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GRAPHS WITH SMALL SPECTRAL GAP[*]

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Abstract. It is conjectured that connected graphs with given number of vertices and minimum spectral gap (i.e., the difference between their two largest eigenvalues) are double kite graphs. The conjecture is confirmed for connected graphs with at most 10 vertices, and, using variable neighbourhood metaheuristic, there is evidence that it is true for graphs with at most 15 vertices. Several spectral properties of double kite graphs are obtained, including the equations for their first two eigenvalues. No counterexamples to the conjecture are obtained. Some numerical computations and comparisons that indicate its correctness are also given. Next, 3 lower and 3 upper bounds on spectral gap are derived, and some spectral and structural properties of the graphs that minimize the spectral gap are given. At the end, it is shown that in connected graphs any double kite graph has a unique spectrum.

1. Introduction. All graphs considered are simple and undirected. For a graph G, $n = n(G)$ and $m = m(G)$ as usual denote its order (the number of vertices) and size (the number of edges). If $A = A(G)$ is the adjacency matrix of G, then the eigenvalues of G, $\lambda_1 = \lambda_1(G) \geq \lambda_2 = \lambda_2(G) \geq \cdots \geq \lambda_n = \lambda_n(G)$, are just the eigenvalues of $A(G)$. The difference between the first two eigenvalues $\delta(G) = \lambda_1(G) - \lambda_2(G)$ will be called the *spectral gap* of G (it is also called the *separator* of G), while the first eigenvalue is usually called the *index* of G, and if G is connected then $\lambda_1(G) > \lambda_2(G)$, i.e., $\delta(G) > 0$. Due to this property we shall assume that the graph considered is connected. Eigenvectors that correspond to the first two eigenvalues will be denoted by $x = (x_1, x_2, \ldots, x_n)^T$ and $y = (y_1, y_2, \ldots, y_n)^T$, respectively. Note that x can be taken to be positive whenever G is connected. In addition, if $x^T x = 1$ then x is called the *principal eigenvector* of G.

For two graphs G_1 and G_2 we define $G_1 \cup G_2$ to be their disjoint union, while pG denotes disjoint union of p copies of G. The join $G_1 \nabla G_2$ is a graph obtained by joining every vertex of G_1 with every vertex of G_2. The line graph $L(G)$ is a

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ELA

http://math.technion.ac.il/iic/ela

418   Z. Stanić

graph whose vertices are the edges of G with two vertices being adjacent whenever the corresponding edges in G are incident with the same vertex. In this case, we say that G is the *root* graph of $L(G)$.

For other notions not defined in this paper, the reader is referred to [6, 7].

The spectral gap is mainly investigated for the class of (connected) regular graphs since it is known that regular graphs with large spectral gap have high connectivity properties which make them relevant in several branches of theoretical computer sciences (see [7, pp. 392–394] and the references cited therein). Conversely, in this paper, we consider graphs with small spectral gap. In the next section, we conjecture that the minimum spectral gap is attained for the *double kite graphs*. The double kite graph is obtained by taking an $(l + 2)$-vertex path P_{l+2} $(l \geq 0)$, two copies of a k-vertex complete graph K_k $(k \geq 1)$, and by identifying one terminal vertex of P_{l+2} with a vertex of one copy of K_k and the other terminal vertex with a vertex of the other copy of K_k (see Fig. 1 in the next section). This graph will be denoted by $DK(k,l)$ and it has $n = 2k + l$ vertices and $m = 2\binom{k}{2} + l + 1$ edges. Note that $DK(1,l)$ and $DK(2,l)$ are isomorphic to paths P_{l+2} and P_{l+4}, respectively.

We indicate some similarities between the spectral gap and the algebraic connectivity, which is defined as the second smallest eigenvalue of the Laplacian of a graph. This invariant is very frequently investigated – see the survey [1] and the corresponding references. It is known that for regular graphs the algebraic connectivity coincides with the spectral gap, and connected regular graphs of degree 3 with minimum algebraic connectivity (and therefore, minimum spectral gap) are determined in [4]. It is conjectured in [2] that the graphs with given order and size and minimum algebraic connectivity are so-called path-complete graphs defined as follows: They consist of a complete graph, a path, and one or several edges joining one endvertex of the path with one or several vertices of the complete graph. It is proved in [11] that for trees with given order and diameter the algebraic connectivity is minimized for paths with stars of (almost) equal size attached to both ends. Notice that the graphs conjectured in [2] have obvious similarity to double kite graphs, while the resulting graphs of [11] with equal stars are in fact the root graphs of double kite graphs.

The paper is organized as follows. In Section 2, we derive the equations for the first two eigenvalues of double kite graphs along with some spectral properties, inequalities, and numerical data. In Section 3, we obtain 3 lower bounds on spectral gap in terms of order and size, and another 3 upper bounds in terms of coordinates of the corresponding principal eigenvector. We also give some structural and spectral properties of graphs that minimize the spectral gap. In Section 4, we prove that in connected graphs any double kite graph has a unique spectrum.

ELA

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2. Spectral gap of double kite graphs. We start with the following conjecture.

CONJECTURE 2.1. *Of all connected graphs with given number of vertices, the spectral gap is minimized for some double kite graph.*

REMARK 2.2. The conjecture is based on underlying results confirmed by use of computer, some spectral properties of double kite graphs obtained in Propositions 2.3 and 2.6, and numerical data given in Table 1.

