On the normalized Laplacian energy and general Randić index R_{-1} of graphs

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Abstract

In this paper, we consider the energy of a simple graph with respect to its normalized Laplacian eigenvalues, which we call the $\mathcal{L}$-energy. Over graphs of order n that contain no isolated vertices, we characterize the graphs with minimal $\mathcal{L}$-energy of 2 and maximal $\mathcal{L}$-energy of $2\lfloor n/2 \rfloor$. We provide upper and lower bounds for $\mathcal{L}$-energy based on its general Randić index $R_{-1}(G)$. We highlight known results for $R_{-1}(G)$, most of which assume G is a tree. We extend an upper bound of $R_{-1}(G)$ known for trees to connected graphs. We provide bounds on the $\mathcal{L}$-energy in terms of other parameters, one of which is the energy with respect to the adjacency matrix. Finally, we discuss the maximum change of $\mathcal{L}$-energy and $R_{-1}(G)$ upon edge deletion.

Key words: normalized Laplacian matrix, graph energy, general Randić index.
AMS Classification: 05C50; 05C90; 15A18; 15A42.

1. Introduction

Throughout this paper, all graphs are simple and have no isolated vertices. We will use d_x^G to denote the degree of a vertex x in G. If there is only one graph in question, we simply write d_x. Let A be the adjacency matrix of a graph G and D be the diagonal matrix of vertex degrees. The *normalized Laplacian matrix* of a graph G, denoted by $\mathcal{L}$, is defined to be the matrix with entries

$$\mathcal{L}(x,y) = \begin{cases} 1 & \text{if } x = y \text{ and } d_y \neq 0, \\ -\dfrac{1}{\sqrt{d_x d_y}} & \text{if } x \text{ and } y \text{ are adjacent in } G, \\ 0 & \text{otherwise.} \end{cases}$$

Note that $\mathcal{L}$ has the following relationship to A and D:

$$\mathcal{L} = I - D^{-1/2} A D^{-1/2}.$$

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[1]Research supported in part by an NSERC PGS D.
[2]Research supported in part by an NSERC Research Grant.
[3]Research supported in part by an NSERC Discovery Grant.

It is well known that 0 is an eigenvalue of $\mathcal{L}$ and that the remaining eigenvalues lie in the interval $[0, 2]$ (see [3] for other properties of the eigenvalues of $\mathcal{L}$).

For convenience, if M is a real symmetric matrix of order n, we order and denote the eigenvalues by $\lambda_1(M) \leq \ldots \leq \lambda_n(M)$ and the singular values by $\sigma_1(M) \leq \ldots \leq \sigma_n(M)$. If G is a graph and M is a real symmetric matrix associated with G, then the *M-energy* of G is

$$E_M(G) = \sum_{i=1}^{n} \left| \lambda_i(M) - \frac{tr(M)}{n} \right|, \tag{1}$$

where $tr(M)$ is the trace of M. Gutman [8] introduced the energy of a graph in 1978. Recently, the adjacency energy [9], Laplacian energy [11], signless Laplacian energy, distance energy [21] and incidence energy [10] of a graph has received much interest. Along the same lines, the energy of more general matrices and sequences has been studied (see [1, 17]). The goal of this paper is to analyze the $\mathcal{L}$-energy of a graph, and determine how graph structure relates to $\mathcal{L}$-energy. Formally, using (1) with M taken to be $\mathcal{L}$, the *normalized Laplacian energy* (or *$\mathcal{L}$-energy*) of a graph G is

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1|.$$

It is easy to see that this is equivalent to

$$\begin{aligned} E_{\mathcal{L}}(G) &= \sum_{i=1}^{n} |\lambda_i(I - \mathcal{L})|, & (2) \\ &= \sum_{i=1}^{n} \sigma_i(I - \mathcal{L}). & (3) \end{aligned}$$

It should be noted that Nikiforov [17] defines the energy of a matrix M of order n to be

$$\mathcal{E}(M) = \sum_{i=1}^{n} \sigma_i(M),$$

in which case by (3) we are interested in $\mathcal{E}(I - \mathcal{L})$. In this paper we use the M-energy definition in (1) when referring to the energy of a real symmetric matrix.

Let G be a graph of order n (with no isolated vertices). A convenient parameter of G is the *general Randić index* $R_\alpha(G)$, defined as

$$R_\alpha(G) = \sum_{x \sim y} (d_x d_y)^\alpha, \tag{4}$$

where the summation is over all (unordered) edges xy in G, and $\alpha \neq 0$ is a fixed real number. In 1975, Randić [22] proposed a topological index R (with $\alpha = -\frac{1}{2}$) under the name 'branching index'. In 1998, Bollobás and Erdős [2] generalized this index by replacing the $-1/2$ with any real number α (as defined in (4)). The papers [14, 15] survey recent results on the general Randić index of graphs with an emphasis on trees and chemical graphs.

In Section 2, we will see that the $\mathcal{L}$-energy of G can be bounded in terms of $R_{-1}(G)$. We then highlight some relevant results on the parameter $R_{-1}(G)$ that appear in the literature.

We provide an upper bound on $R_{-1}(G)$ in the case that G is a connected graph. Finally, we discuss how $R_{-1}(G)$ changes when an edge is deleted.

In Section 3, we show

$$2 \leq E_{\mathcal{L}}(G) \leq 2 \left\lfloor \frac{n}{2} \right\rfloor,$$

and characterize the graphs attaining these bounds. If G is connected, then the upper bound on the $\mathcal{L}$-energy can be improved to $E_{\mathcal{L}}(G) < \sqrt{\frac{15}{28}}(n+1)$. We provide a class of connected graphs attaining $\mathcal{L}$-energy $E_{\mathcal{L}}(G) = \frac{n}{\sqrt{2}} + O(1)$ and ask if this class has maximal $\mathcal{L}$-energy over all connected graphs. Finally, we discuss other bounds for $E_{\mathcal{L}}(G)$ and how edge deletion affects $\mathcal{L}$-energy.

2. Bounds on $R_{-1}(G)$ and its relationship to $\mathcal{L}$-energy

We begin with two other formulations of $R_{-1}(G)$. By analyzing the entries in $(I - \mathcal{L})^2$ and using (4) with $\alpha = -1$, observe that

$$R_{-1}(G) = \frac{tr((I - \mathcal{L})^2)}{2}. \tag{5}$$

By rewriting (4) with $\alpha = -1$ we get,

$$R_{-1}(G) = \frac{1}{2} \sum_{y \in V} \frac{1}{d_y} \sum_{\substack{x \\ x \sim y}} \frac{1}{d_x}, \tag{6}$$

where

$$\sum_{\substack{x \\ x \sim y}} f(x, y)$$

represents the sum over all (unordered) edges xy in G that are incident to a fixed vertex y in the vertex set V of G. Using (4), the quantity $R_{-1}(G)$ can be found by putting a weight of $\frac{1}{d_x d_y}$ on each edge xy of G (which we call the *weight of edge* xy), and then summing the weights over all the edges of G. Alternatively, using (6), $R_{-1}(G)$ can be found by putting a weight of

$$\frac{1}{2d_y} \sum_{\substack{x \\ x \sim y}} \frac{1}{d_x}$$

on each vertex y of G (which we call the *weight of vertex* y), and then summing the weights over all the vertices of G.

In the next lemma we see the importance of $R_{-1}(G)$ when analyzing the $\mathcal{L}$-energy of a graph.

