Cayley sum graphs and eigenvalues of $(3, 6)$-fullerenes

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Abstract

We determine the spectra of cubic plane graphs whose faces have sizes 3 and 6. Such graphs, "(3,6)-fullerenes", have been studied by chemists who are interested in their energy spectra. In particular we prove a conjecture of Fowler, which asserts that all their eigenvalues come in pairs of the form $\{\lambda, -\lambda\}$ except for the four eigenvalues $\{3, -1, -1, -1\}$. We exhibit other families of graphs which are "spectrally nearly bipartite" in this sense. Our proof utilizes a geometric representation to recognize the algebraic structure of these graphs, which turn out to be examples of Cayley sum graphs.

Keywords: (3,6)-cage, fullerene, spectrum, Cayley sum graph, Cayley addition graph, geometric lattice, flat torus.
MSC: 05C50, 05C25, 05C10

1 Introduction

A $(3, 6)$-*fullerene* is a cubic plane graph whose faces have sizes 3 and 6. These graphs have received recent attention from chemists due to their similarity to ordinary fullerenes. (Such graphs are sometimes called $(3, 6)$-*cages* in that community, but in graph theory this term already has a different, well-established meaning.) In 1995, Patrick Fowler (see [7]) conjectured the following result, which we prove here. Prior to this work, this result had been established for several subfamilies of $(3, 6)$-fullerenes [7, 5, 14]. Recall that the *spectrum* of a graph is the multiset of eigenvalues of its adjacency matrix.

Theorem 1.1. *If G is a $(3, 6)$-fullerene, then the spectrum of G has the form $\{3, -1, -1, -1\} \cup L \cup -L$ where L is a multiset of nonnegative real numbers, and $-L$ is the multiset of their negatives.*

*Supported by a Canada NSERC Discovery Grant
†Supported in part by ARRS Research Grant P1–0297, by an NSERC Discovery Grant, and by the CRC program.

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§Supported by PIMS postdoctoral fellowship.

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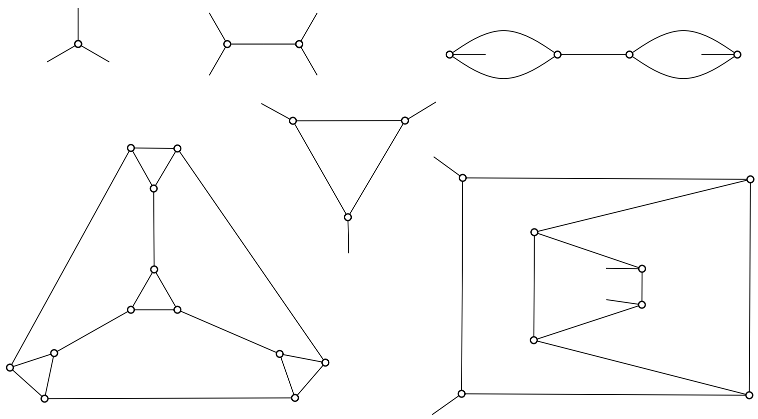

Figure 1: Examples of some small $(0, 3, 6)$-fullerenes.

In fact we prove an extended conjecture of Fowler *et al.* [7]. They propose that a generalized class of graphs called $(0, 3, 6)$-*fullerenes* also exhibit this "spectrally nearly bipartite" behavior. A *semiedge* of a graph is an edge with one endpoint, but unlike a loop, a semiedge contributes just one to both the valency of its endpoint and the corresponding diagonal entry of the adjacency matrix. In a plane embedding, a semiedge s with endpoint v is drawn as an arc with one end at v which sits in a face f, and s contributes one to the length of f. Figure 1 displays some examples of small $(0, 3, 6)$-fullerenes.

The outline of our proof is as follows. We show that every $(0, 3, 6)$-fullerene can be represented as a quotient of a certain lattice-like graph in the plane. This geometric description allows us to prove that these graphs are Cayley sum graphs. Then we call on a theorem which describes the spectral behavior of Cayley sum graphs in terms of the characters of the group.

In fact, the geometric description of $(0, 3, 6)$-fullerenes which is inherent in our proof is just a slight extension of a construction for $(3, 6)$-fullerenes which has been discovered by several authors [5, 7, 16], and follows easily from a deep theorem on the intrinsic metric of polygonal surfaces by Alexandrov [1]. In Section 4, we give a proper exposition of this construction, and a proof that it is universal.

With this construction in hand, it is possible to explicitly compute the spectrum of $(0, 3, 6)$-fullerenes, and in Section 5 we detail precisely how this computation can be made. Finally, in Section 6, we generalize to an arbitrary dimension, and expose the connection between this type of geometric graphs and Cayley sum graphs.

2 Cayley sum graphs

Let Γ be a finite additive abelian group, and let $S \subseteq \Gamma$. We define the *Cayley sum graph* $\mathrm{CayS}(\Gamma, S)$ to be the graph (V, E) with $V = \Gamma$, and $uv \in E$ if and only if $u + v \in S$. If S is a multiset, then $\mathrm{CayS}(\Gamma, S)$ contains multiple edges, and if there exists $u \in \Gamma$ with $2u \in S$, then the edge uu is a semiedge. This definition is a variation of the well-studied *Cayley graph* $\mathrm{Cay}(\Gamma, S)$, in which uv forms an edge if and only if $u - v \in S$.

In contrast with Cayley graphs, there are only a few appearances of Cayley sum graphs in the literature (see [9] and references therein). For this reason we state some of their elementary properties. The graph $G = \mathrm{CayS}(\Gamma, S)$ is $|S|$-regular. While G is not generally vertex-transitive, the map $x \mapsto x + t$ is an isomorphism from G to $\mathrm{CayS}(\Gamma, S + 2t)$, for every $t \in \Gamma$. Finally, the squared graph $G^{(2)}$, which has an edge for each walk of length 2 in G, is the ordinary Cayley graph $\mathrm{Cay}(\Gamma, S - S)$ where $S - S$ is the multiset $\{s_1 - s_2 \mid s_1, s_2 \in S\}$.

