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SPECTRAL UPPER BOUND ON THE QUANTUM K-INDEPENDENCE NUMBER OF A GRAPH*

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Abstract. A well-known upper bound for the independence number $\alpha(G)$ of a graph G, due to Cvetković, is that

$$\alpha(G) \leq n^0 + \min\{n^+, n^-\},$$

where (n^+, n^0, n^-) is the inertia of G. We prove that this bound is also an upper bound for the quantum independence number α_q(G), where $\alpha_q(G) \geq \alpha(G)$ and for some graphs $\alpha_q(G) \gg \alpha(G)$. We identify numerous graphs for which $\alpha(G) = \alpha_q(G)$, thus increasing the number of graphs for which α_q is known. We also demonstrate that there are graphs for which the above bound is not exact with any Hermitian weight matrix, for $\alpha(G)$ and $\alpha_q(G)$. Finally, we show this result in the more general context of spectral bounds for the quantum k-independence number, where the k-independence number is the maximum size of a set of vertices at pairwise distance greater than k.

Key words. Graph, Quantum independence number, Eigenvalues, Inertia bound.

1. Introduction and motivation. Elphick and Wocjan [9] proved that many spectral lower bounds for the chromatic number, $\chi(G)$, are also lower bounds for the quantum chromatic number, $\chi_q(G)$. This was achieved using the linear algebra tools of pinching and twirling and a combinatorial definition of $\chi_q(G)$ due to Mančinska and Roberson [17]. In a different paper, Mančinska and Roberson [18] defined the quantum independence number $\alpha_q(G)$, using quantum homomorphisms, where $\alpha_q(G) \geq \alpha(G)$. Analogously to $\chi_q(G)$, the *quantum independence number* $\alpha_q(G)$ is the maximum integer t for which two players sharing an entangled quantum state can convince an interrogator that the graph G has an independent set of size t. There exist graphs G for which there is an exponential separation between the independence number $\alpha(G)$ and $\alpha_q(G)$ [18].

The subject of quantum graph parameters has been extensively studied in the past decade, due to its connections to a number of subjects, including quantum information theory, operator theory, combinatorics and optimisation. The motivation for studying quantum graph parameters is described, for example, by Cameron *et al.* [6] and in [18] and [9, 10]. We add to this subject by defining an extension of the usual quantum independence number of a graph, called the quantum k-independence number, which is also motivated by its classical counterpart, the k-independence number of a graph. The *k-independence number of a graph*, $\alpha_k(G)$, is the maximum size of a set of vertices at pairwise distance greater than k. Upper bounds on this graph parameter appeared in [13, 12, 4, 3, 20, 1]. Note that $\alpha_1(G) = \alpha(G)$. The quantum k-independence number can be regarded as a generalisation of the (classical) k-independence number. As set out in Definition 2.1, $\alpha_{kq}(G)$ is defined using d-dimensional orthogonal projectors, and $\alpha_k(G)$ corresponds to $d = 1$. It is also worth mentioning that in quantum information theory, $(\alpha_{kq}(G) - \alpha_k(G))$ can be seen and used as a measure of the benefit of entanglement.

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The inertial bound on the independence number of a graph, $\alpha(G) \leq n^0 + \min\{n^+, n^-\}$, is a well-known upper bound on the independence number of a graph due to Cvetković [7]. In this article, we show that it also upper bounds the quantum independence number $\alpha_q(G)$ of a graph. As a consequence of our result, we obtain that $\alpha(G) \leq \alpha_q(G) \leq$ inertialbound, and this allows us to determine the quantum independence number for all graphs for which $\alpha(G)$ equals the inertial bound, substantially increasing the number of graphs for which we can determine the value of $\alpha_q(G)$ (recall that it is not known whether quantum counterparts of $\alpha(G)$ or $\chi(G)$ are computable functions [18]). Moreover, we show that the result mentioned above follows as a special case of a more general upper bound on the quantum k-independence number (where one considers vertices at pairwise distance greater than k). As a consequence of this more general result (the inertial bound is also valid to upper bound the quantum k-independence number), for $k > 1$ one can use the linear optimization methods proposed in [1, 2], which depend on finding the best polynomials of degree k, to optimize our inertial bound and find exact values for α_{kq} for the graphs for which the inertial bound is tight (for some examples, see [1, Tables 2 and 4]).

2. Definitions and notation.

Throughout this paper, $G = (V, E)$ will denote a graph (undirected, simple and loop-less) on vertex set V with n vertices, edge set E and adjacency matrix A with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$.

