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Energy of Signed Spongy Hypercubes

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ABSTRACT

A spongy hypercube is a Cartesian product of a d-connected polyhedral graph and a k-dimensional hypercube. The aim of this paper is to compute the energies of signed spongy hypercubes $T\square Q_k$ and $O\square Q_k$, where T and O are tetrahedron and octahedron, respectively.

1 INTRODUCTION

All graphs considered in this paper will be finite and simple. For a graph G, its vertex and edge sets are denoted by $V(G)$ and $E(G)$, respectively. The adjacency matrix $A(G) = [a_{ij}]$ of G is a zero-one matrix such that $a_{ij} = 1$ if and only if the vertices i and j are adjacent in G, see [1] for details. The eigenvalues of this matrix are called the eigenvalues of G. The sum of the absolute value of all eigenvalues of G is called the **graph energy** of G. This graph parameter was introduced by Ivan Gutman [3,4] who continued his pioneering work in graph energy by finding lower and upper bounds on this quantity in terms of the number of vertices and/or edges. He also characterized the extremalgraphs with respect to the energy. We encourage the interested readers to consult [5] for a survey on different types of graph energy and [6] for a theoretical treatment of cycle-effects on total π-electron energy of molecules.

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Based on some motivation from social psychology, in [8] Harary introduced the notion of a **signed graph** Γ as a graph in which the edges are divided into two disjoint classes, called + and − edges. In an exact phrase, suppose G is a finite simple graph and σ is a function from the edge set of G to $\{1,-1\}$; then the pair (G,σ) is called a **signed graph**, abbreviated by **sigraph**. The graph G is called the **underlying graph** of (G,σ) and σ is its **edge function**.

Suppose G is a simple undirected graph, $\Gamma = (G,\sigma)$ and $U \subset V(G)$. The induced subgraph $\Gamma[U]$ denotes the signed subgraph induced by U and $\Gamma - U$ is used for the signed subgraph induced by $V(G) - U$, i.e. $\Gamma - U = \Gamma[V(G) - U]$. A cycle in Γ containing an even number of negatives edges is called **balanced**. If all cycles in Γ are balanced, then the signed graph Γ is said to be balanced. In other cases, the graph Γ is unbalanced. We use the notation $\sigma(\Gamma)$ for product of signs in all cycles of Γ. Define Γ^U to be the signed graph constructed from Γ by reversing the signature of edges in the cut $[U, V(G) - U]$. We say that the signed graph Γ^U is **signature switching equivalent** (switching equivalent forshort) to Γ. If Γ_1 and Γ_2 are isomorphic and switching equivalent signed graphs, then we say that they are switching isomorphic graphs and their signatures are said to be equivalent. It is well-known that if C is a cycle in Γ, then $\sigma_\Gamma(C) = \sigma_{\Gamma^U}(C)$.

Suppose $\Gamma = (G,\sigma)$ is a signed graph and $A(G) = (a_{ij})$ its adjacency matrix. The matrix $A(G) = (a^{\sigma}{}_{ij})$ given by $a^{\sigma}_{ij} = \sigma(ij)a_{ij}$, is called the **signed adjacency matrix** of Γ. It is easy to see that the switching equivalent signed graphs have similar adjacency and Laplacian matrices.

Pîrvan−Moldovan and Diudea [9] illustrated the Euler characteristic formula in figure counting of polyhedral graphs designed by operations on maps. They calculated this number for truncated cubic network and hypercube. The spongy hypercubes was introduced and studied by Diudea [10]. They are defined as Cartesian products of polyhedral graphs and hypercubes. More precisely, let $G(d,v)$ be a d-connected polyhedron on v vertices and Q_k the k-dimensional hypercube. Then the Cartesian product $G(d,v)\square Q_k$ is called a **spongy hypercube**. The spongy hypercubes that arise by taking $G(d,v)$ to be the tetrahedron, and the octahedron, respectively, are the main subject of our paper. The two generating graphs are shown in Figure 1.

Figure 1 . Tetrahedron and octahedron graphs.