Lemma 1. *Let G be a graph of order n with no isolated vertices. Then*

$$2R_{-1}(G) \leq E_{\mathcal{L}}(G) \leq \sqrt{2nR_{-1}(G)}.$$

Proof. By the Cauchy-Schwartz inequality with (2) (using vectors $(1,\dots,1)^T$ and $(|\lambda_1(I-\mathcal{L})|,\dots,|\lambda_n(I-L)|)^T$) along with (5) we obtain the upper bound

$$E_{\mathcal{L}}(G) \le \sqrt{n\sum_{i=1}^{n}[\lambda_i(I-\mathcal{L})]^2} = \sqrt{n \cdot tr((I-\mathcal{L})^2)} = \sqrt{2nR_{-1}(G)}.$$

Note that the eigenvalues of $I-\mathcal{L}$ lie in the interval $[-1,1]$. Thus, $[\lambda_i(I-\mathcal{L})]^2 \le |\lambda_i(I-\mathcal{L})|$, giving,

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n}|\lambda_i(I-\mathcal{L})| \ge \sum_{i=1}^{n}[\lambda_i(I-\mathcal{L})]^2 = tr((I-\mathcal{L})^2) = 2R_{-1}(G).$$

□

Thus, determining how the structure of a graph relates to $R_{-1}(G)$ will provide information about $E_{\mathcal{L}}(G)$. In the remainder of this section we look at bounds on $R_{-1}(G)$. We first highlight a few known results that can be found in the literature. By considering the minimum and maximum degrees of G, Shi [23] has obtained upper and lower bounds for $R_{-1}(G)$.

Theorem 2. *[23, Theorem 2.2 & 2.3] Let G be a graph of order n with no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$\frac{n}{2d_{\max}} \le R_{-1}(G) \le \frac{n}{2d_{\min}}.$$

Equality occurs in both bounds if and only if G is a regular graph.

Li and Yang [16] provide bounds on $R_{-1}(G)$ given strictly in terms of the order of G. Note that the *length* of a path is the number of edges that the path uses.

Theorem 3. *[16, Theorem 3.2] Let G be a graph of order n with no isolated vertices. Then*

$$\frac{n}{2(n-1)} \le R_{-1}(G) \le \left\lfloor \frac{n}{2} \right\rfloor,$$

with equality in the lower bound if and only if G is a complete graph, and equality in the upper bound if and only if either

(i) n is even and G is the disjoint union of $n/2$ paths of length 1, or
(ii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and one path of length 2.

If G is a disconnected graph with k connected components, in particular, $G_1, G_2, \dots, G_k$, then

$$R_{-1}(G) = \sum_{i=1}^{k} R_{-1}(G_i).$$

Thus, it is interesting to know how $R_{-1}(G)$ behaves for the class of connected graphs. In [4], Clark and Moon provide bounds on $R_{-1}(T)$, for a tree T of order n. They showed that

$$1 \le R_{-1}(T) \le \frac{5n+8}{18}.$$

In [13], Hu, Li and Yuan refine this upper bound, however, gaps were found in their proof (see [18]). Then Pavlović, Stojanvoić and Li gave a sound proof in [19].

Theorem 4. *[13, 19] For a tree T of order $n \geq 103$,*

$$R_{-1}(T) \leq \frac{15n-1}{56}.$$

See [20] for a further refinement (which we omit here), giving a sharp upper bound for $R_{-1}(T)$ amongst all trees T of order n, for $n \geq 720$. Also, see [14, 15] for many other results concerning bounds for $R_{-1}(T)$. In what follows, we will see that the bound $R_{-1}(G) \leq \frac{15(n+1)}{56}$ holds for any connected graph G of order $n \geq 3$.

We say G has a *suspended path* from u to w, if uvw is a path with $d_u^G = 1$ and $d_v^G = 2$. Note that we don't require $d_w^G \geq 3$ as in [4]. A $(t, s+t)$-*system centered at* r is an induced subgraph of G, such that there are t suspended paths to vertex r and $d_r^G = s+t$. This is illustrated in Figure 1.

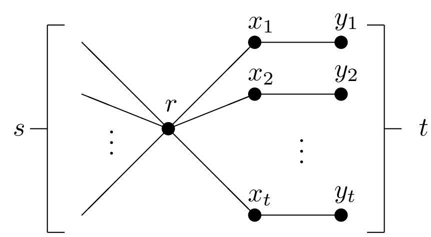

Figure 1: A $(t, s+t)$-system centered at r.

A $(k, t, s+k)$-*system centered at* R is an induced subgraph of G that has k vertex disjoint $(t, t+1)$-systems centered at $r_1, r_2, \ldots, r_k$, such that R is adjacent to each r_i and $d_R^G = s+k$. This is illustrated in Figure 2.

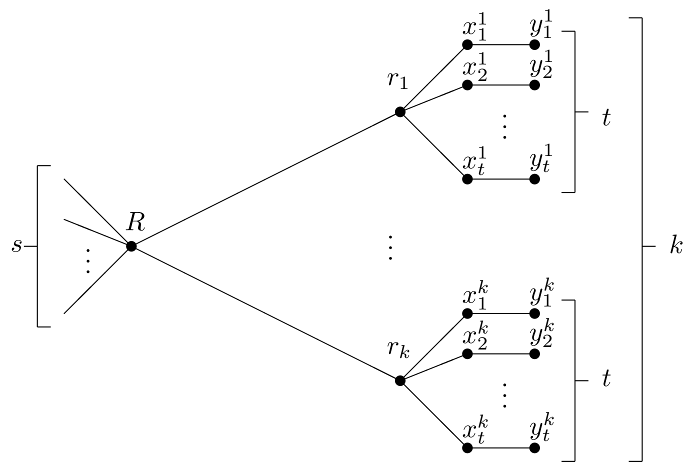

Figure 2: A $(k, t, s+k)$-system centered at R.

The set of all $(t, s+t)$-systems of G, for $s \geq 0$ and $t \geq 1$, and $(k, t, s+k)$-systems of G, for $s \geq 0$ and $k, t \geq 1$, is referred to as the *collection of systems* of G. Any object in this collection is referred to as a *system* of G. Note that a vertex z of G may be the center of many different systems.

One question to ask is if there is always a tree on n vertices that maximizes $R_{-1}(G)$ over all connected graphs of order n. If the answer is yes, then the bound for connected graphs would follow immediately. A first approach would be to look at the spanning trees of G and see if $R_{-1}(G) \leq R_{-1}(T)$ for some spanning tree T of G. However, it is interesting to note that there exist graphs G such that for every spanning tree T of G, the inequality $R_{-1}(T) < R_{-1}(G)$ holds.

Let G be the graph described as follows: Let $t > 16$ be a natural number and consider a cycle with 3 vertices a_1, a_2, a_3 each with degree 4 and with each of a_1, a_2, a_3 being the center of a $(2, t, 4)$-system. The order of G is $12t+9$ and the only spanning trees of G are obtained by removing an edge on the cycle (namely, a_1a_2, a_2a_3 or a_1a_3). If T is any spanning tree of G then,

$$R_{-1}(G) - R_{-1}(T) = \left(\frac{1}{t} + \frac{3}{16}\right) - \left(\frac{4}{3t} + \frac{1}{6}\right) = \frac{t-16}{48t}.$$

Thus, for $t > 16$, we have that for every spanning tree T of G, $R_{-1}(T) < R_{-1}(G)$.

To prove that $R_{-1}(G) \leq \frac{15(n+1)}{56}$ for connected graphs G of order $n \geq 3$, we take the same approach as done in the tree case. An inductive argument will be used. Let S be a subset of vertices of G. We denote the graph obtained by deleting all the vertices in S and their incident edges by $G \backslash S$. We begin with an inequality relating $R_{-1}(G)$ to $R_{-1}(G \backslash S)$. Note that deleting vertices (and edges) of G changes the degree sequence, and so the weighted graph associated with $G \backslash S$ will *not* be an induced weighted subgraph of the weighted graph associated with G.