The spectrum of a (finite abelian) Cayley graph $\mathrm{Cay}(\Gamma, S)$ is easy to describe (see [10, Ex. 11.8] or [11], where the nonabelian case is dealt with). Every character χ of Γ is a (complex-valued) eigenvector corresponding to the eigenvalue

$$\chi(S) := \sum_{s \in S} \chi(s)\,.$$

We may assume $\Gamma = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_u}$, where $|\Gamma| = \prod_i n_i$ and $\mathbb{Z}_k$ denotes the cyclic group of order k. To each $a = (a_1, \ldots, a_u) \in \Gamma$ we associate the group character

$$\chi_a : (x_1, \ldots, x_u) \mapsto \exp\left(2\pi i \sum_j \frac{a_j x_j}{n_j}\right).$$

The characters for a and $-a$ satisfy $\chi_{-a}(x) = \overline{\chi_a(x)}$, so χ_a is a real-valued (indeed ± 1-valued) eigenvector of $\mathrm{Cay}(\Gamma, S)$ if and only if a is an involutive group element. If a is not involutive, then the real and imaginary parts of χ_a provide real-valued eigenvectors for the conjugate pair of eigenvalues $\chi_a(S), \chi_{-a}(S)$.

Cayley sum graphs exhibit a similar phenomenon. Let $R = \{\chi_a \mid a + a = 0\}$ be the real-valued characters of Γ, and let C be a set containing exactly one character from each conjugate pair $\{\chi_a, \chi_{-a}\}$ (where $a \in \Gamma$ and $a + a \neq 0$). So the set of characters of Γ is $R \cup \{\chi, \overline{\chi} \mid \chi \in C\}$. Versions of the following result can be found in the literature [6, 2].

Theorem 2.1. *Let $G = \mathrm{CayS}(\Gamma, S)$ be a Cayley sum graph on a finite abelian group Γ, and let R, C be as above. The multiset of eigenvalues of G is*

$$\{\chi(S) \ :\ \chi \in R\} \cup \{\pm|\chi(S)| \ :\ \chi \in C\}.$$

The corresponding eigenvectors are χ (for $\chi \in R$), and the real and the imaginary parts of $\alpha\chi$ (for $\chi \in C$ with a suitable complex scalar α which depends only on $\chi(S)$).

Proof. Let χ be a character of Γ and $u \in \Gamma$ a vertex of $\mathrm{CayS}(\Gamma, S)$. Then

$$\sum_{v \in N(u)} \chi(v) = \sum_{s \in S} \chi(s - u) = \chi(S)\overline{\chi(u)}\,.$$

This shows that every real-valued character is an eigenvector corresponding to the eigenvalue $\chi(S)$. If $\chi \in C$, then χ is not an eigenvector. In this case we choose a complex number α such that $|\alpha| = 1$ and $\alpha^2\chi(S) = |\chi(S)|$ and we define $x(v) = \alpha\chi(v)$. It follows that for every $u \in \Gamma$,

$$\sum_{v \in N(u)} x(v) = \alpha^2\chi(S) \cdot \alpha^{-1}\overline{\chi(u)} = |\chi(S)| \cdot \overline{x(u)}.$$

Consequently, $\mathrm{Re}\, x$ and $\mathrm{Im}\, x$ are real eigenvectors corresponding to eigenvalues $|\chi(S)|$ and $-|\chi(S)|$, respectively. Both of these vectors are nonzero, as they generate the same 2-dimensional (complex) vector space as $\{\chi, \overline{\chi}\}$. This, together with the orthogonality of characters, implies that we have described the complete set of eigenvectors, and thus the entire spectrum of $\mathrm{CayS}(\Gamma, S)$. ∎

3 $(0,3,6)$-fullerenes as Cayley sum graphs

The goal of this section is to prove that $(0,3,6)$-fullerenes are Cayley sum graphs, and to subsequently prove Fowler's conjecture regarding their spectra.

The proof of Theorem 3.1 utilizes structural properties of 3-regular hexangulations of the torus. This class of graphs was classified by Altshuler [4] and studied by many others (e.g., Thomassen [15]). In a recent work of Alspach and Dean [3], it is shown that they are indeed Cayley graphs, and a description of the group is given. Although the properties we require of these graphs are similar to those found elsewhere, our approach is novel since it is inherently geometric.

A *polygonal surface* $\mathcal{H}$ is a connected 2-manifold without boundary which is obtained from a collection of disjoint simple polygons in $\mathbb{E}^2$ by identifying them along edges of equal length. Thus we view $\mathcal{H}$ both (combinatorially) as an embedded graph with vertices, edges, and faces, and as a manifold with a (local) metric inherited from $\mathbb{E}^2$.

Theorem 3.1. *Every $(0,3,6)$-fullerene is isomorphic to a Cayley sum graph for an abelian group which can be generated by two elements.*

Proof. Let G be a cubic $(0,3,6)$-fullerene with vertex set V. Let $G_2 = G \times K_2$ (the categorical graph product). Let $(V_\bullet, V_\circ)$ be the corresponding bipartition of $V(G_2)$, and for every $v \in V$, let $v_\bullet \in V_\bullet$ and $v_\circ \in V_\circ$ be the vertices of G_2 which cover v. Every semiedge $vv \in E(G)$ lifts to the edge $v_\bullet v_\circ$ in G_2. Each facial walk of G bounding a face of size 6 lifts to two closed walks of length 6 in G_2, and each facial walk of G bounding a face of size 3 lifts to a closed walk of length 6 in G_2. Accordingly, we may extend G_2 to a polygonal surface $\mathcal{H}$ by treating all edges as having equal length and adding a regular hexagon to each closed walk which is the pre-image of a facial walk of G, with clockwise orientation as given by the clockwise orientation of that face. Now, $\mathcal{H}$ is an orientable polygonal surface, all vertices have degree three, and all faces are regular hexagons, so $\mathcal{H}$ is a regular hexangulation of the flat torus. Let $\widetilde{\mathcal{H}}$ be the universal cover of $\mathcal{H}$ and let $\mathbf{p} : \widetilde{\mathcal{H}} \to \mathcal{H}$ be the covering map. Then $\widetilde{\mathcal{H}}$ (with the metric inherited from $\mathcal{H}$) is the regular hexangulation of the Euclidean plane. We define $\widetilde{V}_\bullet = \mathbf{p}^{-1}(V_\bullet)$, $\widetilde{V}_\circ = \mathbf{p}^{-1}(V_\circ)$, and $\tilde{x} = \mathbf{p}^{-1}(x)$ for $x \in V_\bullet \cup V_\circ$.

