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Spectra of Toroidal Graphs

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Dedicated to Professor Nenad Trinajstić on the occasion of his 70$^{\text{th}}$ birthday

Abstract

An n-fold periodic locally finite graph in the euclidean n-space may be considered the parent of an infinite class of n-dimensional toroidal finite graphs. An elementary method is developed which allows the characteristic polynomials of these graphs to be factored, in a uniform manner, into smaller polynomials, all of the same size.

Applied to the hexagonal tessellation of the plane (the graphite sheet), this method enables the spectra and corresponding orthonormal eigenvector systems for all toroidal fullerenes and $(3,6)$–cages to be explicitly calculated. In particular, a conjecture of P.W. Fowler on the spectra of $(3,6)$–cages is proved.

Key words: Graph spectra, periodical graph, toroidal cage, toroidal fullerene, toroidal graph, $(3,6)$–cage

Introduction

A *toroidal 6-cage* S is a trivalent graph embedded in (the surface of) a torus all of whose faces are hexagons (Figure 1). Reflecting the structure of (hypothetical) toroidal carbon molecules such graphs are, in a chemical context, also called *toroidal fullerenes*.

In Hückel's model of hydrocarbons (LCAO-MO theory), the eigenvalues and eigenvectors of the adjacency matrix of S correspond to the energy levels and orbitals of the

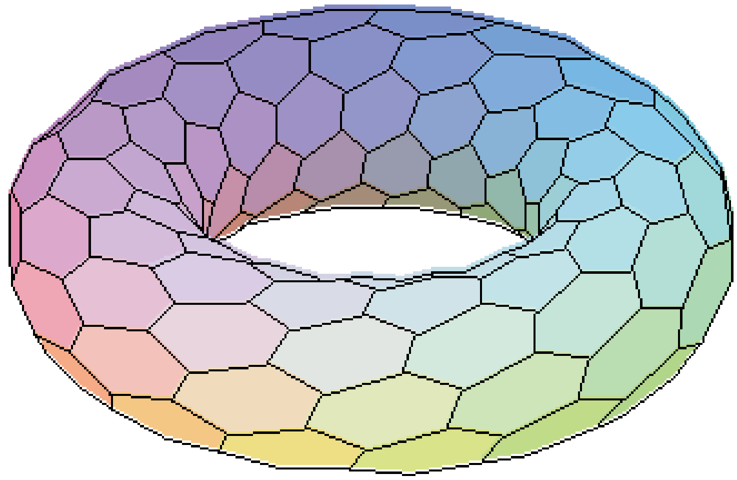


Figure 1

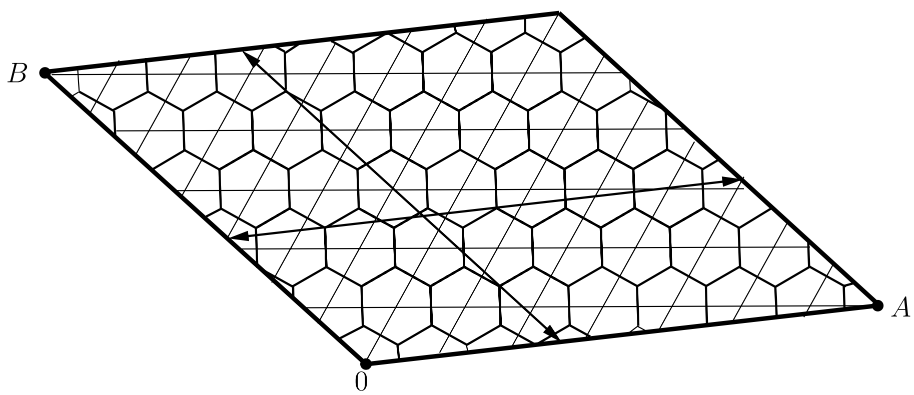


Figure 2

molecule represented by S, respectively. Therefore, a (simple) method that enables these quantities to be determined is required.

It is important to note that, by suitable point identification, all toroidal 6-cages can be derived from a common parent, namely, from the regular hexagonal tessellation of the plane (the graphite lattice) making use of the twofold periodicity of this structure (Figure 2; for details see Part II).

The first, seminal paper on the spectrum of toroidal fullerenes appeared in 1993. Its authors, E.C. Kirby, R.B. Mallion and P. Pollak [6], developed a method (unfortunately, not too simple) that allows the eigenvalues and eigenvectors for all toroidal fullerenes with up to 3600 hexagons, and many others, to be calculated.

The second paper on this topic appeared in 2000. A. Ceulemans, L.F. Chibotaru, S.A. Bovin and P.W. Fowler [1] describe a general method based on solid-state physics: considering the graphite sheet as a crystal, they construct its first Brillouin zone and, folding it twice according to the parameters of the fullerene, develop a procedure for determining spectrum and eigenspaces.

Simplifying and generalizing these procedures we shall in Part I describe a new method for factoring the characteristic polynomial of any graph of n-dimensional toroidal structure derivable from some n-dimensional locally finite n-fold periodic parent.

Part II is devoted to the spectral theory of toroidal fullerenes.

In Part III the results are used to determine explicitly spectrum and eigenvectors of $(3,6)$-cages. A $(3,6)$-cage is a trivalent polyhedron that has only hexagons and triangles as its faces.

Part I. Spectra and eigenvectors of n–dimensional toroidal graphs: general theory

I.1 Preliminaries

We shall consider graphs $\mathbf{G} = (\mathbf{V}, \mathbf{E})$ whose vertex set $\mathbf{V}$ is a set of points in the n-dimensional euclidean space $\mathbb{S}^n$; the edge set $\mathbf{E}$ is a set of pairs of these points which may be represented by straight line segments.

$\mathbf{G}$ is *n-fold periodic* iff there are n translations T_ν of $\mathbb{S}^n$ represented by linearly independent vectors $\mathbf{p}_\nu$ (periods) that leave $\mathbf{G}$ unchanged, i.e., such that $T_\nu\mathbf{G}$ is congruent and isomorphic to $\mathbf{G}$, $\nu = 1, 2, \ldots, n$. The concepts of *primitive period system, fundamental region* etc. are defined as usual.

In what follows we shall assume that $\mathbf{G}$ is n-fold periodic and locally finite: then all fundamental regions contain the same finite number of vertices. For the sake of convenience we shall restrict our exposition to the case $n = 2$: it is not difficult to see that and how the relevant concepts, proofs and theorems generalize for any value of n (including $n = 1$). Thus the graphs to be considered may be interpreted as *drawings* (not necessarily embeddings) on the euclidean plane.