The quantum independence number $\alpha_q(G)$ was originally defined using quantum homomorphisms and can also be defined using nonlocal games. In this work, we require a combinatorial definition of $\alpha_q(G)$, such as the one which appears in [15] (see Definition 2.8). This is generalised to the quantum k-independence number $\alpha_{kq}(G)$ as follows. The special case $k = 1$ corresponds to the quantum independence number $\alpha_q(G)$.

Recall that for matrices $X, Y \in \mathbb{C}^{d\times d}$, their trace inner product (also called Hilbert-Schmidt inner product) is defined as

$$\langle X, Y\rangle_{\mathrm{tr}} = \mathrm{tr}(X^\dagger Y)\,.$$

Definition 2.1. *The quantum k-independence number of a graph $G = (V, E)$, denoted by $\alpha_{kq}(G)$, is the maximum integer t for which there exists a collection of orthogonal projectors $\{P^{(u,i)} \in \mathbb{C}^{d\times d} : u \in V(G), i \in [t]\}$ for some dimension d satisfying the following conditions:*

$$\sum_{u\in V} P^{(u,i)} = I_d \quad \text{for all } i \in [t], \tag{2.1}$$

$$\langle P^{(u,i)}, P^{(u,j)}\rangle_{\mathrm{tr}} = 0 \quad \text{for all } i \neq j \in [t],\ \text{for all } u \in V(G), \tag{2.2}$$

$$\langle P^{(u,i)}, P^{(v,j)}\rangle_{\mathrm{tr}} = 0 \quad \text{for all } i \neq j \in [t],\ \text{for all } u, v \in V(G) \text{ with } \mathrm{dist}(u,v) \leq k. \tag{2.3}$$

We can simplify the proof of our upper bound for $\alpha_{kq}(G)$ by defining a k-projective packing number of a graph, denoted by $\alpha_{kp}(G)$. We will then prove that $\alpha_{kq}(G) \leq \alpha_{kp}(G)$, and that our spectral bound is an upper bound for $\alpha_{kp}(G)$.

Definition 2.2. *A d-dimensional k-projective packing of a graph $G = (V, E)$ is a collection of orthogonal projectors $\{P^{(u)} \in \mathbb{C}^{d\times d} : u \in V(G)\}$ such that*

$$\langle P^{(u)}, P^{(v)}\rangle_{\mathrm{tr}} = 0, \tag{2.4}$$

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for all pairs of distinct vertices[1] $u, v \in V(G)$ *at distance at most* k. *The value of the projective packing is defined as*

$$\frac{1}{d}\sum_{u\in V} r^{(u)},$$

where $r^{(u)}$ *denotes the rank of the projector* $P^{(u)}$. *The* k*-projective packing number* $\alpha_{kp}(G)$ *of a graph* G *is defined as the supremum taken over all* d *of the values over all projective packings of the graph* G. *If* $k = 1$, *then* $\alpha_{kp}(G) = \alpha_p(G)$, *which is the projective packing number of* G.

In order to prove our main result, we need the following two lemmas.

LEMMA 2.3. $\alpha_{kq}(G) \leq \alpha_{kp}(G)$.

Proof. Let $G^{[k]}$ denote the graph formed by making all pairs of vertices of G at distance at most k adjacent. By definition it is clear that $\alpha_{kq}(G) = \alpha_q(G^{[k]})$ and $\alpha_{kp}(G) = \alpha_p(G^{[k]})$. Using that $\alpha_q(G^{[k]}) \leq \alpha_p(G^{[k]})$ [19], it holds that $\alpha_{kq}(G) \leq \alpha_{kp}(G)$. ◻

We will use the following result to reformulate the conditions on the orthogonal projectors of a k-projective packing as conditions on their eigenvectors. We omit the proof of this basic result.

LEMMA 2.4. *Let* $P, Q \in \mathbb{C}^{d\times d}$ *be two arbitrary orthogonal projectors of rank* r *and* s, *respectively. Let*

$$P = \sum_{k\in[r]} |\psi_k\rangle\langle\psi_k| \quad \text{and} \quad Q = \sum_{\ell\in[s]} |\phi_\ell\rangle\langle\phi_\ell|,$$

denote their spectral resolutions, respectively. Then, the following two conditions are equivalent:

$$\langle P, Q\rangle_{\mathrm{tr}} = 0, \tag{2.5}$$

$$\langle\psi_k|\phi_\ell\rangle = 0 \quad \text{for all} \quad k \in [r], \ell \in [s]\,. \tag{2.6}$$

3. Spectral bound for $\alpha_{kq}(G)$ and $\alpha_q(G)$. Let A denote the adjacency matrix of G. Take $p_k(x) \in \mathbb{R}_k[x]$, then $p_k(A)$ denotes a polynomial function of A of degree at most k. Let

$$W(p_k) = \max_{u\in V}\{p_k(A)_{uu}\},$$
$$w(p_k) = \min_{u\in V}\{p_k(A)_{uu}\}.$$

If $p_k(A) = A^k$, then $W(p_k)$ is the number of closed walks of length k containing a given vertex v maximized over all vertices v, and $w(p_k)$ is the number of closed walks of length k containing a given vertex v minimized over all vertices v.