2. MAIN RESULTS

Suppose $\Gamma_1 = (G_1, \sigma_1)$ and $\Gamma_2 = (G_2, \sigma_2)$ are two signed graphs. The Cartesian product $G_1 \square G_2$ is a graph with vertex set $V(G_1) \times V(G_2)$ in which two vertices (a, b) and (x, y) are adjacent if and only if $a = x$ and by $\in E(G_2)$ or $b = y$ and $ax \in E(G_1)$. The Cartesian product of two signed graphs Γ_1 and Γ_2, $\Gamma_1 \square \Gamma_2$, has the Cartesian product $G_1 \square G_2$ as its underlying graph and the sign function σ is defined as:

$$\sigma\big((u_i, v_j)(u_k, v_l)\big) = \begin{cases} \sigma_1(u_i u_k) & if\ j = l \\ \sigma_2(v_j v_l) & if\ i = k \end{cases}.$$

Germina et al. [2], computed the eigenvalues and energies of the Cartesian product of the signed graph. To explain their result, we assume that $\Gamma = \Gamma_1 \square \Gamma_2$ is the Cartesian product of two signed graphs $\Gamma_1 = (G_1, \sigma_1)$ and $\Gamma_2 = (G_2, \sigma_2)$. They proved that if G_1 has exactly n vertices and G_2 has exactly m vertices then $A(\Gamma) = A(\Gamma_1) \otimes I_m + I_n \otimes A(\Gamma_2)$. Here the tensor product $A \otimes B$ of two matrices A and B is defined as the following matrix:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1p}B \\ a_{21}B & a_{22}B & \cdots & a_{2p}B \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mp}B \end{bmatrix}$$

The eigenvalues of this graph can be computed as $\lambda_{ij}(\Gamma) = \lambda_i(\Gamma_1) + \lambda_j(\Gamma_2)$, where $\lambda_1(\Gamma_1), \ldots, \lambda_n(\Gamma_1)$ are eigenvalues of Γ_1 and $\lambda_1(\Gamma_2), \ldots, \lambda_m(\Gamma_2)$ are eigenvalues of Γ_2. Therefore, the energy of this graph is given by $\varepsilon(\Gamma) = \sum_{i=1}^{n} \sum_{j=1}^{m} |\lambda_i(\Gamma_1) + \lambda_j(\Gamma_2)|$.

It is well-known that the distinct eigenvalues of a k-dimensional hypercube are given by $\lambda_i = -k + 2i$, for $i = 0, \ldots, 2k$, and the multiplicity of λ_i is equal to $\binom{k}{i}$. In the next two subsections, different switching equivalent classes and their energies for signed tetrahedron and octahedron graphs are computed.

2.1 ENERGY OF SIGNED TETRAHEDRON GRAPHS

The aim of this section is to find all switching equivalent classes of signed tetrahedron graph. In order to do this, we consider all possible signs of each edge, resulting in 2^m cases for which some signs are switching equivalent. Then we find characteristic polynomial of every class, and finally the eigenvalues and energies. Note that it is possible that for two different classes we have the same spectra and energy, but if two graphs have the same spectra, it still does not mean that they must be in the same class.

By using the above method we find three different switching equivalent classesof signed tetrahedron graph, as listed below:

1. Graph does not have negative cycle. This graph is switchingequivalent with graph (T,+) in which all edges are positive. In this case the eigenvalues of signed tetrahedron graph are equal to $(1,-1,-1,3)$ or$(-1^3,3^1)$. In this case we consider $\sigma = +$.
2. All cycles of graph are negative. So the eigenvalues are $(-3,1,1,1)$ and $\sigma = -$.
3. Two cycles are positive and two others are negative. Hence, the spectrum is $(-\sqrt{5},-1,1,\sqrt{5})$ and $\sigma = \pm$.

Note that the graph $(T\square Q_k,-)$ is in the same switching equivalent class as the graph in which all edges have the negative sign. Hence, the two graphs $(T\square Q_k,+)$ and $(T\square Q_k,-)$ have the same absolute values of their eigenvalues, and, consequently, the same energy. Examples of $(T\square Q_k,-)$ for some small values of k are shown in Figure 2.