Let $\mathfrak{C}$ be a cartesian coordinate system for the plane such that to point X there corresponds a vector $\mathbf{x} = (x_1, x_2)$ which may be identified with X.

$X \equiv Y$, or $\mathbf{x} \equiv \mathbf{y}$, $\mod (\mathbf{p}_1, \mathbf{p}_2)$ means that there are integers r_1, r_2 such that

$$\mathbf{x} - \mathbf{y} = r_1\mathbf{p}_1 + r_2\mathbf{p}_2.$$

Let $\mathbf{G}$ be twofold periodic and assume that $\mathfrak{C}$ has been so chosen that $\mathbf{p}_1 = (1, 0)$, $\mathbf{p}_2 = (0, 1)$ is a primitive pair of periods. Let P^* be the fundamental parallelogram spanned by $\mathbf{p}_1, \mathbf{p}_2$, let $P_\mathbf{o}$ be the parallelogram parallel and congruent to P^* with its centre at $\mathbf{0}$, and denote the configuration consisting of $P_\mathbf{o}$ and the part of $\mathbf{G}$ drawn on it by $P_\mathbf{o}^\mathbf{G}$: clearly, $\mathbf{G}$ is determined by $P_\mathbf{o}^\mathbf{G}$ (Figures 3a,b).

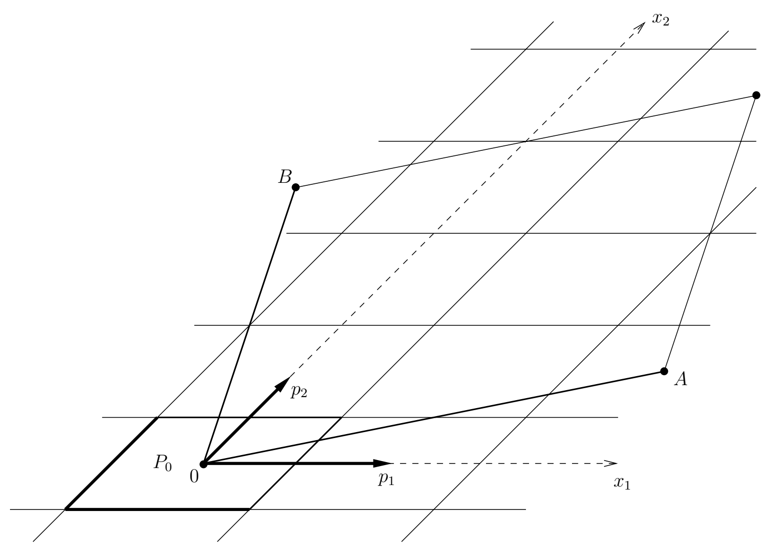


Figure 3a

Define $\mathbf{X} = \{x_1\mathbf{p}_1 + x_2\mathbf{p}_2 \mid x_1, x_2 \text{ integers}\}$ to be the integer coordinate point grid of the plane generated by $\mathbf{p}_1, \mathbf{p}_2$ and consider the tessellation T generated by $P_\mathbf{o}$ with parallelograms $P_\mathbf{x}$ centered at $\mathbf{x} \in \mathbf{X}$ (Figure 3a). Set $[m] = \{1, 2, \ldots, m\}$ and let

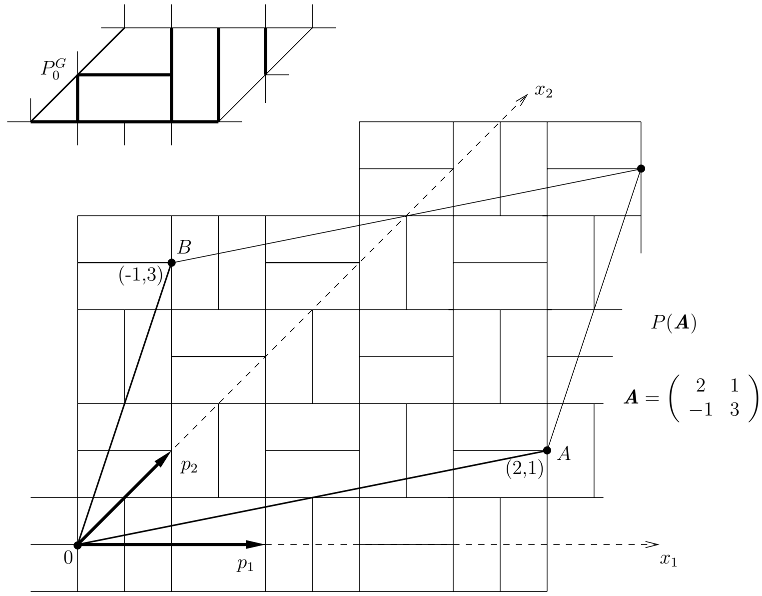


Figure 3b

$\{v_j \mid j \in [m]\}$ be the set of vertices of $\mathbf{G}$ contained in $P_{\mathbf{o}}$. Tessellation T partitions the vertex set of $\mathbf{G}$ into classes in two ways:

class $C'_{\mathbf{x}}$ consists of the m vertices contained in $P_{\mathbf{x}}$ (i.e., $C'_{\mathbf{x}} = \mathbf{V} \cap P_{\mathbf{x}}$), $\mathbf{x} \in \mathbf{X}$;

class C''_j consists of all vertices $v \equiv v_j \bmod (\mathbf{p}_1, \mathbf{p}_2)$, $\quad j \in [m]$.

Every vertex v being determined by the pair of classes $C'_{\mathbf{x}}$, C''_j that it belongs to we shall briefly write

$$v = (\mathbf{x}; j) = (x_1, x_2; j).$$

Let $\mathbf{a} = (a_1, a_2)$, $\mathbf{b} = (b_1, b_2)$ be any pair of vectors with integer components (i.e., $\mathbf{a}, \mathbf{b} \in \mathbf{X}$), set

$$\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} = A, \qquad |\det A| = \triangle$$

and assume $\triangle > 0$: then $(\mathbf{a}, \mathbf{b})$ is a period pair which is primitive if and only if A is unimodular ($\triangle = 1$). Let $\mathfrak{A}$ denote the set of all matrices with the above properties.

