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Eigenvalues of subgraphs of the cube

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ABSTRACT

We consider the problem of maximising the largest eigenvalue of subgraphs of the hypercube Q_d of a given order. We believe that in most cases, Hamming balls are maximisers, and our results support this belief. We show that the Hamming balls of radius $o(d)$ have largest eigenvalue that is within $1 + o(1)$ of the maximum value. We also prove that Hamming balls with fixed radius maximise the largest eigenvalue exactly, rather than asymptotically, when d is sufficiently large. Our proofs rely on the method of compressions.

1. Introduction

In the last few decades much research has been done on spectra of graphs, i.e. the eigenvalues of the adjacency matrices of graphs; see Finck and Grohmann [10], Hoffman [16,17], Nosal [25], Cvetković, Doob and Sachs [6], Neumaier [20], Brigham and Dutton [3,4], Brualdi and Hoffman [5], Stanley [30], Shearer [29], Powers [26], Favaron, Mahéo and Saclé [8,9], Hong [18], Liu, Shen and Wang [19], Nikiforov [21–24], and Cvetković, Rowlinson and Simić [7] for a small selection of relevant publications. Perhaps the most basic property of the spectrum of a graph is its radius, i.e. the maximum eigenvalue: this has received especially much attention. Here we shall mention a small handful of these results.

In what follows, $A(G)$ denotes the adjacency matrix of a graph G and $\lambda_1(G)$ denotes the largest eigenvalue of $A(G)$. As usual, we write $e(G)$ for the number of edges, $\Delta(G)$ for the maximum degree and $\overline{d}(G)$ for the average degree. Trivially, $\overline{d}(G) \leq \lambda_1(G) \leq \Delta(G)$; in particular, if G is d-regular then $\lambda_1(G) = d$. In 1985, Brualdi and Hoffman [5] gave an upper bound on $\lambda_1(G)$ in terms of $e(G)$:

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if $e(G) \leq \binom{k}{2}$ for some integer $k \geq 1$ then $\lambda_1(G) \leq k-1$, with equality if and only if G consists of a k-clique and isolated vertices. Extending this result, Stanley [30] showed that if $e(G) = m$ then $\lambda_1(G) \leq \frac{1}{2}\left(\sqrt{8m+1}-1\right)$, with equality only as before. In 1993, Favaron, Mahéo and Saclé [9] published an upper bound on $\lambda_1(G)$ in terms of the local structure of G: writing $s(G)$ for the maximum of the sum of degrees of vertices adjacent to some vertex, we have $\lambda_1(G) \leq \sqrt{s(G)}$. Furthermore, if G is connected then equality holds if and only if G is regular or bipartite semi-regular (i.e. vertices in the same class have equal degrees). In particular, if G is a triangle-free graph with m edges then $s(G) \leq m$, so $\lambda_1(G) \leq \sqrt{m}$. This inequality was first proved by Nosal [25] in 1970. The star $K_{1,m}$ shows that this upper bound is best possible.

Our main aim in this paper is to study the maximum eigenvalue of subgraphs of the hypercube Q_d on 2^d vertices, rather than general graphs restricted by their parameters like order and size. To be precise, our aim is to give a partial answer to the following question posed by Fink [11] and in a weaker form by Friedman and Tillich [12].

Question 1. *Given m, $1 \leq m \leq 2^d$, what is the maximum of the largest eigenvalue of $Q_d[U]$, where $|U| = m$?*

This problem can be viewed as a variant of the 'classical' isoperimetric problem in the cube. Indeed, since Q_d is d-regular, the problem of bounding the maximum eigenvalue of the subgraph $Q_d[U]$ of Q_d induced by a set $U \subset V(Q_d) = \{0,1\}^d$ is closely related to the size of the edge boundary of U, the set of edges joining a vertex in U to one not in U. If the maximum eigenvalue of $Q_d[U]$ is λ_1, then $e(Q_d[U]) \leq \lambda_1|U|/2$ (by the bound $\lambda_1(G) \geq \overline{d}(G)$ mentioned above), so the size of the edge boundary of U is at least $(d-\lambda_1)|U|$. Thus, if $\lambda_1 \leq \lambda(m)$ whenever $|U| = m$, then for every set of m vertices of the cube Q_d the edge boundary has size at least $(d-\lambda(m))m$.

The study of eigenvalues as a form of isoperimetric inequality is not new: in 1985, Alon and Milman [1] showed that there is a close relation between the second smallest eigenvalue of the Laplacian of a graph and some expansion properties of the graph. The nature of our problem is very different from this. A vaguely related problem has been studied by Reeves, Farr, Blundell, Gallagher and Fink [27].

Before we state our results, we give some precise definitions. Our ground graph is taken to be Q_d, the *d-dimensional hypercube*, where the vertices are labelled by the 0,1 strings of length d, so that $V(Q_d) = \{0,1\}^d$, and two vertices are joined by an edge if they differ in exactly one coordinate. We shall often use the obvious correspondence between binary strings of length d and subsets of $[d]$, in which a subset corresponds to its characteristic function. A *subcube* of Q_d of dimension i is the graph induced by a subset of the vertices obtained by fixing the values of all but i coordinates. The *Hamming ball* H_d^i is the subgraph of Q_d induced by the vertices with at most i ones in their strings. We note that the subgraphs minimising the sizes of the vertex and edge boundaries among all subgraphs of Q_d of a given order are well known. In particular, Harper (see [13] and [14]) showed in 1966 that the Hamming balls minimise the size of the vertex boundary among subgraphs of the same order. In 1976, Hart [15] proved a similar result, showing that subcubes minimise the size of the edge boundary among subgraphs of the hypercube with the same number of vertices.

As the problem of maximising λ_1 is a form of an isoperimetric problem, it seems natural to believe that either Hamming balls or subcubes should be maximisers of λ_1. Although, intuitively, it may seem that λ_1 is related to the edge boundary, we believe that in most cases, the task of maximising λ_1 is, in fact, more related to minimising the vertex boundary. More precisely, we believe that for most radii sufficiently smaller than $d/2$, Hamming balls maximise λ_1 among subgraphs of Q_d with the same order.

We prove several results in this direction. Our first result, which is relatively easy, gives a precise answer when the number of vertices is at most the dimension of the hypercube.

Theorem 2. *Let G be an induced subgraph of Q_d with $n \leq d$ vertices. Then, for $n \geq 105$, $\lambda_1(G) \leq \sqrt{n-1}$, with equality if and only if G is a star.*

We note that the conclusion of Theorem 2 does not hold for all n. Indeed, for $n = 4$, the largest eigenvalue of Q_2 (or C_4) is 2, which is larger than $\sqrt{3}$, the largest eigenvalue of the star $K_{1,3}$.

In order to obtain more general results we evaluate the largest eigenvalue of the Hamming ball H_d^i for radii tending to infinity with the dimension of the cube.

Theorem 3. *If $d, i \to \infty$ and $i \le \frac{d+1}{2}$ then*

$$\lambda_1(H_d^i) = 2\sqrt{i(d+1-i)}\left(1 + O\left(\sqrt{\frac{\log i}{i}}\right)\right).$$

Our first main result is a generalisation of Theorem 2. We prove that for a wide range of radii, the Hamming balls have largest eigenvalues which are asymptotically largest among all subgraphs of the cube of the same order. We note that Samorodnitsky [28] obtained an equivalent result for a wider range of radii (namely for radii i satisfying $i \to \infty$; however, our proof works also if i is bounded). His proof methods are very different from ours.

Theorem 4. *Let $i = i(d) = o(d)$ and let G be a subgraph of Q_d with $n = O\left(\left|H_d^i\right|\right)$ vertices. Then $\lambda_1(G) \le (1 + o(1))\, \lambda_1(H_d^i)$.*

Finally, our second main result gives an exact answer when the radius is fixed.

Theorem 5. *For every i there is $d_0 = d_0(i)$ such that for $d \ge d_0$ the Hamming ball H_d^i maximises the largest eigenvalue among subgraphs of Q_d of the same order.*

1.1. Notation

Given a graph G and a vertex u, the degree of u in G is denoted by $d_G(u)$; when it is not likely to cause confusion, we drop the subscript and write $d(u)$. We denote the base 2 logarithm by $\log(x)$ and the base e logarithm by $\ln(x)$. We use the notation $[d]^{(i)}$ to denote the collection of subsets of $[d]$ of size i, and, similarly, $[d]^{(\le i)}$ denotes the collections of subsets of $[d]$ of size at most i. We note that if H is a subgraph of G then $\lambda_1(H) \le \lambda_1(G)$, due to the monotonicity of λ_1. We may thus concentrate on *induced* subgraphs of Q_d; hence, throughout the paper, we implicitly assume that the subgraphs of Q_d that we consider are induced subgraphs of Q_d.

1.2. Structure of the paper

In the next section, Section 2, we state and prove results about compressions which will be used in the proofs of the above theorems. We prove Theorem 2 in Section 3. In Section 4 we prove Theorem 3 as well as other bounds on the largest eigenvalue of certain subgraphs of the cube. We prove our first main result, Theorem 4, in Section 5 and our second main result, Theorem 5, is proved in Section 6. We conclude with some remarks and open problems in Section 7.

2. Compressions

In this section we prove the results about compressions that we shall need. We start by introducing notation. Let G be an induced subgraph of Q_d, and let $v \in \mathbb{R}^{V(G)} \subseteq \mathbb{R}^{V(Q_d)}$. Then $\langle A(G)v, v\rangle = \langle A(Q_d)v, v\rangle$, since the support of v is contained in $V(G)$. Hence

$$\max_{|G|=n}\{\lambda_1(G)\} = \max_{|G|=n,\ \|v\|=1}\{\langle A(G)v, v\rangle\} = \max_{\|v\|=1,\ \mathrm{supp}(v)=n}\{\langle A(Q_d)v, v\rangle\}.$$

We consider a notion of *compressions* acting on vectors in $\mathbb{R}^{V(Q_d)}$. Let $U, V \subseteq [d]$ be disjoint and let $v \in \mathbb{R}^{V(Q_d)}$. We define $C_{U,V}(v) \in \mathbb{R}^{V(Q_d)}$ as follows, where $S \subseteq [d]$.

$$\left(C_{U,V}(v)\right)_S = \begin{cases} \max\{v_S, v_{S\triangle(U\cup V)}\} & V \subseteq S \text{ and } U \cap S = \emptyset \\ \min\{v_S, v_{S\triangle(U\cup V)}\} & U \subseteq S \text{ and } V \cap S = \emptyset \\ v_S & \text{otherwise.} \end{cases}$$

Note that $C_{U,V}$ applies a $U - V$ compression to the support of v, leaving the multiset of entries of v unchanged. In particular, it preserves the size of the support of v and its norm. For an illustration of compressions, see Figs. 1 and 2.

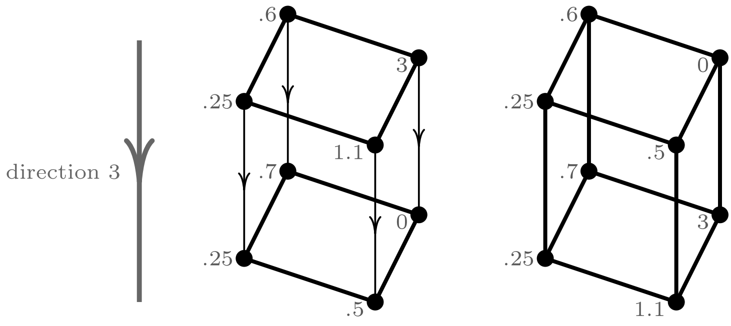

Fig. 1. A $C_{\{3\},\emptyset}$-compression in Q_3. (In each edge marked by an arrow, the coordinates of the two vertices are swapped if the coordinate at the starting point is larger than the coordinate at the end point.)

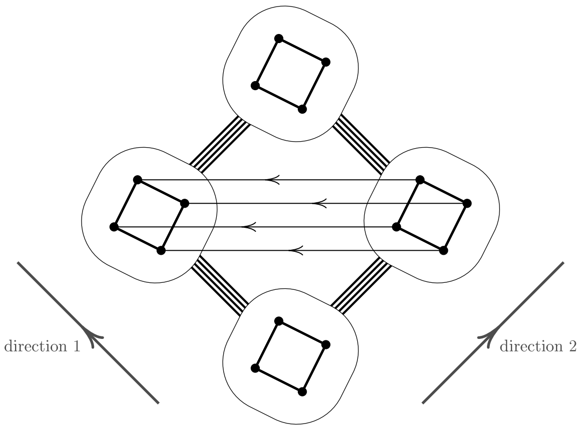

Fig. 2. A $C_{\{2\},\{1\}}$-compression in Q_4.

The *infinite-dimensional hypercube* Q_∞ is the graph whose vertices are the finite subsets of $\mathbb{N}$, where ST is an edge if and only if $|S \triangle T| = 1$. Note that by viewing Q_n as a graph on the subsets of $[n]$, Q_∞ can be viewed as the union $\cup_{n\geq 1} Q_n$. The *binary order* on Q_∞ is defined as follows: $S < T$ if and only if $\max(S \triangle T) \in T$, where $S, T \in V(Q_\infty)$. It is easy to see that the binary order is a total order. An *initial segment* in the binary order is the set of the first m elements in the order, for some m. For example, $V(Q_n)$ is an initial segment. We define the binary i-compression $C_i(v)$ to rearrange the values $(v_S)_{i\in S}$ to be decreasing in the binary order restricted to the subcube $\{S : i \in S\}$, and rearrange the values $(v_S)_{i\notin S}$ to be decreasing in the binary order restricted to $\{S : i \notin S\}$. We define C_i^+ and C_i^- to be the restrictions of v to sets containing i and not containing i, respectively. Note that C_i^+ and C_i^- commute with C_i.