Fix a vertex $u_\bullet \in V_\bullet$, and treat $\widetilde{\mathcal{H}}$ as a regular hexangulation of $\mathbb{E}^2$ with $\mathbf{p}((0,0)) = u_\bullet$. This equips $\widetilde{\mathcal{H}}$ with an (additive abelian) group structure. The point set $\widetilde{V}_\bullet$ is a geometric lattice. The point set $\tilde{u}_\bullet$ is a sublattice of $\widetilde{V}_\bullet$. Any fundamental parallelogram of $\tilde{u}_\bullet$ is a fundamental region of the cover $\mathbf{p}$. We may identify $\mathcal{H}$ with $\widetilde{\mathcal{H}}/\tilde{u}_\bullet$, and this equips $\mathcal{H}$ with a group structure whose identity is $u_\bullet$.

For every $y \in \mathcal{H}$ ($y \in \widetilde{\mathcal{H}}$) the map $x \mapsto x + y$ is an isometry of $\mathcal{H}$ ($\widetilde{\mathcal{H}}$, respectively). This map may or may not preserve the combinatorial structure of $\mathcal{H}$ ($\widetilde{\mathcal{H}}$). An isometry $\mu : \mathcal{H} \to \mathcal{H}$ is *respectful* if μ is an automorphism of the embedded graph associated with $\mathcal{H}$. An isometry $\tilde{\mu} : \widetilde{\mathcal{H}} \to \widetilde{\mathcal{H}}$ is *respectful* if it is a lift of a respectful isometry of $\mathcal{H}$. Now, for every $y \in \widetilde{V}_\bullet$ the map $x \mapsto x + y$ is a respectful isometry of $\widetilde{\mathcal{H}}$. Accordingly, $V_\bullet$ is a subgroup of $\mathcal{H}$ with identity $u_\bullet$, and for every $y \in V_\bullet$ the map $x \mapsto x + y$ is a respectful isometry of $\mathcal{H}$.

Let ρ be the automorphism of the graph G_2 given by the rule $\rho(v_\circ) = v_\bullet$ and $\rho(v_\bullet) = v_\circ$ for every $v \in V$. Now, ρ extends naturally to a respectful isometry of $\mathcal{H}$ which preserves the orientation of the hexagons, but interchanges $V_\circ$ and $V_\bullet$. We choose a respectful isometry $\tilde{\rho}$ of $\mathbb{E}^2$ so that ρ lifts to $\tilde{\rho}$. Because $\tilde{\rho}$ preserves the orientation of $\mathbb{E}^2$, the isometry $\tilde{\rho}$ is either a rotation or translation.

Since $\tilde{\rho}$ is respectful and maps $\widetilde{V}_\bullet$ to $\widetilde{V}_\circ$, it easily follows that ρ is either a rotation by π about the center of an edge or face, or ρ is a rotation by $\pi/3$ about the center of a face F.

We first consider the latter case. Here, all three vertices of $\widetilde{V}_\bullet$ which are on the boundary of F, lie in the same orbit of $\tilde{\rho}^2$. Since ρ^2 is the identity, all three vertices cover the same vertex, say $v_\bullet$ in $\mathcal{H}$. The other three vertices of F cover $v_\circ$. In this case G_2 is the theta-graph with vertex set $\{v_\bullet, v_\circ\}$. Here we have $G \cong \mathrm{CayS}(\{0\}, \{0,0,0\})$, the graph with one vertex and three semiedges, and there is nothing left to prove.

We henceforth assume that $\tilde{\rho}$ is a rotation by π. Let $x, y \in V_\bullet$ and choose $\tilde{x}, \tilde{y} \in \widetilde{V}_\bullet$ which project (respectively) to x, y. Then (using the fact that $\tilde{\rho}$ is a rotation by π) we find that

$$\begin{aligned}\rho(\rho(x)+y) &= \mathbf{p}(\tilde{\rho}(\tilde{\rho}(\tilde{x})+\tilde{y}))\\ &= \mathbf{p}(\tilde{x}-\tilde{y})\\ &= x-y.\end{aligned}$$

In other words, for any fixed $y \in V_\bullet$, conjugating the map on $\mathcal{H}$ given by $x \mapsto x+y$, by ρ yields the map $x \mapsto x-y$.

We define a labeling $\ell : V_\bullet \cup V_\circ \to V_\bullet$ by the rule $\ell(v_\bullet) = \ell(v_\circ) = v_\bullet$. We regard ℓ to be a labeling of $V(G_2)$ by elements of the abelian group $V_\bullet$. Let $v \in V$ and let $y \in V_\bullet$. Then we have

$$\ell(v_\bullet + y) = \ell(v_\bullet) + y$$

and

$$\begin{aligned}\ell(v_\circ + y) &= \ell(\rho(v_\circ + y))\\ &= \ell(\rho(\rho(v_\bullet)+y))\\ &= \ell(v_\bullet - y)\\ &= \ell(v_\circ) - y.\end{aligned}$$

That is, the group $V_\bullet$ acts on the labels of points in $V_\bullet$ by addition and on the labels of points in $V_\circ$ by subtraction. Let S be the multiset of labels of the three vertices in $V_\circ$ which are adjacent to $u_\bullet$ (recall that $u_\bullet$ is the group identity for $V_\bullet$). Then, for every $v_\bullet \in V_\bullet$, the three neighbors of $v_\bullet$ in G_2 have labels $S - v_\bullet$. In particular, v and v' are adjacent vertices in G if and only if $\ell(v_\bullet) + \ell(v'_\circ) \in S$. It follows immediately from this that $G \cong \mathrm{CayS}(V_\bullet, S)$. Since $\widetilde{V}_\bullet$ can be generated by two elements, $V_\bullet = \widetilde{V}_\bullet / \tilde{u}_\bullet$ can also be generated by two elements, and this completes the proof. □

We need only one quick observation before we resolve Theorem 1.1 and the extended conjecture of Fowler et al. If G is a cubic plane graph with s semiedges, and f_i faces of size i for every $i \geq 1$, then $3|V(G)| = 2|E(G)| - s = \sum_{i \geq 1} i f_i$. Applying Euler's formula, we find that $\sum_{i \geq 1}(6-i) f_i = 12 - 3s$. In particular, every $(0,3,6)$-fullerene satisfies

$$s + f_3 = 4. \tag{1}$$

Theorem 3.2. *If G is a $(0,3,6)$-fullerene with s semiedges, then the spectrum of G may be partitioned as $\{M, L, -L\}$ where one of the following holds:*

(a) $s = 0$ *and* $M = \{3, -1, -1, -1\}$,
(b) $s = 2$ *and* $M = \{3, -1\}$,
(c) $s = 3$ *and* $M = \{3\}$, *or*
(d) $s = 4$ *and* $M = \{3, 1\}$.