Consider the parallelogram $P = P(\mathbf{a}, \mathbf{b}) = P(A)$ spanned by $\mathbf{a}, \mathbf{b}$; of the boundary of P only the points $t\mathbf{a}$, $t\mathbf{b}$ $(0 \leq t < 1)$ belong to P (Figures 3). Note that the area of P is

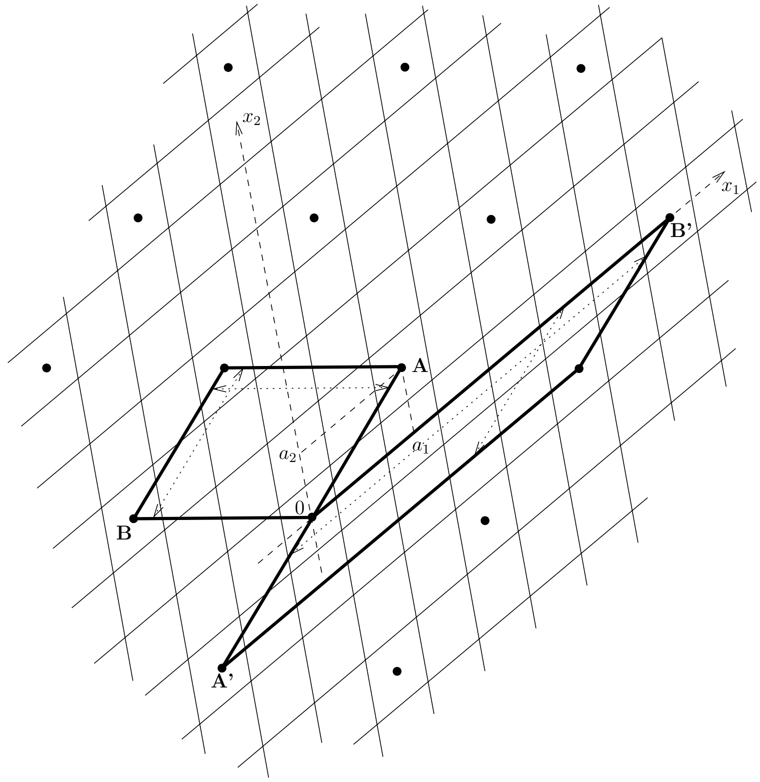


Figure 4

$\triangle$ times the area of $P_{\mathbf{o}}$, in other words, P covers (the area of) $\triangle$ fundamental regions.

Turning to topology, identify any two boundary points of P that lie on opposite sides of P in analog position (Figures 2,4) to obtain a torus $\mathbf{T}$ with a graph $\mathbf{G}(A)$ on $m\triangle$ vertices drawn on it. The vertex set of $G = \mathbf{G}(A)$ is $V = \mathbf{V}(A) = \mathbf{V} \cap P(A)$. Graph $\mathbf{G}(A)$ may also be considered the result of identifying any points of the plane being congruent $\bmod\,(\mathbf{a}, \mathbf{b})$. The partitioning of the vertex set into classes $C'_{\mathbf{x}}$, C''_j is maintained (but shrinked) by replacing each $\mathbf{x}$ by its residue class $\mathbf{x} \bmod (\mathbf{a}, \mathbf{b})$: classes $C'_{\mathbf{x}}$ and $C'_{\mathbf{x}}$ $(\mathbf{x} \bmod (\mathbf{a}, \mathbf{b}))$ have the same number m of elements whereas their number shrinks from infinity to $\triangle$; the number of classes C''_j and $C''_j(\mathbf{x} \bmod (\mathbf{a}, \mathbf{b}))$ is the same – namely, m – whereas the number of elements shrinks from infinity to $\triangle$. Note that $\mathbf{G}$ is the universal cover of all $\mathbf{G}(A)$ and every $\mathbf{G}(A)$ is a cover of $\mathbf{G}(I)$, $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. If matrix A' is derived from A by a unimodular transformation then graphs $\mathbf{G}(A)$ and $\mathbf{G}(A')$

are isomorphic which means that the toroidal realization $\mathbf{G}(A)$ is not unique (Figure 4) (toroidal 6-cages depend on only three parameters); nevertheless for our purposes this is the appropriate representation.

If $\mathbf{G}$ is plane then $\mathbf{G}(A)$ is embedded in $\mathbf{T}$: such embedded graphs will be called *toroidal cages*.

Let $\mathbf{G}$ be a twofold periodic fixed graph and consider the class of graphs $\mathbf{G}(A)$ $(A \in \mathfrak{A})$. We shall split up the task of calculating the spectrum of $\mathbf{G}(A)$ into two simpler tasks:

Task 1, using only the parameters of A and having nothing to do with the structure of $\mathbf{G}$, has an elementary algorithmic solution;

Task 2, depending on the outcome of task 1, consists in solving $\triangle$ eigenvalue problems each of size m which, in many cases of practical significance (especially, in the case of toroidal fullerenes), can be solved simultaneously. In particular, the method allows the characteristic polynomial of $\mathbf{G}(A)$, which is of degree $m\triangle$, to be factored into $\triangle$ polynomials each of degree m.

I.2 Spectra of graphs representable on a torus

Given a twofold periodic graph $\mathbf{G}$ and a matrix $A \in \mathfrak{A}$, set $\mathbf{G}(A) = G = (V, E)$. The problem to be solved is to find all vectors $\mathbf{e} = \{e(v) \mid v \in V\}$ (the eigenvectors of G) and corresponding values λ (the eigenvalues of G) satisfying

$$\sum_{v' \in N(v)} e(v') = \lambda\, e(v), \quad v \in V \tag{1}$$

where $N(v)$, the neighbourhood of vertex v, is the set of vertices in G adjacent to v.

We extend the vector $\mathbf{e}$ to the vertex set $\mathbf{V}$ of $\mathbf{G}$ such that $e(v)$ is twofold periodic with the period pair $(\mathbf{a}, \mathbf{b})$ and, following Kirby et al. [6], make the following

Ansatz:

$$e(v) = \varrho_1^{x_1}\varrho_2^{x_2}u_j \qquad (v = (\mathbf{x};j) = (x_1,x_2;j);\ \mathbf{x}\in\mathbf{X},\ j\in[m]). \tag{2}$$

This immediately entails two conditions for $\varrho_1, \varrho_2;\ u_1, u_2, \ldots, u_m$:

1) For fixed u_j the function $\varrho_1^{x_1}\varrho_2^{x_2}u_j$ must be twofold periodic in $\mathbf{x} = (x_1, x_2)$ with the periods $\mathbf{a}, \mathbf{b}$. That means that we have to determine ϱ_1, ϱ_2 such that the function $\varphi(\mathbf{x}) = \varrho_1^{x_1}\varrho_2^{x_2}$ has the period pair $(\mathbf{a}, \mathbf{b})$. As $\varphi(\mathbf{o}) = \varrho_1^0\varrho_2^0 = 1$, and because the points 0, A and B of the plane (Figures 3) represent the same point of the torus, we must have

$$\varrho_1^{a_1}\varrho_2^{a_2} = \varrho_1^{b_1}\varrho_2^{b_2} = 1. \tag{3}$$

This necessary condition is also sufficient for periodicity: indeed, (3) implies

$$\begin{aligned}\varphi(\mathbf{x}+p\mathbf{a}+q\mathbf{b}) &= \varrho_1^{x_1+pa_1+qb_1}\cdot\varrho_2^{x_2+pa_2+qb_2}\\ &= \varrho_1^{x_1}\varrho_2^{x_2}\left(\varrho_1^{a_1}\varrho_2^{a_2}\right)^p\left(\varrho_1^{b_1}\varrho_2^{b_2}\right)^q = \varrho_1^{x_1}\varrho_2^{x_2} = \varphi(\mathbf{x}).\end{aligned}$$