Abiad *et al.* [3] proved the following result.

THEOREM 3.1 ([3]). *Let* $\lambda_1 \geq \ldots \geq \lambda_n$ *denote the eigenvalues of the adjacency matrix* A *of a graph* G, *and let* $p_k \in \mathbb{R}_k[x]$. *Then,*

$$\alpha_k(G) \leq \min\{|i : p_k(\lambda_i) \geq w(p_k)|\,, |i : p_k(\lambda_i) \leq W(p_k)|\}\,.$$

[1] It's important to require that $u \neq v$.

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If we let $k = 1$ and $p_k(A) = A$, this reduces to the well-known inertia bound due to Cvetković [7]:

THEOREM 3.2 ([7]). *The independence number of a graph is bounded from above by*

$$\alpha(G) \leq n^0(A) + \min\{n^+(A), n^-(A)\},$$

where (n^0, n^-, n^+) *are the numbers of zero, negative and positive eigenvalues of* A.

Our principal result is as follows.

THEOREM 3.3. *Let* $\lambda_1 \geq \ldots \geq \lambda_n$ *denote the eigenvalues of the adjacency matrix* A *of a graph* G*, and let* $p_k \in \mathbb{R}_k[x]$*. Then*

$$\alpha_{kq}(G) \leq \alpha_{kp}(G) \leq \min\left\{|i : p_k(\lambda_i) \geq w(p_k)|\,,\, |i : p_k(\lambda_i) \leq W(p_k)|\right\}.$$

Proof. The inequality $\alpha_{kq}(G) \leq \alpha_{kp}(G)$ was addressed in Lemma 2.3.

We now prove the upper bound on $\alpha_{kp}(G)$. Using Lemma 2.4 we obtain an equivalent formulation of a k-projective packing in terms of vectors instead of projectors. Define the orthonormal vectors

$$|\Psi^{(u,i)}\rangle = |u\rangle \otimes |\psi^{(u,i)}\rangle,$$

where the spectral resolutions of the projectors $P^{(u)}$ are given by

$$P^{(u)} = \sum_{i=1}^{r^{(u)}} |\psi^{(u,i)}\rangle\langle\psi^{(u,i)}|.$$

Due to the block structure of the vectors $|\Psi^{(u)}\rangle$ and the matrix $p_k(A) \otimes I_d$, we have

$$\langle\Psi^{(u,i)}|(p_k(A) \otimes I)|\Psi^{(v,j)}\rangle = p_k(A)_{uv} \cdot \langle\psi^{(u,i)}|\psi^{(v,j)}\rangle. \tag{3.7}$$

We now examine the values that occur on the right-hand side for all possible combinations of (u, i) and (v, j). First, consider two arbitrary vertices $u, v \in V(G)$ at distance strictly greater than k from each other. Then, we have $(p_k(A))_{uv} = 0$ since $p_k(A)$ is a linear combination of the powers $A^0, \ldots, A^k$. Second, consider two different vertices $u, v \in V(G)$ at distance less or equal to k from each other. The term $(p_k(A))_{uv}$ can be non-zero in this case, but due to the orthogonality condition we have $\langle\psi^{(u,i)}|\psi^{(v,j)}\rangle = 0$ for all $i \in [r^{(u)}]$ and $j \in [r^{(v)}]$. Finally, we consider the case $u = v$. In this case, the right-hand side is equal to $d^{(u)} \cdot \delta_{ij}$, where

$$d^{(u)} = (p_k(A))_{uu}.$$

Now let S denote the matrix whose columns are $|\Psi^{(u,i)}\rangle$ for $u \in V$ and $i \in [r^{(u)}]$, i.e.,

$$S = \sum_{u \in V(G)} \sum_{i \in [r^{(u)}]} |\Psi^{(u,i)}\rangle\langle(u, i)|,$$

and r denote its rank, which is equal to $\sum_u r^{(u)}$.

