Generation of isospectral graphs

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Abstract: We discuss a discrete version of Sunada's Theorem on isospectral manifolds which allows to generate isospectral simple graphs, i.e. nonisomorphic simple graphs which have the same Laplace spectrum. We also consider additional boundary conditions and Buser's transplantation technique applied to a discrete situation.

1 Introduction

On a simple graph $G = (V, E)$ with vertex set $V = \{x_1, \dots, x_n\}$ and edge set $E \subseteq \{\{x_i, x_j\} : x_i, x_j \in V, x_i \neq x_j\}$, the Laplace or Kirchhoff operator $L = L(G)$ is defined as $L = A - D$ where $A = A(G)$ denotes the adjacency matrix of G, i.e.

$$A_{ij} = \begin{cases} \alpha_{ij} = \alpha_{ji} = 1 & \text{if } \{x_i, x_j\} \in E, \\ \alpha_{ij} = \alpha_{ji} = 0 & \text{otherwise,} \end{cases}$$

and $D = D(G)$ is the valence matrix of G, i.e. D is the diagonal matrix with

$$D_{ii} = \sum_{j=1}^{n} \alpha_{ij} =: d_i\,.$$

The Laplace and the adjacency spectrum of graphs (i.e. the eigenvalue spectrum of $L(G)$ and $A(G)$ respectively) are widely studied (see e.g. [6]). Non-isomorphic graphs (i.e. graphs whose adjacency matrices are not permutation similar) affording the same (adjacency) characteristic polynomial $\det(A - \lambda I)$, I denoting the identity matrix, are called cospectral. Schwenk showed in [15] that almost all trees are cospectral (or more precisely: almost all trees share their adjacency spectrum with another non-isomorphic tree). Botti and Merris generalized the results of Schwenk, McKay [12] and Turner [17] and showed that almost all trees share a complete set of immanental polynomials (see [1] for the precise statement).

Part of the interest in these questions comes from the interpretation of $L(G)$ as the resonance spectrum of molecules (see e.g. [7], [8] and [11]), and on the other hand, results in this area are relevant for numerical reasons because L is the discrete analogue of the (differential) Laplace operator.

In his pioneering work [16] Sunada discovered a routine method to generate non-isometric Riemannian manifolds which have the same Laplace-Beltrami spectrum. We explain this procedure now briefly since our interest is to find a discrete analogue: Let $(\mathfrak{G}, \mathfrak{H}_1, \mathfrak{H}_2)$ be a Gassmann-Sunada triple, i.e. $\mathfrak{G}$ is a finite group and $\mathfrak{H}_1$, $\mathfrak{H}_2$ are subgroups such that for every $g \in \mathfrak{G}$ there holds $\#\{[g] \cap \mathfrak{H}_1\} = \#\{[g] \cap \mathfrak{H}_2\}$, where $[g]$ denotes the conjugacy class $\{c^{-1}gc : c \in \mathfrak{G}\}$ of g and where

$\#S$ means the number of elements of the set S. Now, if $\pi : M \to M_0$ is a normal finite Riemannian covering with covering transformation group $\mathfrak{G}$, and if $\pi_1 : M_1 \to M_0$ and $\pi_2 : M_2 \to M_0$ are the coverings corresponding to $\mathfrak{H}_1$ and $\mathfrak{H}_2$ respectively, then M_1 and M_2 are isospectral manifolds.

Our aim is now to describe to what extent the analogue statement holds for graphs.

2 Sunada's theorem for graphs

First it is necessary to extend the definition of the Laplace operator to graphs which are not simple: Let V denote the vertex set of a finite graph G, E the edge set and $\varphi : E \to \{\{x,y\} : x,y \in V\}$ the edge mapping. Then the Laplace operator on a function $f : V \to \mathbb{R}$ is defined by

$$L(G)f(x) = \Big(\sum_{\substack{e\in E \\ \varphi(e)=\{x,y\}}} f(y)\Big) - \#\{e \in E \,:\, x \in \varphi(e)\}\, f(x).$$

Notice that an edge k with $\varphi(k) = \{x\}$, i.e. a loop, has no effect on the value of $L(G)f(x)$ and we will frequently remove loops without saying explicitly. The zeta function $\zeta_G(s)$ of G is then defined by

$$\zeta_G(s) = \sum (-\lambda_i)^{-s}$$

where $0 > \lambda_1 \geq \lambda_2 \geq \dots$ are the nonzero Laplacian eigenvalues of G counted with their multiplicity. From the discrete maximum principle it follows that the multiplicity of the eigenvalue 0 equals the number of connected components of G. Hence, two connected graphs G_1 and G_2 are isospectral if and only if $\zeta_{G_1}(s) \equiv \zeta_{G_2}(s)$.