Equations (3) will be called the *basic equations*. We shall discuss and solve these equations in Section I.3; let us anticipate:

(I) the basic equations have exactly $\triangle$ pairwise distinct solutions $\boldsymbol{\varrho} = (\varrho_1, \varrho_2)$ (precisely as many as required);

(II) in every solution $\boldsymbol{\varrho}$ the numbers ϱ_1, ϱ_2 are $\triangle^{\text{th}}$ roots of unity, thus $\varrho_1^{-1} = \bar{\varrho}_1$, $\varrho_2^{-1} = \bar{\varrho}_2$.

Let $\mathbb{R} = \mathbb{R}(A)$ denote the set of solutions $\boldsymbol{\varrho}$ of the basic equations (3).

2) Next $u_1, u_2, \ldots, u_m$ must be determined. Consider the vertices in $P_{\mathbf{o}}$, namely, $v_j = (\mathbf{o}, j), j \in [m]$, and their neighbours. According to our ansatz (2), the corresponding

equations of (1), with $v' = (\mathbf{x}'; k)$, become

$$\sum_{\substack{\mathbf{x}'\in\mathbf{X}\\ k\in[m]}} \delta(\mathbf{x}'; k \mid \mathbf{o}; j)\varrho_1^{x_1'}\varrho_2^{x_2'}u_k = \lambda\, u_j, \quad j \in [m] \tag{4}$$

where

$$\delta(v' \mid v) = \begin{cases} 1 & \text{if } v' \in N(v) \\ 0 & \text{otherwise} \end{cases}$$

is the adjacency characteristic function of $G = \mathbf{G}(A)$. Up to a common factor $\varrho_1^{x_1}\ \varrho_2^{x_2}$, the same equations arise if vertices $v_j = (\mathbf{o}; j)$ are replaced by vertices $(\mathbf{x}; j)$ ($\mathbf{x}$ fixed, $j \in [m]$). This means that our ansatz has been successful: every solution to equations (3) and (4) yields an eigenvalue λ and corresponding (complex) eigenvector $\mathbf{e}$ with components $e(x_1, x_2; j) = \varrho_1^{x_1}\varrho_2^{x_2}u_j$. By (I), (3) has precisely $\triangle$ solutions. By (II), for every fixed $\boldsymbol{\varrho} \in \mathbb{R}(A)$, the corresponding coefficients matrix of equations (4) is Hermitean implying that equations (4) have precisely m (independent) solutions. Thus we have obtained a system of $m\triangle = |V|$ eigenvalues $\lambda = \lambda(\mu; \boldsymbol{\varrho})$ and corresponding eigenvectors $\mathbf{e} = \mathbf{e}(\mu; \boldsymbol{\varrho})$ ($\mu \in [m]$) of G.

In order to prove that this system is complete we shall show that if the eigenvectors $\mathbf{u}$ (the solutions of (4)) chosen are orthonormal then the eigenvectors $\mathbf{e}$ are pairwise orthogonal with common norm $\triangle$.

We need some preparation.

In what follows $A \in \mathfrak{A}$ is arbitrary but fixed. In order to avoid confusion we shall write down the eigenvalues, eigenvectors and their components together with all parameters they depend on: so the m solutions of the Hermitean eigenvalue problem (4) that we shall use are

$$\lambda(\mu; \boldsymbol{\varrho}); \qquad \mathbf{u}(\mu; \boldsymbol{\varrho}) = \{u_j(\mu; \boldsymbol{\varrho}) \mid j \in [m]\}$$

satisfying

$$\mathbf{u}(\mu;\boldsymbol{\varrho})\cdot\mathbf{u}(\nu;\boldsymbol{\varrho})=\delta_{\mu\nu} \tag{5}$$

$(\boldsymbol{\varrho}\in\mathbb{R}(A);\ \mu,\nu\in[m])$. [1]

Lemma 1. *Under the multiplication rule*

$$(\varrho_1,\varrho_2)\cdot(\sigma_1,\sigma_2)=(\varrho_1\sigma_1,\varrho_2\sigma_2)$$

the set $\mathbb{R}=\mathbb{R}(A)$ *is an abelian group* (immediate).

In particular: $(1,1)\in\mathbb{R}$ and with $\boldsymbol{\varrho},\boldsymbol{\sigma}\in\mathbb{R}$ also $\boldsymbol{\varrho}\boldsymbol{\sigma}\in\mathbb{R}$ and $\boldsymbol{\varrho}^{-1}=(\varrho_1^{-1},\varrho_2^{-1})=(\bar{\varrho}_1,\bar{\varrho}_2)=\bar{\boldsymbol{\varrho}}\in\mathbb{R}$.

Let $\mathbf{X}\cap P(A)=\mathbf{X}(A)$. Note that

$$V=\mathbf{V}(A)=\{(\mathbf{x};j)\mid \mathbf{x}\in\mathbf{X}(A), j\in[m]\}=\mathbf{X}(A)\times[m].$$

Lemma 2. [2] *For any* $\boldsymbol{\varrho}\in\mathbb{R}(A)$, $\sum\limits_{\mathbf{x}\in\mathbf{X}(A)}\varrho_1^{x_1}\varrho_2^{x_2}=\begin{cases}\triangle & \textit{if } \varrho_1=\varrho_2=1,\\ 0 & \textit{otherwise.}\end{cases}$

Proof. W.l.o.g., we may assume $\mathfrak{C}$ to be the usual orthogonal coordinate system. Consider the grids Γ_1, Γ_2 generated by vector pairs $\mathbf{a}=(a_1,a_2)$, $\mathbf{b}=(b_1,b_2)$ and $\mathbf{p}=(\triangle,0)$, $\mathbf{q}=(0,\triangle)$, respectively. As $\mathbf{p}=b_2\mathbf{a}-a_2\mathbf{b}$, $\mathbf{q}=-b_1\mathbf{a}+a_1\mathbf{b}$, Γ_2 is a subgrid of Γ_1. If points congruent mod $(\mathbf{p},\mathbf{q})$ are considered equivalent, the square Q spanned by $\mathbf{p},\mathbf{q}$, with area $\triangle^2$, after due exchange of area, covers $\triangle$ parallelograms $P_1=P(A),P_2,\dots,P_\triangle$ each congruent to $P(A)$ of area $\triangle$ (Figure 5). For any $\boldsymbol{\varrho}\in\mathbb{R}(A)$ the function $\varrho_1^{x_1}\varrho_2^{x_2}$ is

