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ON RELATION BETWEEN SPECTRA OF GRAPHS AND THEIR DIGRAPH DECOMPOSITIONS

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Abstract. A graph, consisting of undirected edges, can be represented as a sum of two digraphs, consisting of oppositely oriented directed edges. Gutman and Plath in [J. Serb. Chem. Soc. 66 (2001), 237–241] showed that for annulenes, the eigenvalue spectrum of the graph is equal to the sum of the eigenvalue spectra of respective two digraphs. Here we exhibit a number of other graphs with this property.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Following [**1**], in the standard graph representation of organic molecules, edges represent covalent chemical bonds, which are assumed to be undirected, as is the entire graph. However, each undirected edge may be alternatively viewed as a pair of oppositely oriented directed edges. In this way, whole undirected graph G may always be decomposed into a pair of digraphs, $\overrightarrow{G}$ and $\overleftarrow{G}$, consisting of oppositely oriented directed edges, such that $V(\overrightarrow{G}) = V(\overleftarrow{G}) = V(G)$ and $E(G) = E(\overrightarrow{G}) \cup E(\overleftarrow{G})$.

In [**1**], Gutman and Plath showed that graphs of annulenes, undirected cycles, have an interesting property: each eigenvalue of an undirected cycle is equal to the sum of the corresponding eigenvalues of directed cycles from its digraph decomposition.

The spectrum $\mathrm{Sp}[\overrightarrow{G}]$ of a digraph $\overrightarrow{G}$ is the collection of eigenvalues of its adjacency matrix $A(\overrightarrow{G})$. The adjacency matrix $A(\overleftarrow{G})$ is the transpose of $A(\overrightarrow{G})$. Therefore, the digraphs $\overrightarrow{G}$ and $\overleftarrow{G}$ have equal spectra. Since $A(\overrightarrow{G})$ is not symmetric, its eigenvalues may be complex numbers. However, if a complex number z is an eigenvalue of $\overrightarrow{G}$, then also its complex conjugate $\overline{z}$ is an eigenvalue of $\overrightarrow{G}$. Note that

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if $\overrightarrow{G}$ does not possess directed cycles, then all its eigenvalues are equal to zero [**1**, Theorem 3.(a)]. Namely, if $\overrightarrow{G}$ has n vertices, then the characteristic polynomial of $A(\overrightarrow{G})$ may be written in the form

$$\phi(G,\lambda) = \lambda^n + \sum_{k=1}^{n} a_k \lambda^{n-k}. \tag{1.1}$$

Then, by the Sachs' theorem for digraphs [**2, 3, 4**],

$$a_k = \sum_S (-1)^{p(S)},$$

where the summation goes over all k-vertex subgraphs S of G that consist entirely of directed cycles, the number of directed cycles in S being $p(S)$. Thus, if $\overrightarrow{G}$ has no directed cycles, we have $a_k = 0$ for all $k = 1, 2, \ldots, n$ and the characteristic polynomial (1.1) is equal to $\phi(G,\lambda) = \lambda^n$, whose all roots are equal to zero.

Next, denote the eigenvalues of $\overrightarrow{G}$ by $\lambda_1(\overrightarrow{G})$, $\lambda_2(\overrightarrow{G})$, $\ldots \lambda_n(\overrightarrow{G})$. The eigenvalues of $\overleftarrow{G}$ may always be labelled such that $\lambda_k(\overrightarrow{G}) + \lambda_k(\overleftarrow{G})$ is a real number [**1**, Theorem 2]. Simply, if $\lambda_k(\overrightarrow{G})$ is real, choose $\lambda_k(\overleftarrow{G})$ to be equal to $\lambda_k(\overrightarrow{G})$, and if $\lambda_k(\overrightarrow{G})$ is not real, choose $\lambda_k(\overleftarrow{G})$ to be equal to the complex conjugate of $\lambda_k(\overrightarrow{G})$, which is also an eigenvalue of $\overrightarrow{G}$. Note that this labelling implies

$$\lambda_k(\overrightarrow{G}) + \lambda_k(\overleftarrow{G}) = 2\,\mathrm{Re}\,\lambda_k(\overrightarrow{G}).$$

We will implicitly assume this type of labelling for the eigenvalues of $\overleftarrow{G}$ in the sequel.