An isomorphism on the graph G is a permutation p on V such that there exists a permutation q of E with $\varphi \circ q = (p \times p) \circ \varphi$. If q' is another permutation on E with $\varphi \circ q' = (p \times p) \circ \varphi$ then $\varphi \circ q \circ (q')^{-1} = \varphi$. Hence q is unique up to permutation of edges connecting the same vertices. In order to define a canonical permutation q (depending on p) we first order the set $E = \{e_1, \dots, e_k\}$ by $e_i \leq e_j :\iff i \leq j$ and then define the canonical q with $\varphi \circ q = (p \times p) \circ \varphi$ to be the order preserving permutation, i.e. $\varphi(e_i) = \varphi(e_j)$ and $e_i \leq e_j \implies qe_i \leq qe_j$.

Now, let $\mathfrak{G}$ be a group acting as isomorphisms on the graph G. Two vertices x, z in V are called equivalent with respect to $\mathfrak{G}$ if $x = gz$ for a $g \in \mathfrak{G}$. Two edges h and k are called equivalent if the canonical permutation q of some $g \in \mathfrak{G}$ has the property $h = qk$. The graph $G/\mathfrak{G}$ is defined as follows: The vertex set of the quotient $G/\mathfrak{G}$ is defined as the set of equivalence classes $\{[x] \,:\, x \in V\}$ and the edge set of $G/\mathfrak{G}$ is the set of equivalence classes $\{[e] \,:\, e \in E\}$. The edge map $\varphi/\mathfrak{G}$ of $G/\mathfrak{G}$ is defined by $\varphi/\mathfrak{G}([e]) = \{[x],[z]\}$ if $\varphi(e) = \{x, z\}$.

In order to formulate our main theorem, we need to define the following technical conditions:

A group $\mathfrak{G}$ acting as isomorphisms on the graph G is said to fulfill

- the *weak fixed point condition in* $x \in V$ iff for all $h \in \mathfrak{G}$ the following implication holds: if $e, k \in E$ with $\varphi(e) = \{x, y\}$, $\varphi(k) = \{x, z\}$ with $y \notin [x]$ and $z = hy \neq y$ and if x is a fixed point of $g \in \mathfrak{G}$, i.e. $gx = x$, then $gy \neq z$,

- the *weak fixed point condition* iff $\mathfrak{G}$ satisfies the weak fixed point condition in every $x \in V$,
- the *strong fixed point condition* iff no element $g \in \mathfrak{G}$ (except the identity) has a fixed point $x \in V$.

Of course, the strong fixed point condition implies the weak fixed point condition.

Theorem 1 *Let G be a finite, connected graph and $\mathfrak{G}$ be a group of isomorphisms acting on G. If $(\mathfrak{G}, \mathfrak{H}_1, \mathfrak{H}_2)$ is a Gassmann-Sunada triple, then the zeta functions $\zeta_{G/\mathfrak{H}_1}$ and $\zeta_{G/\mathfrak{H}_2}$ are identical and hence $G/\mathfrak{H}_1$ and $G/\mathfrak{H}_2$ are isospectral graphs, provided $\mathfrak{H}_1$ and $\mathfrak{H}_2$ satisfy the weak fixed point condition.*

Remarks: (i) It may happen, even if $\mathfrak{H}_1$ and $\mathfrak{H}_2$ are not conjugate, that the quotients $G/\mathfrak{H}_1$ and $G/\mathfrak{H}_2$ are isomorphic.

(ii) Without the weak fixed point condition the assertion of the theorem is in general false, as we will see afterwards.

(iii) Note that there is no fixed point condition whatsoever in the original version of Sunada's Theorem which deals with Riemannian manifolds instead of graphs.

The proof of Theorem 1 is based upon Sunada's Proposition 1 below and the compatibility Proposition 2 which we will both present first.