[1] $\mathbf{x}\cdot\mathbf{y}$, the scalar product of vectors $\mathbf{x}=\{x_i\mid i\in\mathfrak{I}\}$, $\mathbf{y}=\{y_i\mid i\in\mathfrak{I}\}$, is $\mathbf{x}\cdot\mathbf{y}=\sum\limits_{i\in\mathfrak{I}}x_i\bar{y}_i$; $\delta_{\mu\nu}=\begin{cases}1 & \text{if } \mu=\nu,\\ 0 & \text{otherwise.}\end{cases}$

[2] The authors did not find this proposition in the literature.

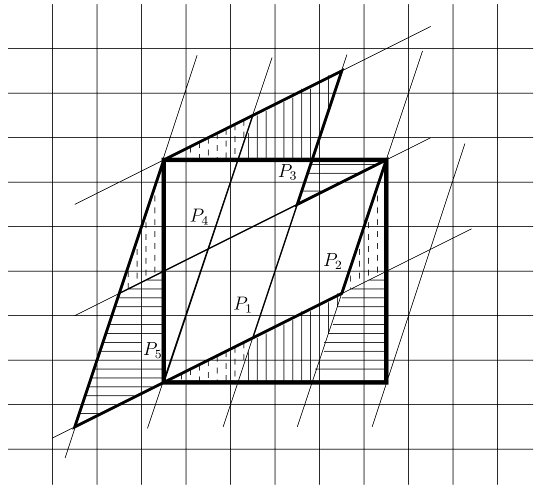


Figure 5

twofold periodic mod $(\mathbf{a},\mathbf{b})$ and mod $(\mathbf{p},\mathbf{q})$, thus

$$\sum_{\mathbf{x}\in\mathbf{X}\cap Q}\varrho_1^{x_1}\varrho_2^{x_2}=\sum_{i=1}^{\triangle}\sum_{\mathbf{x}\in\mathbf{X}\cap P_i}\varrho_1^{x_1}\varrho_2^{x_2}=\triangle\sum_{\mathbf{x}\in\mathbf{X}\cap P(A)}\varrho_1^{x_1}\varrho_2^{x_2}=\triangle\sum_{\mathbf{x}\in\mathbf{X}(A)}\varrho_1^{x_1}\varrho_2^{x_2}.$$

On the other hand,

$$\sum_{\mathbf{x}\in\mathbf{X}\cap Q}\varrho_1^{x_1}\varrho_2^{x_2}=\sum_{x_1=0}^{\triangle-1}\sum_{x_2=0}^{\triangle-1}\varrho_1^{x_1}\varrho_2^{x_2}=\sum_{x_1=0}^{\triangle-1}\varrho_1^{x_1}\sum_{x_2=0}^{\triangle-1}\varrho_2^{x_2}=\begin{cases}\triangle^2 & \text{if } \varrho_1=\varrho_2=1,\\ 0 & \text{otherwise.}^3\end{cases}$$

The claim follows. $\square$

By Lemma 1, for $\boldsymbol{\varrho},\boldsymbol{\sigma}\in\mathbb{R}(A)$ also $\boldsymbol{\varrho}\boldsymbol{\sigma}^{-1}\in\mathbb{R}(A)$, thus Lemma 2 is equivalent to

Lemma 2′. *For any* $\boldsymbol{\varrho},\boldsymbol{\sigma}\in\mathbb{R}(A)$,

$$\sum_{\mathbf{x}\in\mathbf{X}(A)}\varrho_1^{x_1}\varrho_2^{x_2}\sigma_1^{-x_1}\sigma_2^{-x_2}=\begin{cases}\triangle & \textit{if } \boldsymbol{\varrho}=\boldsymbol{\sigma},\\ 0 & \textit{otherwise.}\end{cases}$$

[3] For $\varrho_i\neq 1$, $1+\varrho_i+\varrho_i^2+\cdots+\varrho_i^{\triangle-1}=(\varrho_i^{\triangle}-1)/(\varrho_i-1)=0$.

Return to the $m\triangle$ eigenvectors we have found by our ansatz for $\mathbf{G}(A)$, namely,

$$\mathbf{e}(\mu;\boldsymbol{\varrho}) = \{\varrho_1^{x_1}\varrho_2^{x_2}u_j(\mu;\boldsymbol{\varrho}) \mid (\mathbf{x},j) \in \mathbf{V}(A)\} \quad (\boldsymbol{\varrho} \in \mathbb{R}(A), \mu \in [m]).$$

For $\boldsymbol{\varrho},\boldsymbol{\sigma} \in \mathbb{R}(A)$ and $\mu,\nu \in [m]$ we have

$$\mathbf{e}(\mu;\boldsymbol{\varrho}) \cdot \mathbf{e}(\nu;\boldsymbol{\sigma}) = \sum_{(\mathbf{x},j)\in\mathbf{V}(A)} \varrho_1^{x_1}\varrho_2^{x_2}u_j(\mu;\boldsymbol{\varrho})\sigma_1^{-x_1}\sigma_2^{-x_2}\overline{u_j(\nu;\boldsymbol{\sigma})}.$$

Recall: $\mathbf{V}(A) = \mathbf{X}(A) \times [m]$. Thus the last summation may be carried out as follows:

$$\sum_{(\mathbf{x},j)\in\mathbf{V}(A)} \cdots = \sum_{(\mathbf{x},j)\in\mathbf{X}(A)\times[m]} \cdots = \sum_{\mathbf{x}\in\mathbf{X}(A)}\sum_{j\in[m]} \cdots .$$

Therefore, $\mathbf{e}(\mu;\boldsymbol{\varrho}) \cdot \mathbf{e}(\nu;\boldsymbol{\sigma}) = \sum_1 \cdot \sum_2$ where

$$\sum\nolimits_1 = \sum_{j\in[m]} u_j(\mu;\boldsymbol{\varrho})\overline{u_j(\nu;\boldsymbol{\sigma})}, \qquad \sum\nolimits_2 = \sum_{\mathbf{x}\in\mathbf{X}(A)} \varrho_1^{x_1}\varrho_2^{x_2}\sigma_1^{-x_1}\sigma_2^{-x_2}.$$