Using the analysis of the different cases above, we obtain

$$\begin{aligned} S^\dagger(p_k(A) \otimes I_d)S &= \sum_{u \in V(G)} \sum_{i \in [r^{(u)}]} \sum_{v \in V(G)} \sum_{j \in [r^{(v)}]} \langle\Psi^{(u,i)}|(p_k(A) \otimes I)|\Psi^{(v,j)}\rangle \cdot |(u, i)\rangle\langle(v, j)| \\ &= \operatorname{diag}\left(d^{(u)} : u \in V, i \in [r^{(u)}]\right). \end{aligned}$$

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We use D to denote the above diagonal matrix. Let $w(p_k)$ denote the minimum of $d^{(u)}$ for $u \in V$. Using interlacing (see for instance [14]), it now follows that there must be at least r eigenvalues of $p_k(A) \otimes I_d$ that are larger than the smallest eigenvalue of D. The latter is equal to $w(p_k)$ by definition. Equivalently, there must be at least r/d eigenvalues of $p_k(A)$ that are at least $w(p_k)$.

This yields the first upper bound

$$\alpha_{kp}(G) \leq |\{j : p_k(\lambda_j) \geq w(p_k)\}| .$$

Let $W(p_k)$ denote the maximum of $(p_k(A))_{uu}$ for $u \in V$. The second upper bound

$$\alpha_{kp}(G) \leq |\{j : p_k(\lambda_j) \leq W(p_k)\}| ,$$

is proved analogously. □

Remark 3.4. We say that a hermitian matrix $W = (w_{uv})$ is a *weighted adjacency matrix* of G if the following holds:

$$\forall u, v \in V(G) : a_{uv} = 0 \Rightarrow w_{uv} = 0. \tag{3.8}$$

Observe that a weighted adjacency matrix W can always be obtained by considering the Hadamard (entry-wise) product of A and an arbitrary Hermitian matrix H, that is, $W = H \odot A$.

The proof of Theorem 3.3 also holds for any weighted adjacency matrix (even allowing nonzero diagonals). The reason that the proof generalizes is as follows. Let $u, v \in V(G)$ be two vertices at distance strictly larger than k. Then, $(W^\ell)_{uv} = 0$ for all $0 \leq \ell \leq k$.

In this work, we restrict to polynomials in the adjacency matrix of G (or polynomials in a weighted adjacency matrix of G), since we are interested in practically computing bounds for specific graphs.

Letting $p_1(A) = A$ in Theorem 3.3, we immediately obtain that:

Corollary 3.5.

$$\alpha(G) \leq \alpha_q(G) \leq \alpha_p(G) \leq n^0(A) + \min\{n^+(A), n^-(A)\}.$$

Abiad *et al.* [4] proved that, when we restrict to the case of $p_k(A) = A^k$, the spectral bound from Theorem 3.3 is tight for $\alpha_k(G)$ for a certain infinite family of graphs (see Section 3.1 in [4]). Since the quantum k-independence number is sandwiched between the classical k-independence number and our spectral bound, we can say that for that family of graphs the above bound for α_{kq} is also tight and the classical and quantum parameters α_k and α_{kq} coincide.

4. Alternative upper bounds for $\alpha_q(G)$. It is known (see for example Section 6.18 of [22]) that:

$$\alpha(G) \leq \alpha_q(G) \leq \lfloor \vartheta'(G) \rfloor \leq \vartheta'(G) \leq \vartheta(G) \leq \vartheta^+(G) \leq \lceil \vartheta^+(G) \rceil \leq \chi_q(\overline{G}) \leq \chi(\overline{G}) ,$$

where ϑ', ϑ, and ϑ^+ are the Schrijver, Lovász and Szegedy theta functions.

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Hoffman, in an unpublished paper, proved that for Δ-regular[2] graphs:

$$\alpha(G) \leq \frac{n|\lambda_n|}{\Delta + |\lambda_n|},$$

where λ_n is the smallest eigenvalue of the adjacency matrix A. This result is typically proved using interlacing of a quotient matrix associated with a vertex partition into the independent set and the remaining vertices and is known as the Hoffman bound or ratio bound.

Lovász [16, Theorem 9] proved that for Δ-regular graphs:

$$\vartheta(G) \leq \frac{n|\lambda_n|}{\Delta + |\lambda_n|}.$$

It is therefore immediate that the Hoffman bound is an upper bound for $\alpha_q(G)$ for regular graphs.