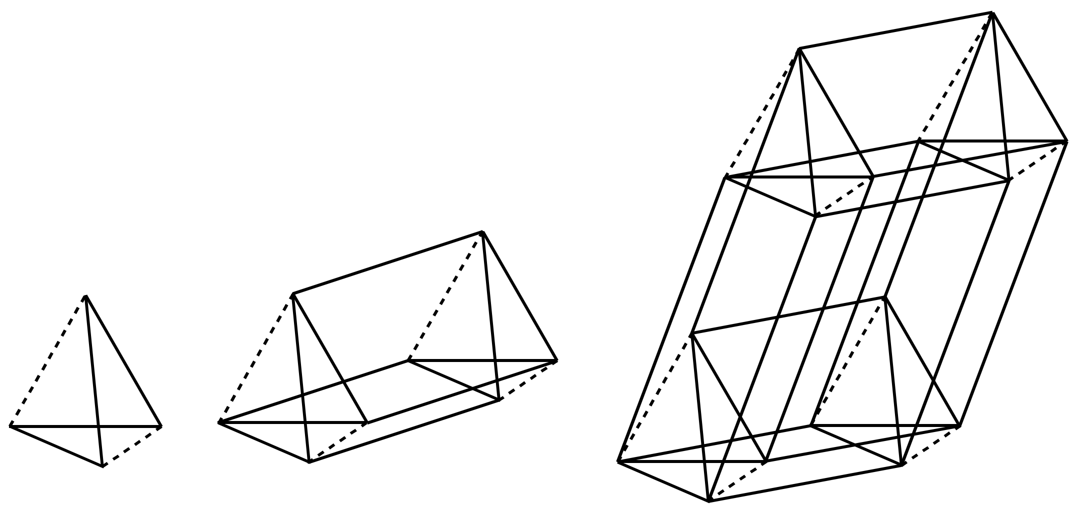

Figure 2. The signed graphs $(T\square Q_0,-)$, $(T\square Q_1,-)$ and $(T\square Q_2,-)$.

Therefore, it suffices to consider the following two cases:

- **Case 1:** Suppose $\sigma = +$. The eigenvalues and their multiplicities of the Cartesian product of this graph with Q_k, for some small values of k, are shown in Table 1. Now we can use the Khayyam-Pascal triangle to obtain explicit formulas for the energy of $(T\square Q_k,+)$ (and hence also for $(T\square Q_k,-)$.

$$\varepsilon(T\square Q_k,+) = 3\sum_{i=0}^{k}\binom{k}{i}|-k-1+2i| + \sum_{i=0}^{k}\binom{k}{i}|-k+3+2i|$$
$$= \sum_{i=0}^{k}\binom{k}{i}(3|-k-1+2i| + |-k+3+2i|).$$

Table 1. Eigenvalues and their multiplicity of graph $(T\square Q_k, +)$.

k	Eigenvalues	Multiplicity
0	−1,3	3,1
1	−2,0,2,4	3,3,1,1
2	−3, −1,1,3,5	3,6,4,2,1
3	−4, −2,0,2,4,6	3,9,10,6,3,1
4	−5, −3, −1,1,3,5,7	3,12,19,16,9,4,1
5	−6, −4, −2,0,2,4,6,8	3,15,31,35,25,13,5,1

Let us look at the expression in square brackets. We denote it by A_i. For a given even integer $k = 2m$, the list of A_i looks as $4k,\ 4k-8,\ \ldots,\ 16,\ 10,\ 6,\ 8, 16, \ldots, 4k-8, 4k$. It can be shown by a straightforward calculations that the pattern $A_i = 4|k-2i|$ is broken only for $i \in \{\frac{k}{2}-1, \frac{k}{2}, \frac{k}{2}+1\}$. By grouping symmetric terms and by correcting for the mid-range anomaly, we obtain

$$\varepsilon(T\square Q_{2m}, +) = 8\sum_{i=0}^{m}(2m-2i)\binom{2m}{i} + 6\binom{2m}{m} + 2\binom{2m}{m+1}.$$

The resulting expression is then readily simplified to a compact form,

For an odd $k = 2m+1$, the $A_i = 4|k-2i|$ pattern is broken only for $i \in \{\frac{k-1}{2}, \frac{k+1}{2}\}$ .Again, by grouping the symmetric terms and by correcting for the mid-range deviation, we obtain

$$\varepsilon(T\square Q_{2m+1}, +) = 8\sum_{i=0}^{m}(2m+1-2i)\binom{2m+1}{i} + 4\binom{2m+1}{m+1},$$

that further simplifies to

Now we can state our results in terms of the hypercube dimension k.