By Lemma 2′, $\sum_2 = \begin{cases} \triangle & \text{if } \boldsymbol{\varrho} = \boldsymbol{\sigma}, \\ 0 & \text{otherwise.} \end{cases}$

Assume $\boldsymbol{\varrho} = \boldsymbol{\sigma}$; then by (5), $\sum_1 = \delta_{\mu\nu}$. We conclude that

$$\mathbf{e}(\mu;\boldsymbol{\varrho}) \cdot \mathbf{e}(\nu;\boldsymbol{\sigma}) = \begin{cases} \triangle & \text{if } \boldsymbol{\varrho} = \boldsymbol{\sigma} \text{ and } \mu = \nu, \\ 0 & \text{otherwise.} \end{cases}$$

Thus we have proved

Theorem 1. *Given a twofold periodic graph* $\mathbf{G}$*, a matrix* $A \in \mathfrak{A}$ *and the corresponding toroidal graph* $G = \mathbf{G}(A)$*:*

Let, for $\boldsymbol{\varrho} \in \mathbb{R}(A)$*, the eigenvalue problem* (4) *have eigenvalues* $\lambda(\mu;\boldsymbol{\varrho})$ *and corresponding orthonormal eigenvectors* $\mathbf{u}(\mu;\boldsymbol{\varrho})$ $(\mu \in [m])$*. Then the numbers* $\lambda(\mu;\boldsymbol{\varrho})$ *and* *vectors*

$$\mathbf{e}(\mu;\boldsymbol{\varrho}) = \{\varrho_1^{x_1}\varrho_2^{x_2}u_j(\mu;\boldsymbol{\varrho}) \mid (\mathbf{x};j) \in \mathbf{V}(A)\} \quad (\boldsymbol{\varrho} \in \mathbb{R}(A), \mu \in [m])$$

form the spectrum and a complete eigenvector system for the graph G, the $\mathbf{e}(\mu;\boldsymbol{\varrho})$ being pairwise orthogonal with common norm $\triangle$.

Note that the solutions $\boldsymbol{\varrho}$ of the basic equations are the dominant parameters determining the spectrum and a particular system of orthogonal eigenvectors (not just the eigenspaces determined by the eigenvalues).

I.3 Solution of the basic equations

We shall first show that both ϱ_1 and ϱ_2 are $\triangle^{\text{th}}$ roots of unity.

ϱ_1, ϱ_2 satisfying the basic equations

$$\varrho_1^{a_1}\varrho_2^{a_2} = \varrho_1^{b_1}\varrho_2^{b_2} = 1 \tag{3}$$

we also have

$$(\varrho_1^{a_1}\varrho_2^{a_2})^{b_2} = \varrho_1^{a_1b_2}\varrho_2^{a_2b_2} = 1, \quad (\varrho_1^{b_1}\varrho_2^{b_2})^{-a_2} = \varrho_1^{-a_2b_1}\varrho_2^{-a_2b_2} = 1$$

which, by multiplication, yield

$$\varrho_1^{a_1b_2-a_2b_1} = 1 \quad \text{implying} \quad \varrho_1^{|a_1b_2-a_2b_1|} = \varrho_1^{\triangle} = 1;$$

analogously, $\varrho_2^{\triangle} = 1$, as claimed. Thus ϱ_1, ϱ_2 uniquely determine, and are determined by, integers k_1, k_2 satisfying

$$\varrho_1 = \varepsilon_{\triangle}^{k_1}, \quad \varrho_2 = \varepsilon_{\triangle}^{k_2} \qquad (0 \le k_1,\, k_2 < \triangle)$$

where ε_r is an abbreviation for $e^{\frac{2\pi i}{r}}$, a primitive r^{th} root of unity. Therefore, the basic equations are equivalent to the *basic congruences*

$$(6)\qquad \left\{\begin{array}{rcl} a_1k_1 + a_2k_2 & \equiv & 0, \\ b_1k_1 + b_2k_2 & \equiv & 0, \end{array}\right. \text{briefly,}\quad A\,\mathbf{k} \equiv \mathbf{o}, \bmod \triangle.$$

To solve these congruences, we shall first transform them using a variant of Euclid's algorithm[4]. Note that the set of solutions of (6) as well as $\triangle = |\det A|$ remain unchanged under the following elementary transformations of matrix A:

- interchange of the rows,
- multiplication of a row by -1,
- subtraction of one row from the other.

Therefore, we may assume $a_1 > 0$, $b_1 \geq 0$.

Apply the following algorithm:

(i) if $b_1 = 0$: stop;

(ii) if $0 < b_1 < a_1$: substract the second row from the first;

(iii) if $b_1 \geq a_1$: substract the first row from the second;

(iv) return.

The procedure stops when the transform of A has attained the form $\begin{pmatrix} a_1' & a_2' \\ 0 & b_2' \end{pmatrix}$; it can, of course, be accelerated by using integer division with remainder in steps (ii) and (iii). Note that a_1' is the greatest common divisor of a_1 and b_1. Setting $\alpha = |b_2'|$, $\beta = a_1'$, $\gamma = -a_2'$ we have $\triangle = \alpha\beta$ and the congruences to be solved become

$$\left\{\begin{array}{rcl} \beta k_1 - \gamma k_2 & \equiv & 0, \\ \alpha k_2 & \equiv & 0, \end{array}\right. \bmod \triangle.$$

[4]This idea (which repeatedly applied also settles the n-dimensional case) is due to W. Rausch and T. Böhme (Ilmenau).

Starting from the second congruence we obtain

$$\begin{cases} k_2 \equiv \dfrac{\triangle}{\alpha}\nu = \beta\nu, \\ k_1 \equiv \dfrac{\gamma k_2}{\beta} + \dfrac{\triangle}{\beta}\mu = \alpha\mu + \gamma\nu, \end{cases} \quad \mathrm{mod}\triangle, \quad \mu = 0, 1, \ldots, \beta - 1, \quad \nu = 0, 1, \ldots, \alpha - 1.$$

Result. The basic congruences (6) have precisely $\alpha\beta = \triangle$ solutions, namely,

$$\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} \equiv \begin{pmatrix} \alpha\mu + \gamma\nu \\ \beta\nu \end{pmatrix}, \ \mathrm{mod}\triangle, \quad \mu = 0, 1, \ldots, \beta - 1, \quad \nu = 0, 1, \ldots, \alpha - 1.$$