Observation 5. *Let S be a subset of vertices of G, then,*

$$R_{-1}(G) \quad \leq \quad R_{-1}(G \backslash S) + \sum_{\substack{x \sim y \\ x \in S, y \notin S}} \frac{1}{d_x^G d_y^G} + \sum_{\substack{x \sim y \\ x, y \in S}} \frac{1}{d_x^G d_y^G}.$$

In [13], to prove the upper bound on $R_{-1}(T)$, the edge weights of T were summed up at the end of the proof. In general, for connected graphs it is more beneficial to use the formulation (6) of $R_{-1}(G)$ and sum up the vertex weights (as seen in the final case of the proof below). Some of the cases in [13, 19, 20] can be extended to general graphs, but for completeness of this paper we provide the full proof in the general case. Note that in Cases (0)-(iii) we use $1/4$ instead of $15/56$ in our manipulations of the second term.

Theorem 6. *Let G be a connected graph on $n \geq 3$ vertices. Then*

$$R_{-1}(G) \leq \frac{15(n+1)}{56}.$$

Proof. The proof is by induction on the number of vertices. If $n = 3$, then the path of length 2 and the triangle both satisfy the inequality. Let G be a connected graph on $n \geq 4$ vertices, and assume that the inequality holds for connected graphs on fewer than n vertices.

Case (0): If G has minimum degree at least 2 then by Theorem 2, we have $R_{-1}(G) \leq n/4$, and so the inequality holds.

Case (i): Let x be a vertex of degree 1 that is adjacent to a vertex y with $d_y \geq 4$. Deleting the vertex x does not disconnect the graph, thus, using $S = \{x\}$ in Observation 5 along with induction, we have

$$\begin{aligned} R_{-1}(G) &\leq R_{-1}(G\backslash\{x\}) + \frac{1}{d_y}, \\ &\leq \frac{15}{56}n + \frac{1}{4}, \\ &< \frac{15}{56}(n+1). \end{aligned}$$

Case (ii): Let z be a vertex of degree 2 such that $z \sim x$, $z \sim y$, $d_x \leq d_y$.

(a) Suppose $x \not\sim y$ in G and either $d_x = 1, d_y \leq 2$, or $d_y \geq d_x \geq 2$. Then form a graph H by deleting z and adding the edge xy. Note that $d_x^H = d_x$ and $d_y^H = d_y$. Thus,

$$R_{-1}(G) = R_{-1}(H) + \frac{1}{2d_x} + \frac{1}{2d_y} - \frac{1}{d_x d_y}.$$

Since H has $n-1$ vertices and is connected, we have by induction that

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}n + \frac{d_x + d_y - 2}{2d_x d_y}, \\ &< \frac{15}{56}(n+1) + \frac{2d_x + 2d_y - d_x d_y - 4}{4d_x d_y}, \\ &= \frac{15}{56}(n+1) + \frac{(d_x-2)(2-d_y)}{4d_x d_y}. \end{aligned}$$

If $d_x = 1, d_y \leq 2$ or $d_y \geq d_x \geq 2$, then $R_{-1}(G) < \frac{15}{56}(n+1)$.

(b) Suppose $x \sim y$ in G (and hence $d_y \geq d_x \geq 2$), then

$$R_{-1}(G) \leq R_{-1}(G\backslash\{z\}) + \frac{1}{2d_x} + \frac{1}{2d_y} + \frac{1}{d_x d_y} - \frac{1}{(d_x-1)(d_y-1)}.$$

Since deleting z does not disconnect the graph, we have by induction that

$$R_{-1}(G) < \frac{15}{56}(n+1) - \frac{f(d_x, d_y)}{4d_x d_y (d_x-1)(d_y-1)},$$

where

$$f(x,y) = (x-1)(x-2)y^2 - (3x+1)(x-2)y + 2(x+2)(x-1).$$

Our goal is to show that $f(x,y) \geq 0$, for $y \geq x \geq 2$ (with x, y integral). Note that $f(2,y) = 8$, for all y. Fix $x = x_0 \geq 3$ and view f as a parabola in y opening upward. The vertex of the parabola occurs with horizontal coordinate $\frac{3}{2} + \frac{2}{x_0-1} \leq 2.5$. As $f(x_0, 3) = 2x_0^2 - 10x_0 + 20 \geq 0$, for $x_0 \geq 3$, we have that $f(x_0, y) \geq 0$, for $y \geq 3$. Thus, $R_{-1}(G) < \frac{15}{56}(n+1)$.

Case (iii): Assume we have vertices u, v, x, y with $d_u = 1$, $d_v = 3$, $u \sim v$, $v \sim y$, $v \sim x$ and $d_x \leq d_y$.

(a) If $d_x = 1$ and $d_y \geq 5$, then let H denote the graph obtained from G by deleting vertices x, v, and u. Note that H is a connected graph with $n-3 \geq 3$ vertices. Thus, induction gives

$$R_{-1}(G) \leq \frac{15}{56}(n-2) + \frac{1}{3} + \frac{1}{3} + \frac{1}{15} < \frac{15}{56}(n-2) + \frac{3}{4} < \frac{15}{56}(n+1).$$

(b) Suppose $x \not\sim y$. If either: $d_x = 1, d_y \leq 4$, or $d_y \geq d_x \geq 2$, then form a new graph H obtained from G by deleting u and v and adding the edge xy. Notice that $d_x^H = d_x$ and $d_y^H = d_y$. Then

$$R_{-1}(G) = R_{-1}(H) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} - \frac{1}{d_x d_y}.$$

If $d_x = d_y = 1$, then G is a star on 4 vertices and the inequality holds. Otherwise, H is a connected graph with $n-2 \geq 3$ vertices, and by induction we have

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} - \frac{1}{d_x d_y}, \\ &< \frac{15}{56}(n+1) + \frac{2d_x + 2d_y - d_x d_y - 6}{6d_x d_y}, \\ &= \frac{15}{56}(n+1) + \frac{(2-d_x)d_y + 2(d_x-3)}{6d_x d_y}. \end{aligned}$$

If $d_x = 1, d_y \leq 4$, then the numerator of the second term is nonpositive. If $d_x = 2$ or $d_x = 3$, then the the numerator of the second term is negative. If $d_y \geq d_x \geq 4$, then

$$(2-d_x)d_y + 2(d_x - 3) \leq -2d_y + 2(d_y - 3) < 0.$$

Hence, $R_{-1}(G) < \frac{15}{56}(n+1)$ holds.

(c) Suppose $x \sim y$ and $d_y \geq d_x \geq 2$. Form a graph H by deleting u and v. Note that $d_x^H = d_x - 1$ and $d_y^H = d_y - 1$. Keeping track of the weight of edge xy in G and H gives

$$R_{-1}(G) < R_{-1}(H) + \frac{1}{3} + \frac{1}{3d_x} + \frac{1}{3d_y} + \frac{1}{d_x d_y} - \frac{1}{(d_x-1)(d_y-1)}.$$

Deleting u and v and using induction gives

$$R_{-1}(G) < \frac{15}{56}(n+1) - \frac{f(d_x, d_y)}{6d_x d_y (d_x-1)(d_y-1)},$$

where

$$f(x,y) = (x-1)(x-2)y^2 - (3x^2 - 5x - 4)y + 2(x-1)(x+3).$$

Our goal is to show that $f(x,y) \geq 0$, for $y \geq x \geq 2$ (with x, y integral). Note that $f(2,y) \geq 0$, for $y \geq 2$. Fix $x = x_0 \geq 3$ and view f as a parabola in y opening upward. The vertex occurs with horizontal coordinate $\frac{3}{2} + \frac{4x_0 - 10}{2(x_0-1)(x_0-2)} \leq 2$, for $x_0 = 2$ and $x_0 \geq 3$. As $f(x_0, 3) = 2x_0^2 - 8x_0 + 24 \geq 0$ for $x_0 \geq 3$, we have that $f(x_0, y) \geq 0$, for $y \geq 3$. Thus, $R_{-1}(G) < \frac{15}{56}(n+1)$.