Theorem 2.1: $\varepsilon(T\square Q_k, +) = \varepsilon(T\square Q_k, -) = (\mathrm{k}+3)\binom{k+2}{\left\lfloor\frac{k+2}{2}\right\rfloor}$.

- **Case 2:** Now we consider the case that two cycles of graph are balanced (positive) and two others are unbalanced (negative). In the signed graph $(T, \pm)$ we have 4 distinct eigenvalues and two of them are integer. Table 2 shows the relevant information for this case. The formula of energy of signed graph $(T\square Q_k, \pm)$ can be written as follows:

$$\begin{aligned}\varepsilon(T\square Q_k, \pm) &= \sum_{i=0}^{k}\binom{k}{i}|-k-1+2i| + \sum_{i=0}^{k}\binom{k}{i}|-k+1+2i| \\ &+ \sum_{i=0}^{k}\binom{k}{i}\left(|-k+\sqrt{5}+2i| + |-k-\sqrt{5}+2i|\right) \\ &= \sum_{i=0}^{k}\binom{k}{i}\left(|-k-1+2i| + |-k+1+2i|\right. \\ &\left.+|-k+\sqrt{5}+2i| + |-k-\sqrt{5}+2i|\right).\end{aligned}$$

Table 2. Eigenvalues and their multiplicity of graph $(T\square Q_k, \pm)$.

k	Eigenvalues	Multiplicity
0	$-\sqrt{5},-1,1,\sqrt{5}$	1,1,1,1
1	$-\sqrt{5}-1,-\sqrt{5}+1,-2, 0, 2,\sqrt{5}-1 ,\sqrt{5}+1$	1,1,1,2,1,1,1
2	$-\sqrt{5}-2, -\sqrt{5} ,-\sqrt{5}+2 ,-3, -1,1,3,$ $\sqrt{5}-2, \sqrt{5} ,\sqrt{5}+2$	1,2,1,1,3,3,1,1,2,1
3	$-\sqrt{5}-3, -\sqrt{5}-1-\sqrt{5}+1, -\sqrt{5}+3, -4, -2,0,$ $2,4, \sqrt{5}-3, \sqrt{5}-1, \sqrt{5}+1, \sqrt{5}+3$	1,3,3,1,1,4,6,4,1,1,3,3,1

By the same reasoning as in the previous case, we can show that the expression in square brackets, let us call it B_i, has the form $B_i = 4|k-2i|$ for almost all i. The only exceptions are $i \in \left\{\frac{k}{2}-1, \frac{k}{2}, \frac{k}{2}+1\right\}$ for an even k and $i \in \{\frac{k-1}{2}, \frac{k+1}{2}\}$ for an odd k. The exceptional cases are the only ones containing $\sqrt{5}$. By grouping together symmetric terms, multiplying by the corresponding multiplicities and correcting for the exceptional cases, we obtain explicit expressions for the energies of $(T\square Q_k, \pm)$ as follows:

Theorem 2.2.

$$\varepsilon(T\square Q_{2m}, \pm) = 4(2m+\sqrt{5})\binom{2m}{m-1} + 2(1+\sqrt{5})\binom{2m}{m};$$

$$\varepsilon(T\square Q_{2m+1}, \pm) = 4(2m+\sqrt{5}+1)\binom{2m+1}{m}.$$

In Table 3, we list the values of energy for different signs of graph $(T\square Q_k, \sigma)$ for the first few values of k.