Example: $\begin{pmatrix} -4 & -5 \\ 6 & 3 \end{pmatrix}$; $\triangle = 18$;

$$\begin{pmatrix} -4 & -5 \\ 6 & 3 \end{pmatrix} \longrightarrow \begin{pmatrix} 4 & 5 \\ 6 & 3 \end{pmatrix} \longrightarrow \begin{pmatrix} 4 & 5 \\ 2 & -2 \end{pmatrix} \longrightarrow \begin{pmatrix} 2 & 7 \\ 2 & -2 \end{pmatrix} \longrightarrow \begin{pmatrix} 2 & 7 \\ 0 & -9 \end{pmatrix}$$

$\alpha = 9,\ \beta = 2,\ \gamma = -7;\quad k_1 \equiv 9\mu - 7\nu;\ k_2 \equiv 2\nu,\ \mathrm{mod}\,18,\quad \mu = 0, 1;\ \nu = 0, 1, 2, 3, 4, 5, 6, 7, 8.$

I.4 An example

Let $\mathbf{H}$ be the twofold periodic graph part $P^{\mathbf{H}}_{\mathbf{o}}$ of which is displayed (bold face) in Figure 6. With the abbreviations

$$1 + \varrho_1 + \varrho_2 = \alpha,\ 1 + \bar{\varrho}_1 + \varrho_2 = \beta$$

the corresponding eigenvalue problem (4) becomes

$$(7) \qquad \begin{cases} \qquad\qquad \alpha u_3 + \beta u_4 = \lambda u_1 \\ \qquad\qquad \bar{\beta} u_3 + \bar{\alpha} u_4 = \lambda u_2 \\ \bar{\alpha} u_1 + \beta u_2 \qquad\qquad = \lambda u_3 \\ \bar{\beta} u_1 + \alpha u_2 \qquad\qquad = \lambda u_4 \end{cases}$$

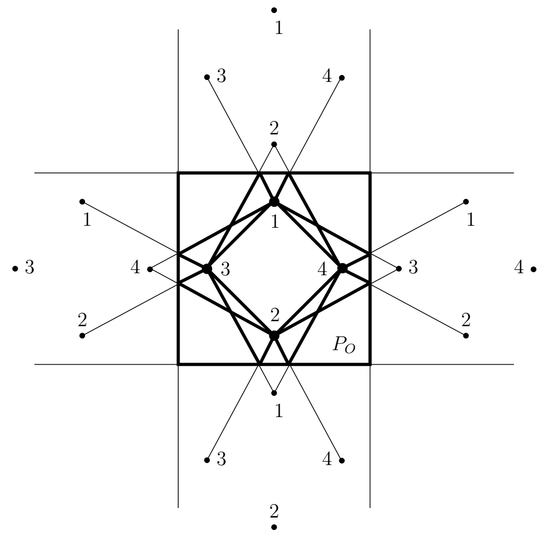


Figure 6

with characteristic polynomial

$$
(8) \qquad \varphi(\boldsymbol{\varrho};\lambda) = \begin{vmatrix} \lambda & 0 & -\alpha & -\beta \\ 0 & \lambda & -\bar{\beta} & -\bar{\alpha} \\ -\bar{\alpha} & -\beta & \lambda & 0 \\ -\bar{\beta} & -\alpha & 0 & \lambda \end{vmatrix}
$$

$$
= \lambda^4 - 2(\alpha\bar{\alpha} + \beta\bar{\beta})\lambda^2 + (\alpha\bar{\alpha} - \beta\bar{\beta})^2
$$

$$
= (\lambda - |\alpha| - |\beta|)(\lambda - |\alpha| + |\beta|)(\lambda + |\alpha| - |\beta|)(\lambda + |\alpha| + |\beta|).
$$

The characteristic polynomial of the toroidal graph $H = \mathbf{H}(A)$ $(A \in \mathfrak{A})$ is

$$
(9) \qquad f_H(\lambda) = \prod_{\boldsymbol{\varrho} \in \mathbb{R}(A)} \varphi(\boldsymbol{\varrho};\lambda).
$$

As an example, let $A = \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}$ (Figure 7). With

$$
\triangle = 5,\ \varepsilon = e^{\frac{2\pi i}{5}} = \frac{1}{4}(\sqrt{5} - 1) + i\frac{1}{4}\sqrt{2(5 + \sqrt{5})}
$$