We used the library of programs Nauty [15] to generate the graphs and confirm the conjecture for those with at most 10 vertices.

Seeking counterexamples we used the facilities of the AutoGraphiX system [12] (an efficient tool based on a variable neighbourhood search metaheuristic for producing extremal graphs with given parameters). We applied several approaches to impose the direction to possible solutions, but we did not found any counterexample with at most 15 vertices.

In the sequel, we give the equations for the first two eigenvalues of double kite graphs, determine certain spectral properties, and conclude the section with some numerical data.

Using the eigenvalue interlacing [7, Theorem 0.10], we get that $\lambda_2(DK(k,l))$ is a simple eigenvalue greater than $k-2$; if $l>0$ then it is greater than $k-1$. We prove a proposition.

PROPOSITION 2.3. *$DK(k,l)$ is a unique graph with minimum index within the set of all connected n-vertex graphs ($n \geq 2k$) which contain (not necessarily induced) subgraph equal to either $2K_k$, or $K_1\nabla 2K_{k-1}$.*

Proof. If $k < 2$ the proof follows from the fact that within the set of all trees with given number of vertices, the path has minimum index [7, p. 78].

If $k \geq 3$ then any graph, say H, belonging to the described set contains a subgraph equal to either $K_1\nabla 2K_{k-1}$, or $DK(k,l')$ ($l' \leq l$). In the first case since both $DK(k,l)$ and H have at least $2k$ vertices, using [7, Theorem 0.7] and the result concerning the index of graphs with an internal path (cf. [13]), we get $\lambda_1(H) > \lambda_1(K_1\nabla 2K_{k-1}) > \lambda_1(D(k,l))$. In the latter case, by the same argumentation, we get $\lambda_1(H) \geq \lambda_1(DK(k,l')) \geq \lambda_1(DK(k,l))$ with the equalities iff $H = DK(k,l)$. ☐

PROPOSITION 2.4. *If $\lambda_2(DK(k,l)) > 2$ then $\lambda_1(DK(k,l))$ and $\lambda_2(DK(k,l))$ are equal to $2\cosh(2t)$ where t is respectively equal to the unique positive root of*

$$(2.1) \qquad 2(k-2)\cosh t\cosh((l+2)t) - \cosh((l+5)t) = 0$$

ELA

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420   Z. Stanić

Fig. 1: $DK(k,l)$ with vertex labelling.

and

$$(2.2) \qquad (2 - k + 2\cosh(2t)) \left(2\cosh(2t) - \frac{\sinh((l-1)t)}{\sinh((l+1)t)} \right) - k + 1 = 0.$$

Proof. Let $n = 2k + l$, and $x = (x_1, x_2, \ldots, x_n)^T$ and $y = (y_1, y_2, \ldots, y_n)^T$ be the eigenvectors which correspond to $\lambda_1 = \lambda_1(DK(k,l))$ and $\lambda_2 = \lambda_2(DK(k,l))$, respectively. Assume that the vertices are labelled as in Fig. 1, and the coordinates x_i, y_i correspond to vertex i $(i = 1, \ldots, 2k + l)$. We have

$$(2.3) \qquad \lambda_1 x_i = \sum_{i \sim j} x_j \quad \text{and} \quad \lambda_2 y_i = \sum_{i \sim j} y_j \quad (i = 1, \ldots, 2k + l).$$

In what follows, we construct the eigenvectors x and y, i.e., we determine all of their coordinates such that both equalities above hold. Using these equalities we get

$$(2.4)\ x_i - \lambda_1 x_{i+1} + x_{i+2} = 0 \ \text{ and } \ y_i - \lambda_2 y_{i+1} + y_{i+2} = 0 \ (i = k, \ldots, k + l - 1).$$

We have $x > 0$ (since it corresponds to the largest eigenvalue) and, by [6, Proposition 5.3.1], there are exactly 2 connected subgraphs of $DK(k,l)$ such that y is positive in one and negative in the other. The symmetry of the graph considered and the equalities (2.3) allow us to assume

$$(2.5) \qquad \begin{aligned} &x_1 = x_2 = \cdots = x_{k-1} = x_{k+l+2} = x_{k+l+3} = \cdots = x_{2k+l} \\ &y_1 = y_2 = \cdots = y_{k-1} = -y_{k+l+2} = -y_{k+l+3} = \cdots = -y_{2k+l}, \end{aligned}$$

and

$$(2.6) \qquad x_{k+i} = x_{k+l+1-i} \quad \text{and} \quad y_{k+i} = -y_{k+l+1-i} \quad \left(i = 0, \ldots, \left\lfloor \frac{l}{2} \right\rfloor \right).$$

Since any eigenvector is determined up to a multiplying constant we can take $x_1 = \lambda_1$ and $y_1 = \lambda_2$ (it is clear that $y_1 \neq 0$). Substituting these values into (2.5) we

ELA

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get that if the equalities (2.3) hold for $1 \le i \le k - 1$ and for $k + l + 2 \le i \le 2k + l$ then

(2.7) $x_k = x_{k+l+1} = \lambda_1(\lambda_1 - k + 2)$ and $y_k = -y_{k+l+1} = \lambda_2(\lambda_2 - k + 2),$

must hold.