Proof. By the previous theorem, there is an abelian group Γ which can be generated by two elements so that $G \cong \mathrm{CayS}(\Gamma, S)$ for some $S \subseteq \Gamma$ with $|S| = 3$. By Theorem 2.1, we may partition the eigenvalues of G into multisets $M, L, -L$ where $M = \{\chi(S) : \chi \in R\}$ and R is the set of ± 1-valued characters of Γ. Every eigenvalue in M is the sum of three integers in $\{\pm 1\}$. The identity character corresponds to $3 \in M$. Since G is not bipartite, we have $-3 \notin M$, so every other element of M is ± 1. The trace of the adjacency matrix is equal to s, and is also equal to the sum of the eigenvalues. Since L and $-L$ sum to 0, we conclude that $s = \sum M$.

We have $|R| \in \{1, 2, 4\}$ because Γ has 2^k involutive elements, for some $k \leq 2$. If $|R| = 1$, then $M = \{3\}$ and $s = 3$ as in the statement. If $|R| = 2$, then $s = \sum M = 3 \pm 1$, so we have either the case $s = 2$ or $s = 4$ of the statement. Finally, we assume $|R| = 4$. By Equation (1) we have $s \leq 4$, so $\sum M \in \{0, 2, 4\}$. If $\sum M = 0$, then $s = 0$ (G is a $(3, 6)$-fullerene), and we have case (a). Finally, if $\sum M \in \{2, 4\}$, then M contains both a 1 and a -1. By transferring these two entries from M to the multisets L and $-L$, we find ourselves again in either the case $s = 2$ or the case $s = 4$ of the statement. This completes the proof. $\square$

We remark that there are infinitely many $(0, 3, 6)$-fullerenes with s semiedges, for each $s = 0$, 2, 3, 4. As shown by Theorem 3.2, there are none with $s = 1$, a fact that is non-trivial to prove from the first principles (compare Theorem 2 (with $k = 3$) in [8, Sec. 13.4, p. 272]).

4 An explicit construction

It is known that all $(3, 6)$-fullerenes arise from the so-called *grid construction*. Roughly speaking, the grid construction expresses the dual plane graph, which is a triangulation of the sphere, as a quotient of the regular triangular grid. The grid construction is also used by physicists [5, 14] (sometimes without formal justification) since it a convenient way to classify $(3, 6)$-fullerenes and compute their invariants.

We describe an extension of the grid construction and show that it characterizes the $(0, 3, 6)$-fullerenes. The construction makes clear how semiedges arise. The group structure of $(0, 3, 6)$-fullerenes is explicitly determined as a quotient of the A_2 lattice group. With this, we can easily find the Cayley sum graph representation via standard lattice computations, and thereby determine the spectrum and the eigenvectors of every $(0, 3, 6)$-fullerene.

In the following, $\mathcal{T}$ is the infinite triangular grid, whose vertices (called *gridpoints*) are points in the A_2 lattice. The midpoint of any edge in $\mathcal{T}$ is called an *edgepoint*. The *dual* G^* of a plane graph G with semiedges is defined as an obvious extension of the dual of an ordinary graph; every semiedge in G which is incident with vertex v and face f corresponds to a semiedge in G^* which is incident with the dual vertex f^* and the dual face v^*.

Construction 4.1. *The following procedure results in a* $(0, 3, 6)$*-fullerene,* G.

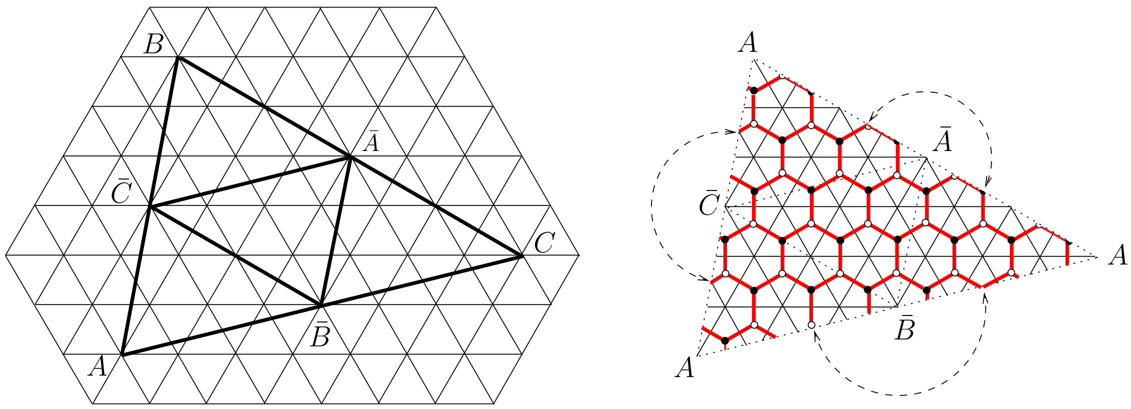

Figure 2: An example of Construction 4.1.

1. *Let $\triangle ABC$ be a triangle having no obtuse angle, and whose vertices are gridpoints of $\mathcal{T}$. Let $\bar{A}$, $\bar{B}$, $\bar{C}$ be the midpoints of the edges which are opposite to A, B, C (respectively) in $\triangle ABC$.*

2. *Optionally, translate $\triangle ABC$ so that A coincides with an edgepoint of $\mathcal{T}$.*

3. *From $\triangle ABC$, we fold an (isosceles) tetrahedron $Q = A\bar{A}\bar{B}\bar{C}$ by identifying the boundary segment $\bar{A}B$ with $\bar{A}C$, $\bar{B}C$ with $\bar{B}A$, and $\bar{C}A$ with $\bar{C}B$ (so A, B, and C are identified into a single vertex in Q). The portion of $\mathcal{T}$ lying within $\triangle ABC$ becomes a finite graph G^*, possibly with semiedges, and drawn on the surface of Q.*

4. *Let G be the dual of the plane graph G^*.*

Every gridpoint within or on the boundary of $\triangle ABC$, except A, $\bar{A}$, $\bar{B}$, and $\bar{C}$, has degree 6 in G^*, and corresponds to a hexagonal face of G. After Step 2, each of A, $\bar{A}$, $\bar{B}$, $\bar{C}$ is either a gridpoint or an edgepoint of $\mathcal{T}$. If $X \in \{A, \bar{A}, \bar{B}, \bar{C}\}$ is a gridpoint, then X becomes a vertex of degree 3 in G^*, and corresponds to a triangular face in G. If X is an edgepoint, then X becomes one end of a semiedge in G^*, which corresponds to a semiedge in G. It follows that Construction 4.1 results in a $(0, 3, 6)$-fullerene.

