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Cheeger-type inequalities for the second largest spectral gap from 1 of the normalized Laplacian

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Abstract

We study the second largest spectral gap from 1 of the normalized Laplacian of a graph, a quantity that appears in the literature in connection with random walks, expander graphs, and Ramanujan graphs. We relate it to the classical Cheeger and dual Cheeger constants, and we introduce a new Cheeger-type constant admitting a probabilistic interpretation in terms of two-step random walks. For this constant, we establish sharp inequalities analogous to the classical Cheeger inequalities.

Note added in v2. A referee pointed out that the bounds in Corollary 5.5 and Theorem 6.1 follow from the Cheeger inequalities for weighted graphs [2]. Indeed, the matrix M from (3) is the transition matrix of the random walk on the weighted graph with adjacency matrix $DM = AD^{-1}A$, whose Cheeger constant is $1 - \tilde{h}$, while the second largest eigenvalue of M is τ^2. We are grateful to the referee for this observation, which unfortunately means that these inequalities (as well as most results from Section 4) are not new. Nevertheless, our direct and self-contained proof of Theorem 6.1 yields a characterization of its equality case which, to the best of our knowledge, is new. We also believe that the probabilistic interpretation of $\tilde{h}$ and the formulation of the inequalities in terms of τ may still be of interest. In light of this, we decided to keep the paper on arXiv, but not to submit it to a journal.

1 Introduction

Let G be a simple graph on n nodes with no isolated vertices, and let

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \leq 2$$

denote the eigenvalues of its normalized Laplacian. Since the foundational work of Fan Chung [5], these eigenvalues have been extensively studied and are known to encode important geometric and combinatorial properties of graphs. In particular, the classical Cheeger inequalities relate the eigenvalue λ_2 to the Cheeger constant h [5], while the largest eigenvalue λ_n is linked to the dual Cheeger constant $\overline{h}$ through the dual Cheeger inequalities [1, 2, 4].

In [10], the smallest spectral distance from 1,

$$\varepsilon := \min_{i \neq 1} |1 - \lambda_i|$$

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was investigated, and the sharp bound $\varepsilon \leq 1/2$ was established for connected graphs on $n \geq 3$ vertices. Here, we study instead the second largest spectral distance from 1,

$$\tau := \max_{i \neq 1} |1 - \lambda_i|,$$

which controls the rate of convergence of a random walk on G to its stationary distribution, as explained in Remark 2.2. This quantity also appears in Fan Chung's book [5, Chapters 1.5, 5, and 6], in relation to random walks and expander graphs.

Among other results, in Proposition 3.1 we show that

$$\tau = \max\{1 - \lambda_2, \lambda_n - 1\},$$

and as a consequence we relate τ to the classical Cheeger and dual Cheeger constants in Proposition 3.2. We further introduce a new Cheeger-type constant $\tilde{h}$ which admits an interpretation in terms of the probability of returning to a set of vertices after two steps (Definition 3.5 and Remark 3.6) for which we establish the following sharp inequalities (Corollary 5.5 and Theorem 6.1):

$$2\tilde{h} - 1 \leq \tau^2 \leq \sqrt{1 - (1 - \tilde{h})^2}.$$

Our work is also related to Ramanujan graphs [13, 15]. In fact, if G is d-regular, then the normalized Laplacian eigenvalues satisfy $\lambda_i = 1 - \mu_i/d$, where μ_i are the eigenvalues of the adjacency matrix. Since, by definition, a Ramanujan graph is a d-regular graph satisfying

$$\max_{i \,:\, \mu_i \neq \pm d} |\mu_i| \leq 2\sqrt{d-1},$$

Ramanujan graphs can equivalently be characterized as d-regular graphs such that

$$\max_{i \,:\, \lambda_i \neq 0,2} |1 - \lambda_i| \leq \frac{2\sqrt{d-1}}{d}.$$

For non-bipartite connected graphs, this is equivalent to

$$\tau \leq \frac{2\sqrt{d-1}}{d}. \tag{1}$$

Structure of the paper

The paper is organized as follows. In Section 2, we recall the necessary background on the normalized Laplacian and the relevant eigenvalue inequalities. In Section 3, we introduce τ and $\tilde{h}$, and we relate τ to the classical Cheeger and dual Cheeger constants. In Section 4 we study basic properties of $\tilde{h}$ and pose two questions for future research. We then derive lower bounds for τ^2 in Section 5, and upper bounds in Section 6. Since the proof of the main upper bound is rather long, we dedicate Section 7 entirely to it.

2 Background

Fix a simple graph $G = (V, E)$ on n nodes and m edges, with no isolated vertices, and let $v_1, \ldots, v_n$ denote the vertices of G. The *adjacency matrix* of G is the $n \times n$ matrix $A := A(G)$ with entries

$$A_{ij} := \begin{cases} 1 & \text{if } v_i \sim v_j \\ 0 & \text{otherwise.} \end{cases}$$

The *normalized Laplacian* of G is the matrix

$$L := L(G) := \mathrm{Id} - D^{-1}A,$$

where Id denotes the $n \times n$ identity matrix, and $D := D(G) := \mathrm{diag}(\deg v_1, \ldots, \deg v_n)$ is the *degree matrix* of G. We denote the eigenvalues of L by

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \leq 2.$$

Now, let $C(V)$ denote the vector space of functions $f : V \to \mathbb{R}$, and, given $f, g \in C(V)$, let

$$\langle f, g \rangle := \sum_{v \in V} \deg v \cdot f(v) \cdot g(v). \tag{2}$$

We can see then see the normalized Laplacian L as an operator $C(V) \to C(V)$ such that

$$Lf(v) = f(v) - \frac{1}{\deg v} \sum_{w \sim v} f(w).$$

Moreover, L is self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle$, i.e.,

$$\langle Lf, g \rangle = \langle f, Lg \rangle \quad \forall f, g \in C(V).$$

In analogy with [10] (proof of Lemma 3), we note that the values $(1-\lambda_1)^2, \ldots, (1-\lambda_n)^2$ are precisely the eigenvalues of the matrix

$$M := (\mathrm{Id} - L)^2 = (D^{-1}A)^2, \tag{3}$$

whose entries are

$$M_{vu} = \sum_{w \in V} (D^{-1}A)_{vw}(D^{-1}A)_{wu} = \sum_{w \in \mathcal{N}(v) \cap \mathcal{N}(u)} \frac{1}{\deg v \, \deg w}, \quad \text{for } v, u \in V. \tag{4}$$

In particular, ε^2 is the smallest eigenvalue of M, while τ^2 is the second largest. Moreover, similarly to L, M is also self-adjoint with respect to the weighted inner product in (2), implying that its eigenvalues can be characterized using the Courant–Fischer–Weyl min-max Principle via the Rayleigh Quotients

$$\mathrm{RQ}(f) := \frac{\langle Mf, f \rangle}{\langle f, f \rangle} = \frac{\sum_{w \in V} \frac{1}{\deg w} \left(\sum_{v \in \mathcal{N}(w)} f(v) \right)^2}{\sum_{w \in V} \deg w \cdot f(w)^2},$$

for functions $f \in C(V) \setminus \{\mathbf{0}\}$. In particular,

$$\varepsilon^2 = \min_{f \in C(V) \setminus \{\mathbf{0}\}} \mathrm{RQ}(f),$$

while

$$\tau^2 = \max_{\substack{f \in C(V) \setminus \{\mathbf{0}\}: \\ \sum_{w \in V} \deg w \cdot f(w) = 0}} \mathrm{RQ}(f). \tag{5}$$

Remark 2.1. The approach adopted here differs slightly from that in [10]. In particular, instead of working with the matrix $(D^{-1/2}AD^{-1/2})^2$, here we consider $M = (D^{-1}A)^2$, together with the weighted inner product in (2). This allows us to work within the same framework as L, as they are self-adjoint with respect to the same inner product. Nevertheless, the characterization obtained above for ε^2 is equivalent to that of Lemma 3 in [10]. The characterization of τ^2 can be derived analogously by observing that τ^2 is the second largest eigenvalue of M, while the eigenfunctions corresponding to the largest eigenvalue of M (which is $(1-\lambda_1)^2 = 1$) are precisely the constant functions. Hence, by the Courant–Fischer–Weyl min-max Principle, τ^2 is obtained by maximizing the Rayleigh Quotient over all functions that are orthogonal to the constant functions with respect to the inner product in (2), namely over all $f \in C(V)$ such that

$$\langle f, \mathbf{1} \rangle = \sum_{w \in V} \deg w \cdot f(w) = 0.$$

Remark 2.2. Let $T := D^{-1}A$. Then,

$$T_{vu} = \begin{cases} \frac{1}{\deg v} & \text{if } v \sim u \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, T is the transition probability matrix of a random walk on G, while $M = T^2$ is the two-step transition probability matrix of the random walk. In particular, M_{vu} in (4) is the probability that a random walk starting at v is at u after two steps. Moreover, since τ is the absolute value of the second largest eigenvalue of T, it controls the rate of convergence of a random walk on G to its stationary distribution (see for instance Section 2.2 in [9], Section 12.2 in [12], or Section 9 in [2]).

We now recall the classical geometric quantities associated with λ_2 and λ_n, namely the Cheeger and dual Cheeger constants, together with the corresponding inequalities relating them to λ_2 and λ_n. To this end, we first introduce some preliminary notation.

Definition 2.3. Let $U, S \subseteq V$. We denote by

$$E(U,S) := \Big\{ \{u,s\} \in E : u \in U,\ s \in S \Big\}$$

the set of edges between U and S, and we let

$$e(U,S) := |E(U,S)|.$$

Similarly, for $w \in V$, we define $E(w,S) := E(\{w\},S)$ and we let $e(w,S) := |E(w,S)|$ denote its cardinality. Moreover, we let $\bar{S} := V \setminus S$ denote the *complement* of S, and we let

$$\operatorname{vol} S := \sum_{v \in S} \deg v$$

be the *volume* of S. Finally, the *neighborhood* of S is defined as

$$\mathcal{N}(S) := \{w \in V : E(w,S) \neq \emptyset\}.$$

We can now define the Cheeger and dual Cheeger constants.