Consider now the remaining coordinates. Solving the systems (2.4) we get

$$x_i = a_1 r_1^{i-k+1} + b_1 r_1^{-(i-k+1)} \quad \text{and}$$
$$y_i = a_2 r_2^{i-k+1} + b_2 r_2^{-(i-k+1)} \quad (i = k, \ldots, k + l + 1),$$

where $r_j = \frac{\lambda_j + \sqrt{\lambda_j^2 - 4}}{2}$ $(j = 1, 2)$. Using (2.6) we get $b_1 = a_1 r_1^{l+3}$ and $b_2 = -a_2 r_2^{l+3}$, which yields

(2.8)
$$x_i = a_1 \left(r_1^{i-k+1} + r_1^{-(i-k-l-2)} \right) \quad \text{and}$$
$$y_i = a_2 \left(r_2^{i-k+1} - r_2^{-(i-k-l-2)} \right) \quad (i = k, \ldots, k + l + 1),$$

In particular, putting $i = k$, we get

$$x_k = a_1 \left(r_1 + r_1^{l+2} \right) \quad \text{and} \quad y_k = a_2 \left(r_2 - r_2^{l+2} \right),$$

while (2.7) gives another equalities for x_k and y_k respectively, which together with these above give

$$a_1 = \frac{\lambda_1(\lambda_1 - k + 2)}{r_1 + r_1^{l+2}} \quad \text{and} \quad a_2 = \frac{\lambda_2(\lambda_2 - k + 2)}{r_2 - r_2^{l+2}}.$$

Substituting the expression of a_1 into the first equality of (2.8), and putting $\lambda_1 = 2\cosh(2t), t > 0$ (i.e., $r_1 = e^{2t}$), we get

(2.9) $x_i = 2 \frac{e^{i-k+1} + e^{-(i-k-l-2)}}{1 + e^{l+2}} \cosh(2t)(2\cosh(2t) - k + 2)$ $(i = k, \ldots, k + l + 1).$

In this way, we obtain the solutions of the first system of (2.4). In fact, all the solutions x_i $(k + 1 \le i \le k + l)$ satisfy the first equality of (2.3). It remains to find the appropriate values of x_k and x_{k+l+1}. In this purpose, we apply (2.9) to $\lambda_1 x_k = (k - 1)\lambda_1 + x_{k+1}$, and we get that x_k is determined by a positive root of

$$\frac{e^{l+3}}{e^2(1 + e^{l+2})} \left(2(k - 2) \cosh t \cosh((l + 2)t) - \cosh((l + 5)t) \right) = 0.$$

Since $\frac{e^{l+3}}{e^2(1+e^{l+2})} > 0$, the root of the above equation is the root of (2.1), and this equation clearly has a positive real root (the left hand side is a function with a different sign in 0 and k, for example). Moreover, this is the unique positive real

$$\boxed{\textbf{ELA}}$$

root (since otherwise we would have two non-collinear eigenvectors corresponding to a simple eigenvalue). The value of x_{k+l+1} is obtained in the same way and it is equal to x_k. Therefore, we have just collected all coordinates of x corresponding to $\lambda_1 = 2\cosh(2t)$, where t is the unique positive root of (2.1), i.e., we get the first assertion of the theorem.

Substituting the expression of a_2 into the second equality of (2.8), and using the same substitutions $\lambda_2 = 2\cosh(2t)$ $(t > 0)$, $r_2 = e^{2t}$ we get the solutions of the second system of (2.4):

$$y_i = 2\frac{e^{i-k+1}-e^{-(i-k-l-2)}}{1-e^{l+2}}\cosh(2t)(2\cosh(2t) - k + 2)$$

$$(i = k, \ldots, k + l + 1).$$

Considering the coordinates y_k and y_{k+l+1} we get that the first one is determined by the unique positive root of (2.2), while $y_{k+l+1} = -y_k$, and the proof is complete. $\square$

REMARK 2.5. Notice that both functions on the left hand side of the equations (2.1) and (2.2) are even; since both eigenvalues, λ_1 and λ_2, are equal to $2\cosh(2t)$ (for the appropriate t), we get that the unique positive and the unique negative root of both equations produce the same solution for the corresponding eigenvalue. Notice also that the condition $\lambda_2(D(k,l)) > 2$ in Proposition 2.4 holds whenever $k \geq 4$ or $k = 3$, $l \geq 2$. In addition, statements of the same proposition hold even if any of the first two eigenvalues is less than 2 with caveat that in this case, t is a complex root of the corresponding equation. In this way, we allow the special case when the double kite graph reduces to a path.

Using Proposition 2.4, we prove the following results.

PROPOSITION 2.6. $\delta(DK(k,l)) > \delta(DK(k,l+1))$.

Proof. First, if $k < 3$ then the inequality is easily proven by examination of the corresponding eigenvalues of paths P_n and P_{n+1}.

If $k \geq 3$, then we have $\lambda_1(DK(k,l)) > \lambda_1(DK(k,l+1))$ [13].

Next, let $\lambda_2(DK(k,l)) = 2\cosh(2\hat{t})$. Since $\sinh((l-1)t)/\sinh((l+1)t)$ is an increasing function in $l \geq 0$ we get that

$$f(t) = (2 - k + 2\cosh(2t))\left(2\cosh(2t) - \frac{\sinh(lt)}{\sinh((l+2)t)}\right) - k + 1$$

is negative in $\hat{t}$. Moreover, f increases in $t \geq \hat{t}$ and $lim_{t\to\infty}f(t) = \infty$, which yields that f is equal to zero in some point greater than $\hat{t}$. Thus, $\lambda_2(DK(k,l)) < \lambda_2(DK(k,l+1))$.