Case (iv): Let $t \geq 1$ and suppose there is a $(t, s+t)$-system of G with $s + t \geq 14$. Label the vertices as in Figure 1. Then deleting x_1 and y_1, and using induction gives,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \frac{1}{2} + \frac{1}{2d_r}, \\ &\leq \frac{15}{56}(n+1) - \frac{30}{56} + \frac{1}{2} + \frac{1}{28}, \\ &= \frac{15}{56}(n+1). \end{aligned}$$

Case (v): Suppose there is a $(t, s+t)$-system of G with $s \geq 0$ and $t \geq 4$. Label the vertices as in Figure 1. This system has a subgraph that is a $(4,4)$-system (that includes the vertices x_1 and y_1). By keeping track of the edge weight changes in the $(4,4)$-system subgraph and deleting x_1 and y_1, we get

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \left(2 + \frac{4}{2d_r}\right) - \left(\frac{3}{2} + \frac{3}{2(d_r-1)}\right), \\ &= \frac{15}{56}(n+1) - \frac{(d_r-7)(d_r-8)}{28d_r(d_r-1)}, \\ &\leq \frac{15}{56}(n+1), \end{aligned}$$

since d_r is an integer.

Case (vi): Suppose there is a $(k, 3, s+k)$-system with $s+k \leq 14$ and $k \geq 1$. Label the vertices as in Figure 2. This system has a subgraph that is a $(1,3,1)$-system with center R (that includes the vertices x_1^1 and y_1^1). By keeping track of the edge weight changes in the $(1,3,1)$-system and deleting x_1^1 and y_1^1, we get

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n-1) + \left(\frac{3}{2} + \frac{3}{8} + \frac{1}{4d_R}\right) - \left(1 + \frac{1}{3} + \frac{1}{3d_R}\right), \\ &= \frac{15}{56}(n+1) + \frac{d_R - 14}{168d_R}, \\ &\leq \frac{15}{56}(n+1), \end{aligned}$$

since $d_R = s + k \leq 14$.

Case (vii): Suppose there is a $(k, 2, k+1)$-system of G, for some fixed $k \geq 2$. Label the vertices as in Figure 2. Let $u \neq r_j$, $1 \leq j \leq k$, be a vertex adjacent to R. Form a new graph H obtained from G by deleting the vertices of each $(2,3)$-system with center r_j, for $j \geq 2$, deleting R, and adding the edge ur_1. Note that deleting vertex R from G disconnects the graph, but by adding the edge ur_1 (and deleting each $(2,3)$-system with centers r_j, for $j \geq 2$) we ensure that H is connected. The degree of u and r_1 are the same in both G and H. Hence,

$$R_{-1}(G) - R_{-1}(H) = \frac{4(k-1)}{3} + \frac{k-1}{3(k+1)} + \frac{1}{3(k+1)} + \frac{1}{d_u(k+1)} - \frac{1}{3d_u}.$$

As we deleted $5(k-1)+1$ vertices to form H, we have by induction,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n+1) - \frac{d_u(k^2 - 11k + 44) + 56(k-2)}{168d_u(k+1)}, \\ &< \frac{15}{56}(n+1), \end{aligned}$$

since $k^2 - 11k + 44 > 0$ and $k \geq 2$.

Case (viii): Let $k \geq 1$ and $t \in [1,3]$.

(a) Suppose there is a $(k, 2, k+t+1)$-system of G with center R such that R is also the center of a $(t, k+t+1)$-system (note $d_R = k+t+1$). Let u be the vertex adjacent to R that is not a vertex of one of the systems with center R. Create a new graph H by deleting the vertex R and the vertices of all the systems with center R, and adding a $(1,2,d_u)$-system with center vertex u. A total of $5(k-1)+2t+1$ vertices have been deleted. Thus, we have by induction,

$$\begin{aligned} R_{-1}(G) &\leq \frac{15}{56}(n+1)-(5k+2t-4)\frac{15}{56}+\frac{4k}{3}+\frac{k}{3(k+t+1)}+ \\ &\quad \frac{t}{2}+\frac{t}{2(k+t+1)}+\frac{1}{d_u(k+t+1)}-\frac{4}{3}-\frac{1}{3d_u}, \\ &= \frac{15}{56}(n+1)-\frac{(k^2-11k+44+6t^2+7kt-34t)d_u+56(k+t-2)}{168d_u(k+t+1)}, \\ &< \frac{15}{56}(n+1), \end{aligned}$$

for $t \in [1,3]$ and $k \geq 1$.

(b) Suppose G has a $(k,2,k+t)$-system with center R such that R is also the center of a $(t,k+t)$-system (note $d_R = k+t$). Then $n = 5k+2t+1$ and every vertex of G belongs to either the $(k,2,k+t)$-system or the $(t,k+t)$-system. Then,

$$\begin{aligned} R_{-1}(G) &= \frac{4k}{3}+\frac{k}{3(k+t)}+\frac{t}{2}+\frac{t}{2(k+t)}, \\ &= \frac{15(n+1)}{56}-\frac{k^2+7kt+34k+6t^2+6t}{168(k+t)}, \\ &< \frac{15(n+1)}{56}. \end{aligned}$$

Final Case: By Cases (i)-(iii), we may assume that every vertex of degree 1 in G is adjacent to a vertex of degree 2, and further, every vertex of degree 2 in G is adjacent to both a vertex of degree 1 and a vertex of degree at least 3. Thus, every vertex with degree 1 or 2 is contained in a system of G.

Note that if G is a (t,t)-system then $n = 2t+1$ and $R_{-1}(G) < \frac{15(n+1)}{56}$. Thus, any $(t,s+t)$-system of G (with $s \neq 1$) must have $s \geq 2$, $s+t \leq 13$ and $t \leq 3$, by Cases (iv) and (v). Any $(t,s+t)$-system with $s=1$ belongs to a (k,t,d)-system of G.
Any $(k,t,s+k)$-system of G must have $2 \leq t \leq 3$ by Cases (ii) and (v):

- $t=3$: For $(k,3,d)$-systems, we must have $d \geq 15$, by Case (vi). Note that if $d=k$, then the graph is a $(k,3,k)$-system which has $R_{-1}(G) \leq \frac{15(n+1)}{56}$.
- $t=2$: Note that if the graph is a $(k,2,k)$-system then $R_{-1}(G) < \frac{15}{56}(n+1)$. If G has a $(1,2,2)$-system, then the center of this system has degree 2 forcing G to be a $(3,3)$-system (which has $R_{-1}(G) < \frac{15}{56}(n+1)$). Thus, for $(k,2,s+k)$-systems, by Case (vii) we must have $s \geq 2$.

Thus, in G, the center vertex of a $(k,2,d)$-system and $(k',3,d)$-system may coincide, as with the center vertex of a $(k,2,d)$-system and a (t,d)-system (but not a $(k,3,d)$-system and (t,d)-system).

We can partition the vertices of the graph G so as to separate the systems. By Case (0), G has at least one system.