Van Dam and Haemers [8] proved that for *any* graph

$$\alpha(G) \leq \frac{n(\mu_1 - \delta)}{\mu_1},$$

where δ is the minimum degree of G and μ_1 is the largest eigenvalue of the Laplacian matrix of G. This bound equals the Hoffman bound for regular graphs.

Bachoc *et al.* subsequently proved (see section 5 in [5]), in the context of simplicial complexes, that for any graph:

$$\vartheta(G) \leq \frac{n(\mu_1 - \delta)}{\mu_1}.$$

It is therefore immediate that the van Dam and Haemers bound is an upper bound for $\alpha_q(G)$.

5. Implications for $\alpha_q(G)$ and for $\alpha(G)$. It follows from Theorem 3.3 that any graph with $\alpha(G) = n^0 + \min(n^+, n^-)$ has $\alpha_q = \alpha$. This is the case for numerous graphs, including odd cycle, perfect, folded cube, Kneser, Andrasfai, Petersen, Desargues, Grotzsch, Heawood, Clebsch and Higman-Sims graphs. Furthermore, if the inertia bound is tight with an appropriately chosen weight matrix, then again $\alpha_q = \alpha$. This is the case for all bipartite graphs. There are also many graphs, including Chvatal, Hoffman-Singleton, Flower Snark, Dodecahedron, Frucht, Octahedron, Thomsen, Pappus, Gray, Coxeter and Folkman for which $\alpha = \lfloor \vartheta \rfloor$, so again $\alpha_q = \alpha$. For all such graphs, there are no benefits from quantum entanglement for independence. The Clebsch graph demonstrates that the inertia bound is not an upper bound for $\lfloor \vartheta'(G) \rfloor$.

Elzinga and Gregory [11] asked whether there exists a real symmetric weight matrix W for every graph G such that:

$$\alpha(G) = n^0(W) + \min(n^+(W), n^-(W))? \tag{5.9}$$

They demonstrated experimentally that this is true for all graphs with up to 10 vertices, and for vertex transitive graphs with up to 12 vertices. Sinkovic [24] subsequently proved that there is no real symmetric

[2] We use the unconventional symbol Δ instead of d for the degree of regular graphs because d is the dimension of the Hilbert space used in the definition of the quantum independence number.

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weight matrix for which (5.9) is tight for Paley 17. This leaves open, however, whether there is always a Hermitian weight matrix for which (5.9) is exact.

It follows from Theorem 3.3 that every graph with $\alpha < \alpha_q$ is a counter-example to (5.9) for real symmetric and Hermitian weight matrices. This leads to the question of whether (5.9) is true for α_q or α_p. It follows from Theorem 3.3 that the answer is no, because for some graphs, such as the line graph of the cartesian product of K_3 with itself, the projective packing number is non-integral [23].

There are also numerous regular graphs for which the Hoffman bound on $\alpha(G)$ is exact, but the unweighted inertia bound is not. Examples include the Shrikhande, Tesseract, Hoffman and Cuboctahedral graphs. There are also many regular graphs where the floor of the Hoffman bound is exact, but the unweighted inertia bound is not. Examples include some circulant, cubic and quartic graphs. For all of these graphs, $\alpha_q = \alpha$.

Appendix A in [4] demonstrates, however, that it is hard to find well-known graphs for which there is equality in Theorem 3.3 when $k \geq 2$ and $p_k(A) = A^k$.

It would be interesting to find the graph with the smallest number of vertices that has $\alpha(G) < \alpha_q(G)$. Such a graph must have at least 11 vertices (given the experimental results due to Elzinga and Gregory). The smallest such graph that we know of is due to Piovesan (see Figure 3.1 in [21]), which has 24 vertices, with $\chi = \alpha = 5, \chi_q = 4$ and $\alpha_q \geq 6$.

6. Conclusion. To conclude, we illustrate the differences between classical and quantum graph parameters, by summarising results in [18] for orthogonality graphs. The orthogonality graph $\Omega(n)$ has vertex set the set of ± 1-vectors of length n, with two vertices adjacent if they are orthogonal. With n a multiple of 4, $\chi_q(\Omega(n)) = n$ but $\chi(\Omega(n))$ is exponential in n. Similarly, $\alpha_q(\Omega(n)\Box K_n) = 2^n$ but $\alpha(\Omega(n)\Box K_n) \leq n(2-\epsilon)^n$, for some $\epsilon > 0$, where $\Box$ denotes the Cartesian product [18].

Therefore, the spectral bounds in this paper and in [9] for quantum graph parameters demonstrate the weaknesses of such bounds for classical graph parameters for some families of graphs.

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