Definition 2.4. The *Cheeger constant* of G is

$$h := h(G) := \min_{\emptyset \neq S \subsetneq V} \frac{e(S,\overline{S})}{\min\{\operatorname{vol} S, \operatorname{vol} \overline{S}\}}.$$

The *dual Cheeger constant* of G is

$$\bar{h} := \bar{h}(G) := \max_{\substack{\text{partitions} \\ V = S_1 \sqcup S_2 \sqcup S_3 : \\ S_1, S_2 \neq \emptyset}} \frac{2 \cdot e(S_1, S_2)}{\operatorname{vol} S_1 + \operatorname{vol} S_2}.$$

Remark 2.5. A set S realizing the Cheeger constant corresponds to a sparse edge cut $E(S, \overline{S})$ which separates the graph into two parts of comparable volume. Thus, small values of h indicate that the graph is close to being disconnected. Moreover, we always have $0 \leq h \leq 1$, with $h = 0$ if and only if G is disconnected.

Similarly, a partition $V = S_1 \sqcup S_2 \sqcup S_3$ realizing the dual Cheeger constant corresponds to a large set of edges between S_1 and S_2, with relatively few edges inside S_1 and S_2. Thus, large values of $\bar{h}$ indicate that a large portion of the graph is close to bipartite. Moreover, by Theorem 3.1 in [2], since we are not admitting isolated vertices, we always have $0 < \bar{h} \leq 1$, and $\bar{h} = 1$ if and only if G is bipartite.

The Cheeger inequalities [5, 11] state that

$$1 - \sqrt{1 - h^2} \leq \lambda_2 \leq 2h, \tag{6}$$

while the dual Cheeger inequalities [1, 2, 4] state that

$$2\overline{h} \leq \lambda_n \leq 1 + \sqrt{1 - \left(1 - \overline{h}\right)^2}. \tag{7}$$

We conclude this section by introducing additional notation that will be used throughout the paper.

Definition 2.6. Let $U \subseteq V$. The *indicator function* $\mathbb{1}_U \colon V \to \mathbb{R}$ is defined as

$$\mathbb{1}_U(v) := \begin{cases} 1, & \text{if } v \in U, \\ 0, & \text{if } v \notin U. \end{cases}$$

3 The quantities τ and $\tilde{h}$

In this section, we study basic properties of τ and introduce the new Cheeger-type constant $\tilde{h}$. We again let $G = (V, E)$ be a simple graph on n nodes with no isolated vertices, and we let

$$0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \leq 2$$

denote the eigenvalues of its normalized Laplacian L. Recall that, in the Introduction, we defined

$$\tau := \max_{i \neq 1} |1 - \lambda_i|.$$

Moreover, in (5), we established the characterization

$$\tau^2 = \max_{\substack{f \in C(V): \\ \sum_{w \in V} \deg w \cdot f(w) = 0}} \operatorname{RQ}(f).$$

We also note that an estimate for τ was obtained in [10, Proposition 2], where it was shown that

$$\frac{1}{n-1} \leq \tau \leq 1.$$

We now characterize τ as follows.

Proposition 3.1. *For every graph G,*

$$\tau = \max\{1 - \lambda_2, \lambda_n - 1\}.$$

Proof. By definition of τ, and since $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \leq 2$, we have that

$$\tau = \max\left\{|1 - \lambda_2|, \ldots, |1 - \lambda_n|\right\} = \max\left\{|1 - \lambda_2|, |1 - \lambda_n|\right\}.$$

Moreover, since $\sum_{i=1}^{n} \lambda_i = n$ for all graphs, it follows that $\lambda_n > 1$. In fact, if $\lambda_n \leq 1$, then $\lambda_i \leq 1$ for all i, and therefore

$$\sum_{i=1}^{n} \lambda_i = \sum_{i=2}^{n} \lambda_i \leq n - 1 < n,$$

which is a contradiction. Hence,

$$\tau = \max\left\{|1 - \lambda_2|, \lambda_n - 1\right\}. \tag{8}$$

We now consider two cases.

- Case 1: $\lambda_2 \leq 1$. In this case, $|1 - \lambda_2| = 1 - \lambda_2$, and therefore, by (8),

  $$\tau = \max\{1 - \lambda_2, \lambda_n - 1\}.$$

- Case 2: $\lambda_2 > 1$. In this case, $|1 - \lambda_2| = \lambda_2 - 1 \leq \lambda_n - 1$. Therefore, by (8),

  $$\tau = \max\{|1 - \lambda_2|, \lambda_n - 1\} = \lambda_n - 1.$$

  Moreover, since $1 - \lambda_2 < 0$ in this case, it is also true that

  $$\tau = \lambda_n - 1 = \max\{1 - \lambda_2, \lambda_n - 1\}.$$

This proves the claim.

□

Now, let $\widehat{h} := \min\left\{h, 1 - \bar{h}\right\}$. Combining the Cheeger inequalities in (6) with the dual Cheeger inequalities in (7), we can infer the following.

Proposition 3.2. *For every graph,*

$$1 - \sqrt{1 - \widehat{h}^2} \leq 1 - \tau \leq 2\widehat{h},$$

or equivalently,

$$1 - 2\widehat{h} \leq \tau \leq \sqrt{1 - \widehat{h}^2}.$$

The proof of Proposition 3.2 uses the following observations.

Remark 3.3. If $a \leq A$ and $b \leq B$, then $\min\{a, b\} \leq a \leq A$ and $\min\{a, b\} \leq b \leq B$, therefore

$$\min\{a, b\} \leq \min\{A, B\}.$$

Remark 3.4. If a function f is increasing on an interval I, then for all $a, b \in I$,

$$\min\{f(a), f(b)\} = f(\min\{a, b\}).$$

Proof of Proposition 3.2. Since the two statements are clearly equivalent, it suffices to prove the first one. By Proposition 3.1, $\tau = \max\{1-\lambda_2, \lambda_n - 1\}$, implying that

$$1 - \tau = \min\{\lambda_2, 2 - \lambda_n\}.$$

Moreover, by (7), we have that

$$1 - \sqrt{1 - \left(1 - \overline{h}\right)^2} \leq 2 - \lambda_n \leq 2(1 - \overline{h}). \tag{9}$$

By (6) and (9), together with Remark 3.3, we infer that

$$1 - \tau = \min\{\lambda_2, 2 - \lambda_n\} \leq \min\{2h, 2(1 - \overline{h})\} = 2\widehat{h}$$

and

$$1 - \tau = \min\{\lambda_2, 2 - \lambda_n\} \geq \min\left\{1 - \sqrt{1 - h^2}, 1 - \sqrt{1 - \left(1 - \overline{h}\right)^2}\right\}.$$

Thus, it remains to show that

$$\min\left\{1 - \sqrt{1 - h^2}, 1 - \sqrt{1 - \left(1 - \overline{h}\right)^2}\right\} = 1 - \sqrt{1 - \widehat{h}^2},$$

This follows from Remark 3.4, together with the fact that the function

$$f(x) := 1 - \sqrt{1 - x^2}$$

is increasing on $[0, 1]$, which implies that

$$\min\{f(h), f(1 - \overline{h})\} = f(\min\{h, 1 - \overline{h}\}) = f(\widehat{h}).$$

□

Proposition 3.2 bounds τ in terms of $\widehat{h} := \min\left\{h, 1 - \overline{h}\right\}$, and therefore in terms of both h and $\overline{h}$. Our goal is instead to establish sharp inequalities for τ (or τ^2) involving a single geometric quantity. To this end, we introduce the following new Cheeger-type constant.

Definition 3.5. Given a nonempty set $S \subseteq V$, we let

$$\tilde{h}(S) := \frac{1}{\operatorname{vol} S} \cdot \sum_{w \in V} \frac{e(w, S)^2}{\deg w} = \frac{1}{\operatorname{vol} S} \cdot \sum_{w \in \mathcal{N}(S)} \frac{e(w, S)^2}{\deg w}.$$

Moreover, we let

$$\tilde{h} := \max_{\substack{\emptyset \neq S \subseteq V: \\ \operatorname{vol} S \leq \operatorname{vol} V/2}} \tilde{h}(S).$$

Remark 3.6. The quantity $\tilde{h}(S)$ becomes large when the vertices in $\mathcal{N}(S)$ devote a large proportion of their degrees to edges connecting to S. Moreover,

$$\tilde{h}(S) = \sum_{w \in V} \frac{e(w, S)}{\operatorname{vol} S} \cdot \frac{e(w, S)}{\deg w},$$

where $e(w, S)/\operatorname{vol} S$ is the probability that a one-step random walk starting from S reaches w, assuming that the starting vertex in S is selected with probability proportional to its degree,

while $e(w,S)/\deg w$ is the probability of returning from w to S in one step. Therefore, the quantity $\tilde{h}(S)$ can be interpreted as the probability that a random walk starting in S returns to S after two steps. This probabilistic interpretation suggests a deep connection between $\tilde{h}$ and τ^2 in view of Remark 2.2. Moreover, the Cheeger constant of G (Definition 2.4) can be written as

$$h = \min_{\substack{\emptyset \neq S \subseteq V: \\ \operatorname{vol} S \leq \operatorname{vol} V/2}} h(S),$$

where

$$h(S) := \frac{e(S,\overline{S})}{\operatorname{vol} S}$$

is the probability that a one-step random walk starting from S leaves S, and therefore $1-h(S)$ is the probability that a one-step random walk starting from S remains in S. Hence, $\tilde{h}$ may be seen as a two-step analogue of $1-h$.

In Section 4, we investigate several properties of $\tilde{h}$. Sections 5, 6 and 7 are devoted to proving the following sharp inequalities:

$$2\tilde{h} - 1 \leq \tau^2 \leq \sqrt{1-(1-\tilde{h})^2}.$$

4 Properties of $\tilde{h}$

This section is devoted to investigating properties of $\tilde{h}$. We begin by proving the sharp upper bound $\tilde{h} \leq 1$, before deriving several lower bounds, discussing a few examples and posing two open questions. Also in this section, all graphs are assumed to be simple and to have no isolated vertices.