Table 3. The energy of signed graphs $(T\square Q_k, \sigma)$.

k	$\varepsilon(T\square Q_k, +)$	$\varepsilon(T\square Q_k, -)$	$\varepsilon(T\square Q_k, \pm)$
0	6	6	$2 + 2\sqrt{5}$
1	12	12	$4\sqrt{5} + 4$
2	30	30	$8\sqrt{5} + 12$
3	60	60	$12\sqrt{5} + 36$
4	140	140	$28\sqrt{5} + 76$
5	280	280	$40\sqrt{5} + 200$

2.2 DIFFERENT SWITCHING EQUIVALENT CLASSES AND THEIR ENERGY IN SIGNEDOCTAHEDRON GRAPH

In this section we find different switching equivalent classes of signed graph $(O\square Q_k, \sigma)$ for all possible signs. By using the fact that two graphs are switching equivalent if and only if they have the same signs of cycles, we can find all switching equivalent classes of this graph. By numbering all cycles, Figure 3, we find 14 different classes. Note that the cycle number 8 contains edges 45, 46 and 56.

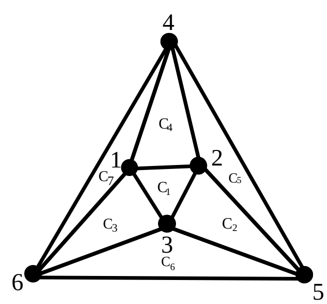

Figure 3. Cycles in the octahedron graph.

We have the following general result:

Theorem2.3. Let O be a signed octahedron graph with distinct eigenvalues $\lambda_1, \ldots, \lambda_s$ with multiplicities $m(\lambda_i)$, $j = 1, \ldots, s$. Then

$$\varepsilon(O\square Q_k, \sigma) = \sum_{j=1}^{s} \sum_{i=0}^{k} \binom{k}{i} m(\lambda_j)| - k + \lambda_j + 2i|.$$

In order to find all possible switching equivalent classes in the signed octahedron graph, we have checked all 2^{12} different sign choices. We have found exactly 14 different switching equivalent classes. Since all graphs in a switching equivalent class have the same characteristic polynomial and energy, we consider the graphs that have the smallest number of negative edges in each class. Note that some of those classes have the same energy. As an example, one graph in every class is shown in Figure 4. In Table 4, we calculate their characteristic polynomials and the corresponding energies. Also in the last column of this table an example of every case is shown.

It turns out that graphs 1, 2, and 14 of Table 4 have integral spectrum, and for them we obtain explicit formulas for energies of their Cartesian products with Q_k in the same way as was used in the previous subsection. For someother graphs we could obtain formulas involving quadratic irrationalities as in the case of Theorem 2.2. Obviously, the classes represented by graphs 1 and 2 will have the same energy and we consider them first. It suffices to look at the graph 1. Its eigenvalues are −2, 0, and 4, with multiplicities 2, 3, and 1, respectively. Hence,

$$\begin{aligned}\varepsilon(O\square Q_k,+) &= \sum_{i=0}^{k} 2\binom{k}{i}|-k-1+2i| + \sum_{i=0}^{k} 3\binom{k}{i}|-k+2i| + \sum_{i=0}^{k}\binom{k}{i}|-k-1+2i| \\ &= \sum_{i=0}^{k}\binom{k}{i}\left[2|-k-2+2i| + 3|-k+2i| + |-k-1+2i|\right]\end{aligned}$$

The expression in the square brackets, denote it by D_i, is of the form $D_i = 6|k-2i|$ for $i = 1, \dots, k$, with the only exceptions around the mid-range. More precisely, for every k, the pattern is valid for all $i \notin \{m-1, m, m+1\}$. Now, as in the previous subsection, by grouping symmetric terms and accounting for the mid-range exceptions, we obtain

$$\varepsilon(O\square Q_{2m},+) = 2\sum_{i=0}^{m} 12(m-i)\binom{2m}{i} + 28\binom{2m}{m-1} + 8\binom{2m}{m}$$

and

$$\varepsilon(O\square Q_{2m+1},+) = 2\sum_{i=0}^{m-2} 6(2m+1-2i)\binom{2m+1}{i} + 38\binom{2m+1}{m-1} + 22\binom{2m+1}{m}.$$

The above expressions are then readily simplified as

$$\varepsilon(O\square Q_{2m},+) = 4(3m+4)\binom{2m}{m-1} + 8\binom{2m}{m}$$

and

$$\varepsilon(O\square Q_{2m+1},+) = 2(6m+13)\binom{2m+1}{m-1} + 22\binom{2m+1}{m}$$

for even and odd k, respectively.