In general, the eigenvalues $\lambda_k(G)$ of undirected graph G are not related to the eigenvalues of digraphs from its digraph decomposition. Gutman and Plath [**1**, Theorem 4] showed that for the decomposition of undirected cycle $C_n = \overrightarrow{C_n} \cup \overleftarrow{C_n}$ in two directed cycles, the eigenvalues of undirected cycle may be labelled such that

$$\lambda_k(C_n) = \lambda_k(\overrightarrow{C_n}) + \lambda_k(\overleftarrow{C_n}) = 2\,\mathrm{Re}\,\lambda_k(\overrightarrow{C_n}), \quad \text{for } k = 1, 2, \ldots, n,$$

or, shorter,

$$\mathrm{Sp}[C_n] = 2\,\mathrm{Re}\,\mathrm{Sp}[\overrightarrow{C_n}].$$

Concluding [**1**], Gutman and Plath said: "The discovery of more graphs G satisfying

$$\mathrm{Sp}[G] = 2\,\mathrm{Re}\,\mathrm{Sp}[\overrightarrow{G}] \tag{1.2}$$

would, however, be of much greater importance."

Our main task here is to exhibit a number of graphs satisfying (1.2). The plan of the paper is as follows: in Section 2 we exhibit all such graphs with up to 8 vertices and 14 edges, in Section 3 we show how new instances may be obtained from existing ones using NEPS, and in Section 4 we present a family of graphs satisfying (1.2) which may not be obtained using the method of Section 3.

2. Small instances

We have enumerated all digraph decompositions of connected graphs with at most 8 vertices and 14 edges and, besides cycles, we have found seven other graphs satisfying (1.2). In addition, our experiments show that the complete bipartite graph $K_{4,4}$ has two distinct decompositions each satisfying (1.2). For each of these eight graphs, a digraph $\overrightarrow{G_i}$ is given in Figure 1, while the spectra of $\overrightarrow{G_i}$ and $G_i = \overrightarrow{G_i} \cup \overleftarrow{G_i}$ are as follows (where parenthesized numbers in exponents denote multiplicities):

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_1}) &= [2, -0.5 \pm i\,1.538842, -0.5 \pm i\,0.363271]\\
\mathrm{Sp}(G_1) &= [4, -1^{(4)}]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_2}) &= [\pm 1.414214, \pm i\,1.414214, 0^{(2)}]\\
\mathrm{Sp}(G_2) &= [2.828427, 0^{(4)}, -2.828427]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_3}) &= [1.618034, -0.618034, -0.809017 \pm i\,1.401259, 0.309017 \pm i\,0.535233]\\
\mathrm{Sp}(G_3) &= [3.236068, 0.618034^{(2)}, -1.236068, -1.618034^{(2)}]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_4}) &= [2, 0^{(3)}, -1 \pm i\,1.732051]\\
\mathrm{Sp}(G_4) &= [4, 0^{(3)}, -2^{(2)}]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_5}) &= [2, 0.400969 \pm i\,0.193096, -0.277479 \pm i\,1.215715, -1.123490 \pm i\,1.408812]\\
\mathrm{Sp}(G_5) &= [4, 0.801938^{(2)}, -0.554958^{(2)}, -2.246980^{(2)}]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_6}) &= [\pm 1.732051, \pm i\,1.732051, 0^{(4)}]\\
\mathrm{Sp}(G_6) &= [3.464102, 0^{(6)}, -3.464102]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_7}) &= [\pm 1.618034, \pm i\,1.618034, \pm 0.618034, \pm i\,0.618034]\\
\mathrm{Sp}(G_7) &= [3.236068, 1.236068, 0^{(4)}, -1.236068, -3.236068]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_8}) &= [\pm 2, \pm 2i, 0^{(4)}]\\
\mathrm{Sp}(G_8) &= [4, 0^{(6)}, -4]
\end{aligned}$$

$$\begin{aligned}
\mathrm{Sp}(\overrightarrow{G_9}) &= [\pm 2, \pm i\,\sqrt{2}^{(2)}, 0^{(2)}]\\
\mathrm{Sp}(G_9) &= [4, 0^{(6)}, -4]
\end{aligned}$$