We may naturally apply these maps to the indicator function of a set F to obtain another indicator function, coinciding with the usual definitions of these maps on sets. We suppress explicit usage of the indicator function where this can be done without confusion.

Given $i \in [d]$, we abuse notation by denoting the singleton $\{i\}$ by i where this is not likely to cause confusion. Furthermore, if $S \subseteq [d]$ we denote $S \cup \{i\}$ by $S + i$ and similarly we denote $S \setminus \{i\}$ by $S - i$. The following two results show that the application of a $C_{i,\emptyset}$ compression or a $C_{i,j}$ compression to a vector v does not decrease the inner product $\langle A(Q_d)v, v\rangle$.

Lemma 6. *Let $i \in [d]$ and $v \in \mathbb{R}^{V(Q_d)}$ and denote $A = A(Q_d)$ and $\bar{v} = C_{i,\emptyset}(v)$. Then $\langle Av, v\rangle \leq \langle A\bar{v}, \bar{v}\rangle$.*

Proof. Consider an edge $ST \in E(Q_d)$ with $S \subset T$. If $T \setminus S = \{i\}$, then v_S and v_T are either swapped or not, and in either case the contribution of ST to the inner product is unchanged. All other edges have either $i \in S \cap T$ or $i \notin S \cup T$. These edges come in pairs $(S, S+j), (S+i, S+i+j)$. By the rearrangement inequality and the definition of $C_{i,\emptyset}$, the contribution of this pair of edges to the inner product is at most as large in $C_{i,\emptyset}(v)$ as it is in v. □

Lemma 7. *Let $i, j \in [d]$ be distinct, let $v \in \mathbb{R}^{V(Q_d)}$, and denote $A = A(Q_d)$ and $\bar{v} = C_{i,j}(v)$. Then $\langle Av, v\rangle \le \langle A\bar{v}, \bar{v}\rangle$.*

Proof. Consider an edge $ST \in E(Q_d)$ with $S \subseteq T$. The function $C_{i,j}$ is a composition of conditional swaps, and each vertex of Q_d is involved in at most one of these swaps. If neither S nor T are involved in a swap, then the contribution of the edge ST to the inner product is unchanged.

If both S and T are involved in a swap, then if $i \in S$ then $j \notin S$ and, also, $i \in T$ and $j \notin T$, and we have v_S potentially being swapped with v_{S-i+j} and v_T potentially being swapped with v_{T-i+j}; if $i \notin S$ then $j \in S$, so v_S and v_T are potentially swapped with v_{S-j+i} and v_{T-j+i} respectively. Hence edges ST where both vertices are potentially swapped come in pairs $(S, T), (S-i+j, T-i+j)$. By the rearrangement inequality, the contribution of each of these pairs to the inner product is not decreased by $C_{i,j}$.

If only S is involved in a swap, then exactly one of i and j is in S, whilst both i and j are in T. Hence such edges come in pairs $(T-i, T)$ and $(T-j, T)$, and the contribution of such pairs to the inner product is unchanged by $C_{i,j}$. Similarly, the edges where only T is involved in a swap come in pairs $(S, S+i)$ and $(S, S+j)$, and the contribution of such pairs to the inner product is unchanged by $C_{i,j}$. □

We say that a vector $v \in \mathbb{R}^{V(Q_d)}$ is *down-compressed* if $C_{U,\emptyset}(v) = v$ for every $U \subseteq [d]$, and we say that v is *left-compressed* if $C_{i,j}(v) = v$ for every $1 \le j < i \le d$. We say that v is *compressed* if it is down-compressed and left-compressed. It follows from Lemmas 6 and 7 that in order to find the maximum of $\lambda_1(G)$ over subgraphs of the cube of order n, it suffices to consider induced graphs G whose vertex set is compressed. Furthermore, this maximum is the maximum of $\langle Av, v\rangle$ over compressed vectors v with support of size n.

2.1. Counting copies of subcubes

The aim of this subsection is to provide an upper bound on the number of copies of a subcube in a subgraph G of the cube, in terms of $|G|$.

Given a set $U \subseteq V(Q_d)$ and $d' \le d$ we denote the number of copies of $Q_{d'}$ in $Q_d[U]$ by $\#(Q_{d'} \subseteq U)$. The following result, which was proved by Bollobás and Radcliffe [2], shows that the number of copies of $Q_{d'}$ is maximised by initial segments of the binary order. We present a proof here for the sake of completeness.

Lemma 8. *Let $U, I \subseteq V(Q_d)$ with $|U| = |I|$ and I is an initial segment in binary order. Then for any $d' \le d$,*

$$\#(Q_{d'} \subseteq U) \le \#(Q_{d'} \subseteq I).$$

Proof. We prove the lemma by induction on d'. The case $d' = 0$ is trivial, as $|U| = |I|$. Suppose that $d' > 0$. We proceed by induction on $d \ge d'$. For $d = d'$ we have that both $\#(Q_{d'} \subseteq U)$ and $\#(Q_{d'} \subseteq I)$ are 0 if $|U| = |I| < 2^d$ and both are 1 otherwise.

Fix $i \in [d]$. Suppose that $d > d'$ and $C_i(U) = U' \ne U$. For any copy H of $Q_{d'}$ in $Q_d[U]$, one of the following three statements holds: $C_i^+(H) = H$; $C_i^-(H) = H$; or $C_i^-(H) = C_{i,\emptyset}(C_i^+(H))$. Hence by induction the following holds.

$$\begin{aligned}
\#(Q_{d'} \subseteq U) &\le \#(Q_{d'} \subseteq C_i^+U) + \#(Q_{d'} \subseteq C_i^-U) + \\
&\qquad \min\left\{\#(Q_{d'-1} \subseteq C_i^+U), \#(Q_{d'-1} \subseteq C_i^-U)\right\} \\
&\le \#(Q_{d'} \subseteq C_i^+U') + \#(Q_{d'} \subseteq C_i^-U') + \\
&\qquad \min\left\{\#(Q_{d'-1} \subseteq C_i^+U'), \#(Q_{d'-1} \subseteq C_i^-U')\right\} \\
&= \#(Q_{d'} \subseteq U').
\end{aligned}$$

The last equality follows from the fact that $C_i^- U'$ and $C_{i,\emptyset}(C_i^+ U')$ are *nested*, i.e. one of these sets is contained in the other.

Define a finite sequence $\{U_k : k = 0, \dots, K\}$ by taking $U_0 = U$ and $U_{k+1} = C_i U_k$ for the least i such that $C_i U_k \neq U_k$, if such an i exists. It is easy to verify that this sequence cannot be infinite. Denote $W = U_K$. Then $\#(Q_{d'} \subseteq U) \leq \#(Q_{d'} \subseteq W)$ and $C_i W = W$ for every $i \in [d]$. If $W = I$ the proof is complete, thus we may assume that $W \neq I$.

Since $W \neq I$, W is not an initial segment in binary order, so there exists $S < T$ with $S \notin W$ and $T \in W$. Since $C_i^+ W$ and $C_i^- W$ are both initial segments, we have that $i \in S \triangle T$ for every $i \in [d]$. In other words, $S = T^c$, and there is at most one such pair (S, T), so T is the successor of S in binary order and is the maximal element of W. Hence $T = \{d\}$ and $S = [d-1]$. But then T is in at most one $Q_{d'}$ in W, whilst S is in $\binom{d-1}{d'} \geq 1$ copies of $Q_{d'}$ in $W - T + S$. Hence $I = W - T + S$ has at least as many $Q_{d'}$ subgraphs as W, completing the proof. $\square$

The following upper bound on the number of copies of a subcube follows easily.

Lemma 9. *Let U be a subset of $V(Q_D)$ of size n, for some D. Then, for every $d \leq D$,*

$$\#(Q_d \subseteq U) \leq \frac{n}{2^d}\binom{\log n + 1}{d}.$$

Proof. By Lemma 8, we may assume that U is initial in binary order, so U is contained in a cube of dimension $\lceil \log n \rceil$. Hence each vertex is in at most $\binom{\log n+1}{d}$ copies of Q_d and each copy of Q_d is counted 2^d times. $\square$

In fact, one can prove a smooth version of the above upper bound. We define $\binom{x}{d} = \mathbb{1}_{\{x \geq d-1\}} \frac{x(x-1)\cdot\ldots\cdot(x-d+1)}{d!}$ for $x \geq 0$ and d integer; in particular, $\binom{x}{d} \geq 0$ for every $x \geq 0$ and d integer.

Lemma 10. *Let U be a subset of $V(Q_D)$ of size n, for some D. Then, for every $d \leq D$,*

$$\#(Q_d \subseteq U) \leq \frac{n}{2^d}\binom{\log n}{d}.$$

Proof. Let $T_{n,d} = \#(Q_d \subseteq I_n)$, where I_n is initial in binary order in Q_∞ with $|I| = n$. We prove that $T_{n,d} \leq \frac{n}{2^d}\binom{\log n}{d}$ by induction on d. It is clear for $d = 0$ so we assume $d > 0$. Note that we may assume that $n \geq 2^d$ because, otherwise, I_n contains no copies of Q_d.

We proceed by induction on the number of non-zero digits in the binary representation of n. If n is a power of 2, I_n is a cube of dimension $\log n$ and we have $T_{n,d} = \frac{n}{2^d}\binom{\log n}{d}$.

Now suppose that n has $l > 1$ non-zero digits in the binary representation. Write $n = 2^{k_1} + \cdots + 2^{k_l}$ where $k_1 > \cdots > k_l$ and let $r = 2^{k_1}$ and $m = n - r$. Then by the definition of binary order and by induction we obtain the following inequality.

$$T_{n,d} = T_{r,d} + T_{m,d} + T_{m,d-1} \leq \frac{r}{2^d}\binom{\log r}{d} + \frac{m}{2^d}\binom{\log m}{d} + \frac{m}{2^{d-1}}\binom{\log m}{d-1}.$$

Note that if $m < 2^{d-1}$ then $T_{m,d} = T_{m,d-1} = 0$, so $T_{n,d} = T_{r,d} \leq \frac{r}{2^d}\binom{\log r}{d} \leq \frac{n}{2^d}\binom{\log n}{d}$, as required, so we may assume that $m \geq 2^{d-1}$. It remains to prove the following inequality.

$$\frac{r}{2^d}\binom{\log r}{d} + \frac{m}{2^d}\binom{\log m}{d} + \frac{m}{2^{d-1}}\binom{\log m}{d-1} \leq \frac{n}{2^d}\binom{\log n}{d}. \tag{1}$$

Writing $r = (1+\alpha)m$ and rearranging (1), we need to show that the following expression is non-negative for $m \geq 2^{d-1}$ and $\alpha > 0$.

$$\frac{(2+\alpha)m}{2^d}\binom{\log((2+\alpha)m)}{d} - \frac{(1+\alpha)m}{2^d}\binom{\log((1+\alpha)m)}{d} - \frac{m}{2^d}\binom{\log m}{d} - \frac{m}{2^{d-1}}\binom{\log m}{d-1}.$$

Writing $\beta = \log m$, we need to show that the following expression is non-negative for $\alpha > 0$ and $\beta \geq d-1$.

$$\begin{aligned} f_\beta(\alpha) &= (2+\alpha)\binom{\log(2+\alpha)+\beta}{d} - (1+\alpha)\binom{\log(1+\alpha)+\beta}{d} \\ &\quad - \binom{\beta}{d} - 2\binom{\beta}{d-1}. \end{aligned}$$

Substituting $\alpha = 0$ we obtain

$$f_\beta(0) = 2\binom{\beta+1}{d} - \binom{\beta}{d} - \binom{\beta}{d} - 2\binom{\beta}{d-1} = 0.$$

The derivative $f'_\beta(\alpha)$ at $\alpha > 0$ is

$$\begin{aligned} &\frac{1}{d!\ln 2}\sum_{i=0}^{d-1}\left(\prod_{0\leq j\leq d-1, j\neq i}(\log(2+\alpha)+\beta-j) - \prod_{0\leq j\leq d-1, j\neq i}(\log(1+\alpha)+\beta-j)\right) \\ &\quad + \binom{\log(2+\alpha)+\beta}{d} - \binom{\log(1+\alpha)+\beta}{d} \geq 0. \end{aligned}$$

We have shown that $f_\beta(0) = 0$ and $f'_\beta(\alpha) \geq 0$ for every $\alpha > 0$. It follows that $f_\beta(\alpha) \geq 0$ for every $\alpha \geq 0$, as required. $\square$

3. The star is best for $n \leq d$

In this section we prove Theorem 2, thus showing that the star on d vertices maximises the largest eigenvalue among subgraphs of the cube Q_d with at most d vertices.