For the energy of the $14th$ case, denote it by $(O\square Q_k,\pm)$, we have:

$$\varepsilon(O\square Q_k, \pm) = \sum_{i=0}^{k} 3\binom{k}{i}|-k-2+2i| + \sum_{i=0}^{k} 3\binom{k}{i}|-k+2+2i|$$
$$= \sum_{i=0}^{k} 3\binom{k}{i}[|-k-2+2i| + |-k+2+2i|],$$

since the eigenvalues of the $14th$ signed octahedron are -2 and 2, each with multiplicity of 3. Therefore, we have $\varepsilon(O\square Q_{2m}, \pm) = 2.3\sum_{i=0}^{m-1} 4(m-i)\binom{2m}{i} + 3.4\binom{2m}{m}$ and $\varepsilon(O\square Q_{2m+1}, \pm) = 2.3\sum_{i=0}^{m-1} 2(2m+1-2i)\binom{2m+1}{i} + 3.2.4\binom{2m+1}{m}$. We now simplifythis expression to $\varepsilon(O\square Q_{2m}, \pm) = 12(m+1)\binom{2m}{m}and\varepsilon(O\square Q_{2m+1}, \pm) = 12(m+2)\binom{2m+1}{m}$, for even and odd k, respectively. Now we can state our results in terms of the hypercube dimension k.

Theorem2.4. $\varepsilon(O\square Q_k, \pm) = 12(\left\lceil\frac{k}{2}\right\rceil + 1)\binom{k}{\left\lfloor\frac{k}{2}\right\rfloor}$.

Table 4. The characteristic polynomial and energy of signed graphs$(O\square Q_k, \sigma)$.

	Characteristic Polynomial	Energy	Negative Cycles
1	$\lambda^6 - 12\lambda^4 - 16\lambda^3$	8	_ _ _ _ _ _
2	$\lambda^6 - 12\lambda^4 + 16\lambda^3$	8	$C_1, C_2, C_3, C_4, C_5, C_6, C_7, C_8$
3	$\lambda^6 - 12\lambda^4 + 16\lambda^2$	8.944	C_1, C_3, C_4, C_7
4	$\lambda^6 - 12\lambda^4 + 32\lambda^2$	9.656	C_1, C_2, C_7, C_8
5	$\lambda^6 - 12\lambda^4 - 8\lambda^3 + 20\lambda^2 + 16\lambda$	9.837	C_1, C_4
6	$\lambda^6 - 12\lambda^4 + 8\lambda^3 + 20\lambda^2 - 16\lambda$	9.837	$C_1, C_3, C_4, C_6, C_7, C_8$
7	$\lambda^6 - 12\lambda^4 - 8\lambda^3 + 32\lambda^2 + 32\lambda$	10.472	C_1, C_5
8	$\lambda^6 - 12\lambda^4 + 8\lambda^3 + 32\lambda^2 - 32\lambda$	10.472	$C_1, C_2, C_3, C_4, C_6, C_8$
9	$\lambda^6 - 12\lambda^4 - 8\lambda^3 + 36\lambda^2 + 48\lambda + 16$	10.928	C_1, C_8
10	$\lambda^6 - 12\lambda^4 + 36\lambda^2 - 16$	10.928	C_2, C_3, C_4, C_5
11	$\lambda^6 - 12\lambda^4 + 8\lambda^3 + 36\lambda^2 - 48\lambda + 16$	10.928	$C_1, C_3, C_4, C_5, C_6, C_8$
12	$\lambda^6 - 12\lambda^4 + 32\lambda^2 - 16$	10.837	C_1, C_2, C_4, C_7
13	$\lambda^6 - 12\lambda^4 + 36\lambda^2 - 32$	11.313	C_1, C_5, C_6, C_8
14	$\lambda^6 - 12\lambda^4 + 48\lambda^2 - 64$	12	C_1, C_5, C_6, C_7