We remark that Construction 4.1 works even if $\triangle ABC$ has an obtuse angle (although it does not yield a geometric tetrahedron). However, this does not give any new $(0, 3, 6)$-fullerenes, as the following theorem shows. By forbidding obtuse triangles, we lose no generality and gain canonicality.

Theorem 4.2. *Every $(0, 3, 6)$-fullerene arises from Construction 4.1.*

Proof. Let G be a $(0, 3, 6)$-fullerene. If G has just one vertex, then G arises from the construction when $\triangle ABC$ is a triangular face of $\mathcal{T}$. We assume G has at least two vertices. The proof of Theorem 3.1 shows that the direct product $G_2 = G \times K_2$ is a bipartite hexangulation $\mathcal{H}$ of the flat torus, where $\mathcal{H}$ is the image of a covering map $\mathbf{p} : \widetilde{\mathcal{H}} \to \mathcal{H}$ from a hexagonal tessellation of the plane.

We further recall that there is an isometry ρ of $\mathcal{H}$ which is respectful of G_2 and interchanges its partite sets $V_\bullet$ and $V_\circ$. This isometry lifts to an isometry of $\widetilde{\mathcal{H}}$ which is a rotation $\tilde{\rho}$ by π about a point, say $A \in \widetilde{\mathcal{H}}$, which is either the center of a hexagonal face, or the midpoint of an edge of $\widetilde{\mathcal{H}}$. (More precisely $\tilde{\rho} : x \mapsto 2A - x$ is the central symmetry through A.) The kernel of $\mathbf{p}$ is a geometric lattice Λ in $\widetilde{\mathcal{H}}$, and rotation by π about any point in in the scaled lattice $\frac{1}{2}\Lambda$ also projects to ρ. Let B, C be points in $\widetilde{\mathcal{H}}$ such that the vectors AB, AC form lattice basis for Λ. By possibly translating C by a (unique) integer multiple of AB, we can assume that $\triangle ABC$ has no obtuse angles. This lattice basis defines a fundamental parallelogram $ABDC$ where $AD = AB + AC$. Scaling the parallelogram by $\frac{1}{2}$ results in a fundamental parallelogram for $\frac{1}{2}\Lambda$ whose vertices we may label $A\bar{C}\bar{A}\bar{B}$ as in Construction 4.1.

Now each vertex v of G lifts to a unique pair of vertices $v_\bullet, v_\circ$ in the (half-open) parallelogram $ABDC$, where $v_\bullet, v_\circ$ are centrally symmetric about $\bar{A}$. By representing v with the vertex in $\{v_\bullet, v_\circ\}$ which lies in $\triangle ABC$, and identifying boundary segments of $\triangle ABC$ as in Step 3 of the construction, we obtain an isomorphic copy of G. Finally, Construction 4.1 is stated in terms of the triangular grid $\mathcal{T}$, which is the plane dual of $\widetilde{\mathcal{H}}$. □

We remark that Construction 4.1 in fact produces a $(0, 3, 6)$-fullerene G rooted at a triangle or semiedge labeled with A. Two triangles drawn in $\mathcal{T}$ result in isomorphic pairs (G, A) if and only if the triangles are congruent. Therefore the map $\triangle ABC \mapsto G$ is at most 4-to-1 up to symmetries of $\mathcal{T}$.

5 Computing the spectrum

In this section, we use Construction 4.1 to compute the group and spectrum of any particular $(0, 3, 6)$-fullerene G.

The faces of $\mathcal{T}$ consist of *up-triangles* (Δ) and *down-triangles* (∇). We regard $\Lambda_\bullet$ to be an A_2-lattice generated by unit-length vectors $\mathbf{a}, \mathbf{b}$ with $\angle\mathbf{ab} = \pi/3$. With A being the gridpoint selected in Step 1 of Construction 4.1, we shall assume that the origin of $\Lambda_\bullet$ is (the center of) the up-triangle $u_\bullet := \triangle A(A + \mathbf{a})(A + \mathbf{b})$. Note that $\Lambda_\bullet$ is a translation of the gridpoints of $\mathcal{T}$ and corresponds to $\widetilde{V}_\bullet$ in the proof of Theorem 3.1. We denote by Λ the sublattice of $\Lambda_\bullet$ generated by vectors $\overrightarrow{AB}$ and $\overrightarrow{AC}$. (A translation of Λ is used in the proof of Theorem 4.2.) In Step 2, we translate $\triangle ABC$ by a vector

$$\mathbf{c} := \frac{p_1}{2}\mathbf{a} + \frac{p_2}{2}\mathbf{b} \tag{2}$$

for integers p_1, p_2. We may assume without loss of generality that $p_1, p_2 \in \{0, 1\}$, so, after Step 2, the point A is either a vertex or an edgepoint on the boundary of $u_\bullet$. Let p, q, r, s be integers satisfying

$$AB = p\mathbf{a} + q\mathbf{b}, \qquad AC = r\mathbf{a} + s\mathbf{b}. \tag{3}$$

Let $\bar{A}$, $\bar{B}$, $\bar{C}$ and T be as in the construction of G.

To express G as a Cayley sum graph we label the faces of $\mathcal{T}$ with elements of the finite abelian group presented as $\Gamma = \langle\, \alpha, \beta \mid p\alpha + q\beta = 0,\ r\alpha + s\beta = 0 \,\rangle$. We define $f : \Lambda_\bullet \to \Gamma$ by

$$f(i\mathbf{a} + j\mathbf{b}) = i\alpha + j\beta, \tag{4}$$

and extend f to the down-triangles in such a way that triangles which are centrally symmetric with respect to A receive the same value of f. The kernel of f is (a translation of) the lattice Λ generated by AB and AC. We observe the following properties:

- f assigns the same value to triangles that are identified during the 'folding' stage of the construction. This is because the triangles that are identified are symmetric with respect to each of $\bar{C}$, $\bar{B}$, and $\bar{A}$; each of these symmetries is a composition of the negation map $\Lambda_\bullet \mapsto -\Lambda_\bullet$ and a translation by an element of $\Lambda = \ker f$.