Proposition 4.1. *For any graph,*

$$\tilde{h} \leq 1,$$

with equality if and only if G is bipartite or disconnected.

Proof. Let $S \subset V$ be a nonempty subset such that $\operatorname{vol} S \leq \operatorname{vol} V/2$. Then,

$$\begin{aligned}
\operatorname{RQ}(\mathbb{1}_S) &= \frac{\sum_{w\in V} \frac{1}{\deg w} \left(\sum_{v \in \mathcal{N}(w)} \mathbb{1}_S(v) \right)^2}{\sum_{w \in V} \deg w \cdot \mathbb{1}_S(w)^2} \\
&= \frac{\sum_{w\in V} \frac{1}{\deg w} \cdot e(w,S)^2}{\sum_{w\in S} \deg w} \\
&= \frac{1}{\operatorname{vol} S} \sum_{w \in V} \frac{e(w,S)^2}{\deg w} \\
&= \tilde{h}(S).
\end{aligned}$$

Since $0 \leq \operatorname{RQ}(f) \leq 1$ for all functions $f \in C(V) \setminus \{\mathbf{0}\}$, it follows immediately that $\tilde{h}(S) \leq 1$, and consequently, $\tilde{h} \leq 1$.

Moreover, $\tilde{h} = 1$ if and only if there exists a nonempty set of vertices S such that $\operatorname{vol} S \leq \operatorname{vol} V/2$ and $\operatorname{RQ}(\mathbb{1}_S) = 1$. As $\mathbb{1}_S \neq \mathbf{1}$, this can occur if and only if either the normalized

Laplacian admits 0 as an eigenvalue with multiplicity at least 2, in which case the graph G is disconnected, or the normalized Laplacian has eigenvalue 2, in which case a connected component of G is bipartite. In the case where the graph is connected, it must therefore be bipartite, and the statement follows. □

Remark 4.2. Proposition 4.1 is consistent with the probabilistic interpretation of $\tilde{h}$ discussed in Remark 3.6. In fact, since $\tilde{h}(S)$ is the probability that a random walk starting in S returns to S after two steps, it is clear that $\tilde{h}(S) \leq 1$. Moreover, equality can occur only when the random walk returns to S after two steps with probability 1, which corresponds precisely to disconnected or bipartite cases.

The main lower bound for $\tilde{h}$ in this section is the following.

Proposition 4.3. *For any graph,*

$$\tilde{h} \geq \max_{\substack{\emptyset \neq S \subseteq V: \\ \operatorname{vol} S \leq \operatorname{vol} V/2}} \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)}.$$

Remark 4.4. The quantity $\operatorname{vol} S / \operatorname{vol} \mathcal{N}(S)$ in Proposition 4.3 becomes larger when the vertices in $\mathcal{N}(S)$ devote a larger fraction of their degrees to edges connecting to S. This is in line with Remark 3.6, and helps us understand the geometric intuition behind $\tilde{h}$. This quantity also appears in Lemma 6.2 in [5], which shows that, if G is not a complete graph and $S \subseteq V$, then

$$\tau^2 + (1-\tau^2) \cdot \frac{\operatorname{vol} S}{\operatorname{vol} V} = 1 - (1-\tau^2) \cdot \frac{\operatorname{vol} \overline{S}}{\operatorname{vol} V} > \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)}.$$

In particular, if $\operatorname{vol} S \leq \operatorname{vol} V/2$, this implies that

$$\frac{\tau^2+1}{2} > \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)},$$

therefore

$$\frac{\tau^2+1}{2} > \max_{\substack{\emptyset \neq S \subseteq V: \\ \operatorname{vol} S \leq \operatorname{vol} V/2}} \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)}.$$

Interestingly, Corollary 5.5 below will show that $(\tau^2+1)/2 \geq \tilde{h}$.

Proof of Proposition 4.3. By Sedrakyan's inequality, given real numbers $u_1, \ldots, u_n$ and positive real numbers $v_1, \ldots, v_n$,

$$\sum_i \frac{u_i^2}{v_i} \geq \frac{\left(\sum_i u_i\right)^2}{\sum_i v_i}.$$

Therefore, given a nonempty set $S \subseteq V$,

$$\begin{aligned}
\tilde{h}(S) &= \frac{1}{\operatorname{vol} S} \cdot \sum_{w \in \mathcal{N}(S)} \frac{e(w,S)^2}{\deg w} \\
&\geq \frac{1}{\operatorname{vol} S} \cdot \frac{\left(\sum_{w \in \mathcal{N}(S)} e(w,S)\right)^2}{\sum_{w \in \mathcal{N}(S)} \deg w} \\
&= \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)},
\end{aligned}$$

implying that

$$\tilde{h} \geq \max_{\substack{\emptyset \neq S \subseteq V: \\ \operatorname{vol} S \leq \operatorname{vol} V/2}} \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)}.$$

□

Example 4.5. Consider a bipartite graph, and fix the sets S and $\overline{S}$ that give the bipartition. Then, $\overline{S} = \mathcal{N}(S)$, and $\operatorname{vol} S = \operatorname{vol} \mathcal{N}(S)$. Therefore, by Proposition 4.3, $\tilde{h} \geq 1$, while by Proposition 4.1 we have $\tilde{h} \leq 1$. This implies that $\tilde{h} = 1$, and both bounds are sharp in this case.

Remark 4.6. If G is bipartite, then $\lambda_2 \geq 2 - \lambda_n = 0$, implying that $1 - \tau = \min\{\lambda_2, 2 - \lambda_n\} = 0$, and therefore $\tau = 1$. By Example 4.5, this implies that $\tilde{h} = \tau = 1$ for bipartite graphs.

Proposition 4.3 has the following corollaries.

Corollary 4.7. *If there exists a set $S \subseteq V$ such that $\operatorname{vol} S = \operatorname{vol} V/2$, then*

$$\tilde{h} \geq \frac{1}{2}.$$

Proof. By Proposition 4.3, we have that

$$\begin{aligned} \tilde{h} &\geq \tilde{h}(S) \\ &\geq \frac{\operatorname{vol} S}{\operatorname{vol} \mathcal{N}(S)} \\ &\geq \frac{\operatorname{vol} S}{\operatorname{vol} V} \\ &= \frac{1}{2}. \end{aligned}$$

□

Corollary 4.8. *If G is k-regular and n is even, then*

$$\tilde{h} \geq \frac{1}{2}.$$

The next proposition gives a lower bound for $\tilde{h}$ whenever there exists a nonempty set $S \subseteq V$ such that $\operatorname{vol} S \leq \operatorname{vol} V/2$ and the vertices in $\mathcal{N}(S)$ devote the same proportion of their degrees to edges connecting to S.

Proposition 4.9. *Assume that there exist a nonempty set $S \subseteq V$ such that $\operatorname{vol} S \leq \operatorname{vol} V/2$ and a constant $\nu \in (0, 1]$ such that, for each $w \in \mathcal{N}(S)$, $\nu = e(w, S)/\deg w$. Then,*

$$\tilde{h} \geq \nu.$$

Proof. We have that

$$\tilde{h} \geq \tilde{h}(S) = \frac{1}{\operatorname{vol} S} \cdot \sum_{w \in \mathcal{N}(S)} \frac{e(w, S)^2}{\deg w} = \frac{1}{\operatorname{vol} S} \cdot \nu \cdot \left(\sum_{w \in \mathcal{N}(S)} e(w, S) \right) = \nu.$$

□

In spectral graph theory, it is an open problem to characterize all graphs satisfying

$$\lambda_n = \frac{\chi}{\chi - 1},$$

and several classes of graphs for which equality holds are known, including bipartite graphs, complete graphs, and petal graphs [3, 7, 8, 16, 17]. The next corollary of Proposition 4.9 provides a lower bound for $\tilde{h}$ for such graphs.

Corollary 4.10. *If a graph has chromatic number χ and is such that $\lambda_n = \chi/(\chi-1)$, then*

$$\tilde{h} \geq \frac{1}{\chi - 1}.$$

Proof. By Theorem 3.4 in [7], if $\lambda_n = \chi/(\chi-1)$, then for a fixed proper χ-coloring of G with coloring classes $V_1, \ldots, V_\chi$, for each $i \in \{1, \ldots, \chi\}$ and for every vertex w,

$$e(w, V_i) = \begin{cases} \frac{\deg w}{\chi - 1}, & \text{if } w \notin V_i, \\ 0, & \text{if } w \in V_i. \end{cases}$$

Hence, if we fix $i \in \{1, \ldots, \chi\}$, then clearly $\operatorname{vol} V_i \leq \operatorname{vol} V/2$ (since each coloring class is an independent set), and Proposition 4.9 for $\nu = 1/(\chi - 1)$ gives

$$\tilde{h} \geq \frac{1}{\chi - 1}.$$

□

Remark 4.11. For bipartite graphs, $\chi = 2$ and $\lambda_n = 2 = \chi/(\chi - 1)$. Hence, in this case, the bound in Corollary 4.10 is sharp.

Similarly, for the cycle graph on three vertices, $\chi = 3$, $\lambda_n = 3/2 = \chi/(\chi - 1)$, and one can check that $\tilde{h} = 1/2$ (cf. Example 4.13 below). Therefore, the bound in Corollary 4.10 is sharp also in this case.

The next result shows that $\tilde{h}(S)$ is symmetric with respect to taking the complement whenever S and $\overline{S}$ have the same volume.