Theorem 2. *Let G be an induced subgraph of Q_d with $n \leq d$ vertices. Then, for $n \geq 105$, $\lambda_1(G) \leq \sqrt{n-1}$, with equality if and only if G is a star.*

Note that this result is not entirely obvious. Indeed, a natural line of attack is to use the inequality $\lambda_1(G) \leq \sqrt{s(G)}$ of Favaron, Mahéo and Saclé [9] that we mentioned in the introduction, where $s(G)$ is the maximum of the sum of degrees of vertices adjacent to some vertex. Taking a vertex u, its k neighbours, and $\binom{k}{2}$ additional vertices, each joined to two of the k neighbours of u, we get a subgraph G of Q_n with $n = 1+k+\binom{k}{2} = (k^2+k+2)/2$ vertices and $e(G) = s(G) = k^2$. Hence, $\lambda_1(G) \leq \sqrt{s(G)} = k$, which is about $\sqrt{2}$ times as large as $\sqrt{n-1}$, the bound we wish to prove. The problem is, of course, that the inequality we have applied is far from sharp in this case.

We shall use the following bound, relating the problem of maximising the largest eigenvalue to the task of maximising a trace of a matrix.

Lemma 11. *Let G be a bipartite graph with bipartition $\{X, Y\}$ and let $k \geq 1$. Then*

$$\begin{aligned} (\lambda_1(G))^{2k} &\leq \frac{1}{2}\operatorname{tr}\left(A(G)^{2k}\right) \\ &= \#(\textit{closed walks of length } 2k \textit{ starting at a vertex in } X) \\ &= \#(\textit{closed walks of length } 2k \textit{ starting at a vertex in } Y). \end{aligned}$$

In particular,

$$(\lambda_1(G))^4 \leq \#(\textit{edges in } G) + 2\#(\textit{paths of length } 2 \textit{ in } G) + 4\#(C_4 \textit{ in } G).$$

Proof. Let $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A = A(G)$ (A is symmetric and real, so its eigenvalues are all real). Recall that, since G is bipartite, λ is an eigenvalue of A if and only if $-\lambda$ is an eigenvalue of

A (given an eigenvector v with eigenvalue λ, swap the sign in coordinates of v corresponding to one of the sides of G to obtain an eigenvector with eigenvalue $-\lambda$). It follows that $\lambda_n = -\lambda_1$. Hence,

$$2(\lambda_1)^{2k} \le (\lambda_1)^{2k} + \cdots + (\lambda_n)^{2k} = \mathrm{tr}(A^{2k}).$$

We conclude that $(\lambda_1)^{2k} \le \mathrm{tr}(A^{2k})/2$. The rest of the proof is immediate from the fact that $\left(A^k\right)_{i,j}$ is the number of walks of length k from vertex i to vertex j. $\square$

We shall also make use of the following bound on the number of edges and 4-cycles in a $K_{2,3}$-free bipartite graph.

Claim 12. *Let G be a bipartite graph with bipartition $\{X, Y\}$ and assume that G is $K_{2,3}$-free. Set $k = |X|$, $l = |Y|$. Then*

- $\#(C_4 \text{ in } G) \le \binom{l}{2}$.
- $|E(G)| \le \#(2\text{-paths with both ends in } Y) + k \le 2\binom{l}{2} + k$.

Proof. The first part follows directly from the fact that G is $K_{2,3}$-free, so every pair of vertices in Y is contained in at most one 4-cycle. The first inequality in the second part follows from the observation that for every vertex $v \in X$, we have $d(v) \le \#(2\text{-paths in } G \text{ with } v \text{ as the middle vertex}) + 1$. The second inequality again follows from the assumption that G is $K_{2,3}$-free. $\square$

We now proceed to the proof of Theorem 2.

Proof of Theorem 2. Let G be a subgraph of Q_d with $n \le d$ vertices and assume that $\lambda_1(G) \ge \sqrt{n-1}$. Denote by $\{X, Y\}$ the bipartition of the vertices of G where $k = |X| \ge |Y| = l$.

By Lemma 11 and the fact that G is $K_{2,3}$-free, we obtain the following.

$$\begin{aligned}
(n-1)^2 &\le (\lambda_1(G))^4 \\
&\le 2\sum_{v\in V(G)} \binom{d(v)}{2} + |E(G)| + 4\#(C_4 \text{ in } G) \\
&\le 2\left(\binom{k}{2} + \binom{l}{2} + 2\#(C_4 \text{ in } G)\right) + |E(G)| + 4\#(C_4 \text{ in } G) \\
&= 2l^2 - 2nl + n^2 - n + |E(G)| + 8\#(C_4 \text{ in } G).
\end{aligned}$$

Hence,

$$0 \le 2l^2 - 2nl + n - 1 + |E(G)| + 8\#(C_4 \text{ in } G). \tag{2}$$

We replace $|E(G)|$ and $\#(C_4 \text{ in } G)$ by the upper bounds from Lemma 10 to obtain the following inequality.

$$\begin{aligned}
0 &\le 2l^2 - 2nl + n - 1 + (n\log n)/2 + 2n\binom{\log n}{2} \\
&= 2l^2 - 2nl + n\left(\log^2 n - (\log n)/2 + 1\right) - 1.
\end{aligned}$$

Since $l \le n/2$, we deduce the following upper bound on l (we implicitly assume that $n \ge 72$, in which case the expression under the square root sign is non-negative).

$$\begin{aligned}
l &\le \frac{1}{4}\left(2n - \sqrt{4n^2 - 8n\left(\log^2 n - (\log n)/2 + 1\right) + 8}\right) \\
&= \frac{1}{2}\left(n - \sqrt{n^2 - 2n\log^2 n + n\log n - 2n + 2}\right).
\end{aligned} \tag{3}$$

By Claim 12 and by (2),

$$\begin{aligned} 0 &\leq 2l^2 - 2nl + n - 1 + 10\binom{l}{2} + n - l \\ &= (l-1)(7l + 1 - 2n). \end{aligned}$$

If $l \geq 2$ it follows that $l \geq \frac{1}{7}(2n-1)$. Combining this lower bound on l with the upper bound (3), we get the following inequality.

$$\frac{1}{7}(2n-1) \leq l \leq \frac{1}{2}\left(n - \sqrt{n^2 - 2n\log^2 n + n\log n - 2n + 2}\right).$$

This is a contradiction if $n \geq 105$. Thus if $n \geq 105$ we must have $l = 1$, implying that G is a star. □

4. The largest eigenvalue of the Hamming ball

In this section we estimate the largest eigenvalue of the Hamming ball H_d^i for several ranges of i and d. We start by proving Theorem 3, where we give an estimate for the eigenvalue of the Hamming ball when the radius goes to infinity.

Theorem 3. *If $d, i \to \infty$ and $i \leq \frac{d+1}{2}$ then*

$$\lambda_1(H_d^i) = 2\sqrt{i(d+1-i)}\left(1 + O\left(\sqrt{\frac{\log i}{i}}\right)\right).$$

We establish the upper bound of Theorem 3 in the following claim.

Claim 13. *Let d and i be integers satisfying $i \leq \frac{d+1}{2}$. Then $\lambda_1(H_d^i) \leq 2\sqrt{i(d-i+1)}$.*

Proof. Let $G = H_d^i$ and for $j \geq 0$ let $V_j = [d]^{(j)}$. Let $G_j = G[V_j \cup V_{j+1}]$. The graph G_j is a bipartite graph whose vertices in one side (V_j) have degree $d - j$ and the vertices in the other side (V_{j+1}) have degree $j + 1$. Thus $\lambda_1(G_j) = \sqrt{(j+1)(d-j)}$.

Let $v = (v_S)_{S \in V(G)}$ be an eigenvector with norm 1 and eigenvalue $\lambda_1(G)$. Define $\alpha_j^2 = \sum_{S \in V_j} v_S^2$. Note that $E(G) = \bigcup_{0 \leq j \leq i-1} E(G_j)$, hence the following holds (we view G_j as a graph on vertex set $V(G)$, so that the product $A(G_j)v$ is well defined).

$$\begin{aligned} \lambda_1(G) = \langle A(G)v, v\rangle &\leq \sum_{j=0}^{i-1} \langle A(G_j)v, v\rangle \\ &\leq \sum_{j=0}^{i-1} \left(\alpha_j^2 + \alpha_{j+1}^2\right)\lambda_1(G_j) \\ &= \sum_{j=0}^{i-1} \left(\alpha_j^2 + \alpha_{j+1}^2\right)\sqrt{(j+1)(d-j)} \\ &\leq 2\sqrt{i(d-i+1)}. \end{aligned}$$

It follows that $\lambda_1(G) \leq 2\sqrt{i(d-i+1)}$, as required. □

We shall need the following claim in a subsequent section.

Claim 14. *Let t, d and i be integers, and let G be a subgraph of H_d^i whose maximum degree is at most t. Then $\lambda_1(G) \leq 2\sqrt{it}$.*

We do not include the proof here, instead we remark that the proof of Claim 13 can be adapted to prove Claim 14, by defining $G_j = G[V_j \cup V_{j+1}]$ (where $V_j = [d]^{(j)}$), and noting that here $\lambda_1(G_j) \leq \sqrt{(j+1)t}$.

We now turn to the proof of Theorem 3.

Proof of Theorem 3. Denote $\lambda = \lambda_1(H_d^i)$ and $A = A(H_d^i)$. We first note that by Claim 13, we have $\lambda \leq 2\sqrt{i(d+1-i)}$.

We now obtain a lower bound on λ. Given $0 < k < i$, define the vector $v_k \in \mathbb{R}^{V(H_d^i)}$ by $(v_k)_S = \mathbb{1}_{\{S \in [d]^{(i-k)}\}} \binom{d}{i-k}^{-\frac{1}{2}}$. Note that $\|v_k\| = 1$. We obtain the following sequence of inequalities.

$$\begin{aligned}
\lambda^{2k} &\geq \langle A^{2k} v_k, v_k \rangle \\
&= \# \left(2k\text{-walks in } H_d^i \text{ from } [d]^{(i-k)} \text{ to } [d]^{(i-k)}\right) \binom{d}{i-k}^{-1} \\
&\geq \binom{d}{i-k} \# \Big(2k\text{-walks in } [i-2k, i] \text{ from } i-k \text{ to } i-k\Big) \\
&\qquad \cdot \Big((i-2k+1)(d-i+2k)\Big)^k \binom{d}{i-k}^{-1} \\
&\geq \binom{2k}{k} \Big((i-2k+1)(d-i+2k)\Big)^k .
\end{aligned}$$

To see why the second inequality holds, note that to form a $2k$-walk from $[d]^{(i-k)}$ to $[d]^{(i-k)}$ we first pick the starting point (for which there are $\binom{d}{i-k}$ options); then we pick a $2k$-walk in $[i-2k, i]$ from $i-k$ to $i-k$; and, finally, for each move from a set of size r to a set of size $r-1$ we have r options for an edge to go along, and for a move from a set of size $r-1$ to a set of size r there are $d+1-r$ options. We pair each move from a set of size r to a set of size $r-1$ with a move in the opposite direction, from a set of size $r-1$ to a set of size r. The number of possible steps in H_d^i for such a pair is $r(d+1-r)$. Note that the function $r(d+1-r)$ is increasing for $r \leq (d+1)/2$; hence, $r(d+1-r) \geq (i-2k+1)(d-i+2k)$ for every $r \in [i-2k+1, i]$. So, for each choice of a walk in $[i-2k, i]$ from $i-k$ to $i-k$ and a starting point in $[d]^{(i-k)}$, there are at least $\big((i-2k+1)(d-i+2k)\big)^k$ walks corresponding to it in H_d^i. The third inequality holds because each $2k$-walks from $i-k$ to $i-k$ in $[i-2k, i]$ is determined by the set of times in the walk in which we move 'up' (i.e. from r to $r+1$). Since there are exactly k 'up' and k 'down' moves, this number is $\binom{2k}{k}$.

Hence, if $k \to \infty$,

$$\lambda^{2k} \geq \frac{1}{\sqrt{\pi k}} 2^{2k} \Big((i-2k+1)(d-i+2k)\Big)^k (1 + o(1)).$$

Thus,

$$\begin{aligned}
\lambda &\geq k^{-\frac{1}{4k}} 2\sqrt{(i-2k+1)(d-i+2k)} \left(1 + O\left(k^{-1}\right)\right) \\
&= 2\sqrt{(i-2k+1)(d-i+2k)} \left(1 + O\left(k^{-1} \log k\right)\right) \\
&= 2\sqrt{i(d+1-i)} \left(1 + O\left(k^{-1} \log k\right) + O\left(k/i\right)\right).
\end{aligned}$$

Taking $k = \sqrt{i \log i}$, we get $\lambda \geq 2\sqrt{i(d+1-i)} \left(1 + O\left(\sqrt{\frac{\log i}{i}}\right)\right)$, completing the proof of Theorem 3. $\square$

We now consider the case where the radius of the Hamming ball is fixed.