- Let A_1 be the collection of centers of $(1, d)$-systems with $3 \leq d \leq 13$ that do not share a center with any $(2, d)$-system or (k, t, d)-system.
- Let A_2 be the collection of centers of $(2, d)$-systems with $4 \leq d \leq 13$ that do not share a center with any $(3, d)$-system or (k, t, d)-system.
- Let A_3 be the collection of centers of $(3, d)$-systems with $5 \leq d \leq 13$ that do not share a center with any (k, t, d)-system.
- For $k \geq 1$, let B_k be the collection of centers of $(k, 2, d)$-systems with $d \geq k+2$ that do not share a center with any $(k+1, 2, d)$-system, $(k', 3, d)$-system or any (i, d)-system, for $k', i \geq 1$.
- For $k \geq 1$, let C_k be the collection of centers of $(k, 3, d)$-systems with $d \geq k+1$ that do not share a center with any $(k+1, 3, d)$-system or $(k', 2, d)$-system, for $k' \geq 1$.
- For $k_1, k_2 \geq 1$, let D_{k_1,k_2} be the collection of centers R, such that both a $(k_1, 2, d)$-system and a $(k_2, 3, d)$-system have center R, but R is not the center of a $(k_1+1, 2, d)$-system or a $(k_2+1, 3, d)$-system.
- For $i \in [1, 3]$ and $k \in [1, 13-i]$, let E_k^i be the collection of centers R such that both a $(k, 2, d)$-system and (i, d)-system have center R, but R is not the center of a $(k+1, 2, d)$-system or a $(i+1, d)$-system.

The above sets provide a partition of G into its systems. If z is the center of a system of G, then either z appears in exactly one set described above, or z is the center of a $(t, t+1)$-system that belongs to a (k, t, d)-system (whose center belongs to exactly one set described above). Let Q be the vertices of G that are have degree at least 3 and are not the center of a system of G. Then,

$$n = |Q| + 3|A_1| + 5|A_2| + 7|A_3| + \sum_{k\geq 1}(5k+1)|B_k| + \sum_{k\geq 1}(7k+1)|C_k| +$$

$$\sum_{k_1\geq 1}\sum_{k_2\geq 1}(5k_1+7k_2+1)|D_{k_1,k_2}| + \sum_{k=1}^{12}(5k+3)|E_k^1| + \sum_{k=1}^{11}(5k+5)|E_k^2| + \sum_{k=1}^{10}(5k+7)|E_k^3|.$$

By using (6), we will count the weight on each vertex of G. If S is a subset of vertices of G, we write $w(S)$ to denote the sum of the weights of the vertices in S.

Let $y \in Q$. Then y cannot be adjacent to degree 1 or 2 vertices, thus,

$$w(y) \leq \frac{1}{2d_y}\sum_{\substack{x \\ x\sim y}}\frac{1}{3} = \frac{1}{6} < \frac{15}{56}.$$

Let $y \in A_1$ and S_y be the set of vertices of the $(1, d_y)$-system with center y. As $d_y \geq 3$, counting the weight on the degree 1 vertex, degree 2 vertex, and y respectively, gives

$$\frac{w(S_y)}{3} \leq \frac{1}{3}\left[\frac{1}{4} + \frac{1}{4}\left(\frac{1}{d_y}+1\right) + \frac{1}{2d_y}\left(\frac{1}{2}+\frac{d_y-1}{3}\right)\right] = \frac{2d_y+1}{9d_y} < \frac{15}{56}.$$

Let $y \in A_2$ and S_y be the set of vertices of the $(2, d_y)$-system with center y. As $d_y \geq 4$,

$$\frac{w(S_y)}{5} \leq \frac{1}{5}\left[2\left(\frac{1}{4}+\frac{1}{4}\left(\frac{1}{d_y}+1\right)\right)+\frac{1}{2d_y}\left(1+\frac{d_y-2}{3}\right)\right] = \frac{7d_y+4}{30d_y} < \frac{15}{56}.$$

Let $y \in A_3$ and S_y be the set of vertices of the $(3, d_y)$-system with center y. As $d_y \geq 5$,

$$\frac{w(S_y)}{7} \leq \frac{1}{7}\left[3\left(\frac{1}{4}+\frac{1}{4}\left(\frac{1}{d_y}+1\right)\right)+\frac{1}{2d_y}\left(\frac{3}{2}+\frac{d_y-3}{3}\right)\right] = \frac{5d_y+3}{21d_y} < \frac{15}{56}.$$

Let $y \in B_k$ and S_y be the set of vertices of the $(k, 2, d_y)$-system with center y. Then

$$\frac{w(S_y)}{5k+1} \quad \leq \quad \frac{1}{5k+1}\left[k\left(\frac{7}{6}+\frac{1}{6}\left(1+\frac{1}{d_y}\right)\right)+\frac{1}{2d_y}\left(\frac{k}{3}+\frac{d_y-k}{3}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k+1}-\frac{15}{56} \quad \leq \quad \frac{28k-17d_y-kd_y}{168(5k+1)d_y}.$$

As $d_y \geq k+2$, we have that $28k-17d_y-kd_y \leq -(k^2-9k+34)$. When $k=4$ or $k=5$ we have $k^2-9k+34=14$. Hence, $\frac{w(S_y)}{5k+1} < \frac{15}{56}$.

Let $y \in C_k$ and S_y be the set of vertices of the $(k, 3, d_y)$-system with center y. Then,

$$\frac{w(S_y)}{7k+1} \quad \leq \quad \frac{1}{7k+1}\left[k\left(\frac{27}{16}+\frac{1}{8}\left(\frac{3}{2}+\frac{1}{d_y}\right)\right)+\frac{1}{2d_y}\left(\frac{k}{4}+\frac{d_y-k}{3}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{7k+1}-\frac{15}{56} \quad \leq \quad \frac{14k-17d_y}{168(7k+1)d_y}.$$

As $d_y \geq k$, we have that $\frac{w(S_y)}{7k+1} < \frac{15}{56}$.

Let $y \in D_{k_1,k_2}$ and S_y be the set of vertices of the $(k_1, 2, d_y)$-system and $(k_2, 3, d_y)$-system with center y. Then,

$$\begin{aligned}\frac{w(S_y)}{5k_1+7k_2+1} \quad \leq \quad & \frac{1}{5k_1+7k_2+1}\left[k_1\left(\frac{4}{3}+\frac{1}{6d_y}\right)+k_2\left(\frac{15}{8}+\frac{1}{8d_y}\right)\right.\\ & \left.+\frac{1}{2d_y}\left(\frac{k_1}{3}+\frac{k_2}{4}+\frac{d_y-k_1-k_2}{3}\right)\right].\end{aligned}$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k_1+7k_2+1}-\frac{15}{56} \quad \leq \quad -\frac{d_yk_1-28k_1-14k_2+17d_y}{168(5k_1+7k_2+1)d_y}.$$

As $d_y \geq k_1+k_2$, we have

$$d_yk_1-28k_1-14k_2+17d_y \geq k_1^2+k_1k_2+3k_2-11k_1.$$

But $k_2 \geq 15 - k_1$, so

$$k_1^2 + k_1k_2 + 3k_2 - 11k_1 \geq k_1 + 45 > 0.$$

Hence, $\frac{w(S_y)}{5k_1+7k_2+1} < \frac{15}{56}$.

Fix $t \in [1,3]$. Let $y \in E_k^t$ and S_y be the set of vertices of the $(k, 2, d_y)$-system and (t, d_y)-system with center y. Then,

$$\frac{w(S_y)}{5k+2t+1} \quad \leq \quad \frac{1}{5k+2t+1}\left[k\left(\frac{4}{3}+\frac{1}{6d_y}\right)+t\left(\frac{1}{2}+\frac{1}{4d_y}\right)+\frac{1}{2d_y}\left(\frac{d_y-t}{3}+\frac{t}{2}\right)\right].$$

By subtracting $\frac{15}{56}$ from both sides, the right hand side factors as

$$\frac{w(S_y)}{5k+2t+1} - \frac{15}{56} \quad \leq \quad -\frac{kd_y - 28k + 6td_y - 56t + 17d_y}{168(5k+2t+1)d_y}.$$

Since $d_y = k + t + s$ with $s \geq 2$ (by Case (viii)), a simple check verifies that for $t \in [1,3]$, $k \in [1, 13-t]$ and $s \in [2, 13-t-k]$, then

$$kd_y - 28k + 6td_y - 56t + 17d_y > 0.$$

Hence, $\frac{w(S_y)}{5k+2t+1} < \frac{15}{56}$.