Proposition 1 (Sunada) *Let H be a Hilbert space on which a finite group $\mathfrak{G}$ acts as unitary transformations, and let $A : H \to H$ be a self-adjoint operator of trace class, i.e. A is supposed to have finite trace norm, and we assume that A commutes with the $\mathfrak{G}$-action. For a subgroup $\mathfrak{H}$ in $\mathfrak{G}$, we denote by $H^{\mathfrak{H}}$ the subspace consisting of $\mathfrak{H}$-invariant vectors. Then the following is true: If $(\mathfrak{G}, \mathfrak{H}_1, \mathfrak{H}_2)$ is a Gassmann-Sunada triple then* $\mathrm{trace}(A|H^{\mathfrak{H}_1}) = \mathrm{trace}(A|H^{\mathfrak{H}_2})$.

The proof may be found in [16]. Theorem 1 now follows from Proposition 1 and the following proposition which crucially incorporates the weak fixed point condition:

Proposition 2 *Let $\mathfrak{G}$ be a group acting as isomorphisms on the graph G, $x \in V$, and let $\omega : G \to G/\mathfrak{G}$ be the covering projection. Then*

$$L(G)(f \circ \omega)(x) = L(G/\mathfrak{G})f([x])$$

for all $f : G/\mathfrak{G} \to \mathbb{R}$, if and only if $\mathfrak{G}$ satisfies the weak fixed point condition in x.

Proof. We have

$$\begin{aligned} L(G)(f \circ \omega)(x) &= \sum_{\substack{e \in E \\ \varphi(e) = \{x,y\}}} (f \circ \omega)(y) - \#\{e \in E \,:\, x \in \varphi(e)\}(f \circ \omega)(x) \\ &= \sum_{\substack{e \in E \\ \varphi(e) = \{x,y\} \\ y \notin [x]}} (f \circ \omega)(y) - \#\{e \in E \,:\, x \in \varphi(e), y \notin [x]\}(f \circ \omega)(x). \end{aligned}$$

Notice that the weak fixed point condition in x is equivalent to the fact that for $h, k \in \{e \in E : \varphi(e) = \{x,y\}, y \notin [x]\}$ holds $[h] = [k] \implies h = k$. Hence we can write

$$\begin{aligned} L(G)(f \circ \omega)(x) &= \sum_{\substack{[e] \in E/\mathfrak{G} \\ \varphi/\mathfrak{G}([e]) = \{[x],[y]\} \\ [y] \neq [x]}} f([y]) - \#\{[e] \in E/\mathfrak{G} : [x] \in \varphi/\mathfrak{G}([e]), [y] \neq [x]\} f([x]) \\ &= \sum_{\substack{[e] \in E/\mathfrak{G} \\ \varphi/\mathfrak{G}([e]) = \{[x],[y]\}}} f([y]) - \#\{[e] \in E/\mathfrak{G} : [x] \in \varphi/\mathfrak{G}([e])\} f([x]) \\ &= L(G/\mathfrak{G}) f([x]). \end{aligned}$$

On the other hand, if the weak fixed point condition is not satisfied in x, we have $\#\{e \in E : x \in \varphi(e), y \notin [x]\} > \#\{[e] \in E/\mathfrak{G} : [x] \in \varphi/\mathfrak{G}([e]), [y] \neq [x]\}$, and hence for a function f which is equal to 1 in $[x]$ and 0 else, we obtain $L(G)(f \circ \omega)(x) \neq L(G/\mathfrak{G}) f([x])$. □

Proof of Theorem 1. Let us start by fixing an orientation for each edge $k \in E$ (E the edge set of G): If $\varphi(k) = \{x, y\}$, we choose an orientation $\tilde{\varphi}(k) = (x, y)$ or $\tilde{\varphi}(k) = (y, x)$.

Let $\ell^2(V)$ and $\ell^2(E)$ be the finite dimensional Hilbert spaces of all functions $f : V \to \mathbb{R}$ (V the vertex set of G) and $f : E \to \mathbb{R}$ respectively, equipped with the standard inner product $\langle \cdot, \cdot \rangle$. The ∇-operator, $\nabla : \ell^2(V) \to \ell^2(E)$, for $f \in \ell^2(V)$ in an edge $k \in E$ is defined by

$$\nabla f(k) = f(x) - f(y),$$

where $\tilde{\varphi}(k) = (x, y)$. Then there holds

$$\langle L(G) f, g \rangle = -\langle \nabla f, \nabla g \rangle, \qquad (*)$$

and hence the Laplace operator is selfadjoint. Furthermore, since G is connected, $L(G)$ satisfies the discrete maximum principle $L(G) f = 0 \iff f = \text{constant}$.