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The above inequalities on λ_1 and λ_2 give $\delta(DK(k,l)) > \delta(DK(k,l+1))$. □

PROPOSITION 2.7. *If $k \geq 2$, then*

$$\delta(DK(k,0)) = \frac{1}{2}\left(2 - \sqrt{(k-1)(k+3)} + \sqrt{5+k(k-2)}\right).$$

Proof. For $k = 2$ we get the result by direct computation. Using the equalities $2\cosh(2t) = \lambda_j$ and $e^{2t} = \frac{\lambda_j + \sqrt{\lambda_j^2 - 4}}{2}$ $(j = 1, 2)$, and putting $l = 0$, we get the rational expressions of (2.1) and (2.2). Solving them we get

(2.10)
$$\begin{aligned}\lambda_1(DK(k,0)) &= \tfrac{1}{2}\left(\sqrt{5+k(k-2)} + k - 1\right) \quad \text{and} \\ \lambda_2(DK(k,0)) &= \tfrac{1}{2}\left(\sqrt{(k-1)(k+3)} + k - 3\right),\end{aligned}$$

and the proof follows. □

Using the last two propositions we can obtain families of double kite graphs with very small spectral gap. Numerical computation given below confirms this estimation. Before that we compare the spectral gaps of a path P_n (as we pointed out, a special case of double kite graph) and a cycle C_n.

PROPOSITION 2.8. $\delta(P_n) < \delta(C_n)$, *for any $n \geq 3$.*

Proof. Considering the first two eigenvalues of both graphs we get

(2.11) $\quad \delta(P_n) = 2\left(\cos\dfrac{\pi}{n+1} - \cos\dfrac{2\pi}{n+1}\right) \quad$ and $\quad \delta(C_n) = 2\left(1 - \cos\dfrac{2\pi}{n}\right),$

and so

$$\delta(C_n) - \delta(P_n) = 2\left(1 - \cos\frac{\pi}{n+1} + \cos\frac{2\pi}{n+1} - \cos\frac{2\pi}{n}\right) > 0$$

(since $1 > \cos\frac{\pi}{n+1}$, and $\cos\frac{2\pi}{n+1} > \cos\frac{2\pi}{n}$). □

Using the equations (2.1) and (2.2) we determine in the family of double kite graphs with at most 20 vertices those with minimum spectral gap. For $n \leq 6$ the resulting graph is P_n. For $7 \leq n \leq 9$, this is $DK(3,l)$. For $10 \leq n \leq 15$ we get $DK(4,l)$, and for $16 \leq n \leq 20$ we get $DK(5,l)$.

Note that, by Proposition 2.6, the extension of an internal path of any double kite graph (with preserving the complete subgraphs unchanged) necessarily produces the graph with smaller spectral gap. On the other hand, if two double kite graphs of different orders both minimize the spectral gap, then the larger one does not necessarily contain the longer internal path. For example, this occurs for minimizers of order 9 and 10.

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TABLE 2.1
Spectral gap of some graphs.

n	C_n	P_n	$DK(\frac{n-4}{2},4)$	$DK(\frac{n-6}{2},6)$	$DK(4,n-8)$
10	0.3820	0.2365	0.0644	0.2365	0.0640
20	0.0979	0.0665	0.0001	$7.2 \cdot 10^{-6}$	$2.7 \cdot 10^{-6}$
50	0.0158	0.0114	$3.7 \cdot 10^{-7}$	$1.1 \cdot 10^{-9}$	$1.7 \cdot 10^{-15}$
100	0.0039	0.0029	$1.5 \cdot 10^{-8}$	$1.1 \cdot 10^{-11}$	$*$
200	0.0010	0.0007	$2.3 \cdot 10^{-10}$	$7.1 \cdot 10^{-14}$	$*$
500	0.0002	0.0001	$2.1 \cdot 10^{-12}$	$*$	$*$
1000	$3.9 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$	$4.5 \cdot 10^{-13}$	$*$	$*$

Finally, using Proposition 2.4 and equations (2.11), we determine spectral gaps of some graphs with large order. The results are summarized in Table 1. The asterisk stands for a value less than 10^{-16} (very commonly used numerical precision). We note that the unique positive roots of the equations given in Proposition 2.4 are easily determined for any n (by numerical computation). On the other hand, the consideration of the characteristic polynomial of $DK(k,l)$ (its explicit form is given in Lemma 4.3 of Section 4) for the same purpose is more complicated: First it often has many positive roots, and second its two largest roots are almost equal for large n (compare Table 1), and so the rounding in numerical computation can cause possible confusions.

A graph with fixed order and minimum spectral gap may or may not have the double kite structure (some future research will show), but in any case the results of this section can be considered as a contribution to the subject of graphs with small spectral gap.

3. Bounds on spectral gap and properties of minimizers. We derive 2 lower bounds on spectral gap of arbitrary connected graph just in terms of its order and size, and another lower bound when the corresponding graph is bipartite. We also give 3 upper bounds in terms of coordinates of its principal eigenvector. All bounds are obtained by combining known bounds on λ_1 and λ_2. In the second part of this section, we give some properties of graph that minimizes the spectral gap in the family of graphs with given order.