Proposition 4.12. *If a set $S \subseteq V$ is such that $\operatorname{vol} S = \operatorname{vol} V/2$, then*

$$\tilde{h}(S) = \tilde{h}(\overline{S}).$$

Proof. Let S be such that $\operatorname{vol} S = \operatorname{vol} V/2$. In this case, also $\operatorname{vol} \overline{S} = \operatorname{vol} V/2$. Hence,

$$\begin{aligned}
\tilde{h}(\overline{S}) &= \frac{1}{\operatorname{vol} \overline{S}} \cdot \sum_{w \in V} \frac{e(w, \overline{S})^2}{\deg w} \\
&= \frac{1}{\operatorname{vol} \overline{S}} \cdot \sum_{w \in V} \frac{(\deg w - e(w, S))^2}{\deg w} \\
&= \frac{1}{\operatorname{vol} \overline{S}} \cdot \sum_{w \in V} \left(\deg w - 2e(w, S) + \frac{e(w, S)^2}{\deg w} \right) \\
&= \frac{1}{\operatorname{vol} S} \left(\operatorname{vol} V - 2 \cdot \frac{\operatorname{vol} V}{2} + \sum_{w \in V} \frac{e(w, S)^2}{\deg w} \right)
\end{aligned}$$

$$= \frac{1}{\operatorname{vol} S} \sum_{w \in V} \frac{e(w,S)^2}{\deg w}$$
$$= \tilde{h}(S).$$

□

We now consider several examples illustrating the behavior of $\tilde{h}$. We begin by computing $\tilde{h}$ for complete graphs.

Example 4.13. Consider the complete graph K_n on $n \geq 2$ vertices, and let $S \subset V$ with $|S| \leq n/2$. Then,

$$\begin{aligned}
\tilde{h}(S) &= \frac{\sum_{w \in V} e(w,S)^2}{(n-1) \cdot (n-1)|S|} \\
&= \frac{|S|(|S|-1)^2 + (n-|S|) \cdot |S|^2}{(n-1)^2|S|} \\
&= \frac{|S|(|S|^2 - 2|S| + 1) + (n-|S|) \cdot |S|^2}{(n-1)^2|S|} \\
&= \frac{-2|S|^2 + |S| + n|S|^2}{(n-1)^2|S|} \\
&= \frac{|S|(n-2)+1}{(n-1)^2}.
\end{aligned}$$

If n is even, then $\tilde{h}(S)$ is maximal when $|S| = n/2$. Hence,

$$\begin{aligned}
\tilde{h} &= \frac{1}{2} \cdot \frac{n(n-2)+2}{(n-1)^2} \\
&= \frac{1}{2} \cdot \frac{(n-1)^2+1}{(n-1)^2} \\
&= \frac{1}{2}\left(1 + \frac{1}{(n-1)^2}\right).
\end{aligned}$$

Furthermore, if n is odd, then $\tilde{h}(S)$ is maximal if $|S| = (n-1)/2$. Hence, in this case,

$$\begin{aligned}
\tilde{h} &= \frac{1}{2} \cdot \frac{(n-1)(n-2)+2}{(n-1)^2} \\
&= \frac{1}{2}\left(1 - \frac{n-3}{(n-1)^2}\right).
\end{aligned}$$

Summarizing,

$$\tilde{h} = \begin{cases} \frac{1}{2}\left(1 + \frac{1}{(n-1)^2}\right), & \text{if } n \text{ is even,} \\ \frac{1}{2}\left(1 - \frac{n-3}{(n-1)^2}\right), & \text{if } n \text{ is odd.} \end{cases}$$

In particular, this illustrates that Corollary 4.8 does not hold if n is odd.

Example 4.14. The *m-petal graph* on $n = 2m+1$ vertices (Figure 1) is the graph with vertex set

$$V = \{x, v_1, \ldots, v_m, w_1, \ldots, w_m\}$$

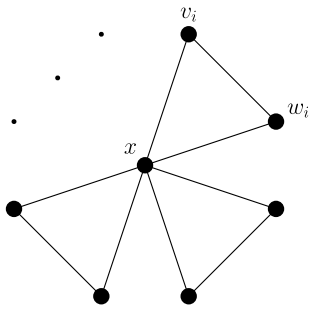


Figure 1: A petal graph.

and edge set

$$E = \bigcup_{i=1}^{m} \Big\{ \{x, v_i\}, \{x, w_i\}, \{v_i, w_i\} \Big\}.$$

Let S be a nonempty subset of its vertices satisfying $\operatorname{vol} S \leq \operatorname{vol} V/2$. Moreover, let $c \in \{0, 1\}$ indicate whether the center vertex belongs to S, and let $k \in \{0, \dots, 2m\}$ denote the number of peripheral vertices in S. Then, $\operatorname{vol} S = 2mc + 2k$. Also, as $\operatorname{vol} S \leq \operatorname{vol} V/2 = 3m$, either $c = 0$ and $k \leq \lfloor 3m/2 \rfloor$, or $c = 1$ and $k \leq \lfloor m/2 \rfloor$.

We compute

$$\begin{aligned} \tilde{h}(S) &= \frac{\sum_{w \in V} \frac{e(w,S)^2}{\deg w}}{\operatorname{vol} S} \\ &= \frac{\frac{k^2}{2m} + k \cdot \frac{(1+c)^2}{2} + (2m-k) \cdot \frac{c^2}{2}}{2mc + 2k} \\ &= \frac{k^2 + km + 2ckm + 2c^2m^2}{4m(k + cm)}. \end{aligned}$$

If $c = 0$, this simplifies to $\tilde{h}(S) = (k + m)/(4m)$. If $c = 1$, we get $\tilde{h}(S) = (k + 2m)/(4m)$ instead. In both cases, $\tilde{h}(S)$ is increasing in k, and therefore we can verify that

$$\tilde{h} = \frac{\lfloor \frac{m}{2} \rfloor + 2m}{4m}.$$

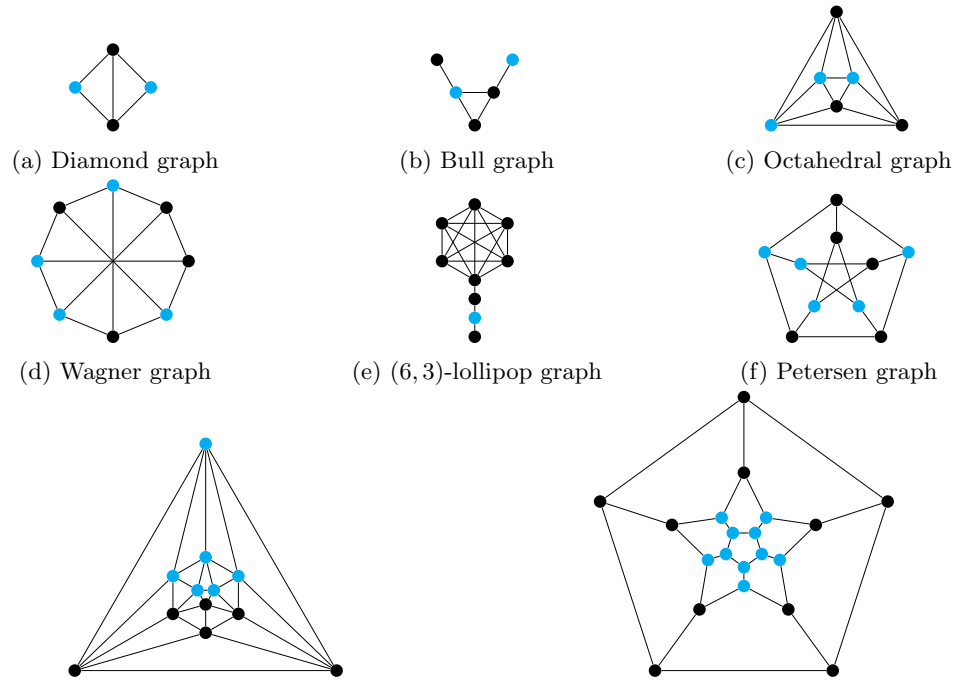
If m is even, we obtain $\tilde{h} = 5/8$. If m is odd, we get $\tilde{h} = (5m - 1)/(8m)$ instead.

By Proposition 4.1 we already know that for even cycles we have $\tilde{h} = 1$, as they are bipartite. We now compute $\tilde{h}$ for odd cycles.

Example 4.15. We consider the odd cycle C_{2m+1} ($m \in \mathbb{N}$), and we let S be a subset of its vertices of size $k > 0$ and volume $\operatorname{vol} S \leq \operatorname{vol} V/2$, that is, satisfying $k \leq m$. Let l be the number of vertices of C_{2m+1} that have two neighbors in S, and note that $l \leq k - 1$. Then, $2k - 2l$ vertices of C_{2m+1} have one neighbor in S, and the rest has no neighbors in S.

We compute

$$\begin{aligned} \tilde{h}(S) &= \frac{\sum_{w \in V} \frac{e(w,S)^2}{\deg w}}{\operatorname{vol} S} \\ &= \frac{l \cdot \frac{2^2}{2} + (2k - 2l) \cdot \frac{1}{2}}{2k} \end{aligned}$$



(a) Diamond graph (b) Bull graph (c) Octahedral graph

(d) Wagner graph (e) $(6,3)$-lollipop graph (f) Petersen graph

(g) Icosahedral graph (h) Dodecahedral graph

Figure 2: The graphs from Table 1. Cyan vertices form sets S for which $\tilde{h}(S) = \tilde{h}$.

$$= \frac{k+l}{2k}.$$

Note that $(k+l)/(2k)$ is an increasing function of l, therefore $\tilde{h}(S) \leq (2k-1)/2k$. As $(2k-1)/2k$ is an increasing function of k, we get $\tilde{h}(S) \leq (2k-1)/2k$.

Hence, $\tilde{h} \leq (2k-1)/2k$. At the same time, by choosing T to be an independent set of size m, we get $\tilde{h}(T) = (2k-1)/2k$. Therefore, for odd cycles,

$$\tilde{h} = \frac{2m-1}{2m}.$$

We now compute $\tilde{h}$ for a selection of small connected non-bipartite graphs. The values in Table 1 below were obtained computationally.

Note that for all graphs in Table 1 and for most graphs in Examples 4.13, 4.14, and 4.15, we have $\tilde{h} > 1/2$. This observation motivates the following question.

Question 1. *Is there a constant $c > 0$ such that $\tilde{h} > c$ for all graphs without isolated vertices? If so, what is the largest such constant?*

If such a constant c exists, it must be strictly smaller than $1/2$, because complete graphs K_n on an odd number of vertices satisfy $\tilde{h} < 1/2$, as shown in Example 4.13. Nevertheless, as $n \to \infty$, the value of $\tilde{h}$ for K_n converges to $1/2$. This observation motivates the following question.

