1}{2} M(1 - c_0) + \varepsilon,$$

and

$$\frac{1}{2} M(1 - c_3) - \varepsilon \geq -a_2 + a_1 \geq -M(1 - c_1) + \varepsilon,$$

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A publication of the International Linear Algebra Society
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which implies that $c_0 + c_2 \leq 1$ and $c_1 + c_3 \leq 1$. The vectors $\boldsymbol{b} = (1, 1, 0, 0)$ and $\boldsymbol{c} = (1, 1, 0, 0)$ satisfy these conditions as well as the other constraints. The corresponding objective value is $1 + \frac{6-3}{3} = 2$, which is not tight, as $\chi_2(G) = 3$. However, if we solve the MILP for all possible values of ℓ using Gurobi, we find that this is the best possible value for the bound in Theorem 4.4.

The algorithm gives a lower bound for the actual maximum of MILP (A.13), as we restricted the optimal polynomial. Nevertheless, there are several graphs for which it gives a tight bound, and hence for which the bound in Theorem 4.4 is tight, such as the Heawood graph, Klein 7-regular graph, and Möbius–Kantor graph.

Like MILP (A.11), MILP (A.13) is tight for the incidence graphs of projective planes $PG(2, q)$, with q a prime power and the prism graphs G_n with $n \neq 2 \mod 4$. Note that the latter are generalized Petersen graphs with parameters $(n, 1)$. The bound is also tight for (generalized) Petersen graphs with $(n, k) \in \{(5, 2), (8, 3), (10, 2)\}$. The second graph is also known as the Möbius–Kantor graph and is walk-regular, but not distance-regular; hence, Delsarte's LP bound [9] is not applicable in this case.

A.3. Optimization of the Hoffman ratio-type bound (Theorem 5.2). Let $G = (V, E)$ have adjacency matrix A and distinct eigenvalues $\theta_0 > \cdots > \theta_d$. Note that we can scale by a positive number and translate the polynomial used in Theorem 5.2 without changing the value of the bound. Hence, we can assume $W(p) - \lambda(p) = 1$. Furthermore, $\lambda(p) < W(p)$, so the scaling does not flip the sign of the bound. Hence, the problem reduces to finding the p that maximizes $p(\lambda_1) - \lambda(p)$, subject to the constraint $W(p) - \lambda(p) = 1$. For each $u \in V$ and $\ell \in [1, d]$, assume that $W(p) = (p(A))_{uu}$, $0 = \lambda(p) = p(\theta_\ell)$ and solve the Linear Program (LP) below. The maximum of these dn solutions then equals the best possible bound obtained by Theorem 5.2.

(A.14)

variables: $(a_0, \dots, a_k)$

input: The adjacency matrix A and its distinct eigenvalues $\{\theta_0, \dots, \theta_d\}$.
A vertex $u \in V$, an $\ell \in [1, d]$. An integer k.

output: $(a_0, \dots, a_k)$, the coefficients of a polynomial p

$$\text{maximize} \quad \sum_{i=0}^{k} a_i \theta_0^i - \sum_{i=0}^{k} a_i \theta_\ell^i$$

$$\text{subject to} \quad \sum_{i=0}^{k} a_i((A^i)_{vv} - (A^i)_{uu}) \leq 0, \ \ v \in V \setminus \{u\}$$

$$\sum_{i=0}^{k} a_i((A^i)_{uu} - \theta_\ell^i) = 1$$

$$\sum_{i=0}^{k} a_i(\theta_0^i - \theta_j^i) > 0, \quad j \in [1, d]$$

$$\sum_{i=0}^{k} a_i(\theta_j^i - \theta_\ell^i) \geq 0, \quad j \in [1, d]$$

Here, the objective function is simply $p(\lambda_1) - \lambda(p)$. The first constraint says $(p(A))_{uu} \geq (p(A))_{vv}$ for all vertices $v \neq u$, which ensures $W(p) = (p(A))_{uu}$. The second constraint gives p the correct scaling and translation such that $W(p) - \lambda(p) = 1$. The third constraint says $p(\theta_0) > p(\theta_j)$ for all $j \in [1, d]$, which ensures $p(\lambda_1) > \lambda(p)$. And the final constraint says $p(\theta_\ell) \leq p(\theta_j)$ for all $j \in [1, d]$, which ensures $\lambda(p) = p(\theta_\ell)$.