PROPOSITION 3.1. *Let G be a connected graph on n ($n \geq 2$) vertices and m edges, then*

$$(3.1) \qquad \delta(G) > \frac{2m - \sqrt{mn(n-2)}}{n},$$

and

$$(3.2) \qquad \delta(G) \geq \frac{4m - n\sqrt{(n+2)(n-2)}}{2n} + 1.$$

Proof. We use $\lambda_1(G) \geq \frac{2m}{n}$ [18], and $\lambda_2(G) < \sqrt{m\frac{n-2}{n}}$ [5] to get

$$\delta(G) = \lambda_1(G) - \lambda_2(G) > \frac{2m}{n} - \sqrt{m\frac{n-2}{n}} = \frac{2m - \sqrt{mn(n-2)}}{n}.$$

The inequality (3.2) is obtained in the similar way by using the same lower bound on $\lambda_1(G)$ and $\lambda_2(G) \leq \frac{\sqrt{(n+2)(n-2)}}{2} - 1$ [14]. □

Comparing the bounds obtained we get that (3.2) is better than (3.1) when $m > \frac{n\left(n^2 - 4\sqrt{(n+2)(n-2)}\right)}{4(n-2)}$. Also, if n is even or G is not a regular nor semiregular bipartite then the equality in (3.2) is not attained (compare the corresponding references).

PROPOSITION 3.2. *Let G be a connected bipartite graph on n vertices and m edges, then*

$$(3.3) \qquad \delta(G) > \frac{8m - n\sqrt{n(n+4)}}{4n}.$$

Proof. We have (compare [16])

$$\lambda_2(G) \leq \begin{cases} \left\lfloor \frac{n}{4} \right\rfloor, & \text{if } n = 0 \,(\mathrm{mod}\,4) \text{ or } n = 1 \,(\mathrm{mod}\,4) \\ \sqrt{\left\lfloor \frac{n}{4} \right\rfloor \left(\left\lfloor \frac{n}{4} \right\rfloor + 1\right)}, & \text{if } n = 2 \,(\mathrm{mod}\,4) \text{ or } n = 3 \,(\mathrm{mod}\,4), \end{cases}$$

and therefore, we have $\lambda_2(G) < \sqrt{\frac{n}{4}\left(\frac{n}{4} + 1\right)}$, for any $n \geq 1$. Next, we get $\delta(G) = \lambda_1(G) - \lambda_2(G) > \frac{2m}{n} - \sqrt{\frac{n}{4}\left(\frac{n}{4} + 1\right)} = \frac{8m - n\sqrt{n(n+4)}}{4n}$. □

For bipartite graphs, (3.3) gives better estimation than (3.2) for any $n \geq 7$.

PROPOSITION 3.3. *Let G be a connected graph with distinct vertices u, v, t, and w, and let x_u, x_v, x_t, and x_w be the corresponding coordinates of its principal eigenvector.*

(i) Let G' be the graph obtained from G by replacing edges uv, tw with non-edges vw, tu. If $(x_t - x_v)(x_u - x_w) < 0$ and $\lambda_1(G) \leq \lambda_1(G')$, then

$$\delta(G) \leq \frac{(x_t - x_v)^2 + (x_u - x_w)^2}{(x_t - x_v)(x_w - x_u)}.$$

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(ii) *Let G' be the graph obtained from G by replacing edge uv with non-edge tw. If $x_t x_w - x_u x_v < 0$ and $\lambda_1(G) \leq \lambda_1(G')$, then*

$$\delta(G) \leq \frac{x_u^2 + x_v^2 + x_t^2 + x_w^2}{2(x_u x_v - x_t x_w)}.$$

(iii) *Let G' be the graph obtained from G by replacing edge uv with non-edge uw. If $x_w - x_v < 0$ and $\lambda_1(G) \leq \lambda_1(G')$, then*

$$\delta(G) \leq \frac{2x_u^2 + (x_v - x_w)^2}{2x_u(x_v - x_w)}.$$

Proof. All three statements are contrapositives of the corresponding parts of Propositions 6.4.2, 6.4.5, and 6.4.7 from [8]. □

We illustrate the previous theorem in an example.

EXAMPLE. Let G be a connected semiregular bipartite graph with n_1 (resp., n_2) vertices in the first (resp., second) colour class, and let us assume that $n_1 > n_2$. Then, the first n_1 of coordinates of its principal eigenvector are equal to $1/\sqrt{2n_1}$, while the remaining coordinates are equal to $1/\sqrt{2n_2}$. If we consider the graph G' obtained in the way described in Proposition 3.3 (iii) where u, w belong to the first colour class, and v belongs to the second then, in general case, the inequality $\lambda_1(G) \leq \lambda_1(G')$ may or may not hold, but if it does hold then we have

$$\delta(G) \leq \frac{n_1 - 2\sqrt{n_1 n_2} + 3n_2}{2\sqrt{n_1 n_2} - 2n_2},$$

which can be good estimation in some cases.

From now on, H_n will denote a graph with minimum spectral gap in the family of connected graphs with n vertices. Since the minimizers of order at most 10 are determined by computer search, we also assume that $n > 10$.