Question 2. *Is there a function $f(n)$ such that $\tilde{h} \geq f(n)$ for all graphs on n vertices, satisfying $\lim_{n\to\infty} f(n) = 1/2$?*

Graph	n	$\tilde{h}$
Diamond graph	4	2/3
Bull graph	5	17/24
Octahedral graph	6	7/12
Wagner graph	8	7/9
$(6,3)$-lollipop graph	9	3/4
Petersen graph	10	31/45
Icosahedral graph	12	3/5
Dodecahedral graph	20	7/9

Table 1: Values of $\tilde{h}$ for several graphs on n vertices depicted in Figure 2.

5 Lower bounds for τ^2

This section is devoted to proving two sharp lower bounds for τ^2. First, in Theorem 5.1 we establish a general lower bound that does not involve $\tilde{h}$. As a consequence, we then derive the sharp inequality in Corollary 5.5 which is expressed in terms of $\tilde{h}$. Again, all graphs are assumed to be simple and to have no isolated vertices.

Theorem 5.1. *For every graph,*

$$\tau^2 \geq \max_{\emptyset \neq S \subsetneq V} \left(\frac{\operatorname{vol} V}{\operatorname{vol} \overline{S}} \cdot \left(\frac{1}{\operatorname{vol} S} \cdot \sum_{w \in V} \frac{e(w,S)^2}{\deg w} \right) - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} \right).$$

Moreover, the inequality is sharp.

The proof of Theorem 5.1 is based on evaluating the Rayleigh Quotient of a function that is constant on S and on its complement. The beginning of the proof is analogous to the classical proof [5] of the upper bound in the Cheeger inequalities (6).

Proof of Theorem 5.1. Fix $\emptyset \neq S \subsetneq V$, let $\alpha := \operatorname{vol} S / \operatorname{vol} \overline{S}$, and let $f : V \to \mathbb{R}$ be such that $f := 1$ on S and $f := -\alpha$ on $\overline{S}$. Then, $\sum_{v \in V} \deg v \cdot f(v) = 0$, implying that

$$\tau^2 \geq \mathrm{RQ}(f) = \frac{\sum\limits_{w \in V} \frac{1}{\deg w} \left(\sum\limits_{v \in \mathcal{N}(w)} f(v) \right)^2}{\sum\limits_{w \in V} \deg w \cdot f(w)^2}. \tag{10}$$

Since $\alpha \operatorname{vol} \overline{S} = \operatorname{vol} S$, the denominator in (10) can be rewritten as

$$\sum_{w \in V} \deg w \cdot f(w)^2 = \operatorname{vol} S + \alpha^2 \operatorname{vol} \overline{S} = (1+\alpha) \operatorname{vol} S.$$

Moreover, the numerator satisfies

$$\sum_{w \in V} \frac{1}{\deg w} \left(\sum_{v \in \mathcal{N}(w)} f(v) \right)^2 = \sum_{w \in V} \frac{1}{\deg w} \left(\sum_{v \in \mathcal{N}(w) \cap S} 1 - \sum_{v \in \mathcal{N}(w) \cap \overline{S}} \alpha \right)^2$$

$$= \sum_{w \in V} \frac{1}{\deg w} \left(e(w,S) - \alpha e(w,\overline{S}) \right)^2.$$

Note also that

$$\operatorname{vol} S = \sum_{v \in S} \deg v = \sum_{w \in V} e(w,S)$$

and, for all $w \in V$,

$$e(w,\overline{S}) = \deg w - e(w,S).$$

Therefore,

$$\begin{aligned}
\mathrm{RQ}(f) &= \frac{\sum_{w \in V} \frac{1}{\deg w} \left(e(w,S) - \alpha e(w,\overline{S}) \right)^2}{(1+\alpha)\operatorname{vol} S} \\
&= \frac{\sum_{w \in V} \frac{1}{\deg w} \left(e(w,S) - \alpha \left(\deg w - e(w,S) \right) \right)^2}{(1+\alpha)\operatorname{vol} S} \\
&= \frac{\sum_{w \in V} \frac{1}{\deg w} \left((1+\alpha) e(w,S) - \alpha \deg w \right)^2}{(1+\alpha)\operatorname{vol} S} \\
&= \frac{\sum_{w \in V} \frac{1}{\deg w} \left((1+\alpha)^2 e(w,S)^2 + \alpha^2 (\deg w)^2 - 2\alpha \deg w (1+\alpha) e(w,S) \right)}{(1+\alpha)\operatorname{vol} S} \\
&= \frac{\sum_{w \in V} \left(\frac{(1+\alpha)^2 e(w,S)^2}{\deg w} + \alpha^2 \deg w - 2\alpha(1+\alpha) e(w,S) \right)}{(1+\alpha)\operatorname{vol} S} \\
&= \sum_{w \in V} \frac{(1+\alpha) e(w,S)^2}{\deg w \cdot \operatorname{vol} S} + \sum_{w \in V} \frac{\alpha^2 \deg w}{(1+\alpha)\operatorname{vol} S} - \sum_{w \in V} \frac{2\alpha e(w,S)}{\operatorname{vol} S} \\
&= \frac{(1+\alpha)}{\operatorname{vol} S} \cdot \left(\sum_{w \in V} \frac{e(w,S)^2}{\deg w} \right) + \frac{\alpha^2 \operatorname{vol} V}{(1+\alpha)\operatorname{vol} S} - 2\alpha.
\end{aligned}$$

Now, observe that

$$1 + \alpha = 1 + \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} = \frac{\operatorname{vol} \overline{S} + \operatorname{vol} S}{\operatorname{vol} \overline{S}} = \frac{\operatorname{vol} V}{\operatorname{vol} \overline{S}}.$$

Hence,

$$\frac{\alpha^2 \operatorname{vol} V}{(1+\alpha)\operatorname{vol} S} = \frac{\operatorname{vol} \overline{S}}{\operatorname{vol} V} \cdot \frac{(\operatorname{vol} S)^2}{(\operatorname{vol} \overline{S})^2} \cdot \frac{\operatorname{vol} V}{\operatorname{vol} S} = \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} = \alpha,$$

and similarly

$$\frac{(1+\alpha)}{\operatorname{vol} S} = \frac{\operatorname{vol} V}{\operatorname{vol} S \cdot \operatorname{vol} \overline{S}}.$$

This implies that

$$\tau^2 \geq \mathrm{RQ}(f) = \frac{\operatorname{vol} V}{\operatorname{vol} S \cdot \operatorname{vol} \overline{S}} \cdot \left(\sum_{w \in V} \frac{e(w,S)^2}{\deg w} \right) - \alpha. \tag{11}$$

This proves the first claim. To show that the inequality is sharp, assume that G is the complete graph. In this case, $\lambda_2 = \lambda_n = n/(n-1)$, implying that

$$\tau = \frac{1}{n-1}.$$

If we let $S = \{x\}$, then $\operatorname{vol} S = n-1$ and $\operatorname{vol} \overline{S} = (n-1)^2$. Hence, (11) becomes

$$\tau^2 \geq \frac{n(n-1)}{(n-1)^3} \cdot \left(\sum_{w \in V \setminus \{x\}} \frac{1}{n-1} \right) - \frac{n-1}{(n-1)^2} = \frac{n}{(n-1)^2} - \frac{n-1}{(n-1)^2} = \frac{1}{(n-1)^2}.$$

Equivalently, $\tau \geq 1/(n-1)$. Since we have shown that $\tau = 1/(n-1)$ in this case, the inequality is sharp. □

Remark 5.2. If G is bipartite, then $\tau = 1$ by Remark 4.6. In this case, the sets S and $\overline{S}$ that give the bipartition satisfy

$$\sum_{w \in V} \frac{e(w,S)^2}{\deg w} = \sum_{w \in \overline{S}} \frac{(\deg w)^2}{\deg w} = \operatorname{vol} \overline{S}.$$

Moreover, in this case $\operatorname{vol} S = \operatorname{vol} \overline{S} = \operatorname{vol} V/2$, hence (11) becomes

$$\tau^2 \geq \frac{\operatorname{vol} V}{\operatorname{vol} S \cdot \operatorname{vol} \overline{S}} \cdot \operatorname{vol} \overline{S} - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} = 1,$$

or equivalently, $\tau \geq 1$. Hence, the inequality from Theorem 5.1 is sharp also in this case.

Remark 5.3. If G is disconnected, then $\tau = 1$, since $\lambda_2 = 0$. In this case, there exists a set $S \subset V$ of volume $\operatorname{vol} S \leq \operatorname{vol} V/2$ that forms the vertex set of a connected component. In this case, Equation (10) becomes

$$\begin{aligned} \tau^2 &\geq \frac{\operatorname{vol} V}{\operatorname{vol} S \cdot \operatorname{vol} \overline{S}} \cdot \left(\sum_{w \in S} \frac{(\deg w)^2}{\deg w} \right) - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} \\ &= \frac{\operatorname{vol} S + \operatorname{vol} \overline{S}}{\operatorname{vol} \overline{S}} - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} \\ &= 1 \end{aligned}$$

or equivalently, $\tau \geq 1$. Hence, the inequality from Theorem 5.1 is also sharp in this case.

Remark 5.4. The expression from the statement of Theorem 5.1 is symmetric in S and $\overline{S}$. To see this, consider f as defined in the proof, and define f' by reversing the roles of S and $\overline{S}$. Then,

$$f' = -\frac{f}{\alpha}.$$

Since f and f' are multiples of one another, they have the same Rayleigh quotient. Hence,

$$\begin{aligned} \operatorname{RQ}(f) &= \frac{\operatorname{vol} V}{\operatorname{vol} \overline{S}} \cdot \left(\frac{1}{\operatorname{vol} S} \cdot \sum_{w \in V} \frac{e(w,S)^2}{\deg w} \right) - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}} \\ &= \operatorname{RQ}(f') \\ &= \left(\frac{\operatorname{vol} V}{\operatorname{vol} S} \cdot \left(\frac{1}{\operatorname{vol} \overline{S}} \cdot \sum_{w \in V} \frac{e(w,\overline{S})^2}{\deg w} \right) - \frac{\operatorname{vol} \overline{S}}{\operatorname{vol} S} \right). \end{aligned}$$

We are now ready to prove the following sharp lower bound for τ^2 in terms of $\tilde{h}$, which follows from Theorem 5.1.