It now follows that $R_{-1}(G) \leq \frac{15}{56}(n+1)$, by summing the weights on each set of vertices in the partition of G. □

Note that by starting the induction at a higher value of n and using some careful consideration, we may improve the bound in Theorem 6 to $\frac{15n+C}{56}$, for some constant $C < 15$. In [19], it is noted there are trees T of every order n such that $R_{-1}(T) = \frac{15}{56}n + O(1)$.

Observe that using $\frac{n}{4}$ instead of $\frac{15(n+1)}{56}$, then Cases (0)-(iii) in the proof of Theorem 6 hold. Thus, we can improve the upper bound in the case that G has no suspended paths.

Observation 7. *Let G be a connected graph on $n \geq 3$ vertices. If G has no suspended paths, then*

$$R_{-1}(G) \leq \frac{n}{4}.$$

We next look at the effect that edge deletion has on $R_{-1}(G)$. If G is a graph and e is an edge of G, we denote by $G - e$ the graph obtained by removing the edge e from G. We call an edge $e = xy$ a *leaf* of G, if either $d_x = 1$ or $d_y = 1$, and a *non-leaf* edge otherwise. Note that deleting a leaf edge of G creates an isolated vertex, thus, in the next two results we assume the edge being deleted is a non-leaf edge.

Lemma 8. *[16, Lemma 3.3] Let G be a graph and let e be an edge whose weight is minimal over all edges in G. If e is a non-leaf edge, then*

$$R_{-1}(G - e) > R_{-1}(G).$$

In the next theorem we determine the maximum change that can occur when deleting an edge.

Theorem 9. *Let G be a graph and let e be a non-leaf edge of G, then*

$$R_{-1}(G) - \frac{1}{4} < R_{-1}(G-e) \leq R_{-1}(G) + \frac{3}{4}.$$

Furthermore, if $G-e$ is connected, then

$$R_{-1}(G-e) \leq R_{-1}(G) + \frac{7}{18}.$$

Proof. Let $e = uv$ and d_u denote d_u^G and d_v denote d_v^G. As e is a non-leaf edge, we have $d_u, d_v \geq 2$. Then

$$R_{-1}(G) - R_{-1}(G-e) = \frac{1}{d_u d_v} - \frac{1}{d_u(d_u-1)} \sum_{\substack{i \neq v \\ i \sim u}} \frac{1}{d_i} - \frac{1}{d_v(d_v-1)} \sum_{\substack{i \neq u \\ i \sim v}} \frac{1}{d_i}.$$

Thus,

$$R_{-1}(G) - R_{-1}(G-e) < \frac{1}{d_u d_v} \leq \frac{1}{4},$$

which gives the first inequality. Similarly, as $d_i \geq 1$,

$$R_{-1}(G) - R_{-1}(G-e) \quad \geq \quad \frac{1}{d_u d_v} - \frac{1}{d_u} - \frac{1}{d_v}.$$

It is not too hard to see that over the integers and for $d_u, d_v \geq 2$, the right hand side is minimal when $d_u = d_v = 2$. Hence,

$$R_{-1}(G) - R_{-1}(G-e) \geq \frac{-3}{4}.$$

If $G-e$ is connected, then there are vertices $\hat{i} \neq v$, $\hat{j} \neq u$ (with possibly $\hat{i} = \hat{j}$) such that $\hat{i} \sim u$, $\hat{j} \sim v$, $d_{\hat{i}} > 1$ and $d_{\hat{j}} > 1$. Thus,

$$R_{-1}(G) - R_{-1}(G-e) \geq \frac{1}{d_u d_v} - \frac{1}{2d_u(d_u-1)} - \frac{d_u-2}{d_u(d_u-1)} - \frac{1}{2d_v(d_v-1)} - \frac{d_v-2}{d_v(d_v-1)}.$$

It is not too hard to see that over the integers and for $d_u, d_v \geq 2$, the right hand side is minimal when $d_u = d_v = 3$. Hence, in the case that $G-e$ is connected,

$$R_{-1}(G) - R_{-1}(G-e) \geq \frac{-7}{18}.$$

□

We illustrate the sharpness of Theorem 9 with three examples.

1. Let G be the path on 4 vertices which has $R_{-1}(G) = 1.25$. Removing the non-leaf edge e of G gives a disconnected graph with $R_{-1}(G-e) = 2$. Thus, in this case, $R_{-1}(G-e) = R_{-1}(G) + \frac{3}{4}$.
2. Let $\hat{G}$ be the path $x_1 x_2 \cdots x_7$ on 7 vertices, and add the edge $e = x_2 x_6$ to form a graph G. Then $\hat{G} = G - e$ is connected and $R_{-1}(G-e) = R_{-1}(G) + \frac{7}{18}$.
3. Let G be the graph of order n composed of a K_{n-2} with a triangle xyz attached to a vertex z of the K_{n-2}. Then using the edge $e = xy$, we have, $R_{-1}(G) - R_{-1}(G-e) = \frac{1}{4} - \frac{1}{n-1}$. By taking $n \to \infty$, the right hand side can be made arbitrarily close to $\frac{1}{4}$.

3. Bounds on the $\mathcal{L}$-energy of a graph

Recall that the $\mathcal{L}$-*energy* of a graph G is

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\lambda_i(\mathcal{L}) - 1|.$$

Using Lemma 1 along with the results in Section 2, bounds can be derived on the $\mathcal{L}$-energy of a graph. If G has k connected components, in particular, $G_1, G_2, \ldots, G_k$, then

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{k} E_{\mathcal{L}}(G_i). \tag{7}$$

We first provide a bound on the $\mathcal{L}$-energy of a graph with k connected components.

Lemma 10. *Let G be a graph of order n with k connected components and no isolated vertices. Then*

$$E_{\mathcal{L}}(G) \leq k + \sqrt{(n-k)(2R_{-1}(G) - k)}.$$

Proof. Note that 1 is an eigenvalue of $I - \mathcal{L}$ with multiplicity k, hence,

$$E_{\mathcal{L}}(G) = k + \sum_{i=1}^{n-k} |\lambda_i(I - \mathcal{L})|.$$

By the Cauchy-Schwartz inequality (using vectors $(1, \ldots, 1)^T$ and $(|\lambda_1(I-\mathcal{L})|, \ldots, |\lambda_{n-k}(I-L)|)^T$) we obtain the upper bound

$$E_{\mathcal{L}}(G) \quad \leq \quad k + \sqrt{(n-k) \sum_{i=1}^{n-k} [\lambda_i(I - \mathcal{L})]^2}.$$

The result now follows by (5). □

We next provide bounds on the $\mathcal{L}$-energy in terms of the minimum and maximum degrees of G.

Corollary 11. *Let G be a graph of order n with k connected components and no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$\frac{n}{n-1} \leq \frac{n}{d_{\max}} \leq E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{d_{\min}}} \leq n.$$

Furthermore,

$$E_{\mathcal{L}}(G) \geq 2k.$$

Proof. Lemma 1 and Theorem 2 gives the first string of inequalities. For the last inequality, by (7), it suffices to prove $E_{\mathcal{L}}(G) \geq 2k$ in the case that $k = 1$. Note that $\lambda_n(I - \mathcal{L}) = 1$, and the trace of $I - \mathcal{L}$ is 0. Thus,

$$E_{\mathcal{L}}(G) = 1 + \sum_{i=1}^{n-1} |\lambda_i(I - \mathcal{L})| \geq 1 + \left| \sum_{i=1}^{n-1} \lambda_i(I - \mathcal{L}) \right| = 1 + |-1| = 2. \tag{8}$$

□

Note that if G is a regular graph of degree r then

$$\frac{n}{r} \leq E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{r}}.$$

Over the graphs of order n with no isolated vertices, we characterize those that have maximal and minimal $\mathcal{L}$-energy.