PROPOSITION 3.4. *H_n has less than $\frac{n\sqrt{(n+2)(n-2)}}{4}$ edges.*

Proof. Assume that H_n has at least $\frac{n\sqrt{(n+2)(n-2)}}{4}$ edges. Substituting this expression for m into (3.2) we get

$$\delta(H_n) \quad \geq \frac{4m - n\sqrt{(n+2)(n-2)}}{2n} + 1 \geq \frac{4(\frac{n\sqrt{(n+2)(n-2)}}{4}) - n\sqrt{(n+2)(n-2)}}{2n} + 1 = 1$$

$$> \delta(DK(3,4)) > \delta(DK(3, n-6)),$$

where the last two inequalities follow from Table 1, and Proposition 2.6, respectively. A contradiction. □

PROPOSITION 3.5. *If H_n is bipartite then it has less than $\frac{n\left(1 + \sqrt{n(n+4)}\right)}{8}$ edges.*

ELA

Proof. Assume that H_n has at least $\frac{n\left(1+\sqrt{n(n+4)}\right)}{8}$ edges. Substituting this expression for m into (3.3) we get

$$
\begin{aligned}
\delta(H_n) \quad &> \frac{8m-n\sqrt{n(n+4)}}{4n} \geq \frac{8\left(\frac{n\left(1+\sqrt{n(n+4)}\right)}{8}\right)-n\sqrt{n(n+4)}}{4n} = \frac{1}{4} \\
&> \delta(DK(3,4)) > \delta(DK(3,n-6)).
\end{aligned}
$$

A contradiction. □

We give a spectral characteristic of H_n.

PROPOSITION 3.6. *If H_n is not a tree then $\lambda_2(H_n)$ is simple eigenvalue.*

Proof. Assume that $\lambda_2(H_n) = \lambda_3(H_n)$. Let uv be an edge which belongs to at least one cycle of H_n (since H_n is not a tree such an edge must exist). Consider the graph $H_n - u + u'$ obtained from H_n by removal of vertex u and addition of vertex u' which is not adjacent to v, but it is adjacent to all remaining neighbours of u. Clearly, the graph obtained is connected and has n vertices; in other words, $H_n - u + u'$ is obtained by deletion of edge uv and then, by [7, Theorem 0.7], we get $\lambda_1(H_n) > \lambda_1(H_n - u + u')$.

On the other hand, by eigenvalue interlacing, we have $\lambda_2(H_n - u) = \lambda_2(H_n)$ (since $\lambda_2(H_n) = \lambda_3(H_n)$), and then $\lambda_2(H_n - u + u') \geq \lambda_2(H_n)$.

Collecting the above inequalities we get $\delta(H_n) > \delta(H_n - u + u')$. A contradiction. □

4. An additional result. We say that two non-isomorphic graphs are cospectral if they are sharing the same spectrum. We give the following result.

PROPOSITION 4.1. *There is no connected graph that is cospectral to $DK(k,l)$ ($k \geq 1$, $l \geq 0$).*

In order to prove the above proposition we need the following results, and the subsequent lemmas. From now on, H will stand for a putative connected graph cospectral to $DK(k,l)$. It is then known that (see [10]):

1. H has $2k + l$ vertices,
2. H has $2\binom{k}{2} + l + 1$ edges,
3. the number of triangles of H is equal to the number of triangles of $DK(k,l)$, i.e., $t(H) = t(DK(k,l)) = 2\binom{k}{3}$.

Recall that a maximal clique of a graph is its complete subgraph that cannot be extended by a vertex to a larger complete subgraph. Since $DK(k,l)$ is a line graph of a tree its least eigenvalue is greater than -2, and the same must hold for the least

ELA

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eigenvalue of H. If so, then H belongs to one of the following classes of graphs (see [9, Theorem 2.3.20]):

1. $\mathcal{L}_1 = \{L(T), \ T \ \text{is a tree}\}$,
2. $\mathcal{L}_2 = \{L(U), \ U \ \text{is an odd unicyclic graph}\}$,
3. $\mathcal{L}_3$ – the graphs obtained by taking $L(T)$, and 2 additional disjoint vertices along with all edges joining these vertices with each vertex of some maximal clique of $L(T)$,
4. $\mathcal{E}$ – the exceptional graphs whose least eigenvalue is greater than -2 (there are 20 such graphs on 6 vertices, 110 on 7 vertices, and 443 on 8 vertices; they can be found in [9, Table A2]).

LEMMA 4.2. *There is no connected graph H that is cospectral to $DK(k, l)$ whenever one of the following holds:*

(i) $k \leq 2$ or $l = 0$,
(ii) $H \in \mathcal{E}$,
(iii) H contains K_{k+1} as an induced subgraph,
(iv) H contains a subgraph equal to either $2K_k$, or $K_1 \nabla 2K_{k-1}$,
(v) H contains $2K_1 \nabla K_{k-1}$ as an induced subgraph.

Proof. (i) If $k \leq 2$ the result follows from the fact that any path is determined by its spectrum [10]. Next, $DK(k, 0)$ is a line graph with exactly two positive eigenvalues, and all such line graphs are determined in [3]. By inspecting their spectra, we get the result.

(ii) Since there is no double kite graphs on 6 vertices with $k \geq 3$, $l \geq 1$, H must have 7 or 8 vertices, and if so then there are exactly 2 double kite graphs to be compared: $DK(3, 1)$, and $DK(3, 2)$. Inspecting the spectra of possible candidates for H we get that none of them coincide with spectrum of any of these 2 graphs.