Corollary 5.5. *For every graph,*

$$\tau^2 \geq 2\tilde{h} - 1.$$

Moreover, the inequality is sharp.

Proof. Fix a nonempty set $S \subseteq V$ such that $\operatorname{vol} S \leq \operatorname{vol} V/2$, or equivalently, $\operatorname{vol} S \leq \operatorname{vol} \overline{S}$. Then, by Theorem 5.1,

$$\tau^2 \geq \frac{\operatorname{vol} V}{\operatorname{vol} \overline{S}} \cdot \tilde{h}(S) - \frac{\operatorname{vol} S}{\operatorname{vol} \overline{S}}.$$

Now, let $\alpha := \operatorname{vol} S / \operatorname{vol} \overline{S}$. Then, $\alpha \leq 1$ and

$$\frac{\operatorname{vol} V}{\operatorname{vol} \overline{S}} = \frac{\operatorname{vol} \overline{S} + \operatorname{vol} S}{\operatorname{vol} \overline{S}} = 1 + \alpha.$$

Hence,

$$\tau^2 \geq (1+\alpha)\tilde{h}(S) - \alpha = \tilde{h}(S) + \alpha(\tilde{h}(S) - 1).$$

Now, the inequalities in the proof of Proposition 4.1 show that $\tilde{h}(S) \leq 1$ for any S. Therefore, $\tilde{h}(S) - 1 \leq 0$, and together with the fact that $\alpha \leq 1$, this implies that

$$\tau^2 \geq \tilde{h}(S) + \alpha(\tilde{h}(S) - 1) \geq \tilde{h}(S) + \tilde{h}(S) - 1 = 2\tilde{h}(S) - 1.$$

Maximizing over all nonempty sets $S \subseteq V$ with $\operatorname{vol} S \leq \operatorname{vol} V/2$ gives

$$\tau^2 \geq 2\tilde{h} - 1.$$

By Remark 4.6, equality holds for bipartite graphs, showing that the inequality is sharp. □

Remark 5.6. For the m-petal graph on $n = 2m + 1$ vertices, with an even number m of petals, we have $\tilde{h} = 5/8$ by Example 4.14, while $\tau^2 = 1/4$ by [10]. Hence, the inequality in Corollary 5.5 is sharp also in this case.

Remark 5.7. If G is a connected non-bipartite d-regular Ramanujan graph, then by (1),

$$\tau^2 \leq \frac{4(d-1)}{d^2}.$$

Together with Corollary 5.5 this implies that, in this case,

$$\tilde{h} \leq \frac{1}{2} + \frac{2(d-1)}{d^2}.$$

6 Upper bounds for τ^2

Also in this section, all graphs are assumed to be simple and to have no isolated vertices. The main upper bound for τ^2 is given by the following theorem, whose proof is presented in Section 7.

Theorem 6.1. *For every graph G,*

$$\tau^2 \leq \sqrt{1 - (1 - \tilde{h})^2}. \tag{12}$$

Moreover, the inequality is an equality if and only if G is bipartite or disconnected.

Applying Bernoulli's inequality in a standard fashion, from Theorem 6.1 one can obtain a weaker upper bound on τ^2 without a square root that is a good approximation when $\tilde{h}$ is close to 1.

Corollary 6.2. *For every graph without isolated vertices we have*

$$\tau^2 \leq 1 - \frac{(1-\tilde{h})^2}{2}.$$

Moreover, the inequality is sharp if and only if G is disconnected or bipartite.

Proof. Bernoulli's inequality states that for any real numbers $r \geq 1$ and $x \geq -1$, we have

$$(1+x)^r \leq 1 + rx.$$

Setting $r = 1/2$ and $x = -(1-\tilde{h})^2$, and applying Bernoulli's inequality to the upper bound on τ^2 from Theorem 6.1, we get

$$\tau^2 \leq \sqrt{1-(1-\tilde{h})^2} \leq 1 - \frac{(1-\tilde{h})^2}{2}, \tag{13}$$

proving the first claim.

If $\tau^2 = 1 - (1-\tilde{h})^2/2$, then from (13) we have in particular $\tau^2 = \sqrt{1-(1-\tilde{h})^2}$. By the equality case from Theorem 6.1, we know that this equality holds if and only if G is disconnected or bipartite, that is, if and only if $\tilde{h} = 1$. Therefore, for $\tau^2 = 1-(1-\tilde{h})^2/2$ to hold, it is necessary that $\tilde{h} = 1$.

On the other hand, if $\tilde{h} = 1$, then $\tau^2 = 1$ (by the equality case of Theorem 6.1), and also $1 - (1-\tilde{h})^2/2 = 1$. Therefore, $\tilde{h} = 1$ is both a necessary and sufficient condition for $\tau^2 = 1 - (1-\tilde{h})^2/2$. Thus, the inequality from the statement is an equality if and only if G is disconnected or bipartite, as claimed. □

We note that while the bound in Corollary 6.2 is weaker than the one in Theorem 6.1, it is not uncommon to use an expression avoiding the square root in the Cheeger inequality

$$1 - \sqrt{1-h^2} \leq \lambda_2.$$

Compare, for example, the quantity $h^2/2$ in Theorem 2.2 in Chung's book [5], with the quantity $1-\sqrt{1-h^2}$ in Theorem 2.3 in the same book [5].

7 Proof of Theorem 6.1

This section is dedicated to proving Theorem 6.1. Much of the proof of Theorem 6.1 uses similar techniques as one of the proofs of the lower bound of the Cheeger inequalities in (6), as presented for example by Luca Trevisan in [18] (other previous work featuring similar arguments includes [14] and [6]). However, our proof has several additional technicalities due to the form of the Rayleigh Quotient of the operator M.

First, we introduce a few results that will be helpful for the proof. We start with the following basic property of fractions.

Remark 7.1. Let $p, r \geq 0$ and $q, s > 0$. Then,

$$\min\left\{\frac{p}{q}, \frac{r}{s}\right\} \leq \frac{p+r}{q+s} \leq \max\left\{\frac{p}{q}, \frac{r}{s}\right\}.$$

Another ingredient is the following lemma, which is essentially Fact 5.2 from [18], differing only in the inequality inside of the probability. Although the proof is almost identical, we reproduce it here for the sake of completeness.

Lemma 7.2. *Let X and Y be random variables such that $\mathbb{P}(Y > 0) = 1$. Then,*

$$\mathbb{P}\left(\frac{X}{Y} \geq \frac{\mathbb{E}X}{\mathbb{E}Y}\right) > 0.$$

Proof of Lemma 7.2. By linearity of expectation, we see that

$$\mathbb{E}\left(X - \frac{\mathbb{E}(X)}{\mathbb{E}(Y)} \cdot Y\right) = \mathbb{E}(X) - \frac{\mathbb{E}(X)}{\mathbb{E}(Y)} \cdot \mathbb{E}(Y) = 0.$$

Therefore,

$$\mathbb{P}\left(X \geq \frac{\mathbb{E}(X)}{\mathbb{E}(Y)} \cdot Y\right) > 0,$$

and the claim follows by dividing both sides of the internal inequality by Y, which we may do because $Y > 0$ almost surely. □

We are now ready to go through the proof of Theorem 6.1, which is divided into several claims in order to make the argument easier to follow.

Proof of Theorem 6.1. Recall that, by (5), we have the following characterization:

$$\tau^2 = \max_{\substack{f \in C(V)\setminus\{\mathbf{0}\}: \\ \sum_{w\in V} \deg w \cdot f(w) = 0}} \mathrm{RQ}(f) = \max_{\substack{f \in C(V)\setminus\{\mathbf{0}\}: \\ \sum_{w\in V} \deg w \cdot f(w) = 0}} \frac{\sum_{w\in V} \frac{1}{\deg w}\left(\sum_{v\in\mathcal{N}(w)} f(v)\right)^2}{\sum_{w\in V} \deg w \cdot f(w)^2}.$$

We first find a convenient function whose Rayleigh Quotient gives an upper bound to τ^2, similarly to Lemma 4.5 in [18].

Claim 1. *There exists a function $f \in C(V) \setminus \{\mathbf{0}\}$ such that*

$$\tau^2 \leq \mathrm{RQ}(f),$$

satisfying

$$\mathrm{vol}\,\mathrm{supp}(f) \in \left(0, \frac{\mathrm{vol}\,V}{2}\right] \quad \textit{and} \quad 1 \in \mathrm{Range}(f) \subset [0, 1].$$

Proof of Claim 1. Let $g \in C(V) \setminus \{\mathbf{0}\}$ be a function satisfying

$$\sum_{w\in V} \deg w \cdot g(w) = 0 \quad \text{and} \quad \tau^2 = \mathrm{RQ}(g).$$

Notice that, as a consequence, g attains at least one positive and one negative value.

For any $c \in \mathbb{R}$, we have $\mathrm{RQ}(g - c\cdot\mathbf{1}) \geq \mathrm{RQ}(g)$. In fact, for $c \neq 0$,

$$\begin{aligned}\mathrm{RQ}(g - c\cdot\mathbf{1}) &= \frac{\langle g - c\cdot\mathbf{1}, M(g - c\cdot\mathbf{1})\rangle}{\langle g - c\cdot\mathbf{1}, g - c\cdot\mathbf{1}\rangle} \\ &= \frac{\langle g, Mg\rangle + \langle -c\cdot\mathbf{1}, M(-c\cdot\mathbf{1})\rangle}{\langle g, g\rangle + \langle -c\cdot\mathbf{1}, -c\cdot\mathbf{1}\rangle}\end{aligned}$$

$$
\begin{aligned}
&= \frac{\langle g, Mg\rangle + c^2\langle \mathbf{1}, M\mathbf{1}\rangle}{\langle g, g\rangle + c^2 \cdot \langle \mathbf{1}, \mathbf{1}\rangle} \\
&\geq \min\left\{ \frac{\langle g, Mg\rangle}{\langle g, g\rangle}, \frac{c^2\langle \mathbf{1}, M\mathbf{1}\rangle}{c^2 \cdot \langle \mathbf{1}, \mathbf{1}\rangle} \right\} \\
&= \min\big\{\mathrm{RQ}(g), \mathrm{RQ}(\mathbf{1})\big\} \\
&= \mathrm{RQ}(g),
\end{aligned}
$$

where we have used Remark 7.1 for the inequality, and afterward used the fact that $1 = \mathrm{RQ}(\mathbf{1})$ is the largest eigenvalue of M.