Note that graphs G_2 and G_6 in Figure 1 are isomorphic to $K_{2,4}$ and $K_{2,6}$, respectively. Having in mind that the cycle C_4, which satisfies (1.2), is isomorphic to $K_{2,2}$, we can arrive to our first expectation: graph $K_{2,2n}$ should have a digraph decomposition satisfying (1.2). Indeed, denote by u and v vertices from two-vertex part of $K_{2,2n}$, and divide the vertices from $2n$-vertex part of $K_{2,2n}$ into two equally

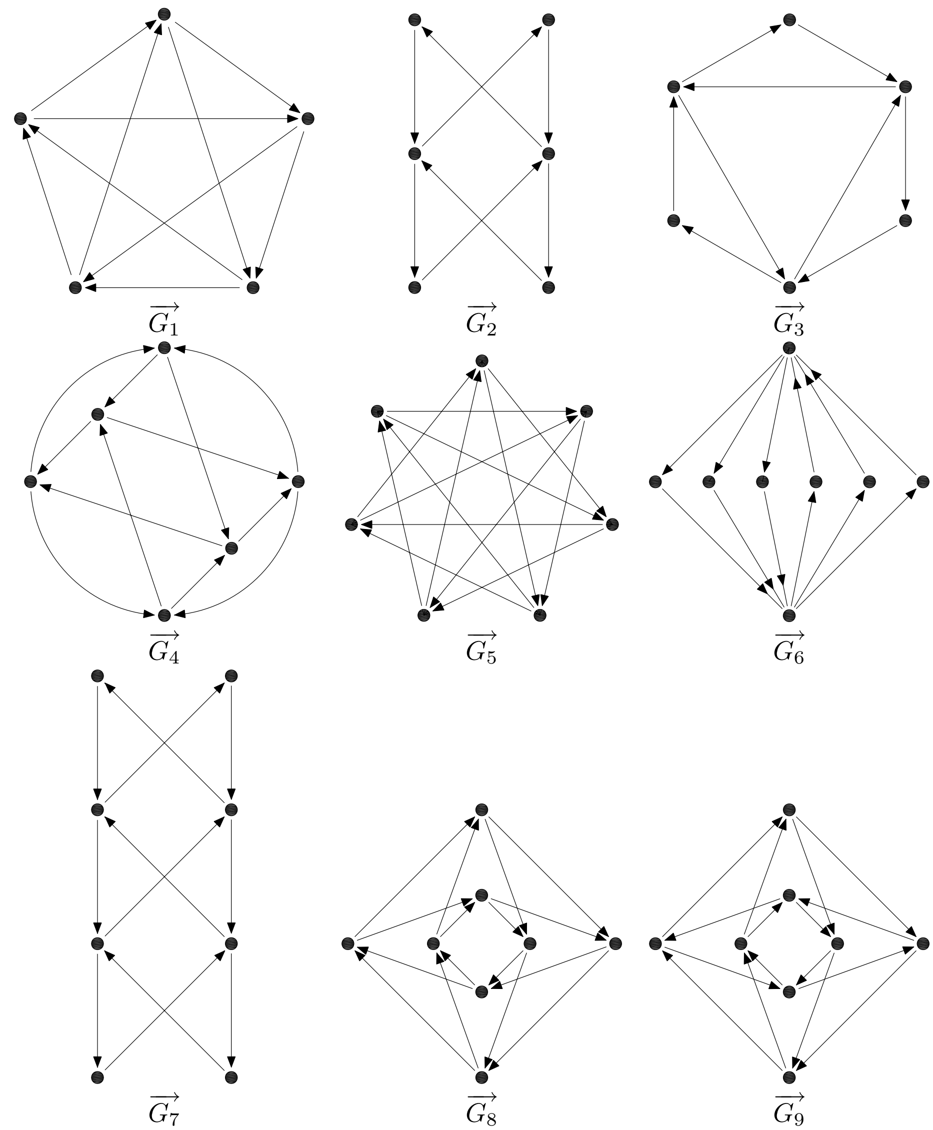

FIGURE 1. Small instances satisfying (1.2).