- f is a bijection from $V(G)$ to Γ. By construction, the up-triangles within the fundamental region $ABDC$ correspond to elements of Γ. The down-triangles within the triangle ABC correspond to up-triangles within DCB.

- If u_1 and u_2 are two up-triangles, then $f(u_2) = f(u_1) + f(u_2 - u_1)$. If d_1 and d_2 are two down-triangles then $f(d_2) = f(d_1) - f(d_2 - d_1)$.

Now let u be any up-triangle and d_1, d_2, d_3 its neighbors. We define the *sum-set* $S = \{f(u)+f(d_i) \mid i = 1, 2, 3\}$. From the above-mentioned properties of f it follows that S does not depend on the choice of u. The symmetry around A shows that we get the same sum-set if we consider neighbors of a down-triangle to define S. It follows that $G \cong \mathrm{CayS}(\Gamma, S)$.

We can explicitly compute Γ and S by applying standard lattice computations. We recall that the *Smith normal form* of a nonsingular integer matrix M is the unique matrix $\mathrm{diag}(\delta_1, \delta_2, \ldots, \delta_k) = UMV$ where U and V are unimodular and the product $\delta_1\delta_2\cdots\delta_i$ is the g.c.d. of the order i subdeterminants of M, $1 \leq i \leq k$ (see, e.g. [12, Section 4.4]).

Lemma 5.1. *Let G be a $(0,3,6)$-fullerene obtained from Construction 4.1, and let $\mathbf{c}$, p, q, r, s be as in* (2) *and* (3). *Let $\mathrm{diag}(m, n) = UMV$ be the Smith normal form of the matrix $M = \begin{pmatrix} p & r \\ q & s \end{pmatrix}$. Let $\mathbf{u}$, $\mathbf{v}$ denote the columns of U. Then $G = \mathrm{CayS}(\Gamma, S)$ where $\Gamma = \mathbb{Z}_m \times \mathbb{Z}_n$ and*

$$S = \{\, (p_1 - 1)\mathbf{u} + p_2\mathbf{v},\ p_1\mathbf{u} + (p_2 - 1)\mathbf{v},\ (p_1 - 1)\mathbf{u} + (p_2 - 1)\mathbf{v} \,\}.$$

Here we interpret each column vector $\binom{x_1}{x_2} \in S$ to be the group element $(x_1 \bmod m,\ x_2 \bmod n) \in \Gamma$.

Proof. The columns of the matrix $B := (\mathbf{a}, \mathbf{b})$ form a lattice basis for $\Lambda_\bullet$ whereas those of BM generate the sublattice Λ. Since U and V are unimodular, the columns of $B' := BU^{-1}$ also generate $\Lambda_\bullet$. Accordingly, Λ is generated by the columns of $BMV = B'\,\mathrm{diag}(m, n)$. It follows that $\Gamma = \Lambda_\bullet/\Lambda \cong \mathbb{Z}_m \times \mathbb{Z}_n$. If we index the up-triangles with respect to the basis B', then the mapping $f : B'\binom{i'}{j'} \mapsto (i' \bmod m, j' \bmod n)$ is the one defined in (4). Changing the basis to $B = B'U$, we find $f(i\mathbf{a} + j\mathbf{b}) = i\mathbf{u} + j\mathbf{v}$.

After Step 1 of the construction, the three down-triangles which are neighbours of $u_\bullet$ reflect through A to the up-triangles at $-\mathbf{a}$, $-\mathbf{b}$ and $-\mathbf{a} - \mathbf{b}$. When A is translated by $\mathbf{c}$ in Step 2, the three up-triangles are accordingly translated by $2\mathbf{c} = p_1\mathbf{a} + p_2\mathbf{b}$. Therefore

$$S = \{f((p_1 - 1)\mathbf{a} + p_2\mathbf{b}),\ f(p_1\mathbf{a} + (p_2 - 1)\mathbf{b}),\ f((p_1 - 1)\mathbf{a} + (p_2 - 1)\mathbf{b})\}$$

as claimed. $\square$

We present a sample computation illustrating the determination of the group and spectrum.

Example 5.2. The example of Figure 2 corresponds to $(p_1, p_2) = (0, 0)$ and $(p, q, r, s) = (6, 2, -2, 6)$. All six integers are even, so the resulting graph G has no semiedges. We compute the Smith normal form to be

$$UMV = \begin{pmatrix} 0 & 1 \\ -1 & -7 \end{pmatrix} \begin{pmatrix} 6 & -2 \\ 2 & 6 \end{pmatrix} \begin{pmatrix} -2 & -3 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 20 \end{pmatrix}.$$

Hence $\Gamma = \mathbb{Z}_2 \times \mathbb{Z}_{20}$. Furthermore, the generating set is

$$S = \{-\mathbf{u} + 0\mathbf{v}, 0\mathbf{u} - \mathbf{v}, -\mathbf{u} - \mathbf{v}\} = \{(0,1), (-1,7), (-1,8)\}.$$

This implies G has eigenvalues $3, -1, -1, -1$, and

$$\{\pm|\varepsilon^b + (-1)^a \varepsilon^{7b} + (-1)^a \varepsilon^{8b}| \,:\, 0 \le a \le 1,\ 1 \le b \le 9\},$$

where $\varepsilon = e^{2\pi i/20}$.

If we were to translate $\triangle ABC$ by $(\frac{1}{2}\mathbf{a}, 0)$, then we get a $(0,3,6)$-fullerene G' with four semiedges. Here we have $(p_1, p_2) = (1, 0)$, which has the effect of translating the generating set by $\mathbf{u}$. That is,

$$G' = \mathrm{CayS}(\, \mathbb{Z}_2 \times \mathbb{Z}_{20}, \{(0,0), (1,6), (1,7)\}\,), \quad \text{and}$$

$$\mathrm{spec}(G') = \{3, 1, 1, -1\} \cup \{\pm|1 + (-1)^a \varepsilon^{6b} + (-1)^a \varepsilon^{7b}| \,:\, 0 \le a \le 1,\ 1 \le b \le 9\}.$$

The four semiedges are incident with the vertices $(0,0), (1,0), (0,10), (1,10) \in \Gamma$.