We now pick c such that

$$
\mathrm{vol}\,\{v : g(v) - c \geq 0\} \geq \frac{\mathrm{vol}\, V}{2} \quad \text{and} \quad \mathrm{vol}\,\{v : g(v) - c \leq 0\} \geq \frac{\mathrm{vol}\, V}{2}.
$$

To see that this can be done, first recall that g attains only finitely many values, say $g_1 < \ldots < g_k$, which then satisfy

$$
\mathrm{vol}\,\{v : g(v) - g_1 \geq 0\} = \mathrm{vol}\, V \quad \text{and} \quad \mathrm{vol}\,\{v : g(v) - g_k \leq 0\} = \mathrm{vol}\, V.
$$

Hence, there exists $i \in \{1 \ldots, k\}$ such that

$$
\mathrm{vol}\,\{v : g(v) - g_i \geq 0\} \geq \frac{\mathrm{vol}\, V}{2} \quad \text{and} \quad \mathrm{vol}\,\{v : g(v) - g_{i+1} \leq 0\} \geq \frac{\mathrm{vol}\, V}{2}.
$$

If neither g_i nor g_{i+1} can be chosen as c, then

$$
\mathrm{vol}\left\{v : g(v) - \frac{g_i + g_{i+1}}{2} < 0\right\} < \frac{\mathrm{vol}\, V}{2} \quad \text{and} \quad \mathrm{vol}\left\{v : g(v) - \frac{g_i + g_{i+1}}{2} > 0\right\} < \frac{\mathrm{vol}\, V}{2},
$$

which contradicts that these two volumes add up to $\mathrm{vol}\, V$, because $(g_i + g_{i+1})/2$ is not in the range of g. Hence, g_i or g_{i+1} can be chosen as c.

In particular, this choice of c also implies that

$$
\mathrm{vol}\,\{v : g(v) - c < 0\} \leq \frac{\mathrm{vol}\, V}{2} \quad \text{and} \quad \mathrm{vol}\,\{v : g(v) - c > 0\} \leq \frac{\mathrm{vol}\, V}{2}.
$$

Set now $\tilde{g} := g - c \cdot \mathbf{1}$, $\tilde{g}^+ := \max\{\tilde{g}, \mathbf{0}\}$, and $\tilde{g}^- := \max\{-\tilde{g}, \mathbf{0}\}$, so that $\tilde{g} = \tilde{g}^+ - \tilde{g}^-$. Then,

$$
\mathrm{vol}\,\mathrm{supp}(\tilde{g}^+) \leq \frac{\mathrm{vol}\, V}{2} \quad \text{and} \quad \mathrm{vol}\,\mathrm{supp}(\tilde{g}^-) \leq \frac{\mathrm{vol}\, V}{2}.
$$

Furthermore, note that $\mathrm{supp}\big(\tilde{g}^+\big) \cap \mathrm{supp}\big(\tilde{g}^-\big) = \emptyset$.

We now claim that at least one $\tilde{f} \in \{\tilde{g}^+, \tilde{g}^-\}$ satisfies $\tilde{f} \neq \mathbf{0}$ and $\mathrm{RQ}(\tilde{g}) \leq \mathrm{RQ}(\tilde{f})$.

First, note that $\tilde{g} \neq 0$ since g attains at least two different values. Now, if $\tilde{g}^+ = 0$, then $\mathrm{RQ}(\tilde{g}) = \mathrm{RQ}(\tilde{g}^-)$, proving the claim. Analogously, if $\tilde{g}^- = 0$, then $\mathrm{RQ}(\tilde{g}) = \mathrm{RQ}(\tilde{g}^+)$.

If both $\tilde{g}^+$ and $\tilde{g}^-$ are nonzero, then

$$
\mathrm{RQ}(\tilde{g}) = \frac{\langle \tilde{g}^+ - \tilde{g}^-, M(\tilde{g}^+ - \tilde{g}^-)\rangle}{\langle \tilde{g}^+ - \tilde{g}^-, \tilde{g}^+ - \tilde{g}^-\rangle}
$$

$$
\begin{aligned}
&= \frac{\langle \tilde{g}^+, M\tilde{g}^+\rangle + \langle \tilde{g}^-, M\tilde{g}^-\rangle - \langle \tilde{g}^+, M\tilde{g}^-\rangle - \langle \tilde{g}^-, M\tilde{g}^+\rangle}{\langle \tilde{g}^+, \tilde{g}^+\rangle + \langle \tilde{g}^-, \tilde{g}^-\rangle - 2\langle \tilde{g}^+, \tilde{g}^-\rangle} \\
&= \frac{\langle \tilde{g}^+, M\tilde{g}^+\rangle + \langle \tilde{g}^-, M\tilde{g}^-\rangle - \langle \tilde{g}^+, M\tilde{g}^-\rangle - \langle \tilde{g}^-, M\tilde{g}^+\rangle}{\langle \tilde{g}^+, \tilde{g}^+\rangle + \langle \tilde{g}^-, \tilde{g}^-\rangle} \\
&\overset{(i)}{\leq} \frac{\langle \tilde{g}^+, M\tilde{g}^+\rangle + \langle \tilde{g}^-, M\tilde{g}^-\rangle}{\langle \tilde{g}^+, \tilde{g}^+\rangle + \langle \tilde{g}^-, \tilde{g}^-\rangle} \\
&\overset{(ii)}{\leq} \max\left\{ \frac{\langle \tilde{g}^+, M\tilde{g}^+\rangle}{\langle \tilde{g}^+, \tilde{g}^+\rangle}, \frac{\langle \tilde{g}^-, M\tilde{g}^-\rangle}{\langle \tilde{g}^-, \tilde{g}^-\rangle} \right\} \\
&= \max\big\{ \mathrm{RQ}\big(\tilde{g}^+\big), \mathrm{RQ}\big(\tilde{g}^-\big) \big\}.
\end{aligned}
$$

In (i), we used the fact that all entries of M are nonnegative by Equation (4), and so are all entries of $\tilde{g}^+$ and $\tilde{g}^-$. Furthermore, in (ii), we used Remark 7.1.

Finally, we set

$$
f := \frac{\tilde{f}}{\max\{\tilde{f}(v) : v \in V\}},
$$

and we note that this is well-defined. The function $f : V \to \mathbb{R}$ then satisfies

$$
\operatorname{vol}\operatorname{supp}(f) \in \left(0, \frac{\operatorname{vol} V}{2}\right] \quad \text{and} \quad 1 \in \operatorname{Range}(f) \subset [0,1],
$$

as well as the chain of (in)equalities

$$
\tau^2 = \mathrm{RQ}(g) \leq \mathrm{RQ}(g - c \cdot \mathbf{1}) \leq \mathrm{RQ}(\tilde{f}) = \mathrm{RQ}(f).
$$

This proves Claim 1. ■

Next, we use f from Claim 1 to find a set $S \subset V$ such that $\operatorname{vol} S \in (0, \operatorname{vol} V/2]$ and

$$
\mathrm{RQ}(f) \leq \sqrt{1 - (1 - \tilde{h}(S))^2}. \tag{14}
$$

To this end, we introduce a random subset S_t of V, following Chapter 5 of Trevisan [18]. Due to the more complicated form of our Rayleigh quotient, our proof then deviates from Trevisan's argument and becomes more involved.

Claim 2. *There is a set S satisfying*

$$
\mathrm{RQ}(f) \leq \sqrt{1 - \Big(1 - \tilde{h}(S)\Big)^2} \quad \textit{and} \quad \operatorname{vol} S \leq \frac{\operatorname{vol} V}{2}.
$$

Proof of Claim 2. To show the existence of such S, we consider the random set

$$
S_t := \{v : f(v) \geq t\},
$$

where t is a random variable distributed as $t^2 \sim U[0,1]$. We thus have

$$
\mathbb{P}(v \in S_t) = \mathbb{P}(f(v) \geq t) = \mathbb{P}(f(v)^2 \geq t^2) = f(v)^2.
$$

Moreover, for two vertices $u, v \in V$, we have

$$
\mathbb{P}(u, v \in S_t) = \min\{f(u)^2, f(v)^2\} \quad \text{and} \quad \mathbb{P}((u \in S_t) \vee (v \in S_t)) = \max\{f(u)^2, f(v)^2\}. \tag{15}
$$

As $\max\{f(v) : v \in V\} = 1$ by Claim 1, we also have that $\mathbb{P}(S_t = \emptyset) = 0$. Moreover, since $\mathbb{P}(t = 0) = 0$, almost surely $S_t \subset \operatorname{supp}(f)$. Therefore, since $\operatorname{vol}\operatorname{supp}(f) \in (0, \operatorname{vol} V/2]$ by Claim 1, it follows that, almost surely, $\operatorname{vol} S_t \in (0, \operatorname{vol} V/2]$. Moreover, since

$$\operatorname{vol} S_t = \sum_{v \in V} \deg v \cdot \mathbb{1}_{S_t}(v),$$

we have that

$$\mathbb{E}\left(\operatorname{vol} S_t\right) = \sum_{v \in V} \deg v \cdot \mathbb{E}\left(\mathbb{1}_{S_t}(v)\right) = \sum_{v \in V} \deg v \cdot \mathbb{P}\left(v \in S_t\right) = \sum_{v \in V} \deg v \cdot f(v)^2.$$

Now, to prove (14), we first bound its left-hand side by rewriting the Rayleigh quotient in a form that is suitable for the Cauchy-Schwarz inequality as follows.