Lemma 15. *There exist constants $\lambda_1 < \lambda_2 < \cdots$ such that $\lambda_1(H_d^i) = \lambda_i \sqrt{d}(1 + O(1/d))$, for fixed i and $d \to \infty$.*

Proof. Let A_i be the $(i+1)\times(i+1)$-matrix defined by

$$(A_i)_{j,k} = \begin{cases} 1 & j = k-1 \\ j & j = k+1 \\ 0 & \text{otherwise.} \end{cases}$$

Denote $\lambda_i = \lambda_1(A_i)$. We show that $\lambda_{i-1} < \lambda_i$, for every $i \geq 2$. Indeed, it follows from the Perron–Frobenius theorem that A_i has only one eigenvector u with eigenvalue $\lambda_1(A_i)$ (up to multiplication by a factor), and that all the coordinates of u are positive (the theorem is applicable here because A_i is a *non-negative irreducible* matrix, i.e. its entries are non-negative, and for every j, k, there is l such that $\left((A_i)_{j,k}\right)^l \neq 0$). Then, since A_{i-1} is a submatrix of A_i,

$$\begin{aligned}\lambda_{i-1} &= \max\left\{\langle A_{i-1}v, v\rangle : v \in \mathbb{R}^i,\ \|v\| = 1\right\} \\ &= \max\left\{\langle A_i(v,0),(v,0)\rangle : v \in \mathbb{R}^i,\ \|v\| = 1\right\} \\ &< \langle A_i u, u\rangle = \lambda_i.\end{aligned}$$

In order to complete the proof of Lemma 15, we show that $\lambda(H_d^i) = \lambda_i\sqrt{d}(1+O(1/d))$.

By symmetry, the eigenvector v of $A(H_d^i)$ with eigenvalue $\lambda_1(H_d^i)$ is uniform on $[d]^{(j)}$ for every $0 \leq j \leq i$ (as there is only one such eigenvector, up to multiplication by a factor, by the Perron–Frobenius theorem). Denote $x_j = v_{[j]}$. The following holds.

$$\lambda_1(H_d^i)\, x_j = \begin{cases} dx_1 & j = 0 \\ jx_{j-1} + (d-j)x_{j+1} & 0 < j < i \\ ix_{i-1} & j = i. \end{cases}$$

Letting $\mu = \lambda_1(H_d^i)/\sqrt{d}$ and $y_j = x_j d^{j/2}$, we obtain

$$\mu y_j = \begin{cases} y_1 & j = 0 \\ jy_{j-1} + (1-j/d)y_{j+1} & 0 < j < i \\ iy_{i-1} & j = i. \end{cases}$$

Recalling the definition of A_i, it follows that μ is the largest eigenvalue of a matrix $A_{d,i}$ whose entries are non-negative and differ (coordinate-wise) from those of A_i by $O(1/d)$. It follows from Observation 16 that $|\mu - \lambda_i| = O(1/d)$. Lemma 15 follows. $\square$

We conclude this section with the following observation, which states that if the entries of two matrices are very close to each other, then so are the largest eigenvalues of the two matrices. This observation was used in Lemma 15, and will be used in Section 6.

Observation 16. *Let A and B be $n \times n$ matrices with non-negative entries, satisfying $|A_{i,j} - B_{i,j}| \leq \varepsilon$ for every $i, j \in [n]$. Then $|\lambda_1(A) - \lambda_1(B)| \leq n\varepsilon$.*

Proof. Let v be an eigenvector of A with eigenvalue $\lambda_1(A)$ and norm 1, whose entries are non-negative (such an eigenvector exists because the entries of A are non-negative). Then the following holds.

$$\begin{aligned}\lambda_1(B) &\geq \langle Bv, v\rangle \\ &= \sum_{i,j\in[n]} B_{i,j}v_iv_j \\ &\geq \sum_{i,j\in[n]} (A_{i,j}-\varepsilon)v_iv_j \\ &= \langle Av, v\rangle - \varepsilon\left(\sum_{i\in[n]} v_i\right)^2 \\ &\geq \lambda_1(A) - n\varepsilon.\end{aligned}$$

The second inequality follows from the assumptions on A and B and uses the fact that the entries of v are non-negative, and the third follows from the Cauchy–Schwarz inequality (using the assumption that the norm of v is 1). By swapping the roles of A and B, Observation 16 follows. □

5. Hamming ball is asymptotically best for $i = o(d)$

In this section we prove Theorem 4, showing that for $i = o(d)$ the Hamming ball H_d^i asymptotically maximises λ_1 among subgraphs of Q_d with about the same number of vertices. Since our proof is rather technical, we start with the special case $i = 1$.

5.1. Proof of Theorem 4 for $i = 1$

Let us first state the result for the special case $i = 1$.

Lemma 17. *Let $c > 0$ be fixed and let G be a subgraph of Q_d with $n \le cd$ vertices. Then $\lambda_1(G) \le \sqrt{d} + O\left(d^{1/4}(\log d)^{1/2}\right)$.*

Our proof strategy is as follows. Using our results about compressions, we may assume that $V(G)$ is compressed. This enables us to partition $V(G)$ into stars, in such a way that the edges not covered by the stars have a small contribution to the eigenvalue, thus enabling us to obtain the required estimate for $\lambda_1(G)$.

Proof. By Lemmas 6 and 7 we can assume that $V(G)$ is compressed. Namely, $V(G)$ is down-compressed (i.e. $C_{U,\emptyset}(V(G)) = V(G)$ for every $U \subset [d]$) and left-compressed (i.e. $C_{i,j}(V(G)) = V(G)$ for every $1 \le j < i \le d$).

We aim to partition $V(G)$ in such a way that each part induces a star and the graph spanned by the edges not contained in any of these parts has small maximum degree. This would imply that $\lambda_1(G)$ is at most the eigenvalue of the star with $d+1$ vertices plus an error term which can be controlled by the maximum degree of the 'leftover' edges.

Let $\varepsilon = \varepsilon(d) = \sqrt{2c/d}$. Let $\mathcal{A}$ be the set of vertices of degree at least εd in G. We call these vertices 'heavy'. To minimise the maximum degree of the leftover graph, we wish to have each heavy vertex as a centre of one of the stars in the partition. However, it may happen, e.g., that $\{1\}, \{2\}$ are heavy and $\{1, 2\}$ is not, in which case $\{1, 2\}$ will have to appear in two stars of the partition. To avoid this from happening, we add vertices to the set of heavy vertices as follows.

Let $\mathcal{B} = \{t \in [d] : \{t\} \in \mathcal{A}\}$. Note that since $V(G)$ is down-compressed, $d(S) \ge d(T)$ for $S, T \in V(G)$ that satisfy $S \subseteq T$; hence, $\mathcal{A}$ is down-compressed. Similarly, $\mathcal{A}$ is left-compressed. It follows that $\mathcal{B}$ is an interval and $\max \mathcal{B} = |\mathcal{B}|$; denote $m = \max \mathcal{B}$. Finally define $\mathcal{D} = \mathcal{P}([m]) \cap V(G)$. Since $\mathcal{A}$ is down-compressed, $\mathcal{A} \subseteq \mathcal{D}$. We show that the maximum degree of $G[\mathcal{A}]$ is at most εd. Indeed, suppose that $v \in \mathcal{A}$ has at least εd neighbours in $\mathcal{A}$. Denote the set of these neighbours by N. Then every vertex in N has at least εd neighbours in $V(G)$. By the structure of Q_d, no vertex is a neighbour of more than two vertices of N. It follows that $|V(G)| > \frac{|N|\varepsilon d}{2} \ge \frac{(\varepsilon d)^2}{2} \ge n$, a contradiction.

For $S \in \mathcal{D}$ define $N^*(S) = \{S\} \cup \left(N(S) \setminus \mathcal{D}\right)$, where $N(S)$ denotes the neighbourhood of S in G. We claim that $N^*(S)_{S\in\mathcal{D}}$ is a collection of disjoint sets. Indeed, by the choice of $\mathcal{D}$, it follows that $\mathcal{D} \subseteq \mathcal{P}([m])$ and any vertex in the neighbourhood of S, where $S \in \mathcal{D}$, which is not in $\mathcal{D}$ must be of the form $S \cup \{s\}$ where $s \notin [m]$ and $S \in \mathcal{D}$. Furthermore, clearly, each of the sets $N^*(S)$ induces a star.

Let $v = (v_S)_{S\in V(G)}$ be an eigenvector of $A(G)$ with eigenvalue $\lambda_1(G)$, whose norm is 1 and whose entries are positive. Note that the edges of G are covered by the edges of the graphs $G[\mathcal{D}]$, $G \setminus \mathcal{D}$ and $\{N^*(S)\}_{S\in\mathcal{D}}$. We thus obtain the following upper bound on $\lambda_1(G)$.

$$\begin{aligned}\lambda_1(G) &= \langle A(G)v, v\rangle \\ &\le \sum_{S\in\mathcal{D}} \langle A(G[N^*(S)])v, v\rangle + \langle A(G[\mathcal{D}])v, v\rangle + \langle A(G\setminus\mathcal{D})v, v\rangle \\ &\le \sum_{S\in\mathcal{D}} \lambda_1(G[N^*(S)]) \sum_{T\in N^*(S)} v_T^2 + \lambda_1(G[\mathcal{D}]) \sum_{S\in\mathcal{D}} v_S^2 + \lambda_1(G\setminus\mathcal{D}) \sum_{S\notin\mathcal{D}} v_S^2.\end{aligned}$$

It remains to obtain upper bounds on the largest eigenvalue of the graphs $G[\mathcal{D}]$, $G \setminus \mathcal{D}$ and $\{N^*(S)\}_{S\in\mathcal{D}}$. By Claim 14, given a subgraph H of Q_d, we have $\lambda_1(H) \le 2\sqrt{\Delta(H)l}$, where $\Delta(H)$ is the maximum degree of H and l is the size of the largest set in $V(H)$. Since $\mathcal{D} \subseteq \mathcal{P}([m])$, the maximum degree of $G[\mathcal{D}]$ is bounded by εd. Also, by definition of $\mathcal{A}$, the maximum degree of $G \setminus \mathcal{D}$ is at most εd. Since $V(G)$ is compressed, the largest set in $V(G)$ has size at most $\log n$. It follows that

$$\lambda_1(G[\mathcal{D}]),\ \lambda_1(G \setminus \mathcal{D}) \le 2\sqrt{\varepsilon d \log n}.$$

Furthermore, $\lambda_1(N^*(S)) \le \sqrt{d}$ since each set $N^*(S)$ is a star on at most $d+1$ vertices. Thus, by the above inequality and using the disjointness of the sets $N^*(S)$, we obtain

$$\lambda_1(G) \le \sqrt{d} + O\left(\sqrt{\varepsilon d \log n}\right) = \sqrt{d} + O\left(d^{1/4}(\log d)^{1/2}\right),$$

thus completing the proof of Lemma 17. □

5.2. Proof of Theorem 4

We now prove Theorem 4 in general.

Theorem 4. *Let $i = i(d) = o(d)$ and let G be a subgraph of Q_d with $n = O\left(\left|H_d^i\right|\right)$ vertices. Then $\lambda_1(G) \le (1+o(1))\,\lambda_1(H_d^i)$.*

Proof. By Lemmas 6 and 7 we can assume that G is compressed. Similarly to the proof for $i = 1$, we partition the vertices into sets that induce subsets of a Hamming ball of radius approximately i. We choose the partition in such a way that the edges not covered by one of these subsets span a graph with small maximum degree. In this way we can bound the eigenvalue of the both subgraphs of G to obtain the required bound. In order to define the partition we need some notation.

Denote $n = |G|$ and let $\frac{\log n}{d} < \varepsilon = \varepsilon(d) < 1/2$ and define the following sets recursively.

$$\mathcal{A}_0 = V(G),$$
$$\mathcal{A}_k = \{S \in \mathcal{A}_{k-1} : S \text{ has at least } \epsilon d \text{ neighbours in } \mathcal{A}_{k-1}\}.$$

Let $M = \max\{k : \mathcal{A}_k \neq \emptyset\}$. We remark that M is well-defined, i.e. $\mathcal{A}_k = \emptyset$ for some k. Indeed, otherwise, G contains a subgraph of minimum degree at least εd; let U be the vertex set of such a subgraph. Then, on the one hand, $e(G[U]) \ge \frac{\varepsilon d|U|}{2}$ and, on the other hand, by Lemma 10 (with $d = 1$) we have

$$e(G[U]) \le \frac{|U|}{2}\log|U| \le \frac{|U|}{2}\log n.$$

Putting the two inequalities together, we find that $\varepsilon \le \frac{\log n}{d}$, a contradiction.

Note that since G is compressed, the sets $(\mathcal{A}_k)_{0\le k\le M}$ are compressed. Indeed, we have that $\mathcal{A}_0 = V(G)$ is down-compressed; by induction, if $\mathcal{A}_k$ is down-compressed then $d_{G[\mathcal{A}_k]}(S) \ge d_{G[\mathcal{A}_k]}(T)$, for $S, T \in \mathcal{A}_k$ satisfying $S \subseteq T$, which implies that $\mathcal{A}_{k+1}$ is down-compressed. A similar reasoning shows that $\mathcal{A}_k$ is left-compressed.

Intuitively, the sets $\mathcal{A}_k$ measure how 'heavy' a vertex is: for a vertex $v \in V(G)$, the larger $\max\{k : v \in \mathcal{A}_k\}$ is, the heavier v is. As in the proof of the special case of $i = 1$, we want to take the heaviest vertices to be the centres of the Hamming balls defining the partition. Since we now have many levels, we first take Hamming balls centred at the heaviest vertices; then we take as centres the heaviest vertices among those that were not covered in the first round; and so on. This process is complicated by the fact that we want each vertex to appear in at most one such Hamming ball. To ensure this, we add some lighter vertices to sets of heavy vertices using the following definitions.