6 The geometry of Cayley sum graphs

In Section 4 we saw how the geometric description of $(0,3,6)$-fullerenes in terms of the A_2 lattice implies that they are Cayley sum graphs. Therefore their eigenvectors are easy to calculate, and their spectra are "nearly bipartite." Here we describe the precise circumstances under which Cayley sum graphs arise from geometric lattices in this manner. In fact we will see that *every* Cayley sum graph arises as a quotient of two cosets of a geometric lattice. We then exhibit some families of Cayley sum graphs which have a recognizable crystallographic local structure.

First we review, in greater generality, the conditions under which a graph G is a Cayley sum graph. Let G_2 be the cover $G \times K_2$ with bipartition $(V_\bullet, V_\circ)$. Note that G_2 has a natural automorphism, ρ, – we call it the *inversion map* – which transposes the two vertices within each fibre. By following the proof of Theorem 1.1, we find that G is a Cayley sum graph on an abelian group Γ if and only if Γ acts regularly on each of $V_\bullet$ and $V_\circ$ as a group of G_2-automorphisms, and this action satisfies

$$\rho^{-1} g \rho = -g, \text{ for each } g \in \Gamma. \tag{5}$$

Our construction proceeds with a sequence of graphs

$$\widetilde{G} \mapsto \widetilde{G}_2 \mapsto G_2 \mapsto G.$$

Let $\Lambda_\bullet \subset \mathbb{E}^d$ be a geometric lattice, and let $\widetilde{G} = \mathrm{CayS}(\Lambda_\bullet, S)$ be a Cayley sum graph with edges drawn as straight line segments. Each generator $s \in S$ corresponds to a set of edges of $\widetilde{G}$ whose midpoints are concurrent at the point $\frac{1}{2}s$. Let $\Lambda_\circ$ be any nontrivial coset of $\Lambda_\bullet$, and let $A \in \mathbb{R}^d$

be such that $\Lambda_\circ = 2A + \Lambda_\bullet$. Let $\tilde{\rho} : x \mapsto 2A - x$ be the inversion map through A. As above, we construct $\widetilde{G}_2 = \widetilde{G} \times K_2$ with partite sets $(\widetilde{V}_\bullet, \widetilde{V}_\circ) = (\Lambda_\bullet, \Lambda_\circ)$, where the fibres of $\widetilde{G}_2$ are the orbits of $\tilde{\rho}$.

The graph $\widetilde{G}_2$ is drawn in Euclidean d-space $\mathbb{E}^d$ with straight line segments for edges. Let $\mathbb{E}^d/\tilde{\rho}$ denote the quotient space (an orbifold) whose points are the $\tilde{\rho}$-orbits $\{x, \tilde{\rho}(x)\}$, $x \in \mathbb{E}^d$. Geometrically speaking, $\mathbb{E}^d/\tilde{\rho}$ is a cone with its apex A having the solid angle of a halfspace. By mapping each point in $\mathbb{E}^d$ to its $\tilde{\rho}$-orbit, we may view $\widetilde{G} \cong \widetilde{G}_2/\tilde{\rho}$ as being naturally embedded in $\mathbb{E}^d/\tilde{\rho}$. Every edge of $\widetilde{G}_2$ whose midpoint is A folds to a semiedge of $\widetilde{G}$. In the case of $(0,3,6)$-fullerenes, $\widetilde{G}_2$ is the plane hexagonal grid, and $\widetilde{G}$ is a grid drawn on a cone where every face is a hexagon except at A, where A is either the midpoint of a triangular face, or the end of a semiedge.

Now let Λ be any sublattice of $\Lambda_\bullet$, and let $\mathbf{p}$ be the be the natural projection from $\mathbb{E}^d$ to the d-torus $\mathbb{E}^d/\Lambda$. Then $G_2 := \mathbf{p}(\widetilde{G}_2)$ is a finite bipartite graph with partite sets $(V_\bullet, V_\circ) := (\mathbf{p}(\Lambda_\bullet), \mathbf{p}(\Lambda_\circ))$, and which is embedded in $\mathbb{E}^d/\Lambda$. Then $\tilde{\rho}$ projects to ρ, a symmetry of order 2 in the d-torus. Evidently ρ is an inversion map for G_2 satisfying (5) with $\Gamma = \Lambda_\bullet/\Lambda$. Therefore $G \cong G_2/\rho$ is a finite Cayley sum graph embedded in the orbifold $\mathbb{E}^d/\rho\Lambda$. Let $\mathcal{A} \subset \mathbb{E}^d/\Lambda$ be the fixed points of ρ. Then $\mathcal{A}$ consists of exactly 2^d points having the form $\mathbf{p}(A + \frac{1}{2}\Lambda)$ and ρ acts on $\mathbb{E}^d/\Lambda$ as an inversion through any point in $\mathcal{A}$. As an orbifold, $\mathbb{E}^d/\rho\Lambda$ is orientable if and only if d is even. To visualize $\mathbb{E}^d/\rho\Lambda$, it is convenient to select a fundamental region for $\mathbb{E}^d/\Lambda$ whose 2^d extreme points belong to $A + \Lambda$. Let T be the part of the region which lies on the positive side of a hyperplane H, which contains the region's centroid. All points in $\mathcal{A}$ lie on the boundary of T so we obtain $\mathbb{E}^d/\rho\Lambda$ by an appropriate gluing of the boundary of T. The graph G is embedded in T with each vertex $\{x, \rho(x)\}$ represented by the unique point in $\{x, \rho(x)\} \cap T$. For example, $\mathbb{E}^2/\rho\Lambda$ is an isosceles tetrahedron, whose four extreme points comprise $\mathcal{A}$. The grid construction of $(0,3,6)$-fullerenes corresponds to selecting H to be a diagonal of a fundamental parallelogram. The Cayley sum graph G has one semiedge for every point of $\mathcal{A}$ which lies on an edge of G_2. Figure 3 summarizes the commuting projections and the four embedded graphs.

Since every finite abelian group is the quotient of two geometric lattices, it follows that every finite Cayley sum graph G arises from a quadruple $(\Lambda_\bullet, S, A, \Lambda)$ as described above. By employing a linear transformation we can even assume that $\Lambda_\bullet = \mathbb{Z}^d$. We do not make this assumption here, since that would obfuscate the following examples. When the sum set S is a set of lattice points which are close to $2A$, then each edge of $\widetilde{G}_2$ is a short line segment, and $\widetilde{G}_2$ is often a recognizable bipartite crystallographic configuration. After selecting Λ and applying the above construction, we obtain a finite Cayley sum graph embedded in T with a local geometry that reflects the crystallographic structure of $\widetilde{G}_2$. We present with some examples.