sized sets A and B. Let $\overrightarrow{K_{2,2n}}$ be the digraph obtained from $K_{2,2n}$ by directing all edges from u to A, from A to v, from v to B and from B to u. Each directed cycle of $\overrightarrow{K_{2,2n}}$ has length 4 and contains vertices u and v. Thus, there are no disjoint directed cycles in $\overrightarrow{K_{2,2n}}$ and from Sachs' theorem we get that the only nonzero coefficient in the characteristic polynomial (except with x^{2n+2}) is the one with $x^{(2n+2)-4}$, which is equal to n^2. Thus, the characteristic polynomial of $\overrightarrow{K_{2,2n}}$ is equal to

$$x^{2n+2} - n^2 x^{2n-2} = x^{2n-2}(x^4 - n^2) = x^{2n-2}(x^2 - n)(x^2 + n),$$

hence, its spectrum is $[\pm\sqrt{n}, \pm i\sqrt{n}, 0^{2n-2}]$, and twice its real part is $[\pm 2\sqrt{n}, 0^{2n}]$, which is just the spectrum of $K_{2,2n}$.

Thus, the graphs $K_{2,2n}$ form our first family of graphs satisfying (1.2), however, their maximum degree increases with the number of vertices, which may not be favorable in chemical applications.

3. NEPS with undirected graphs

The *non-complete extended p-sum* (NEPS) of graphs is a very general graph operation. Many graph operations are special cases of NEPS, to name just the sum, product and strong product of graphs. It is defined for the first time in [**5**], while the following definition is taken from [**3**, p. 66] with minor modification:

Definition. Let $\mathcal{B}$ be a set of binary k-tuples, i.e., $\mathcal{B} \subseteq \{0,1\}^k \setminus \{(0,\dots,0)\}$ such that for every $j = 1,\dots,k$ there exists $\beta \in \mathcal{B}$ with $\beta_j = 1$. The NEPS of graphs $G_1,\dots,G_k$ with basis $\mathcal{B}$, denoted $\mathrm{NEPS}(G_1,\dots,G_k;\mathcal{B})$, is the graph with the vertex set $V(G_1) \times \cdots \times V(G_k)$, in which two vertices $(u_1,\dots,u_k)$ and $(v_1,\dots,v_k)$ are adjacent if and only if there exists $(\beta_1,\dots,\beta_k) \in \mathcal{B}$ such that u_j is adjacent to v_j in G_j whenever $\beta_j = 1$, and $u_j = v_j$ whenever $\beta_j = 0$.

Despite the fact that NEPS is mostly used with undirected graphs, its definition carries over to directed graphs in a straightforward way, as can be seen from the works of Petrić [**6, 7, 8**]. In particular, a relation between spectrum of NEPS and the spectra of its factors holds unchanged (see, e.g., Theorem 2.23 in [**3**]).

Theorem 3.1. *The spectrum of* $\mathrm{NEPS}(G_1,\dots,G_k;\mathcal{B})$ *consists of all possible values* Λ *given by*

$$\Lambda = \sum_{\beta\in\mathcal{B}} \lambda_1^{\beta_1} \cdots \lambda_k^{\beta_k},$$

where λ_j *is an arbitrary eigenvalue of* G_j, $j = 1,\dots,k$.

This enables us to prove the following

Theorem 3.2. *Let* G *be an undirected graph with digraph decomposition* $G = \overrightarrow{G} \cup \overleftarrow{G}$, *and suppose that the eigenvalues of* G *and* $\overrightarrow{G}$ *can be enumerated in such a way that* $\lambda_j(G) = 2\,\mathrm{Re}\,\lambda_j\big(\overrightarrow{G}\big)$ *for each* j. *Further, let* $\mathcal{B}$ *be a set of binary* k*-tuples such that* $\beta_1 = 1$ *for each* $\beta \in \mathcal{B}$, *and let* $G_2,\dots,G_k$ *be arbitrary undirected graphs. Then the eigenvalues of*

$$G^* = \mathrm{NEPS}(G, G_2,\dots,G_k;\mathcal{B}) \quad \textit{and} \quad \overrightarrow{G^*} = \mathrm{NEPS}\big(\overrightarrow{G}, G_2,\dots,G_k;\mathcal{B}\big)$$

may be enumerated in such a way that $\lambda_j(G^*) = 2\,\mathrm{Re}\,\lambda_j\big(\overrightarrow{G^*}\big)$ *for each* j.