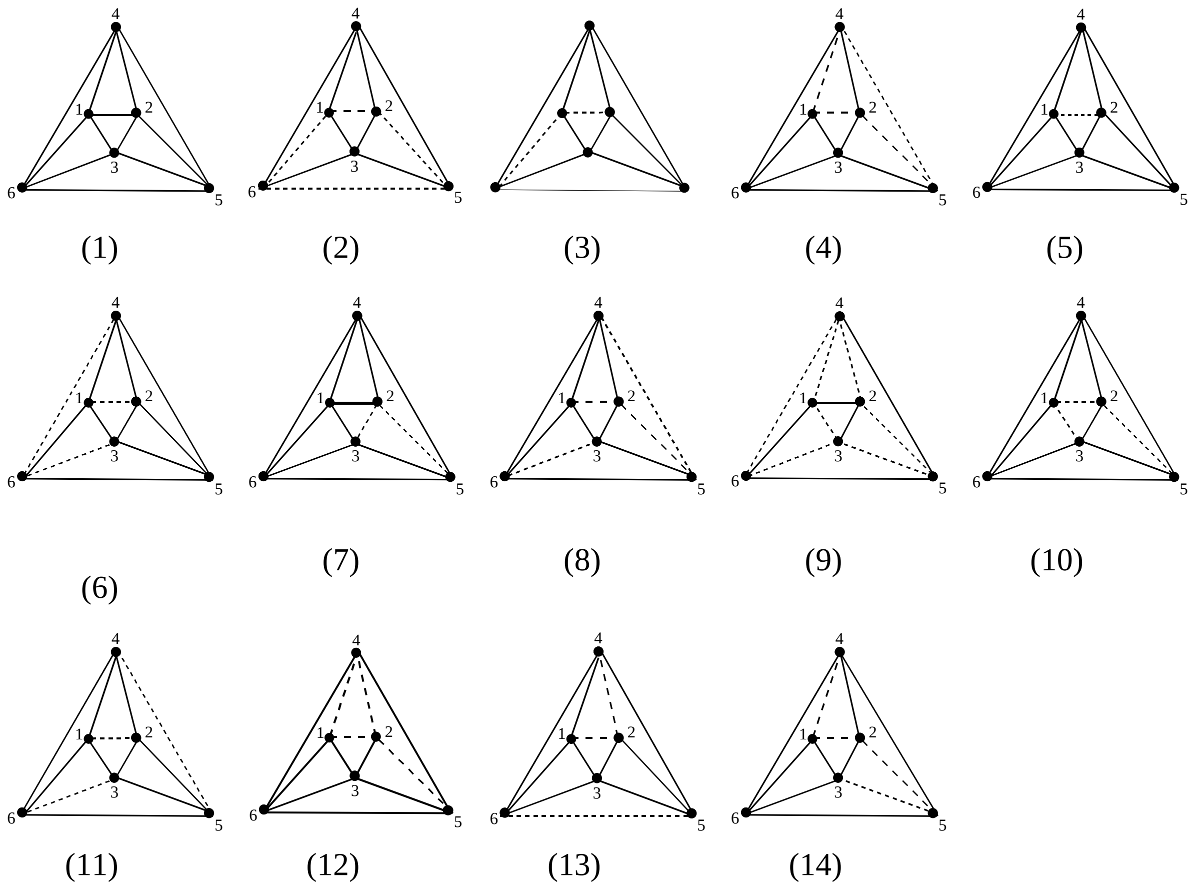

Figure 4. Examples of all switching equivalent classes of signed graphs.

3 CONCLUSION

In this paper we have considered the spongy hypercubes, an interesting classof graphs that arise from Cartesian products of polyhedral graphs andhypercubes. We have looked at the case when the polyhedral graph is thetetrahedron and the octahedron. In both cases we have determined allswitching equivalent classes and computed the corresponding energies. For the tetrahedral spongy hypercubes we were able to determine explicitformulas for the energies in a compact form depending only on the dimensionk of the hypercube. It might be interesting to look at other cases ofspongy hypercubes where the component graphs have integer eigenvalues. Webelieve that our approach would yield explicit formulas for their energiestoo.

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