Now we apply Proposition 1 to the case

$$\begin{aligned} H = H_G &= \{f \in \ell^2(V) : \sum_{x \in V} f(x) = 0\} \\ A = A_G &= (L(G)|H)^{-s}, \quad \operatorname{Re} s > 0. \end{aligned}$$

Note that the maximum principle implies $\operatorname{Ker} L(G) = H^{\perp}$. On the other hand, by $(*)$ we have $\operatorname{Im} L(G) = H$ and hence A is well defined. Now, the operator A is selfadjoint (because $L(G)$ is) and trivially of trace class, commutes with the $\mathfrak{G}$ action (because $L(G)$ does) and $\operatorname{trace} A = \zeta_G(s)$. Since $g \in \mathfrak{G}$ is a permutation of V, g acts as unitary transformation of $\ell^2(V)$. Let ω_i ($i = 1, 2$) denote the covering projection of G onto $G_i = G/\mathfrak{H}_i$, and V_i be the vertex set of G_i. Then the linear mapping

$$f \in \ell^2(V_i) \mapsto (\#\mathfrak{H}_i)^{-1/2} f \circ \omega_i \in \ell^2(V)$$

induces an isometry of Hilbert spaces $\psi_i : H_{G_i} \to H_G^{\mathfrak{H}_i}$ such that, according to Proposition 2, $\psi_i \cdot A_{G_i} = A_G \cdot \psi_i$. Hence, it follows that $\zeta_{G_1}(s) = \operatorname{trace}(A_G | H_G^{\mathfrak{H}_1}) = \operatorname{trace}(A_G | H_G^{\mathfrak{H}_2}) = \zeta_{G_2}(s)$.

□

Now let $\mathfrak{G}$ be a group and $l = \{g_1, \dots, g_n\}$ a subset of the set of elements of $\mathfrak{G}$. Then the Cayley graph $\mathfrak{G}[g_1, \dots, g_n]$ is constructed as follows: The vertex set is the set of elements of $\mathfrak{G}$ and the edge set is $\{\{x, gx\} : x \in \mathfrak{G}, g \in l\}$. Then $\mathfrak{G}$ acts as isomorphisms on $\mathfrak{G}[g_1, \dots, g_n]$ by multiplication from the right. Furthermore the strong (and hence the weak) fixed point condition is fulfilled for any subgroup of $\mathfrak{G}$. Hence we have as a corollary the theorem of Brooks (see [2]).

Corollary 1 (Brooks) *If $\mathfrak{H}_1$ and $\mathfrak{H}_2$ are Gassmann subgroups of $\mathfrak{G}$ then $\mathfrak{G}[g_1, \dots, g_n]/\mathfrak{H}_1$ and $\mathfrak{G}[g_1, \dots, g_n]/\mathfrak{H}_2$ are isospectral graphs.*

3 Reduction of multiple edges

The isospectral graphs obtained by applying Theorem 1 or Corollary 1 to concrete examples are in general not simple, even if the original graph was, and even if loops are eliminated. In this section we show how one may always obtain simple isospectral graphs by introducing suitable new vertices which do not violate the weak fixed point condition. Let us start with the following example:

Example 1 Consider the semidirect product

$$\mathfrak{G} = \mathbb{Z}_8^* \ltimes \mathbb{Z}_8 = \{(x, y) : x = 1, 3, 5, 7;\ y = 0, 1, 2, \dots, 7\}$$

with product structure

$$(x, y) \cdot (x', y') = (xx', xy' + y) \mod 8.$$

The two subgroups

$$\mathfrak{H}_1 = \{(1,0), (3,0), (5,0), (7,0)\},\ \ \mathfrak{H}_2 = \{(1,0), (3,4), (5,4), (7,0)\}$$

have the Gassmann property. Consider the Cayley graph $G = \mathfrak{G}[g_1, g_2, g_3]$ with $g_1 = (3,0)$, $g_2 = (5,0)$ and $g_3 = (1,1)$. Then the graphs $G_1 = G/\mathfrak{H}_1$ and $G_2 = G/\mathfrak{H}_2$ are isospectral. In fact the characteristic polynomial $p(x) = \det(L(G_i) - xI)$ of both graphs is

$$p(x) = 4480x + 10624x^2 + 10360x^3 + 5388x^4 + 1616x^5 + 280x^6 + 26x^7 + x^8.$$

Figure 1 shows G_1 and G_2.