Corollary 12. *Let G be a graph of order n with no isolated vertices. Then*

$$E_{\mathcal{L}}(G) \geq 2,$$

with equality if and only if G is a complete multipartite graph. Further,

$$E_{\mathcal{L}}(G) \leq 2\lfloor n/2 \rfloor,$$

with equality only for the following cases:

(i) n is even and G is the disjoint union of $n/2$ paths of length 1, or

(ii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and one path of length 2, or

(iii) n is odd and G is the disjoint union of $(n-3)/2$ paths of length 1 and a complete graph on 3 vertices.

Proof. Equality in (8) occurs if and only if $\lambda_{n-1}(I - \mathcal{L}) \leq 0$, (equivalently $\lambda_{n-1}(A) \leq 0$). It is known that the adjacency matrix of G has only one positive eigenvalue if and only if G is a complete multipartite graph plus isolated vertices (see [5]).

By Theorem 2, we have $E_{\mathcal{L}}(G) \leq n$. It can be seen that for equality to hold we must have $R_{-1}(G) = n/2$ and G must be regular of degree 1. Thus, G is the disjoint union of $n/2$ paths of length 1, which indeed has $E_{\mathcal{L}}(G) = n$.

Note that both the path of length 2 and the complete graph on 3 vertices have energy 2. Hence, if n is odd, the graphs described in (*ii*) and (*iii*) have energy $n-1$. It is easy to see that if n is odd and $E_{\mathcal{L}}(G) = n-1$, then any even connected component of G must have size 2. If there is an odd connected component $\hat{G}$ of G of size $k \geq 7$, then by Lemma 1 and Theorem 6, $E_{\mathcal{L}}(\hat{G}) < k-1$. If there is a connected component $\hat{G}$ of order 5, and if $\hat{G}$ has no suspended paths, then by Lemma 1 and Observation 7, $E_{\mathcal{L}}(\hat{G}) < 4$. If $\hat{G}$ is of order 5 and has a suspended path, then there are only three such graphs and each has $E_{\mathcal{L}}(\hat{G}) < 4$. Hence, any odd connected component must be of order 3, and since $E_{\mathcal{L}}(G) = n-1$ there can only be one such odd connected component. □

The upper bound in Corollary 12 can be improved for connected graphs by using Lemma 1 and Theorem 6.

Corollary 13. *If G is a connected graph on $n \geq 3$ vertices, then*

$$E_{\mathcal{L}}(G) < \sqrt{\frac{15}{28}}(n+1) < 0.732(n+1).$$

Furthermore, if G has no suspended paths (or more generally, $R_{-1}(G) \leq \frac{n}{4}$), then

$$E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{2}} < 0.7072\ n.$$

One might suspect that over the connected graphs that the path has maximal $\mathcal{L}$-energy, but in general, this is not true. We next provide some common classes of graphs along with their corresponding $\mathcal{L}$-energy.

Example 14. *Let G be a path on n vertices. Using the eigenvalues of $\mathcal{L}$ (see [3]) we get that*

$$E_{\mathcal{L}}(G) = 2 \sum_{k=0}^{\lfloor (n-1)/2 \rfloor} \cos(k\pi/(n-1)).$$

By [7, page 37],

$$\sum_{k=0}^{N} \cos(kx) = \cos\left(\frac{Nx}{2}\right) \sin\left(\frac{N+1}{2}x\right) \csc\left(\frac{x}{2}\right).$$

Thus, for the path, $E_{\mathcal{L}}(G) \sim \frac{2}{\pi}n$.

Example 15. *(a) For n odd, let G be a (t,t)-system with $n = 2t+1$ vertices. The normalized Laplacian matrix of G can be written in block form as*

$$\mathcal{L} = \begin{bmatrix} I_t & -\frac{1}{\sqrt{2}} I_t & \mathbf{0} \\ -\frac{1}{\sqrt{2}} I_t & I_t & -\frac{1}{\sqrt{2t}}\mathbf{1} \\ \mathbf{0}^T & -\frac{1}{\sqrt{2t}}\mathbf{1}^T & 1 \end{bmatrix},$$

where I_t represents the identity matrix of order t, $\mathbf{0}$ represents the 0 vector of size t and $\mathbf{1}$ represents the all ones vector of size t. Thus, the eigenvalues are 0, 1, 2, each with multiplicity 1, and $(1 \pm \frac{1}{\sqrt{2}})$ each with multiplicity $t-1$. Hence, the $\mathcal{L}$-energy is

$$E_{\mathcal{L}}(G) = \frac{n-3}{\sqrt{2}} + 2 \sim \frac{n}{\sqrt{2}}.$$

(b) For $n = 2t+2$ even, let G be the graph obtained by joining a vertex to a leaf of a (t,t)-system. The normalized Laplacian eigenvalues of this graph are 0 and 2 each with multiplicity 1, $(1 \pm \frac{1}{\sqrt{2}})$ each with multiplicity $t-2$, along with four other eigenvalues. This is enough to obtain

$$E_{\mathcal{L}}(G) \sim \frac{n}{\sqrt{2}}.$$

It should be noted that if G is a $(t,3,t)$-system with $n = 7t+1$, then using a computer to test large values of n suggests that $E_{\mathcal{L}}(G) \approx 0.671n$. Similarly, if G is a $(t,2,t)$-system with $n = 5t+1$, then using a computer to test large values of n suggests that $E_{\mathcal{L}}(G) \approx 0.648n$. These values are far from the upper bound given by Corollary 13.

For $n = 3$, the path and triangle each have maximal $\mathcal{L}$-energy 2. For $4 \le n \le 6$, the path has maximal $\mathcal{L}$-energy over the class of connected graphs. Note that for $4 \le n \le 6$, the path falls under the class of graphs described in Example 15. For $7 \le n \le 8$, a computer has verified that over all connected graphs, the class of graphs in Example 15 have maximal $\mathcal{L}$-energy. For $n \ge 9$, it is unknown which graphs have maximal $\mathcal{L}$-energy.

We know of no class of connected graphs on n vertices that has $\mathcal{L}$-energy (asymptotically) larger than $\frac{n}{\sqrt{2}}$. Corollary 13 implies such a graph G would have $R_{-1}(G) > \frac{n}{4}$ and

Observation 7 suggests such a graph should have a large number of suspended paths. We ask the question: Over the connected graphs G of order n, is $E_{\mathcal{L}}(G) \leq \frac{n}{\sqrt{2}} + C$, for some suitable constant C?

We now look at other bounds on $\mathcal{L}$-energy.

Theorem 16. *Let G be a graph of order n with no isolated vertices and let $\Delta = \det(I - \mathcal{L})$. Then*

$$E_{\mathcal{L}}(G) \geq \sqrt{2R_{-1}(G) + n(n-1)\Delta^{2/n}}.$$

Proof. For convenience, we use λ_i to denote $\lambda_i(\mathcal{L})$. Note that

$$E_{\mathcal{L}}(G)^2 \quad = \quad 2R_{-1}(G) + \sum_{i \neq j} |1 - \lambda_i||1 - \lambda_j|.$$

By the arithmetic-geometric mean inequality,

$$\frac{1}{n(n-1)} \sum_{i \neq j} |1 - \lambda_i||1 - \lambda_j| \geq \left(\prod_{i \neq j} |1 - \lambda_i||1 - \lambda_j| \right)^{\frac{1}{n(n-1)}} = \Delta^{2/n}.$$

Hence, the result now follows. □

We next relate the $\mathcal{L}$-energy of a graph G to its A-energy, where A is the adjacency matrix of G. Recall that the A-energy is simply

$$E_A(G) = \sum_{i=1}^{n} |\lambda_i(A)|.$$

This quantity has been well studied by a large number of authors (see, for example, [9]).