$$\begin{aligned}
\mathrm{RQ}(f) &= \frac{\sum\limits_{w \in V} \frac{1}{\deg w} \left(\sum\limits_{v \in \mathcal{N}(w)} f(v) \right)^2}{\sum\limits_{w \in V} \deg w \cdot f(w)^2} \\
&= \frac{\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{f(u) f(v)}{\deg w}}{\sum\limits_{w \in V} \deg w \cdot f(w)^2} \\
&= \frac{\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\min\{f(u), f(v)\} \cdot \max\{f(u), f(v)\}}{\deg w}}{\sum\limits_{w \in V} \deg w \cdot f(w)^2} \\
&\leq \frac{\left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\min\{f(u), f(v)\}^2}{\deg w} \right)^{1/2} \cdot \left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\max\{f(u), f(v)\}^2}{\deg w} \right)^{1/2}}{\sum\limits_{w \in V} \deg w \cdot f(w)^2}, \qquad (16)
\end{aligned}$$

where in (16) we applied the Cauchy-Schwarz inequality to the vectors

$$\left(\frac{\min\{f(u), f(v)\}}{\sqrt{\deg w}} \right)_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \quad \text{and} \quad \left(\frac{\max\{f(u), f(v)\}}{\sqrt{\deg w}} \right)_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}}.$$

We can now use (15), together with linearity of expectation, to further bound $\mathrm{RQ}(f)$ by rewriting (16) as follows:

$$\begin{aligned}
\mathrm{RQ}(f) &\leq \frac{\left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{P}(u, v \in S_t)}{\deg w} \right)^{1/2} \cdot \left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{P}(u \in S_t \vee v \in S_t)}{\deg w} \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)} \\
&= \frac{\left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{E}(\mathbb{1}_{\{u, v \in S_t\}})}{\deg w} \right)^{1/2} \cdot \left(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{E}(\mathbb{1}_{\{u \in S_t \vee v \in S_t\}})}{\deg w} \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)} \\
&= \frac{\left(\mathbb{E}\big(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{1}_{\{u, v \in S_t\}}}{\deg w} \big) \right)^{1/2} \cdot \left(\mathbb{E}\big(\sum\limits_{\substack{w \in V \\ (u,v) \in \mathcal{N}(w)^2}} \frac{\mathbb{1}_{\{u \in S_t \vee v \in S_t\}}}{\deg w} \big) \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)}. \qquad (17)
\end{aligned}$$

Now, note that

$$\mathbb{1}((u \in S_t) \vee (v \in S_t)) = \mathbb{1}(u, v \in S_t) + \mathbb{1}((u \in S_t) \dot{\vee} (v \in S_t)),$$

where $\dot{\vee}$ denotes the exclusive or, and that

$$\sum_{u,v \in \mathcal{N}(w)} \mathbb{1}(u, v \in S_t) = \left(\sum_{v \in \mathcal{N}(w)} \mathbb{1}(v \in S_t) \right)^2 = e(w, S_t)^2.$$

Furthermore,

$$\begin{aligned}\sum_{(u,v) \in \mathcal{N}(w)^2} \mathbb{1}(u \in S_t \dot{\vee} v \in S_t) &= \sum_{(u,v) \in \mathcal{N}(w)^2} \mathbb{1}((u \in S_t) \wedge (v \notin S_t)) + \sum_{(u,v) \in \mathcal{N}(w)^2} \mathbb{1}((u \notin S_t) \wedge (v \in S_t)) \\ &= 2e(w, S_t) \cdot e(w, \bar{S}_t).\end{aligned}$$

The right-hand side of (17) can thus be further rewritten in the following way:

$$\begin{aligned}\mathrm{RQ}(f) &\leq \frac{\left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2}{\deg w} \big) \right)^{1/2} \cdot \left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2 + 2e(w,S_t) \cdot e(w,\overline{S_t})}{\deg w} \big) \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)} \\ &= \frac{\left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2}{\deg w} \big) \right)^{1/2} \cdot \left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2 + 2e(w,S_t)(\deg w - e(w,S_t))}{\deg w} \big) \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)} \\ &= \frac{\left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2}{\deg w} \big) \right)^{1/2} \cdot \left(\mathbb{E}\big(\sum_{w \in V} (\frac{-e(w,S_t)^2}{\deg w} + 2e(w,S_t)) \big) \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)} \\ &= \frac{\left(\mathbb{E}\big(\sum_{w \in V} \frac{e(w,S_t)^2}{\deg w} \big) \right)^{1/2} \cdot \left(-\mathbb{E}(\sum_{w \in V} \frac{e(w,S_t)^2}{\deg w}) + 2 \cdot \mathbb{E}(\operatorname{vol} S_t) \right)^{1/2}}{\mathbb{E}(\operatorname{vol} S_t)}. \end{aligned} \tag{18}$$

We now define two random variables

$$X_t \coloneqq \sum_{w \in V} \frac{e(w, S_t)^2}{\deg w} \quad \text{and } Y_t \coloneqq \operatorname{vol} S_t,$$

and we note that $\mathbb{P}(Y_t > 0) = 1$, since we have seen that $\operatorname{vol} S_t \in (0, \operatorname{vol} V/2]$ almost surely. Using this notation, we can rewrite (18) to obtain

$$\begin{aligned}\mathrm{RQ}(f) &\leq \frac{\left(\mathbb{E}\big(X_t \big) \right)^{1/2} \cdot \left(-\mathbb{E}(X_t) + 2 \cdot \mathbb{E}(Y_t) \right)^{1/2}}{\mathbb{E}(Y_t)} \\ &= \sqrt{-\frac{\mathbb{E}(X_t)^2}{\mathbb{E}(Y_t)^2} + 2\frac{\mathbb{E}(X_t)}{\mathbb{E}(Y_t)}} \\ &= \sqrt{1 - \left(1 - \frac{\mathbb{E}(X_t)}{\mathbb{E}(Y_t)} \right)^2}.\end{aligned}$$

By Lemma 7.2, there is some $t_0 \in [0,1]$ such that

$$\frac{\mathbb{E}(X_t)}{\mathbb{E}(Y_t)} \leq \frac{X_{t_0}}{Y_{t_0}}. \tag{19}$$

Using (19) together with the fact that the function $x \mapsto \sqrt{1-(1-x)^2}$ is increasing on the interval $[0,1]$, we thus immediately get

$$\begin{aligned}\sqrt{1-\left(1-\frac{\mathbb{E}(X_t)}{\mathbb{E}(Y_t)}\right)^2} &\leq \sqrt{1-\left(1-\frac{X_{t_0}}{Y_{t_0}}\right)^2} \\ &= \sqrt{1-\Big(1-\frac{1}{\operatorname{vol} S_{t_0}}\sum_{w\in V}\frac{e(w,S_{t_0})^2}{\deg w}\Big)^2} \\ &= \sqrt{1-(1-\tilde{h}(S_{t_0}))^2}.\end{aligned}$$

This proves the existence of $S = S_{t_0}$ satisfying (14) and $\operatorname{vol} S \leq \operatorname{vol} V/2$. ■

Combining Claims 1 and 2 together with the fact that the function $x \mapsto \sqrt{1-(1-x)^2}$ is increasing on the interval $[0,1]$, we have

$$\tau^2 \leq \mathrm{RQ}(f) \leq \sqrt{1-\left(1-\tilde{h}(S)\right)^2} \leq \sqrt{1-\left(1-\tilde{h}\right)^2},$$

concluding the proof of the upper bound on τ^2.

In the remainder of the proof, we analyze the equality case.

Claim 3. *The inequality from* (12) *is an equality if and only if G is bipartite or disconnected.*

Proof of Claim 3. If the inequality is sharp, then the Cauchy–Schwarz bound in (16) must itself be attained sharply. This occurs if and only if, for every $w \in V$ and every pair $(u,v) \in \mathcal{N}(w)^2$, either

$$\min\{f(u),f(v)\} = t\cdot\max\{f(u),f(v)\} \quad \text{or} \quad t\cdot\min\{f(u),f(v)\} = \max\{f(u),f(v)\},$$

for some $t \geq 0$. In particular, if $u = v$, then necessarily $f(u) = f(v)$, which implies $t = 1$ and thus

$$f(u) = f(v) \text{ for all } w \in V \text{ and all } (u,v) \in \mathcal{N}(w)^2. \tag{20}$$

If G is disconnected, then $\tilde{h} = \tau^2 = 1$, and hence the bound in (12) is an equality.

Therefore, we may assume that G is connected. Fix a vertex $v_0 \in V$. Observe that, by (20), all vertices in the neighborhood $\mathcal{N}(v_0)$ necessarily assume a common function value; we denote this value by a_1. Moreover, the vertices in the neighborhood of $\mathcal{N}(v_0)$, which in particular includes v_0 itself, must assume another common function value; we denote this value by a_0.

This reasoning can be extended inductively to the entire graph. Let S_0 denote the set of vertices at an even distance from v_0, and let S_1 denote the set of vertices at an odd distance from v_0. By construction, every vertex in S_0 has at least one neighbor in S_1 and vice versa, since v_0 has at least one neighbor in S_1, and every vertex $w \neq v_0$ has a neighbor v satisfying $d(v,v_0) = d(w,v_0) - 1$. One obtains that all vertices in S_0 must attain the common function value a_0, and analogously, all vertices in S_1 attain the common function value a_1.

Recall that the function f attains at least two function values by construction (one being equal to zero), from which it follows that $a_0 \neq a_1$. Furthermore, by Equation (20), no vertex can have a neighbor in S_0 and a neighbor in S_1.

We conclude that S_0 and S_1 are independent sets, and that G is bipartite, with bipartition (S_0, S_1).

Conversely, if G is disconnected or bipartite, then $\tau^2 = \tilde{h} = 1$, in which case Equation (12) is an equality. ■

This concludes the proof of Theorem 6.1. □

Tool and computational resource disclosure

The authors used Python to perform computations related to some of the examples presented in this paper. The authors also used a large language model as a tool for language polishing and for identifying possible inconsistencies or errors in preliminary drafts.

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