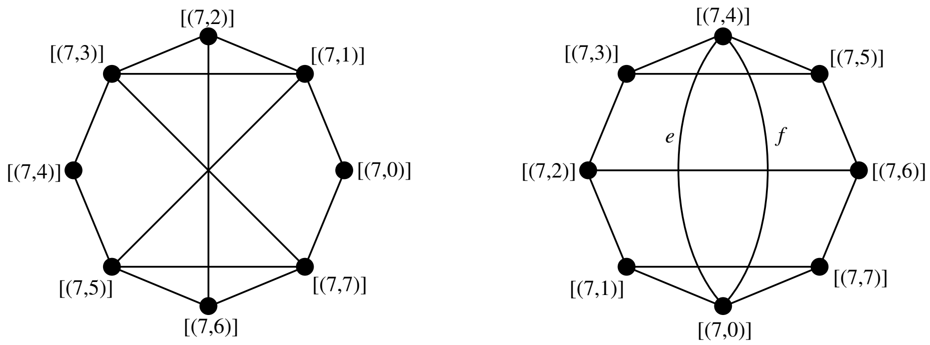

Figure 1: The isospectral graphs G_1 on the left and G_2 on the right.

In the previous example the quotient $G/\mathfrak{H}_2$ has an edge of multiplicity two. The way to reduce this multiplicity is to introduce suitable new vertices in G. In the above example, we introduce on the edge f two vertices (see Figure 1 and 2). This induces in G two vertices on every edge belonging to the equivalence class (with respect to $\mathfrak{H}_2$) of f. This in turn induces two vertices on every edge belonging to the equivalence classes (with respect to $\mathfrak{G}$) of the modified edges of G. We denote this extended graph by $\tilde{G}$. If u and v are the two new vertices on an edge h of G, then the action of $\mathfrak{G}$ on u and v is defined by the action of the canonical permutations on the set of edges: Let h be an edge of the original graph G with $\varphi(h) = \{x, y\}$, $g \in \mathfrak{G}$ and $k = qh$ with q being the canonical permutation related to g. If u is a new vertex on h next to x and v a new vertex on h next to y, then gu is defined as the new vertex on k next to gx and gv is defined as the new vertex on k next to gy. Now, by construction $\mathfrak{G}$ acts as isomorphisms on the extended graph $\tilde{G}$ and $\mathfrak{H}_1$ and $\mathfrak{H}_2$ satisfy the weak fixed point condition also for the extended graph. Moreover the quotient graphs $\tilde{G}_1 = \tilde{G}/\mathfrak{H}_1$ and $\tilde{G}_2 = \tilde{G}/\mathfrak{H}_2$ are, after elimination of loops, simple (by construction) and by Theorem 1 isospectral. The resulting graphs for the previous example are drawn in Figure 2. Notice that we need to introduce *two* new vertices on f. If we only take *one* vertex on f the weak fixed point condition is in general not fulfilled and in fact the resulting graphs in this example would not be isospectral, i.e. we cannot drop the weak fixed point condition.

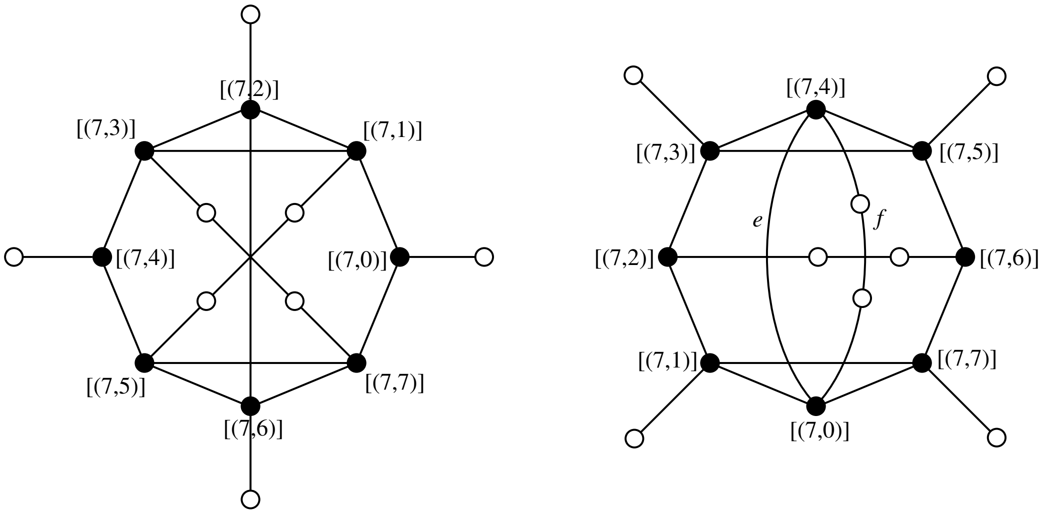

Figure 2: The isospectral simple graphs $\tilde{G}_1$ on the left and $\tilde{G}_2$ on the right.