(iii) If H contains K_{k+1} as an induced subgraph, we have $\lambda_1(H) \geq k$. On the other hand, $\lambda_1(DK(k, l)) \leq \lambda_1(DK(k, 0)) < k$ (cf. (2.10)), which yields $\lambda_1(H) \neq \lambda_1(DK(k, l))$, and the proof follows.

(iv) The proof follows directly from Proposition 2.3.

(v) The eigenvector $(k - 1, k - 1, \lambda_1, \lambda_1, \ldots, \lambda_1)$ corresponds to the eigenvalue $\lambda_1 = \lambda_1(2K_1 \nabla K_{k-1})$, and then, from (2.3), we get $\lambda_1 = \frac{1}{2}\left(\sqrt{k^2 + 4k - 4} + k - 2\right)$. Using Proposition 2.6 and (2.10), we get that

$$\lambda_1(DK(k, l)) < \lambda_1(DK(k, 0)) = \tfrac{1}{2}\left(\sqrt{k(k - 2) + 5} + k - 1\right)$$

$$< \tfrac{1}{2}\left(\sqrt{k^2 + 4k - 4} + k - 2\right) = \lambda_1(2K_1 \nabla K_{k-1})$$

$$\boxed{\textbf{ELA}}$$

holds for any $k \geq 3$, $l \geq 1$, and the proof is complete. $\square$

We need another spectral property of $DK(k,l)$.

LEMMA 4.3. $\lambda_3(DK(k,l)) < 2$.

Proof. Since $DK(k,0)$ belongs to the family of line graphs with exactly 2 positive eigenvalues, we can assume that $l \geq 1$. By eigenvalue interlacing we get that $\lambda_3(DK(k,l)) \leq \max\{\lambda_1(P_l), \lambda_1(K_{k-1})\}$, and therefore we can also assume that $k \geq 4$.

Using the formula for the characteristic polynomial of a graph obtained by inserting an edge between arbitrary vertices of two graphs [7, Theorem 2.12], and the formula for the characteristic polynomial of an l-vertex path $P_{P_l}(t^{1/2} + t^{-1/2}) = \frac{t^{-l/2}(t^{l+1}-1)}{t-1}$ (see, for example, [17]), we can easily get the explicit form of the characteristic polynomial of $DK(k,l)$:

$$P_{DK(k,l)}(t^{1/2} + t^{-1/2}) =$$

$$\frac{\left(1 + \frac{1+t}{\sqrt{t}}\right)^{2k}\left((-2+k+(-2+k)\sqrt{t}-t)^2 t^{3+l} - (-1+(-2+k)(\sqrt{t}+t))^2\right)}{(-1+t)(1+\sqrt{t}+t)^4 t^{\frac{l}{2}}}.$$

By eigenvalue interlacing, we have $\lambda_3(DK(k,l)) \leq k-2$. Computing the limit point $\lim_{t\to 1} P_{DK(k,l)}(t^{1/2} + t^{-1/2})$, we get $P_{DK(k,l)}(2) \neq 0$ (for $k \geq 4$, $l \geq 1$), i.e., $\lambda_3(DK(k,l)) \neq 2$.

We are going to prove that $P_{P_{D(k,l)}}$ is positive at any point $t^{1/2} + t^{-1/2}$ of $(2, k-2]$. Its sign depends only on $(-2+k+(-2+k)\sqrt{t}-t)^2 t^{3+l} - (-1+(-2+k)(\sqrt{t}+t))^2$, and this factor can be rewritten in

$$\left(t^{\frac{l+2}{2}}\left(-t^{\frac{3}{2}} + (-2+k)(t+\sqrt{t})\right)\right)^2 - (-1+(-2+k)(\sqrt{t}+t))^2,$$

which is positive for the corresponding values of t iff

$$f(t) = t^{\frac{l+2}{2}}\left(-t^{\frac{3}{2}} + (-2+k)(t+\sqrt{t})\right) - (-1+(-2+k)(\sqrt{t}+t))$$

is positive. Since $k-2 \geq \sqrt{t}$, putting $k-2 = \sqrt{t}$ into above expression we get

$$f(t) \geq t^{\frac{6+l}{2}} - t^{\frac{3}{2}} - t + 1,$$

and the right hand side is positive at any $t > 1$ (since $l \geq 1$), implying that $f(t) > 0$ for any t satisfying $t^{1/2} + t^{-1/2} \in (2, k-2]$.

Collecting the above results we get that there are no roots of $P_{DK(k,l)}$ ($k \geq 4$, $l \geq 1$) in $[2, k-2]$, which yields $\lambda_3(DK(k,l)) < 2$. $\square$

$$\boxed{\textbf{ELA}}$$

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Recall that a graph is said to be cyclic if it contains at least one cycle.

LEMMA 4.4. *If a connected graph H contains a set of vertices whose removal gives rise to a disconnected graph containing at least 3 cyclic components then $DK(k,l)$ is not cospectral to H.*

Proof. Assume to the contrary, then since the index of any cyclic graph is at least 2, we get $\lambda_3(H) > \lambda_3(DK(k,l))$. ∎

The previous lemma gives very restrictive structural properties of H. For example, if $H \in \mathcal{L}_1$ then it contains at most two maximal cliques of order greater than 4. And if so, then these cliques have at most one common vertex, H does not contain any maximal clique of order 4, the maximal cliques of order 3 are mutually disjoint and each of them has exactly one common vertex with exactly one of two larger cliques. These and similar properties of $H \in \mathcal{L}_2 \cup \mathcal{L}_3$ will be used in the next proof.