We define sets $\mathcal{B}_k, \mathcal{C}_k, \mathcal{D}_k, \mathcal{E}_k$ and numbers m_k for $0 \le k \le M$ as follows. For $k = 0$,

$$\mathcal{B}_0 = \{t \in [d] : \{t\} \in \mathcal{A}_M\} \cup \{1\},$$
$$m_0 = \max \mathcal{B}_0,$$
$$\mathcal{C}_0 = \emptyset,$$
$$\mathcal{E}_0 = \mathcal{D}_0 = \mathcal{P}([m_0]) \cap V(G).$$

For $0 < k \le M$ define recursively

$$\begin{aligned}
\mathcal{B}_k &= \{t > m_{k-1}+1 : \{m_0+1, \dots, m_{k-1}+1, t\} \in \mathcal{A}_{M-k}\} \cup \{m_{k-1}+1\},\\
m_k &= \max \mathcal{B}_k,\\
\mathcal{C}_k &= \{S \cup \{t\} : S \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}, t > m_{k-1}\} \cap V(G),\\
\mathcal{D}_k &= (\mathcal{P}([m_k]) \cap V(G)) \setminus (\mathcal{E}_{k-1} \cup \mathcal{C}_k),\\
\mathcal{E}_k &= \mathcal{C}_0 \cup \dots \cup \mathcal{C}_k \cup \mathcal{D}_0 \cup \dots \cup \mathcal{D}_k.
\end{aligned}$$

Before we proceed with the proof, we try to convey the ideas behind the above definitions. The sets $\mathcal{D}_k$ defined above will be the centres of the Hamming balls and the $\mathcal{C}_k$'s will consist of the other vertices covered by these balls. In each stage we define $\mathcal{C}_k$ to be the set of neighbours of vertices which appeared previously. We define $\mathcal{D}_k$ to be the up-closure (relatively to $V(G) \cap \mathcal{P}([m_k])$) of the vertices in $\mathcal{A}_{M-k}$ which were not covered previously. To this end, in each stage B_k and m_k are defined so that every $t \in S \in \mathcal{A}_{M-k} \setminus \left(\mathcal{E}_{k-1} \cup \mathcal{C}_k\right)$ satisfies $t \le m_k$. Thus $\mathcal{D}_k$ contains $\mathcal{A}_{M-k} \setminus \left(\mathcal{E}_{k-1} \cup \mathcal{C}_k\right)$ and is up-closed in $V(G) \cap \mathcal{P}([m_k])$.

We now define the partition of $V(G)$ into sets inducing subgraphs of Hamming balls with centres in $\bigcup_{0 \le k < M} \mathcal{D}_k$. For a vertex $S \in V(G)$ and $t \ge 1$, let $N_t(S)$ denote the set of vertices of $V(G)$ in distance t from S. For every $0 \le k \le M-1$ and every $S \in \mathcal{D}_k$, let

$$N_S^{(k)} = \{S\} \cup \bigcup_{1 \le j \le M-k} \left(N_j(S) \cap \mathcal{C}_{k+j}\right).$$

In order to show that the sets $N_S^{(k)}$ satisfy our requirement we use the following proposition. Its proof is delayed to the end of this section.

Proposition 18. *The following assertions hold.*

1. *the sets $N_S^{(k)}$, where $0 \le k \le M-1$ and $S \in \mathcal{D}_k$, are pairwise disjoint;*
2. *the sets $\mathcal{C}_k \cup \mathcal{D}_k$, where $0 \le k \le M$, form a partition of $V(G)$;*
3. *$E(G) = \left(\bigcup_{0 \le k \le M} E(G[\mathcal{C}_k \cup \mathcal{D}_k])\right) \cup \left(\bigcup_{0 \le k \le M-1,\ S \in \mathcal{D}_k} E(G[N_S^{(k)}])\right)$;*
4. *the maximum degree of $G[\mathcal{C}_k \cup \mathcal{D}_k]$, where $0 \le k \le M$, is at most εd.*

Let $v = (v_S)_{S \in V(G)}$ be an eigenvector of $A(G)$ with eigenvalue $\lambda_1(G)$, whose entries are positive and whose norm is 1. Define

$$\begin{aligned}
\alpha_k^2 &= \sum_{S \in \mathcal{C}_k \cup D_k} v_S^2 \quad \text{for } 0 \le k \le M,\\
(\beta_{k,S})^2 &= \sum_{T \in N_S^{(k)}} v_T^2 \quad \text{for } 0 \le k < M \text{ and } S \in \mathcal{D}_k.
\end{aligned}$$

By Parts 1 and 2 above, $\sum_{0 \le k < M} \sum_{S \in \mathcal{D}_k} (\beta_{k,S})^2 \le 1$ and $\sum_{k=0}^{M} \alpha_k^2 = 1$. Thus, by Part 3,

$$\begin{aligned}
\lambda_1(G) &= \langle A(G)v, v\rangle\\
&\le \sum_{k=0}^{M} \Big\langle A(G[\mathcal{C}_k \cup \mathcal{D}_k])v,\ v\Big\rangle + \sum_{k=0}^{M-1} \sum_{S \in \mathcal{D}_k} \Big\langle A\left(G\big[N_S^{(k)}\big]\right) v, v\Big\rangle\\
&\le \sum_k \alpha_k^2 \cdot \lambda_1(G[\mathcal{C}_k \cup \mathcal{D}_k]) + \sum_{k,S} (\beta_{k,S})^2 \cdot \lambda_1\left(G\big[N_S^{(k)}\big]\right)\\
&\le \max_k \{\lambda_1(G[\mathcal{C}_k \cup \mathcal{D}_k])\} + \max_{k,S} \left\{\lambda_1(G[N_S^{(k)}])\right\}.
\end{aligned} \tag{4}$$

By Part 4 of Proposition 18, the maximum degree of $G[\mathcal{C}_k \cup \mathcal{D}_k]$ is at most εd. Since $V(G)$ is compressed, the largest set in $V(G)$ has size at most $\log n$. Recall that $n = \Theta\left(\binom{d}{i}\right)$, thus $\log n =$

$(1+o(1))i\log(d/i)$. Claim 14 implies the following upper bound.

$$\lambda_1(G[\mathcal{C}_k \cup \mathcal{D}_k]) \leq 2\sqrt{\varepsilon d \log n} = 2(1+o(1))\sqrt{\varepsilon d i \log(d/i)}. \tag{5}$$

Let us treat first the case where $i \to \infty$. By Claim 14, using the monotonicity of the largest eigenvalue of a graph,

$$\lambda_1\left(G\left[N_S^{(k)}\right]\right) \leq \lambda_1\left(H_d^{M-k}\right) \leq \lambda_1\left(H_d^{M}\right) \leq 2\sqrt{Md}. \tag{6}$$

Substituting (5) and (6) into (4), it follows that

$$\lambda_1(G) \leq 2(1+o(1))\left(\sqrt{\varepsilon d i \log(d/i)} + \sqrt{Md}\right). \tag{7}$$

The following claim will imply that we can choose ε so as to make the above upper bound arbitrarily close to $\lambda_1(H_d^i)$.

Claim 19. *Let $0 < \alpha < 1$ be fixed and set $\varepsilon = \frac{\alpha}{\log(d/i)}$. Then $M \leq (1+o(1))i$.*

We note that for $\varepsilon = \frac{\alpha}{\log(d/i)}$, as is Claim 19, we have $\frac{\log n}{d} < \varepsilon < 1/2$ for large enough d, as required before the definition of the sets $\mathcal{A}_k$. Indeed, the upper bound follows as $i = o(d)$; the lower bound holds since $\frac{\log n}{d} \leq (1+o(1))\frac{\log(d/i)}{d/i} = o\left(\frac{1}{\log(d/i)}\right)$.

Proof. For arbitrary $\beta > 0$ we show that $M \leq (1+\beta)i$ for large enough d. Let $N = (1+\beta)i$ and $D = \varepsilon d$. We need to show that $\mathcal{A}_N = \emptyset$. Assuming the contrary, we may pick $S \in \mathcal{A}_N$. We show that for $0 \leq l \leq N$.

$$|N_l(S) \cap \mathcal{A}_{N-l}| \geq \binom{D}{l}. \tag{8}$$

Indeed, (8) holds trivially for $l = 0$. For $0 \leq l < N$, every vertex in $N_l(S) \cap \mathcal{A}_{N-l}$ has at least D neighbours in $\mathcal{A}_{N-l-1}$, at most l of which are in $N_{l-1}(S)$ and the remaining neighbours are in $N_{l+1}(S)$. Furthermore, every vertex in $N_{l+1}(S) \cap \mathcal{A}_{N-l-1}$ is a neighbour of at most $l+1$ vertices in $N_l(S)$. We conclude that $|N_{l+1}(S) \cap \mathcal{A}_{N-l-1}| \geq |N_l(S) \cap \mathcal{A}_{N-l}| \cdot \frac{D-l}{l+1}$. By induction on l, (8) follows.

It follows from (8) that $n = |V(G)| \geq \binom{D}{N}$. Recall that $i = o(d)$ and note that $\frac{N}{D} = \frac{1+\beta}{\alpha} \cdot \frac{\log(d/i)}{d/i} \leq 1/2$, for sufficiently large d. Thus,

$$\begin{aligned} n \geq \binom{D}{N} &= \frac{D(D-1)\cdot \ldots \cdot (D-N+1)}{N!} \\ &\geq \frac{(D-N)^N}{e\sqrt{N}\left(\frac{N}{e}\right)^N} \\ &\geq \frac{1}{e\sqrt{N}}\left(\frac{eD}{2N}\right)^N. \end{aligned}$$

For the second inequality, we used the inequality $m! \leq e\sqrt{m}\left(\frac{m}{e}\right)^m$, that holds for all m; the third inequality follows since $N/D \leq 1/2$, as explained above. On the other hand,

$$n \leq c\left|[d]^{(\leq i)}\right| = c\left(\binom{d}{0} + \cdots + \binom{d}{i}\right) \leq c\left(2^{-i} + \cdots + 2^{-1} + 1\right)\binom{d}{i} \leq \frac{2c}{\sqrt{2\pi i}}\left(\frac{ed}{i}\right)^i.$$

The first inequality holds since $\binom{d}{x-1} = \binom{d}{x}\frac{x}{d-x+1} \leq \frac{1}{2}\binom{d}{x}$ for $x \leq (d+1)/3$; the second inequality holds since $m! \geq \sqrt{2\pi m}(m/e)^m$ for every m. Combining the two inequalities, we obtain the following inequality.

$$\frac{2c}{\sqrt{2\pi i}}\left(\frac{ed}{i}\right)^i \geq \frac{1}{e\sqrt{N}}\left(\frac{eD}{2N}\right)^N = \frac{1}{e\sqrt{(1+\beta)i}}\left(\frac{e\alpha}{2(1+\beta)} \cdot \frac{d/i}{\log(d/i)}\right)^{(1+\beta)i}.$$

Hence, the following holds, where c_1, c_2 are constants depending on α, β, c.

$$c_2 \geq \left(c_1 \frac{(d/i)^{\frac{\beta}{1+\beta}}}{\log(d/i)} \right)^{(1+\beta)i}.$$

Since $i = o(d)$, we have $\log(d/i) = o\left((d/i)^\gamma\right)$ for every fixed $\gamma > 0$, so we have reached a contradiction. This implies that $M \leq (1+\beta)i$ for large d. $\square$

Assuming still that $i \to \infty$, by (7) with $\varepsilon = \frac{\alpha}{\log(d/i)}$ and Claim 19, we have

$$\lambda_1(G) \;\leq\; 2\,(1+o(1))\left(1+\sqrt{\alpha}\,\right)\sqrt{id}.$$

Since α can be taken arbitrarily close to 0, $i = o(d)$, and $i \to \infty$, it follows from Theorem 3 that

$$\lambda_1(G) \leq 2(1+o(1))\sqrt{i(d+1-i)} = (1+o(1))\lambda_1(H_d^i).$$

This completes the proof of Theorem 4 for $i \to \infty$.

Now suppose that $i \leq \frac{\log d}{4 \log\log d}$. Take $\varepsilon = 2id^{-1/(i+1)}$. It is easy to check that $\frac{\log n}{d} < \varepsilon < 1/2$, satisfying our assumption on ε. Furthermore, one can check that $\binom{\varepsilon d}{i+1} > n$, implying that $M \leq i$, by (8) (which holds for every i and $l \leq N$, assuming that $S \in \mathcal{A}_N$; hence, if $S \in \mathcal{A}_{i+1}$, then $|G| \geq |\mathcal{A}_0| \geq \binom{\varepsilon d}{i+1}$, a contradiction). The following upper bound on $\lambda_1(G)$ follows from (4), (5) and Claim 13.

$$\lambda_1(G) \;\leq\; O\left(\sqrt{i^2 d^{1-\frac{1}{i+1}} \log d}\,\right) + \lambda_1\left(H_d^i\right) \;=\; o\left(\sqrt{d}\right) + \lambda_1\left(H_d^i\right) = (1+o(1))\lambda_1\left(H_d^i\right).$$

Here we used the inequality $i^2 d^{-\frac{1}{i+1}} \log d = o(1)$, which holds for $i \leq \frac{\log d}{4\log\log d}$, and the lower bound $\lambda_1(H_d^i) \geq \sqrt{d}$. This completes the proof of Theorem 4, as we have $\lambda_1(G) \leq (1+o(1))\lambda_1(H_d^i)$ for both $i \leq \frac{\log d}{4\log\log d}$ and for $i \geq \frac{\log d}{4\log\log d}$ (because in the latter case, in particular, $i \to \infty$). $\square$

5.3. *Proof of Proposition 18*

In order to complete the proof of Theorem 4, it remains to prove Proposition 18.