The characteristic polynomial $p(x) = \det(L(\tilde{G}_i) - xI)$ of both graphs is

$$\begin{aligned} p(x) = {} & 36608x + 397952x^2 + 1914944x^3 + 5395872x^4 + 9935152x^5 + \\ & + 12646408x^6 + 11496568x^7 + 7609948x^8 + 3705936x^9 + 1331320x^{10} + \\ & + 350952x^{11} + 66868x^{12} + 8940x^{13} + 794x^{14} + 42x^{15} + x^{16}. \end{aligned}$$

We summarize this result in the following corollary.

Corollary 2 *Let G and $(\mathfrak{G}, \mathfrak{H}_1, \mathfrak{H}_2)$ be as in Theorem 1, $\mathfrak{H}_1$ and $\mathfrak{H}_2$ satisfying the weak fixed point condition. If $G/\mathfrak{H}_1$ or $G/\mathfrak{H}_2$ are not simple then introduction of two new vertices on every multiple edge of $G/\mathfrak{H}_1$ and $G/\mathfrak{H}_2$ generates an extended graph $\tilde{G}$ such that $\tilde{G}/\mathfrak{H}_1$ and $\tilde{G}/\mathfrak{H}_2$ are isospectral and simple (after elimination of loops).*

4 Boundary conditions

Let us declare an arbitrary subset of the vertex set V as boundary $\partial G \subseteq V$. Then, for a map $u : V \to \mathbb{R}$, we may prescribe

(D) Dirichlet boundary conditions: $u = 0$ on ∂G.

It is also possible to model Neumann conditions for an eigenfunction $u : V \to \mathbb{R}$, with $Lu(x) = \lambda u(x)$ on every $x \in V \setminus \partial G$. In this case we require:

(N) Neumann boundary conditions: $2Lu(x) = \lambda u(x)$ on ∂G

Remark: The Neumann boundary condition (N) is a possible discretization of $\partial u/\partial n = 0$ (vanishing normal derivative). One derives (N) by reflecting the graph in points of ∂G as the following figure indicates:

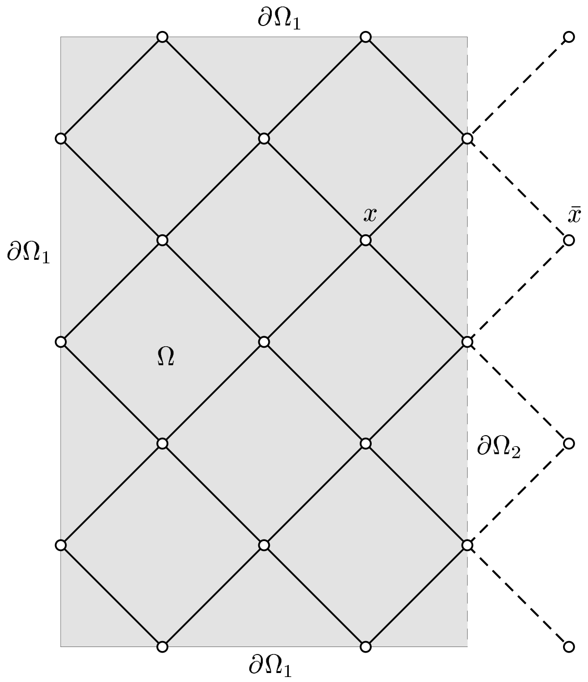

Figure 3: Discrete approximation of $\Delta u = \lambda u$ in a rectangle Ω with mixed boundary conditions $u = 0$ on $\partial\Omega_1$ and $\partial u/\partial n = 0$ on $\partial\Omega_2$. Using the reflection principle, the Neumann condition is equivalent to the assertion that a Laplace eigenfunction f would go into $f \circ \sigma$ if continued as an eigenfunction across the boundary segment $\partial\Omega_2$ where σ is the reflection at $\partial\Omega_2$. Thus the Neumann condition is imposed by introducing the reflected points $\bar{x}_i$ with $\bar{u}_i := u_i$.