Theorem 17. *Let G be a graph of order n with no isolated vertices. Suppose $d_{\min}$ and $d_{\max}$ are the minimum and maximum vertex degrees of G, respectively. Then,*

$$d_{\min} E_{\mathcal{L}}(G) \leq E_A(G) \leq d_{\max} E_{\mathcal{L}}(G).$$

Proof. The proof uses a Theorem due to Ostrowski [12, Theorem 4.5.9]. As $D^{-1/2}$ is nonsingular, for each $k = 1, 2, \ldots, n$, there is a positive real number θ_k such that

$$\frac{1}{d_{\max}} = \lambda_1(D^{-1}) \leq \theta_k \leq \lambda_n(D^{-1}) = \frac{1}{d_{\min}}$$

and

$$\lambda_k(I - \mathcal{L}) = \theta_k \lambda_k(A).$$

Thus,

$$E_{\mathcal{L}}(G) = \sum_{k=1}^{n} \theta_k |\lambda_k(A)|,$$

from which the result now follows. □

Theorem 17 implies that if G is a regular graph of degree r, then $E_A(G) = rE_{\mathcal{L}}(G)$. Since $E_A(G)$ is well studied, many bounds for $E_A(G)$ in the literature can be applied to $E_{\mathcal{L}}(G)$ by way of Theorem 17.

We now look at the effect edge deletion has on $E_{\mathcal{L}}(G)$. We begin with examples to show that $\mathcal{L}$-energy can increase, decrease or remain unchanged upon edge deletion. The examples will also illustrate that the effect edge deletion has on the general Randić index does not necessarily provide direct information about the effect edge deletion has on $\mathcal{L}$-energy.

Example 18. *In this example, we list the $\mathcal{L}$-energy and Randić index (to three decimal places if appropriate) for each graph in Figures 3, 4 and 5.*

(i) The graphs in Figure 3 have a decrease in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second and third) graph, $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.457$ (resp. $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.618$ and $2 = E_{\mathcal{L}}(G-e) < E_{\mathcal{L}}(G) \approx 2.704$). For the first (resp. second and third) graph, $1 = R_{-1}(G-e) > R_{-1}(G) \approx 0.917$ (resp. $R_{-1}(G-e) = R_{-1}(G) = 1$ and $1 = R_{-1}(G-e) < R_{-1}(G) = 1.05$).

(ii) The graphs in Figure 4 have an increase in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second and third) graph, $2.869 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) \approx 2.667$ (resp. $3.076 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) \approx 2.904$ and $3.117 \approx E_{\mathcal{L}}(G-e) > E_{\mathcal{L}}(G) = 3$). For the first (resp. second and third) graph, $1.111 \approx R_{-1}(G-e) > R_{-1}(G) \approx 1.028$ (resp. $R_{-1}(G-e) = R_{-1}(G) \approx 1.007$ and $0.928 \approx R_{-1}(G-e) < R_{-1}(G) \approx 0.978$).

(iii) The graphs in Figure 5 have no change in $\mathcal{L}$-energy upon deleting edge e. For the first (resp. second) graph, $E_{\mathcal{L}}(G-e) = E_{\mathcal{L}}(G) = 2$ (resp. $E_{\mathcal{L}}(G-e) = E_{\mathcal{L}}(G) \approx 2.781$). For the first (resp. second) graph, $1 = R_{-1}(G-e) > R_{-1}(G) = 0.75$ (resp. $R_{-1}(G-e) = R_{-1}(G) = 1.0625$). We are not aware of a graph G, where upon edge deletion, $\mathcal{L}$-energy remains constant while $R_{-1}(G)$ decreases.

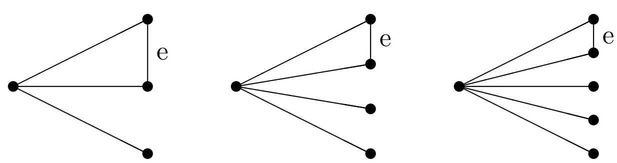

Figure 3: $\mathcal{L}$-energy decreases upon deleting edge e.

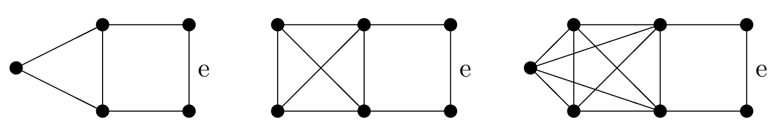

Figure 4: $\mathcal{L}$-energy increases upon deleting edge e.

The next result provides a bound on how much the $\mathcal{L}$-energy can change upon edge deletion.

Theorem 19. *Let G be a graph of order n without isolated vertices and let e be a non-leaf edge of G. Then,*

$$|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq 2\sqrt{\frac{13}{2} - 4\sqrt{2}} \leq 1.8366.$$

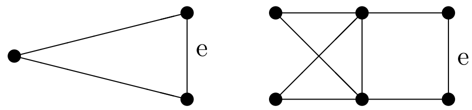

Figure 5: $\mathcal{L}$-energy remains constant upon deleting edge e.

Proof. Let $\mathcal{L}_G$ and $\mathcal{L}_{G-e}$ be the normalized Laplacian matrices of G and $G-e$, and suppose $e = xy$. Let $C = \mathcal{L}_G - \mathcal{L}_{G-e}$. Observe that by [6] (namely $\sum \sigma_i(A+B) \leq \sum \sigma_i(A) + \sum \sigma_i(B)$), we can derive

$$|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq \sum_{i=1}^{n} \sigma_i(C).$$

Note that $rank(C) \leq 4$. Let the eigenvalues of C be 0 with multiplicity $n-4$ and $\lambda_1, \lambda_2, \lambda_3, \lambda_4$.Then,

$$\sum_{i=1}^{n} \sigma_i(C) = |\lambda_1| + |\lambda_2| + |\lambda_3| + |\lambda_4|.$$

By the Cauchy-Schwartz inequality, $|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq 2\sqrt{tr(C^2)}$, which equals:

$$2\sqrt{2}\sqrt{\left(\frac{1}{\sqrt{d_x d_y}}\right)^2 + \sum_{\substack{j \neq y \\ j \sim x}} \left(\frac{1}{\sqrt{d_x d_j}} - \frac{1}{\sqrt{(d_x-1)d_j}}\right)^2 + \sum_{\substack{j \neq x \\ j \sim y}} \left(\frac{1}{\sqrt{d_y d_j}} - \frac{1}{\sqrt{(d_y-1)d_j}}\right)^2},$$

$$\leq 2\sqrt{2}\sqrt{\frac{1}{4} + \frac{\left(\sqrt{d_x-1} - \sqrt{d_x}\right)^2}{d_x} + \frac{\left(\sqrt{d_y-1} - \sqrt{d_y}\right)^2}{d_y}}.$$

The $\frac{1}{4}$ comes from setting $d_x = d_y = 2$, as this is when the first term is maximal, and the other two expressions come from noticing $d_j \geq 1$. The function

$$f(x) = \frac{\left(\sqrt{x-1} - \sqrt{x}\right)^2}{x}$$

has $f'(x) < 0$, for $x > 1$. Thus, as $d_x, d_y \geq 2$, $|E_{\mathcal{L}}(G) - E_{\mathcal{L}}(G-e)| \leq 2\sqrt{\frac{13}{2} - 4\sqrt{2}}$. □

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