- For $d = 1$, if $\widetilde{G}_2$ is the two-way infinite path, then $\widetilde{G}$ is the infinite ray with a semiedge at its origin, and G_2 is an even cycle drawn as a regular polygon. The inversion ρ identifies points reflected in a line which bisects opposite edges of the polygon, so G is a finite path with a semiedge at each end. The spectrum of G takes the form $M \cup L \cup -L$ where $M = \{2\}$ or $M = \{2, 0\}$.

- *(Grid-like examples)* If $\Lambda_\bullet = D_d$, the lattice of integer points of even weight, and $\Lambda_\circ = \Lambda_\bullet + (1, 0, 0, \dots)$, then $\Lambda_\bullet \cup \Lambda_\circ = \mathbb{Z}^d$, and we may take $\widetilde{G}_2$ to be the standard cartesian grid. If $A = (\frac{1}{2}, 0, 0, \dots)$, then applying the construction with any sublattice Λ of $\Lambda_\bullet$ leads to a

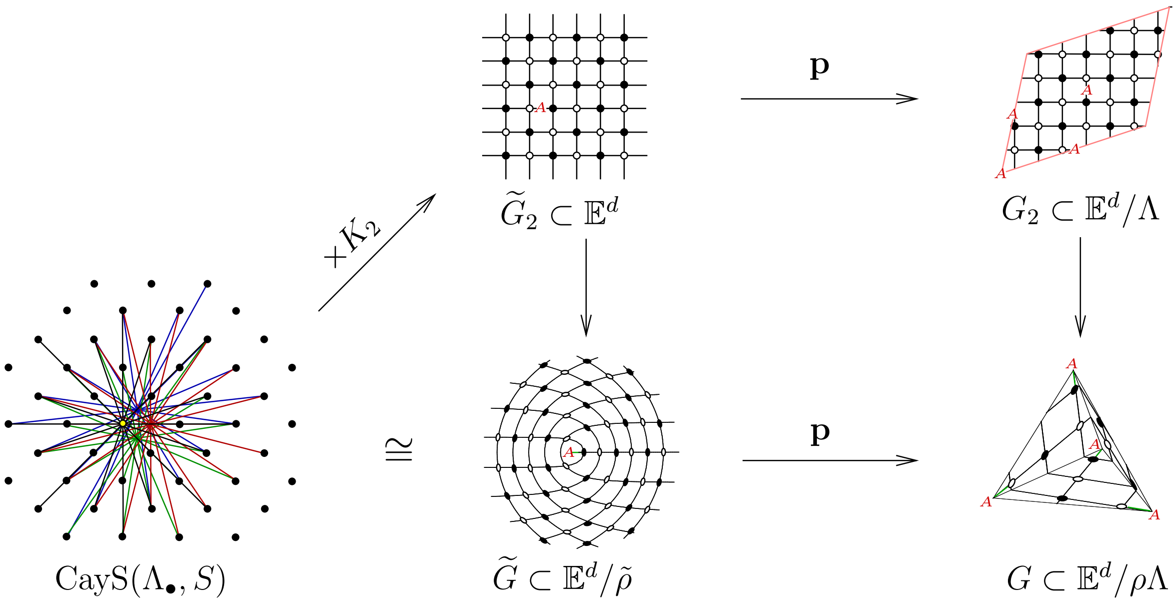

Figure 3: Constructing finite Cayley sum graph from a lattice. Illustrated with the D_2-lattice, resulting in a 28-vertex Cayley sum graph which is also a 4-regular quadrangulation of the tetrahedron.

Cayley sum graph G having exactly 2^d semiedges.

If $d = 2$, then G is a 4-regular quadrangulation of an isosceles tetrahedron, with a semiedge at each tetrahedral vertex. Such an graph illustrates Figure 3. The set of unmatched eigenvalues of G is either $M = \{4\}$ or $M = \{4, 0\}$. Indeed, *every* 4-regular quadrangulation of a sphere can be expressed in this way. To see this fact, we need only adapt the proof of Theorem 3.1.

When d is odd, we may take $A = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \dots)$. Since A is not on an edge of the cubic grid, this results in a grid-like Cayley sum graph G having fewer than 2^d semiedges. Indeed G has no semiedges at all if Λ is a sublattice of $2\Lambda_\bullet$.

- *(Diamond-like examples)* Again we take $\Lambda_\bullet$ to be the D_d-lattice, but put $\Lambda_\circ = \Lambda_\bullet + (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \dots)$. The set $\Lambda_\bullet \cup \Lambda_\circ$ is commonly called the *generalized diamond packing*, and is denoted by D_d^+ (see [13, p. 119]). The *diamond grid* is the graph $\widetilde{G}_2$ in which each point in $\Lambda_\bullet$ is joined to the 2^{d-1} nearest points in $\Lambda_\circ$. Putting $A = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \dots)$ results in a Cayley sum graph having at least 2^{d-1} semiedges. A more attractive option is to put $A = (\frac{5}{4}, \frac{1}{4}, \frac{1}{4}, \dots)$, which lies on no edge of $\widetilde{G}_2$. Provided that Λ is a sublattice of $2\Lambda_\bullet$, this results in a Cayley sum graph having no semiedges. When $d = 3$, this construction gives a class of Cayley sum graphs having the local structure of diamond crystal. Such graphs satisfy $M = \{4, -2, -2\}$ or $M = \{4, 0, -2, -2\}$. Another attractive class is based on D_8^+, otherwise known as the E_8 lattice.

- The 24-dimensional Leech lattice Λ_{24} arises as the union of two cosets of a lattice $h\Lambda_{24}$ which is obtained from the binary Golay code (see [13, p. 124]). This yields a particularly attractive class of crystallographic Cayley sum graphs of high dimension.

We have constructed infinite families of Cayley sum graphs whose spectra have the form $M \cup L \cup -L$, where M is a fixed finite multiset. By taking the categorical products with a fixed graph H, one obtains other "spectrally nearly bipartite" families of graphs. It would be interesting to find other natural examples of this phenomenon.

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