Proposition 18. *The following assertions hold.*

1. *the sets $N_S^{(k)}$, where $0 \leq k \leq M-1$ and $S \in \mathcal{D}_k$, are pairwise disjoint;*
2. *the sets $\mathcal{C}_k \cup \mathcal{D}_k$, where $0 \leq k \leq M$, form a partition of $V(G)$;*
3. $E(G) = \left(\bigcup_{0\leq k\leq M} E(G[\mathcal{C}_k \cup \mathcal{D}_k])\right) \cup \left(\bigcup_{0\leq k\leq M-1,\ S\in\mathcal{D}_k} E(G[N_S^{(k)}])\right)$;
4. *the maximum degree of $G[\mathcal{C}_k \cup \mathcal{D}_k]$, where $0 \leq k \leq M$, is at most εd.*

Proof. We prove the following seven assertions.

1. for every $0 \leq k \leq M$ and $S \in \mathcal{C}_k \cup \mathcal{D}_k$, there are unique $j \leq k$ and $T \in \mathcal{D}_j$, for which there exist distinct $t_{j+1}, \dots, t_k$ satisfying $t_l > m_{l-1}$ (for $j+1 \leq l \leq k$) and $S = T \cup \{t_{j+1}, \dots, t_k\}$;
2. $\mathcal{E}_k$ is compressed for every $0 \leq k \leq M$;
3. $(\mathcal{C}_k \cup \mathcal{D}_k) \cap \mathcal{E}_{k-1} = \emptyset$ for every $1 \leq k \leq M$;
4. there are no edges of G between $\mathcal{E}_k$ and $\mathcal{D}_{k+1} \cup \mathcal{C}_{k+2} \cup \mathcal{D}_{k+2}$ for every $0 \leq k \leq M-2$;
5. the maximum degree of $G[\mathcal{C}_k \cup \mathcal{D}_k]$ is at most m_k, and $m_k \leq \varepsilon d$ for every $0 \leq k \leq M$;
6. $\mathcal{A}_{M-k} \subseteq \mathcal{E}_k$ for every $0 \leq k \leq M$. In particular, $\mathcal{E}_M = V(G)$;
7. the sets $N_S^{(k)}$, where $0 \leq k \leq M-1$ and $S \in \mathcal{D}_k$, are pairwise disjoint.

Note that Proposition 18 follows from these assertions. Indeed, Parts 1 and 4 follow directly from Assertions 7 and 5. Part 2 follows easily from Assertions 3 and 6. To prove Part 3, let ST be an edge of G, where $T = S \cup \{t\}$. Let k be smallest such that $S \in \mathcal{E}_k$ (such k exists because $\mathcal{E}_M = V(G)$). We show that $T \in \mathcal{E}_{k+1}$. Recall that $S \cup \{t'\} \in \mathcal{C}_{k+1}$, for any $t' \notin S$ satisfying $t' > m_k$. We note that there exists such t'

that satisfies $t' \geq t$, because $|S| = o(d)$ (recall that G is compressed, so $|G| \geq 2^{|S|}$ and $|G| = 2^{o(d)}$) and $m_k \leq \varepsilon d < d/2$ (see Assertion 5; recall that $\varepsilon < 1/2$). Since $\mathcal{C}_{k+1} \subseteq \mathcal{E}_{k+1}$, it follows that $S \cup \{t'\} \in \mathcal{E}_{k+1}$, and because $\mathcal{E}_{k+1}$ is compressed (see Assertion 2), we have $T = S \cup \{t\} \in \mathcal{E}_{k+1}$. Also, $T \notin \mathcal{E}_{k-1}$ (since, otherwise, $S \in \mathcal{E}_{k-1}$ because $\mathcal{E}_{k-1}$ is compressed, contrary to the choice of k). Furthermore, $T \notin \mathcal{D}_{k+1}$, by Assertion 4. So, T is either in $\mathcal{C}_k \cup \mathcal{D}_k$, in which case the edge ST is in $G[\mathcal{C}_k \cup \mathcal{D}_k]$; or $T \in \mathcal{C}_{k+1}$. By Assertion 1, $S \in N_{S'}^{(k')}$ for some S' and k'. It is easy to see that, in the latter case, also $T \in N_{S'}^{(k')}$, so $ST \in E(N_{S'}^{(k')})$.

Proof of Assertion 1. We prove Assertion 1 by induction on k. It is trivial for $k = 0$, so we assume $k > 0$. Let $S \in \mathcal{C}_k \cup \mathcal{D}_k$. By the definition of $\mathcal{C}_l$ and by induction, $S = T \cup \{t_{j+1}, \ldots, t_k\}$ for some j, $T \in \mathcal{D}_j$ and $t_u > m_{u-1}$ for all $j + 1 \leq u \leq k$. Suppose that we may also write $S = R \cup \{r_{l+1}, \ldots, r_k\}$, where $R \in \mathcal{D}_l$ and $r_u > m_{u-1}$ for $l + 1 \leq u \leq k$. We show that we must have $l = j$ and $R = T$.

Note that if $j = l = k$, there is nothing to prove. If $j < k$ it follows from the definitions that $S \in \mathcal{C}_k$, thus $S \notin \mathcal{D}_k$ and so $l < k$. By the definitions, there is $s \in S$ with $s > m_{k-1}$ such that $S \setminus \{s\} \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}$. Since $T \subseteq [m_j]$ and $R \subseteq [m_l]$ it follows that $s \in \{t_{j+1}, \ldots, t_k\} \cap \{r_{l+1}, \ldots, r_k\}$. Without loss of generality, $s = t_k = r_k$ (if, say, $s = t_{j'}$, swap $t_{j'}$ with t_k; the property $t_u > m_{u-1}$ for $j + 1 \leq u \leq k$ is maintained). It follows that $T \cup \{t_{j+1}, \ldots, t_{k-1}\} = R \cup \{r_{l+1}, \ldots, r_{k-1}\} \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}$. By induction, $j = l$ and $R = T$, as required.

Proof of Assertion 2. Again we prove the assertion by induction on k. For $k = 0$, we have $\mathcal{E}_0 = \mathcal{P}([m_0]) \cap V(G)$, hence, since G is compressed, $\mathcal{E}_0$ is also compressed. Let $k > 0$, $S \in \mathcal{C}_k \cup \mathcal{D}_k$ and choose $a \in S$, $b < a$ such that $b \notin S$ (if such b exists). Let $T = S \setminus \{a\}$ and $R = S \triangle \{a, b\}$. To prove the assertion we show that $R, T \in \mathcal{E}_k$.

If $S \in \mathcal{D}_k$, the claim follows directly from the definition of $\mathcal{D}_k$ and the fact that G is compressed. Thus we assume $S \in \mathcal{C}_k$, so we can write $S = S_1 \cup \{s\}$ where $s > m_{k-1}$ and $S_1 \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}$. If $a \neq s$, by induction we have $R \setminus \{s\}, T \setminus \{s\} \in \mathcal{E}_{k-1}$, thus $R, T \in \mathcal{E}_k$ (e.g. if $R \setminus \{s\} \in \mathcal{C}_l \cup \mathcal{D}_l$ for some $l \leq k - 1$, then $R \in \mathcal{C}_{l+1}$ by definition of $\mathcal{C}_{l+1}$). We may now assume that $a = s$. Then clearly $T = S_1 \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1} \subseteq \mathcal{E}_k$. It remains to show that $R \in \mathcal{E}_k$.

Let $S = S_2 \cup \{s_{j+1}, \ldots, s_k\}$, where $S_2 \in \mathcal{D}_j$ for some $j \leq k$ and $s_l > m_{l-1}$ and $j + 1 \leq l \leq k$ (by Assertion 1 such a representation exists). Note that we may assume that $s_k = a$ (indeed, $S_2 \subseteq [m_j]$, by definition of $\mathcal{D}_j$, so $a = s_l$ for some $j+1 \leq l \leq k$, but then, since $a = s > m_{k-1}$, we may swap s_l and s_k).

If $b \leq m_j$, it follows that $S_2 \cup \{b\} \in \mathcal{E}_j$ (by definition of $\mathcal{D}_j$). Hence, in this case, $(S_2 \cup \{b\}) \cup \{s_{j+1}, \ldots, s_i\} \in \mathcal{C}_{i-1}$, for every $j + 1 \leq i \leq k$ (by induction and the definition of $\mathcal{C}_l$). In particular, $R = S_2 \cup \{b, s_{j+1}, \ldots, s_{k-1}\} \in \mathcal{C}_{k-1} \subseteq \mathcal{E}_{k-1}$, as required.

It remains to consider the case $b > m_j$. Let $s'_{j+1} < \cdots < s'_k$ be such that $\{s'_{j+1}, \ldots, s'_k\} = \{s_{j+1}, \ldots, s_{k-1}, b\}$. If $s'_u > m_{u-1}$ for every $j + 1 \leq u \leq k$ then $R \in \mathcal{C}_k$. Otherwise let $l = \max\{u : s'_u \leq m_{u-1}\}$ and $S_3 = S_2 \cup \{s'_{j+1}, \ldots, s'_l\}$. Since $S_3 \subseteq [m_{l-1}]$ it follows that $S_3 \in \mathcal{E}_{l-1}$ and $R = S_3 \cup \{s_{l+1}, \ldots, s_k\} \in \mathcal{E}_{k-1}$.

Proof of Assertion 3. From the definitions it follows that $\mathcal{E}_{k-1} \cap \mathcal{D}_k = \emptyset$. Since $\mathcal{D}_0 \cup \cdots \cup \mathcal{D}_{k-1} \subseteq \mathcal{P}([m_{k-1}])$, it follows that $\mathcal{C}_k \cap (\mathcal{D}_0 \cup \cdots \cup \mathcal{D}_{k-1}) = \emptyset$. Thus it remains to show that $\mathcal{C}_j \cap \mathcal{C}_k = \emptyset$ for $0 \leq j < k$. We prove this by induction on k. For $k = 0$ there is nothing to prove. Assume $0 \leq j < k$ and $S \in \mathcal{C}_j \cap \mathcal{C}_k$. Write $s = \max S$ and $S = S_1 \cup \{t_{j+1}, \ldots, t_k\}$, where $S_1 \in \mathcal{D}_j$ and $t_l > m_{l-1}$ for some j and for $j + 1 \leq l \leq k$ (this is possible by Assertion 1). As in the proof of Assertion 2, we may assume that $t_k = s$. It follows from the definition of $\mathcal{C}_l$ that $S \setminus \{s\} \in \mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}$. Similarly, we can show that $S \in \mathcal{C}_{j-1} \cup \mathcal{D}_{j-1}$, so $S \setminus \{s\} \in (\mathcal{C}_{k-1} \cup \mathcal{D}_{k-1}) \cap (\mathcal{C}_{j-1} \cup \mathcal{D}_{j-1})$. As explained above this implies that $S \setminus \{s\} \in \mathcal{C}_{j-1} \cap \mathcal{C}_{k-1}$, contradicting the induction hypothesis.

Proof of Assertion 4. Let $S \in \mathcal{E}_k$ and T be a neighbour of S in G. We show that $T \in \mathcal{E}_k \cup \mathcal{C}_{k+1}$, implying that there are no edges of G between $\mathcal{E}_k$ and $\mathcal{D}_{k+1} \cup \mathcal{C}_{k+2} \cup \mathcal{D}_{k+2}$. If $T \subseteq S$, it follows from Assertion 2 that $T \in \mathcal{E}_k$. So we assume $T = S \cup \{t\}$ and set $s = \max S$. If $t > m_k$, then $T \in \mathcal{C}_{l+1} \subseteq \mathcal{E}_k \cup \mathcal{C}_{k+1}$, where $l \leq k$ is such that $S \in \mathcal{C}_l \cup \mathcal{D}_l$. If $s, t \leq m_k$, then $T \subseteq [m_k]$, so $T \in \mathcal{E}_k$. Finally, we consider the case $t \leq m_k < s$. Since $\mathcal{E}_k$ is compressed, it follows that $T \setminus \{s\} = S \triangle \{s, t\} \in \mathcal{E}_k$. Let $l \leq k$ be such that $T \setminus \{s\} \in \mathcal{C}_l \cup \mathcal{D}_l$. Then, by the definition of $\mathcal{C}_{l+1}$, we have $T \in \mathcal{C}_{l+1} \subseteq \mathcal{E}_k \cup \mathcal{C}_{k+1}$, as required.

Proof of Assertion 5. Let $S, T \in \mathcal{C}_k \cup \mathcal{D}_k$ and $t \in [d]$ be such that $T = S \cup \{t\}$. We note that $t \leq m_k$, because otherwise $T \in \mathcal{C}_{k+1} \cap (\mathcal{C}_k \cup \mathcal{D}_k) = \emptyset$. It follows that the maximum degree of $G[\mathcal{C}_k \cup \mathcal{D}_k]$ is at most m_k.