Proof. Let $\lambda_1(\overrightarrow{G})$ be an arbitrary eigenvalue of $\overrightarrow{G}$, and let λ_j be an arbitrary eigenvalue of G_j for $j = 2, \dots, k$. Then, since $\beta_1 = 1$ for each $\beta \in \mathcal{B}$,

$$\Lambda(\overrightarrow{G^*}) = \sum_{\beta\in\mathcal{B}} \lambda_1^{\beta_1}(\overrightarrow{G})\lambda_2^{\beta_2}\cdots\lambda_k^{\beta_k} = \lambda_1(\overrightarrow{G}) \sum_{\beta\in\mathcal{B}} \lambda_2^{\beta_2}\cdots\lambda_k^{\beta_k} = M\lambda_1(\overrightarrow{G})$$

is an eigenvalue of $\overrightarrow{G^*}$, where $M = \sum_{\beta\in\mathcal{B}} \lambda_2^{\beta_2}\cdots\lambda_k^{\beta_k}$ is a real number (as the eigenvalues $\lambda_2, \dots, \lambda_k$ of undirected graphs must be real [**3**]). Similarly, for $\lambda_1(G) = 2\operatorname{Re}\lambda_1(\overrightarrow{G})$,

$$\Lambda(G^*) = \sum_{\beta\in\mathcal{B}} \lambda_1^{\beta_1}(G)\lambda_2^{\beta_2}\cdots\lambda_k^{\beta_k} = \lambda_1(G) \sum_{\beta\in\mathcal{B}} \lambda_2^{\beta_2}\cdots\lambda_k^{\beta_k} = M\lambda_1(G)$$

is an eigenvalue of G^*. The PROOF then follows from

$$\Lambda(G^*) = M\lambda_1(G) = 2M\operatorname{Re}\lambda_1(\overrightarrow{G}) = 2\operatorname{Re} M\lambda_1(\overrightarrow{G}) = 2\operatorname{Re}\Lambda(\overrightarrow{G^*}). \qquad \square$$

Theorem 3.2 enables us to construct arbitrarily many instances of graphs satisfying (1.2) starting from directed cycles or graphs from Figure 1. For example, the graph $\overrightarrow{G_8}$ is isomorphic to $\mathrm{NEPS}(\overrightarrow{C_4}, K_2; \{(1,0),(1,1)\})$ of directed cycle C_4 and complete graph K_2. Similarly, for any $n \geqslant 3$, $\mathrm{NEPS}(\overrightarrow{C_n}, K_2; \{(1,0),(1,1)\})$ is a graph satisfying (1.2), where each vertex has indegree and outdegree equal to two.

However, the edges of NEPS of $\overrightarrow{G}$ with undirected graphs always follow the direction of edges of $\overrightarrow{G}$. Thus, the directed cycles in such NEPS mimic the directed cycles from $\overrightarrow{G}$, which may not be considered favorably in applications as well.

4. Family of twisted ladders

Inspired by graphs $\overrightarrow{G_2}$ and $\overrightarrow{G_7}$ from Figure 1, in this section we present a family of oriented graphs, which may not be represented as NEPS of an oriented graph with undirected graphs.

For $n \geqslant 2$, let P_n denote the path on n vertices whose vertices are labelled as $1, \dots, n$, such that vertex j is adjacent to vertices $j-1$ and $j+1$ for $j = 2, \dots, n-1$. Next, denote the vertices of complete graph K_2 by 0 and 1. Let

$$TL_n = \mathrm{NEPS}\left(P_n, K_2; \{(1,0),(1,1)\}\right).$$

Let us form the directed graph $\overrightarrow{TL_n}$ from TL_n by orienting edges from (j,k) to $(j+1,k)$ for $j = 1, \dots, n-1$ and $k = 0, 1$, and from (j,k) to $(j-1, 1-k)$ for $j = 2, \dots, n$ and $k = 0, 1$, like in Figure 2. We call $\overrightarrow{TL_n}$ the *twisted ladder*.

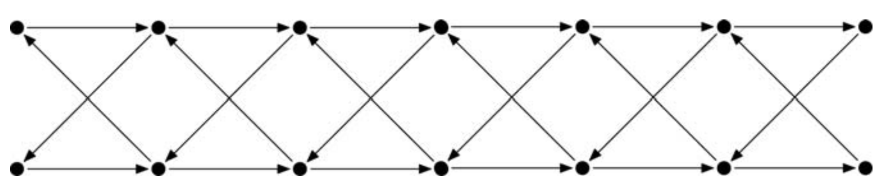

Figure 2. An example of a twisted ladder.