Proof of Proposition 4.1.   Assume to the contrary. Then, by Lemma 4.2 (ii), $H \in \bigcup_{i=1}^3 \mathcal{L}_i$.

Let $H \in \mathcal{L}_1 \cup \mathcal{L}_2$. If X is the vertex set of the corresponding root graph then counting the number of vertices, edges, and triangles of H, we get:

$$n(H) = \frac{1}{2}\sum_{v\in X} \deg(v) \quad = 2k+l$$

(4.1)
$$m(H) = \sum_{v\in X}\binom{\deg(v)}{2} \quad = 2\binom{k}{2}+l+1$$

$$t(H) = \sum_{v\in X}\binom{\deg(v)}{3}+i = 2\binom{k}{3},$$

where $\deg(v)$ is the degree of the corresponding vertex and $i = 0$, unless $H = L(U)$ and U contains a triangle when $i = 1$.

Let a_j denote the number of vertices in X having degree j. By Lemma 4.2 (iii) and (iv), we have $a_j = 0$ for $j > k$, and $a_k \le 1$. Using the result of Lemma 4.4, we get $\sum_{j=5}^k a_j \le 2$, $a_4 \le 2$, and if $a_4 = 2$ then $\sum_{j=5}^k a_j \le 1$.

Let $k \ge 7$. We get $t(H) \le \binom{k}{3}+\binom{k-1}{3}+a_3+i$, and (by Lemma 4.4) $a_3+i \le 2k-1$. Thus $t(H) \le \binom{k}{3}+\binom{k-1}{3}+2k-1 < 2\binom{k}{3}$. A contradiction.

It remains to consider the case $k \in \{3,4,5,6\}$.

If $k = 6$, we get $t(H) < t(DK(6,l))$ whenever $a_5 + a_6 < 2$. So we have $t(H) = \binom{6}{3}+\binom{5}{3}+a_3+i = 2\binom{6}{3}$, giving $a_3 + i = 10$. Computing $m(H)$ and $n(H)$ for $a_6 = a_5 = 1, a_4 = 0$, we get $a_1 = 31 - 3i$. On the other hand, counting the number

ELA

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of terminal vertices in the root graph of H for these parameters we get $a_1 = 19$ (if $H = L(T)$) or $a_1 = 17$ (if $H = L(U)$). A contradiction.

If $k = 5$, from the system (4.1) we get $t(H) = 10a_5 + 4a_4 + a_3 + i = 20$ and $15a_5 + 8a_4 + 3a_3 - a_1 = 22$. Clearly, $t(H) < 20$ unless $a_5 = 1$, and then $a_4 = 1$ or $a_4 = 2$ must hold. In the first case we get $a_3 = 6 - i, a_1 = 19 - 3i$, and $a_3 = 2 - i, a_1 = 15 - 3i$ in the second, but in both cases a_1 does not match the exact number of terminal vertices in the root graph.

If $k = 4$, in the similar way, we get $a_1 = 10 - 3i$, while the number of terminal vertices in T (resp., U) with $a_4 = 1$ is 8 (resp., 6).

Finally, if $k = 3$ then H must contain exactly 2 triangles, but then it is not cospectral to $DK(3, l)$ by Proposition 2.3.

Let $H \in \mathcal{L}_3$. Instead of (4.1) we have the following equations:

$$
\begin{aligned}
n(H) = & \quad \frac{1}{2} \sum_{v \in X} \deg(v) + 2 & = 2k + l \\
(4.2) \qquad m(H) = & \quad \sum_{v \in X} \binom{\deg(v)}{2} + 2d & = 2\binom{k}{2} + l + 1 \\
t(H) = & \sum_{v \in X} \binom{\deg(v)}{3} + i + 2\binom{d}{2} = 2\binom{k}{3},
\end{aligned}
$$

where d denotes the order of the maximal clique related to 2 additional vertices (see definition of $\mathcal{L}_3$). By Lemma 4.2 (v), we get $d \leq k - 2$. Let X again denote the set of vertices of T, and let a_j's be the same as above (along with the inequalities obtained).

Considering the third equation of (4.2) we get $t(H) < t(DK(k, l))$ unless (a) $a_k = a_{k-1} = 1, d \in \{1, 2, 3\}$, (b) $a_k = 0, k \leq 5$, or (c) $a_k = 1, d = k - 2$. In case (a) we get $t(H) < t(DK(k, l))$ unless $d = 1, k \leq 6$, or $d = 2, k \leq 7$, or $d = 3, k \leq 9$. These particular cases and the case (b) are resolved by solving system (4.2) in a_1 and comparing the value obtained with the exact value of a_1. Similarly, in case (c), solving the system we get $a_3 = k - 2, a_1 = 3k - 2$, but considering T we get $a_1 = k + (k - 3) + (k - 2) = 3k - 5$. A contradiction. $\square$

REMARK 4.5. If some double kite graph has nonunique spectral gap then, according to Proposition 4.1, it is not cospectral to other connected graph with equal gap. In other words, if some double kite graph minimizes the spectral gap then it is the unique minimizer or there is another minimizer but with different spectrum.

A graph is determined by its spectrum if it is a unique graph having this spectrum. To show whether a double kite graph is determined by its spectrum, it remains to check

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whether it is cospectral to some disconnected graph or not, but this consideration is beyond the subject of this paper.

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