We now prove by induction on k that $m_k \leq \varepsilon d$. Recall that by the definition of M, the maximum degree of $G[\mathcal{A}_M]$ is at most εd. Thus for $k = 0$ we have $m_0 = \max\{1, d_{G[\mathcal{A}_M]}(\emptyset)\} \leq \varepsilon d$. Now let $k > 0$ and $S = \{m_0 + 1, \dots, m_{k-1} + 1\}$. It follows from the definition of $\mathcal{B}_{k-1}$ that $S \notin \mathcal{A}_{M-(k-1)}$, so $d(S, \mathcal{A}_{M-k}) \leq \varepsilon d$ (we define $d(S, \mathcal{A}_{M-k})$ to be the number of neighbours of S in $\mathcal{A}_{M-k}$). Hence $m_k \leq \max\{t : S \cup \{t\} \in \mathcal{A}_{M-k}\} \leq d(S, \mathcal{A}_{M-k}) \leq \varepsilon d$, and the assertion follows.

Proof of Assertion 6. Let $S \in \mathcal{A}_{M-k}$. Note that if $|S| \leq k$ it can be easily shown by induction that $S \in \mathcal{E}_k$. Thus we assume $|S| \geq k + 1$. Define $t_k = \max S$ and for $0 \leq j < k$, denote $t_j = \max(S \setminus \{t_{j+1}, \dots, t_k\})$. Assume first that $m_j < t_j$ for every $0 \leq j < k$. Since $\mathcal{A}_{M-k}$ is compressed, it follows that $\{m_0 + 1, \dots, m_{k-1} + 1, t_k\} \in \mathcal{A}_{M-k}$. Thus $t_k \leq m_k$, $S \subseteq [m_k]$ and $S \in \mathcal{E}_k$. Otherwise, let $l \geq 0$ be maximal such that $t_l \leq m_l$. It follows from the definitions that $S \cap [m_l] \in \mathcal{E}_l$ and $S \in \mathcal{E}_k$.

Proof of Assertion 7. We show that for every $0 \leq j < k \leq M - 1$ if $S \in \mathcal{C}_k$, $T \in \mathcal{D}_j$ are such that $S \in N_T^{(k-j)}$ then there exist $t_{j+1}, \dots, t_k$ such that $S = T \cup \{t_{j+1}, \dots, t_k\}$ and $t_l > m_{l-1}$ for every $j < l \leq k$. By uniqueness of such a representation (see Assertion 1), it follows that j and T are unique, i.e., if $S \in N_{T'}^{(k-j')}$ for some $1 \leq j' \leq k$ and $T' \in \mathcal{C}_{j'}$ then $j' = j$ and $T' = T$, as required.

By Assertions 2 and 4 the sets $\mathcal{E}_l$ are down-compressed and there are no edges between $\mathcal{E}_l$ and $\mathcal{C}_{l+2} \cup \mathcal{D}_{l+2}$, for every $0 \leq l \leq M - 2$. Thus, since $S \in N_T^{(k-j)}$, S is obtained by adding $k - j$ elements to T, and we can write $S = T \cup \{t_{j+1}, \dots, t_k\}$. Without loss of generality, $t_{j+1} < \cdots < t_k$. We show that $t_l > m_{l-1}$ for $j + 1 \leq l \leq k$. Suppose to the contrary that there is l for which $t_l \leq m_{l-1}$. It follows that $T \cup \{t_{j+1}, \dots, t_l\} \in \mathcal{E}_{l-1}$ and thus $S \in \mathcal{E}_{k-1}$, contradicting our assumptions that $S \in \mathcal{C}_k$. This proves that the required representation exists, thus proving the assertion. $\square$

The proof of Proposition 18 completes the proof of our first main result, Theorem 4.

6. Hamming ball is best for fixed *i*

In this section we prove Theorem 5.

Theorem 5. *For every i there is $d_0 = d_0(i)$ such that for $d \geq d_0$ the Hamming ball H_d^i maximises the largest eigenvalue among subgraphs of Q_d of the same order.*

Let us start with an outline of the proof. We are given a graph G that maximises the largest eigenvalue among subgraphs of Q_d with $|H_d^i|$ vertices. As usual, we assume that G and its eigenvector v with eigenvalue $\lambda_1(G)$ are compressed. Using the proof of Theorem 4, we conclude that by removing the vertices of size at least $i + 1$, the largest eigenvalue does not decrease by much. We infer that G contains almost all vertices of size at most i. By the assumption that G maximises λ_1, and given an eigenvector v, we know that by replacing (in both G and v) any vertex of size at least $i + 1$ with a vertex of size i that is not already in G, the inner product $\langle A(G)v, v\rangle$ does not decrease. This enables us to obtain a lower bound on the coefficient v_S for S in G whose size is largest among vertices in G. Finally, using the relations between the coefficients in v of vertices and their neighbourhoods, and the fact that there are few vertices of size at least $i + 1$, we reach a contradiction to the assumption that v is compressed, by concluding that there is a vertex whose coefficient in v is larger than the coefficient of the empty set.

We now proceed to the proof of the theorem.

Proof of Theorem 5. Let G be a subgraph of Q_d with $|H_d^i|$ vertices and assume $\lambda \triangleq \lambda_1(G)$ is largest among subgraphs of Q_d with the same number of vertices. In light of Claim 13,

$$\lambda = \Omega\left(\sqrt{d}\right). \tag{9}$$

Let $v = (v_S)_{S\in V(G)}$ be a positive vector of norm 1 satisfying $\lambda = \langle A(G)v, v\rangle$. By Lemmas 6 and 7, we can assume that $V(G)$ and v are compressed.

We first show that the graph obtained from G by removing vertices of size at least $i+1$ still has a large maximum eigenvalue.

Claim 20. *Let $U = V(G) \cap [d]^{(\le i)}$. There exists $\eta = \eta(i) > 0$ such that $\lambda_1(Q_d[U]) \ge \lambda_1(H_d^i) - O\big(d^{1/2-\eta}\big)$.*

Proof. We use the proof of Theorem 4. Consider (4) which states the following (we use the definitions of $\mathcal{C}_k$, $\mathcal{D}_k$ and $N_S^{(k)}$ from Section 5).

$$\lambda = \lambda_1(G) \le \max_k \{\lambda_1 (G[\mathcal{C}_k \cup \mathcal{D}_k])\} + \max_{k,S} \left\{\lambda_1\left(G\big[N_S^{(k)}\big]\right)\right\}.$$

As explained after the proof of Claim 19, if $\varepsilon = 2id^{-1/(i+1)}$ then $M \le i$, implying that the sets $N_S^{(k)}$ are subsets of Hamming balls of radius at most i. Recall that each set $N_S^{(k)}$ (where $k \le M-1$ and $S \in \mathcal{D}_k$) is a subset of the set of vertices T in G that contain S and satisfy $|T \setminus S| \le i$. Since G is compressed, it follows that $G[N_S^{(k)}]$ is isomorphic to a subgraph of $Q_d[U]$, hence $\lambda_1(N_S^{(k)}) \le \lambda_1(Q_d[U])$ for every $k \le M-1$ and $S \in \mathcal{D}_k$. Furthermore, for our choice of ε, the following holds (see (5)).

$$\lambda_1(G[\mathcal{C}_k \cup \mathcal{D}_k]) = O\left(\sqrt{d^{1-\frac{1}{i+1}}\log d}\right).$$

Thus, for any $\eta < 1/2(i+1)$, we have

$$\lambda \le O(d^{1/2-\eta}) + \lambda_1(Q_d[U]).$$

Claim 20 follows from the assumption that $\lambda \ge \lambda_1(H_d^i)$. □

We conclude that $\left|V(G) \setminus [d]^{(\le i)}\right|$ is small.

Claim 21. *There exists $\theta = \theta(i) > 0$ such that $\left|V(G) \setminus [d]^{(\le i)}\right| = O\big(d^{i-\theta}\big)$.*

Proof. Define

$$U = \left\{s \in [d] \ : \text{there exists } S \in V(G) \cap [d]^{(i)} \text{ such that } s = \min S\right\}$$
$$\mathcal{U} = \left\{S \in [d]^{(i)} \ : S \cap U \ne \emptyset\right\}.$$

Since G is compressed, it follows that $U^{(i)} \subseteq V(G) \cap [d]^{(i)} \subseteq \mathcal{U}$. Write $|U| = (1-\beta)d$ and let H be the subgraph of Q_d induced by $[d]^{(<i)} \cup \mathcal{U}$. Note that $V(G) \cap [d]^{(\le i)} \subseteq V(H)$. It follows from Claim 20 that for some constant $\eta = \eta(i) > 0$, the following holds.

$$\lambda_1(H) \ge \lambda_1(H_d^i) - O(d^{1/2-\eta}). \tag{10}$$

We shall conclude that $\beta = O(d^{-\theta})$ for some $\theta = \theta(i) > 0$. This would imply that $\left|V(G) \cap [d]^{(i)}\right| \ge \binom{(1-\beta)d}{i} = \binom{d}{i} - O(d^{i-\theta})$, as required.

Note that, by symmetry, the eigenvector u of H with eigenvalue $\lambda_1(H)$ is uniform on vertices of the same size and with the same number of elements in $[(1-\beta)d]$. Let $u_{j,k}$ be the coordinate in u of a vertex from $[d]^{(j)}$ with k elements in $[(1-\beta)d]$, where $(j,k) \in I = \{(j,k) : 0 \le k \le j \le i\} \setminus \{(i,0)\}$ and define $u_{j,k} = 0$ for $(j,k) \notin I$. The following system of equations holds.

$$\begin{aligned}\lambda_1(H)\, u_{j,k} = &(j-k)\, u_{j-1,k} + k\, u_{j-1,k-1} + \\ &((1-\beta)d - k)\, u_{j+1,k+1} + (\beta d - (j-k))\, u_{j+1,k}.\end{aligned}$$

Let A be the matrix whose rows and columns are indexed by I that satisfies the following for $x = (x_{j,k})_{(j,k)\in I}$ (we define $x_{j,k} = 0$ for $(j,k) \notin I$).

$$\begin{aligned}(Ax)_{j,k} = &(j-k)\, x_{j-1,k} + k\, x_{j-1,k-1} + \\ &((1-\beta) - k/d)\, x_{j+1,k+1} + (\beta - (j-k)/d)\, x_{j+1,k}.\end{aligned}$$

We note that the vector w, defined by $w_{j,k} = u_{j,k}d^{j/2}$ for $(j,k) \in I$, is an eigenvector of A with eigenvalue $\lambda(H)/\sqrt{d}$. As all the coordinates in w are positive, it follows that $\lambda_1(A) = \lambda_1(H)/\sqrt{d}$. Denote $\mu = \lambda_1(A)$.

Let B be the matrix whose rows and columns are indexed by $I_+ = I \cup \{(i, 0)\}$, and is defined by the same system of equations as A, but for $(x_{j,k})_{(j,k)\in I_+}$ (where $x_{j,k} = 0$ for $(j, k) \notin I_+$). As before, $\lambda_1(B)\sqrt{d} = \lambda_1(H_d^i)$. So, by Claim 20, we have

$$\lambda_1(B) - \lambda_1(A) = O(d^{-\eta}). \tag{11}$$

We shall show that if $\beta \leq 1/2$, then

$$\lambda_1(B) - \lambda_1(A) = \Omega\left(\beta^{4i}\right). \tag{12}$$

Before proving (12), we show how to complete the proof of Claim 21 under the assumption that (12) holds for $\beta \leq 1/2$. First, suppose that $\beta \leq 1/2$. Then, by (11) and (12), we have $\beta = O(d^{-\eta/4i})$, as required. Now, suppose that $\beta > 1/2$. Let A' be defined as A but with $\beta' = 1/2$ in place of β (to be precise, we need $(1 - \beta')d$ to be integer, which is the case if $\beta' = 1/2$ and d is even; if d is odd we take $\beta' = 1/2 - 1/2d$). Note that $\lambda_1(A) \leq \lambda_1(A')$ (as the graph corresponding to A is a subgraph of the graph corresponding to A'). Now, by (12), applied to A', we have $\lambda_1(B) - \lambda_1(A) \geq \lambda_1(B) - \lambda_1(A') = \Omega((1/2)^{4i}) = \Omega(1)$, a contradiction to (11).

In order to prove (12) for $\beta \leq 1/2$, we use Claim 22 . Consider the graph F on vertex set I, where the neighbourhood of $(j, k) \in I$ is $\{(j + 1, k + 1), (j + 1, k), (j - 1, k), (j - 1, k - 1)\} \cap I$. Every vertex in F is within distance at most i from $(0, 0)$, thus the diameter of F is at most $2i$. The entries in A corresponding to these edges are at least $\beta + O(1/d)$ (as $\beta \leq 1/2$). The following inequality follows from Claim 22 which is proved below (where $\mu = \lambda_1(A)$; using the fact that $\mu = O(1)$ which follows from Lemma 15).

$$w_{j,k} \geq \left(\frac{\beta + O(1/d)}{\mu}\right)^{2i} = \Omega(\beta^{2i}).$$

Let $w_\varepsilon \in \mathbb{R}^{I_+}$ be defined as follows.

$$(w_\varepsilon)_{j,k} = \begin{cases} \sqrt{1-\varepsilon^2}\, w_{j,k} & (j,k) \in I \\ \varepsilon & (j,k) = (i,0). \end{cases}$$

We note that, since w has norm 1, w_ε also has norm 1. Furthermore,

$$\begin{aligned} \lambda_1(B) \geq \langle B w_\varepsilon, w_\varepsilon\rangle &= \left(1 - \varepsilon^2\right)\mu + i\varepsilon\sqrt{1-\varepsilon^2}\, w_{i-1,0} \\ &= \left(1 - \varepsilon^2\right)\mu + \Omega\left(\beta^{2i}\varepsilon\sqrt{1-\varepsilon^2}\right). \end{aligned}$$

By picking $\varepsilon = c\beta^{2i}$ for sufficiently small c, we have $\lambda_1(B) \geq \mu + c^2\beta^{4i}/2$, proving (12). This completes our proof of Claim 21. $\square$

We now state and prove Claim 22, which was used in the proof of Claim 21.