Now we illustrate that Buser's transplantation technique (see [3]) for eigenfunctions works also in the discrete situation.

Example 2 This example is the discrete analogue of an example of Buser, Conway, Doyle and Semmler [4] for planar isospectral domains. Consider the two propeller-shaped regions in Figure 4 which contain the two graphs we want to investigate. Each region consists of seven equilateral triangles. The triangles on the right hand side are labeled by the numbers $0, \dots, 6$.

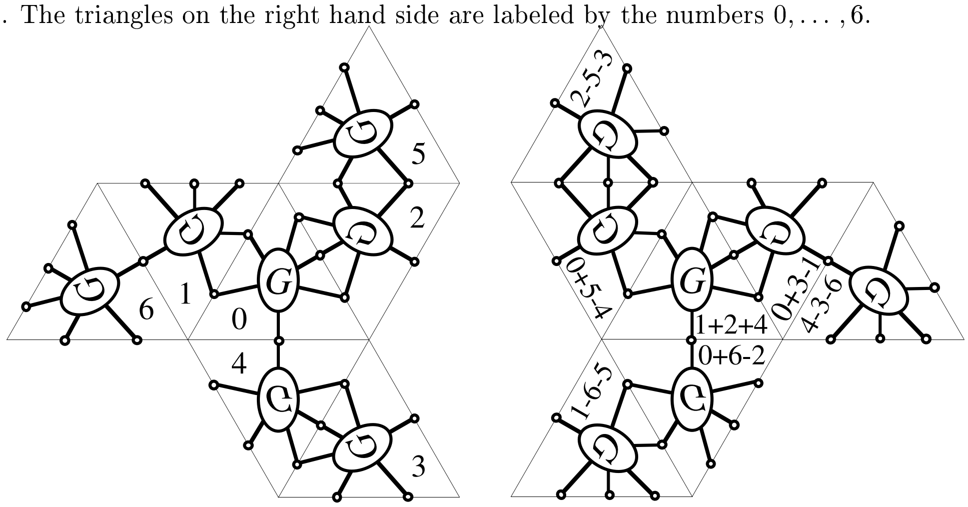

Figure 4

G stands for an arbitrary graph. The subgraphs in two triangles which have a common edge are reflection symmetric with respect to this edge. The boundary of the graphs consists of the edges on the boundary of the regions (thin outer line). Of course, the two graphs are non-isomorphic. On the other hand it is easy to see that they share the same spectrum. The proof is based upon Buser's transplantation principle [3]: Let λ be a real number and u any eigenfunction of the Laplacian with eigenvalue λ for the Dirichlet problem corresponding to the left-hand graph. Let $u_0, \dots, u_6$ denote the functions obtained by restricting u to the triangle with the corresponding number. For brevity we write 0 for u_0, 1 for u_1 etc. On the right in Figure 4, we show how to obtain from u an eigenfunction $\tilde{u}$ of eigenvalue λ for the right-hand graph. In the central triangle we put $\tilde{u}$ to be the function $1+2+4$. By this we mean the function $u_1 \circ \sigma_1 + u_2 \circ \sigma_2 + u_4 \circ \sigma_4$ where σ_1 is the isomorphism which carries the subgraph in triangle 1 on the left to the subgraph of the central triangle on the right and so on. In the remaining triangles we proceed analogously as indicated in the Figure. It is easy to check that for vertices on a common side of two triangles this does not lead to conflicts, the values induced from both triangles coincide. Furthermore everything is arranged such that on the boundary of the right hand graph the Dirichlet condition for $\tilde{u}$ is fulfilled. By linearity, in the interior of each triangle $\tilde{u}$ is a Laplace eigenfunction with eigenvalue λ and for the vertices on the common edge of two triangles the equation $Lu = \lambda u$ is easily checked. Since the same procedure also works in the opposite direction from the right to the left graph, we conclude that the eigenspaces of every eigenvalue λ for both sides coincide, and hence the graphs have the same spectrum and the same characteristic polynomial.

In fact the two graphs are also Neumann isospectral, as can be seen by a similar transplantation proof obtained by replacing every minus sign in the above by a plus sign.

The group behind this example is $PSL(3, 2)$, the automorphism group of the projective plane of order 2. For an explicit presentation see [4] and [5]. ○

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