THEOREM 4.1. *For $n \geqslant 2$,* $\mathrm{Sp}[TL_n] = 2\,\mathrm{Re}\,\mathrm{Sp}\big[\overrightarrow{TL_n}\big]$.

PROOF. Let us recall that the eigenvalues of path P_n are $2\cos\frac{k\pi}{n+1}$ for $k = 1,\dots,n$ (see, e.g., [**3**, Section 2.7]), while $\mathrm{Sp}[K_2] = \{1,-1\}$. Then from Theorem 1, to an arbitrary eigenvalue λ of P_n there correspond eigenvalues

$$\lambda^1 \cdot 1^0 + \lambda^1 \cdot 1^1 = 2\lambda \quad \text{and} \quad \lambda^1 \cdot (-1)^0 + \lambda^1 \cdot (-1)^1 = 0$$

of TL_n. Thus,

$$\mathrm{Sp}[TL_n] = \Big\{4\cos\frac{k\pi}{n+1} \,:\, k = 1,\dots,n\Big\} \cup \{0^{(n)}\}.$$

Next we show that

$$\mathrm{Sp}[\overrightarrow{TL_n}] = \Big\{2\cos\frac{k\pi}{n+1}, 2i\,\cos\frac{k\pi}{n+1} \,:\, k = 1,\dots,n\Big\}, \tag{4.1}$$

from which equality $\mathrm{Sp}[TL_n] = 2\,\mathrm{Re}\,\mathrm{Sp}\big[\overrightarrow{TL_n}\big]$ will immediately follow.

Denote the adjacency matrix $A\big(\overrightarrow{TL_n}\big)$ simply by A. Let $\lambda = 2\cos\frac{k\pi}{n+1}$ be an arbitrary eigenvalue of the path P_n and let x be an eigenvector of P_n corresponding to λ. We will use x to form two eigenvectors of $\overrightarrow{TL_n}$, one for eigenvalue λ and the other for eigenvalue $i\lambda$. First, recall that x satisfies

$$\begin{aligned}
&\lambda x(1) = x(2),\\
&\lambda x(j) = x(j-1) + x(j+1), \quad j = 2,\dots,n-1,\\
&\lambda x(n) = x(n-1).
\end{aligned}$$

Now, let x' be a vector defined on vertices of $\overrightarrow{TL_n}$ by

$$x'(j,0) = x'(j,1) = x(j), \quad j = 1,\dots,n.$$

Then for $j = 2,\dots,n-1$,

$$\begin{aligned}
(Ax')(j,k) &= x'(j-1,1-k) + x'(j+1,k)\\
&= x(j-1) + x(j+1)\\
&= \lambda x(j)\\
&= \lambda x'(j,k),
\end{aligned}$$

and similarly,

$$(Ax')(1,k) = \lambda x'(1,k), \qquad (Ax')(n,k) = \lambda x'(n,k).$$

Thus, λ is indeed an eigenvalue of $\overrightarrow{TL_n}$.

Next, let x'' be a vector defined on vertices of $\overrightarrow{TL_n}$ by

$$x''(j,k) = i^{j+2k} x(j), \qquad j = 1,\dots,n, \qquad k = 0,1.$$

Then

$$\begin{aligned}(Ax'')(j,k) &= x''(j-1,1-k) + x''(j+1,k)\\ &= i^{j+1-2k}x(j-1) + i^{j+1+2k}x(j+1)\\ &= i^{j+1+2k}\lambda x(j)\\ &= i\lambda\, i^{j+2k}x(j)\\ &= i\lambda x''(j,k),\end{aligned}$$

and similarly,

$$(Ax'')(1,k) = i\lambda x''(1,k), \qquad (Ax'')(n,k) = i\lambda x''(n,k).$$

Thus, $i\lambda$ is an eigenvalue of $\overrightarrow{TL_n}$ as well, which shows that (4.1) holds. $\square$

5. Concluding remarks

One might argue that no twisted ladders would be considered favourable for chemical applications, since all their directed cycles are still of length four only. Nevertheless, after exhibiting many graphs satisfying (1.2), other than the cycles, we are tempted to think that it is very likely that there exist graphs whose digraph decompositions will satisfy both (1.2) and the needs of potential chemical applications.

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