Claim 22. *Let A be an $n \times n$ matrix with non-negative entries, and let $\alpha > 0$. Let H be a graph with vertex set $[n]$ for which if $jk \in E(H)$ then $A_{j,k} \geq \alpha$ and $A_{k,j} \geq \alpha$. Suppose, additionally, that H is connected and has diameter r.*

Let $u = (u_j)_{j\in[n]}$ be an eigenvector of A with eigenvalue $\lambda = \lambda_1(A)$, whose norm is 1 and whose entries are non-negative. The $u_j \geq \left(\frac{\alpha}{\lambda}\right)^r \frac{1}{\sqrt{n}}$ for all $j \in [n]$.

Proof. Denote by j_0 an index j that maximises u_j. Then, in particular, $u_{j_0} \geq 1/\sqrt{n}$. Let N_t be the set of vertices in H whose distance from j_0 is t. We shall show that for every $j \in N_t$, we have $u_j \geq \left(\frac{\alpha}{\lambda}\right)^t u_{j_0}$. This statement holds trivially for $t = 0$. Now suppose that it holds for t. Let $j \in N_{t+1}$ and let $k \in N_t$ be a neighbour of j. Then $\lambda u_j = \sum_l A_{j,l}u_l \geq A_{j,k}u_k \geq \alpha\left(\frac{\alpha}{\lambda}\right)^t u_{j_0}$. The statement easily follows, completing the proof of Claim 22. (Note that $\alpha \leq \lambda$, as, otherwise, we reach a contradiction to the maximality of u_{j_0}.) $\square$

Let $l = \max\{j : V(G) \cap [d]^{(j)} \neq \emptyset\}$. Assuming that $V(G) \neq [d]^{(\leq i)}$, we have $l > i$. Note that since G is left-compressed, $[l] \in V(G)$; also, since G is down-compressed, we have

$$l = O(\log d). \tag{13}$$

Claim 23. *If $l > i$ then $v_{[l]} \geq v_{\emptyset}\lambda^{-i}$.*

Proof. We first show that $v_S \geq v_{\emptyset}\lambda^{-|S|}$ for every $S \in V(G)$, by induction on $|S|$. It is trivially true for $S = \emptyset$. Now let $S \neq \emptyset$ and let $a \in S$, $T = S \setminus \{a\}$. Then λv_S is the sum of weights of the neighbours of S, and in particular $\lambda v_S \geq v_T \geq v_{\emptyset}\lambda^{-|T|} = v_{\emptyset}\lambda^{-|S|+1}$, as required.

Since we assume $l > i$, the set $[d]^{(\leq i)} \setminus V(G)$ is non-empty. Pick a minimal element S in it. Consider the graph G' which is induced by $(V(G) \setminus \{[l]\}) \cup \{S\}$. Let v' be the vector in $\mathbb{R}^{V(G')}$ that agrees with v on every coordinate in $V(G) \cap V(G')$, and $v'_S = v_{[l]}$. Note that $|G'| = |G|$, so, by our assumption on G, $\lambda_1(G) \geq \lambda_1(G')$. It follows that $\langle A(G)v, v\rangle = \lambda_1(G) \geq \lambda_1(G') \geq \langle A(G')v', v'\rangle$. Hence,

$$0 \leq \langle A(G)v, v\rangle - \langle A(G')v', v'\rangle = v_{[l]}\left(2\sum_{j\in[l]} v_{[l]\setminus\{j\}} - 2\sum_{j\in S} v_{S\setminus\{j\}}\right).$$

The following inequality follows.

$$\lambda v_{[l]} = \sum_{j\in[l]} v_{[l]\setminus\{j\}} \geq \sum_{j\in S} v_{S\setminus\{j\}} \geq v_{\emptyset}\lambda^{-(|S|-1)} \geq v_{\emptyset}\lambda^{-(i-1)}.$$

This completes the proof of Claim 23. □

We now make a few definitions. Let $\varepsilon = \varepsilon(i)$ be a sufficiently small constant that depends only on i (the constraint determining how small ε should be can be found at the end of the proof of Claim 24). Let

$$t = \min\left\{j : v_{[l-j-1]} \leq \frac{\varepsilon\lambda}{l} \cdot v_{[l-j]}\right\}.$$

In particular, for every $j \leq t$, the following holds.

$$v_{[l-j]} \geq \left(\frac{\varepsilon\lambda}{l}\right)^j v_{[l]}. \tag{14}$$

Define, for $j \geq 0$,

$$\mathcal{A}_j = \left\{S \in V(G) \cap [d]^{(l-t+j)} : [l-t] \subseteq S\right\},$$
$$W_j = \sum_{S\in\mathcal{A}_j} v_S.$$

In the next claim, we prove that $t = i$ and give a lower bound on W_i.

Claim 24. *$t = i$ and $W_i \geq \lambda^i W_0$.*

Before proving Claim 24, we show how it can be used to complete the proof of Theorem 5. By Claim 24, the definition of W_0 and (14), we obtain the following inequality.

$$W_i \geq \lambda^i W_0 = \lambda^i v_{[l-i]} \geq \left(\frac{\varepsilon\lambda^2}{l}\right)^i v_{[l]}. \tag{15}$$

Since G and v are compressed, $v_S \leq v_{[l]}$ for every $S \in \mathcal{A}_i$, and so $W_i \leq |\mathcal{A}_i| v_{[l]}$. It follows that $|\mathcal{A}_i| \geq \left(\frac{\varepsilon\lambda^2}{l}\right)^i$. Since $l = O(\log d)$ and $\lambda = \Omega(\sqrt{d})$ (see (13) and (9)), it follows that $|V(G) \cap [d]^{(l)}| \geq |\mathcal{A}_i| = \Omega\left(\frac{d^i}{(\log d)^i}\right)$. This is a contradiction to Claim 21 (recall that $l > i$, otherwise we are done), thus completing the proof of Theorem 5. □

We now prove Claim 24, which was used in the proof of Theorem 5.

Proof of Claim 24. We first note that $t \leq i$. Indeed, by (14), if $t \geq i+1$, then $v_{[l-i-1]} \geq \left(\frac{\varepsilon\lambda}{l}\right)^{i+1} v_{[l]}$. Recall that, since G and v are compressed, $v_{[l-i-1]} \leq v_{\emptyset}$. Also, by Claim 23, $v_{[l]} \geq v_{\emptyset}\lambda^{-i}$. Putting these three inequalities together, we deduce that

$$v_{\emptyset} \geq v_{[l-i-1]} \geq \left(\frac{\varepsilon\lambda}{l}\right)^{i+1} v_{[l]} \geq \left(\frac{\varepsilon\lambda}{l}\right)^{i+1} v_{\emptyset}\lambda^{-i} \geq \left(\frac{\varepsilon}{l}\right)^{i+1} \lambda v_{\emptyset}.$$

This is a contradiction, as the right-hand side is at least $\Omega\left(\left(\frac{\sqrt{d}}{(\log d)^{i+1}}\right) v_{\emptyset}\right) = \omega(v_{\emptyset})$ (as $\lambda = \Omega(\sqrt{d})$ and $l = O(\log d)$).

Define, for $j \geq 0$ (also, define $\mathcal{A}_{-1} = \emptyset$),

$$\mathcal{B}_j = \left\{T \in \left(V(G) \cap [d]^{(l-t+j-1)}\right) \setminus \mathcal{A}_{j-1} : \text{there exists } S \in \mathcal{A}_j \text{ s.t. } T \subseteq S\right\}$$
$$U_j = \sum_{S \in \mathcal{B}_j} v_S.$$

We obtain the following inequalities, using the fact that every vertex in $\mathcal{A}_j$ has at most $d-j$ neighbours in $\mathcal{A}_{j+1}$.

$$\lambda W_j \leq \begin{cases} W_1 + U_0 & j = 0 \\ (d-j+1)W_{j-1} + (j+1)W_{j+1} + U_j & 0 < j < t \\ (d-t+1)W_{t-1} + U_t & j = t. \end{cases}$$

Define $k = \min\{j : W_{j+1} \leq \lambda W_j\}$. Clearly $k \leq t$ since $W_{t+1} = 0$ (by definition of l). Thus $W_j \geq \lambda^j W_0$ for $0 \leq j \leq k$. We will show that $k = t = i$, thus completing the proof of Claim 24.

Note that $U_0 \leq (l-t)v_{[l-t-1]} \leq l v_{[l-t-1]} \leq \varepsilon\lambda v_{[l-t]} = \varepsilon\lambda W_0$, by the assumption that v is compressed and the definition of t. Also, $\lambda U_j \geq (j+1)U_{j+1} \geq U_{j+1}$ for $0 \leq j \leq t$, thus $U_j \leq \lambda^j U_0 \leq \varepsilon\lambda^{j+1} W_0 \leq \varepsilon\lambda W_j$ for $0 \leq j \leq k$. Hence, the above inequalities can be rewritten as follows.

$$\lambda W_j \leq \begin{cases} W_1 + \varepsilon\lambda W_0 & j = 0 \\ (d-j+1)W_{j-1} + (j+1)W_{j+1} + \varepsilon\lambda W_j & 0 < j < k \\ (d-k+1)W_{k-1} + \varepsilon\lambda W_k & j = k. \end{cases}$$

Denote $W = (W_0, \dots, W_k)^T$, and let A be the matrix with the above coefficients, but with the terms preceded by ε dropped. Note that $\lambda_1(A) = \lambda_1(H_d^k)$ (this follows from the fact that, by symmetry, an eigenvector of H_d^k with eigenvalue $\lambda_1(H_d^k)$ is uniform over all vertices in $[d]^{(j)}$ for every $0 \leq j \leq k$; note that A is the transpose of the matrix $A_{d,i}$ which is described implicitly in Lemma 15). The above inequalities translate to $\lambda W_j \leq (AW)_j + \varepsilon\lambda W_j$, or, equivalently, $(AW)_j \geq (1-\varepsilon)\lambda W_j$. We obtain the following chain of inequalities.

$$\lambda_1\left(H_d^k\right) = \lambda_1(A) \geq \frac{\langle AW, W\rangle}{\langle W, W\rangle} \geq (1-\varepsilon)\lambda \geq (1-\varepsilon)\lambda_1\left(H_d^i\right).$$

The last inequality follows from the assumption that $\lambda = \lambda_1(G)$ is maximal among all subgraphs of Q_d with the same order, so, in particular, $\lambda \geq \lambda_1\left(H_d^i\right)$.

Recall that by Claim 13, $\lambda_1\left(H_d^j\right) = \mu_j\sqrt{d}(1 + O(1/d))$, where $\mu_j < \mu_{j+1}$ for every j. Hence, if ε is chosen to be sufficiently small, then $k \geq i$. In fact, since $k \leq t \leq i$, we conclude that $k = t = i$, as required. □

7. Conclusion

The question of characterising the subgraphs of the cube that maximise λ_1 is far from being completely answered. We have shown that for fixed i and large d, H_d^i maximises λ_1 among subgraphs of Q_d of the same order. It would be interesting to determine if a similar statement holds for a wider range of radii.

Question 25. *For which i does H_d^i maximise λ_1 among all subgraphs of Q_d of the same order?*

For radii tending to infinity with the dimension of the cube, our results as well as Samorodnitsky's results [28] only show that the Hamming balls have largest eigenvalues which are asymptotically largest among subgraphs of the same order. We believe that, similarly to Theorem 2, the Hamming balls maximise the maximum eigenvalues exactly rather than just asymptotically, for large d and a large range of radii.

We point out that for radii that are very close to $d/2$ the Hamming ball does not achieve the largest maximum eigenvalue, as can be seen by the following example.

Example 26. Assume that d is even and consider the Hamming ball of radius $d/2-1$, $H = H_d^{d/2-1}$. We show that $\lambda_1(H) = d-2$. Put $\lambda = d-2$ and let x be the vector with coefficient $x_i = 1 - 2i/d$ on the vertices of size i. The following can be easily verified.

$$\lambda x_i = \begin{cases} dx_1 & i = 0 \\ ix_{i-1} + (d-i)x_{i+1} & 0 < i < d/2 - 1 \\ ix_{i-1} & i = d/2 - 1. \end{cases}$$

Thus we have $A(H)x = (d-2)x$. Since all the coefficients x_i are positive, this implies that $\lambda_1(H) = d-2$. Note that $|H| = 2^{d-1}\left(1 - \Theta\left(1/\sqrt{d}\right)\right) > 2^{d-2}$. Thus, since the largest eigenvalue of the subcube of dimension $d-2$ is $d-2$, we can achieve a larger maximum eigenvalue with a (connected) subgraph on $|H|$ vertices that contains the subcube of dimension $d-2$.

As seen by this example, it may be interesting to consider subgraphs whose largest eigenvalue is very close to d. For instance, determining the range of radii for which the Hamming balls maximise the largest eigenvalue, especially for large radii, seems like a challenging problem. The following weaker problem also seems hard.

Question 27. *Is it true that for every fixed $c > 0$, if a subgraph H of Q_d has $\lambda_1(H) \geq d - c$, then $|H| = \Omega(2^d)$?*

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