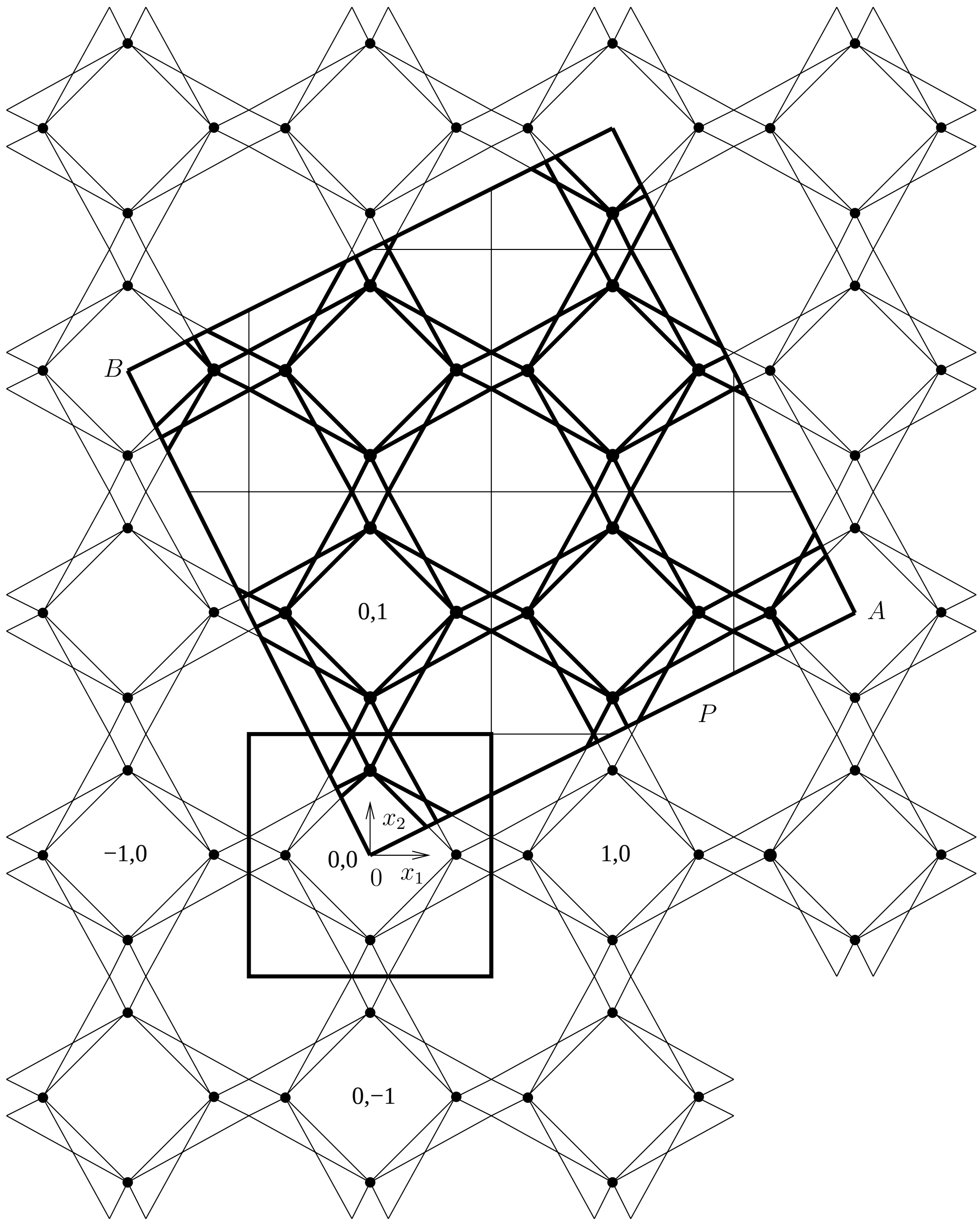


Figure 7

the solutions of (3) are

$$\varrho_1 = \varepsilon^{2\nu},\ \varrho_2 = \varepsilon^{\nu},\ \nu = 0, 1, 2, 3, 4 \quad ,$$

thus

$$\begin{aligned} |\alpha|^2 &= (1+\varepsilon^{2\nu}+\varepsilon^{\nu})(1+\varepsilon^{3\nu}+\varepsilon^{4\nu}) = 1+\varepsilon^{\nu}+\varepsilon^{2\nu}+\varepsilon^{3\nu}+\varepsilon^{4\nu}+(\varepsilon^{2\nu}+\varepsilon^{3\nu})^2, \\ |\beta|^2 &= (1+\varepsilon^{3\nu}+\varepsilon^{\nu})(1+\varepsilon^{2\nu}+\varepsilon^{4\nu}) = 1+\varepsilon^{\nu}+\varepsilon^{2\nu}+\varepsilon^{3\nu}+\varepsilon^{4\nu}+(\varepsilon^{\nu}+\varepsilon^{4\nu})^2 \end{aligned}$$

yielding

for $\nu = 0$: $\quad |\alpha| = |\beta| = 3,$

for $\nu = 1, 4$: $\quad |\alpha| = 2\left|\cos\frac{4\pi}{5}\right| = \frac{1}{2}(\sqrt{5}+1), \quad |\beta| = 2\left|\cos\frac{2\pi}{5}\right| = \frac{1}{2}(\sqrt{5}-1),$

for $\nu = 2, 3$: $\quad |\alpha| = 2\left|\cos\frac{2\pi}{5}\right| = \frac{1}{2}(\sqrt{5}-1), \quad |\beta| = 2\left|\cos\frac{4\pi}{5}\right| = \frac{1}{2}(\sqrt{5}+1)$

which, by (8) and (9), results in

$$f_H(\lambda) = \lambda^2(\lambda-6)(\lambda+6)(\lambda-1)^4(\lambda+1)^4(\lambda^2-5)^4.$$

Having the spectrum, the eigenvectors can now be obtained from equations (7) and (2) (for a simpler example, the eigenvectors will explicitly be calculated in Part II).

I.5 Regular toroidal cages

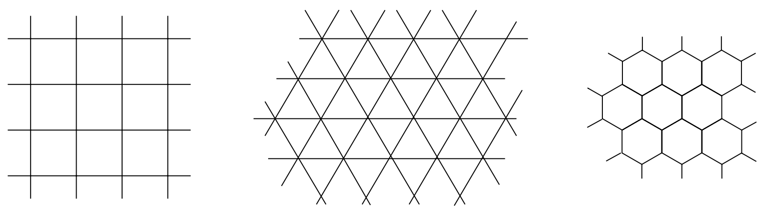
There are three regular tessellations of the plane (Figure 8):

- the tiling by squares whose graph is the **f**our-lattice **F**,
- the tiling by equilateral triangles whose graph is the **t**hree-lattice **T**,

- the tiling by regular hexagons whose graph is the **s**ix-lattice **S**.

S and **T** are duals of each other, **F** is self-dual.

These tessellations generate three classes of regular toroidal cages, namely, $\mathfrak{F} = \{\mathbf{F}(A)\}$, $\mathfrak{T} = \{\mathbf{T}(A)\}$, $\mathfrak{S} = \{\mathbf{S}(A)\}$; $A \in \mathfrak{A}$. For all of them – in particular, for $\mathfrak{F}$ and $\mathfrak{T}$ – the eigenvalue problem becomes most simple. After giving the results for $\mathfrak{F}$ and $\mathfrak{T}$, we shall discuss the class $\mathfrak{S}$ of regular toroidal 6-cages at some length, because of its significance for the chemistry (Hückel theory) of toroidal fullerenes, in Part II.



F T S

Figure 8

Regular toroidal 4-cages (class $\mathfrak{F}$) and 3-cages (class $\mathfrak{T}$)

For $\mathfrak{F}$ and $\mathfrak{T}$ we have $m = 1$ (Figures 9, 10) which means that the eigenvalue problem

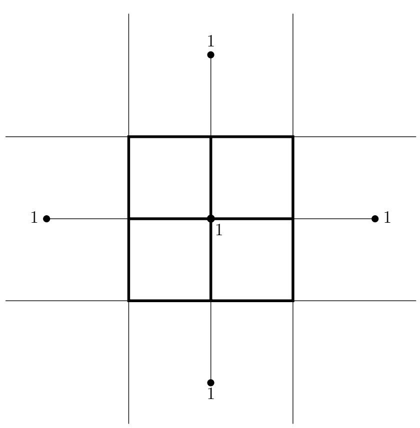


Figure 9

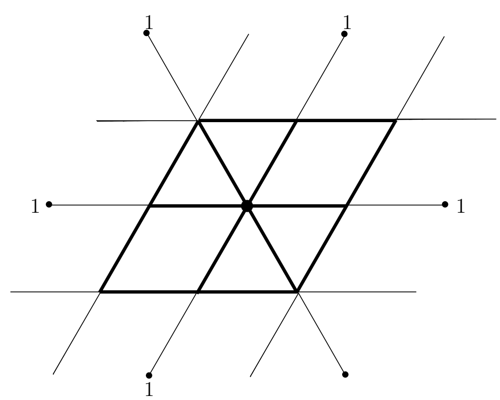


Figure 10

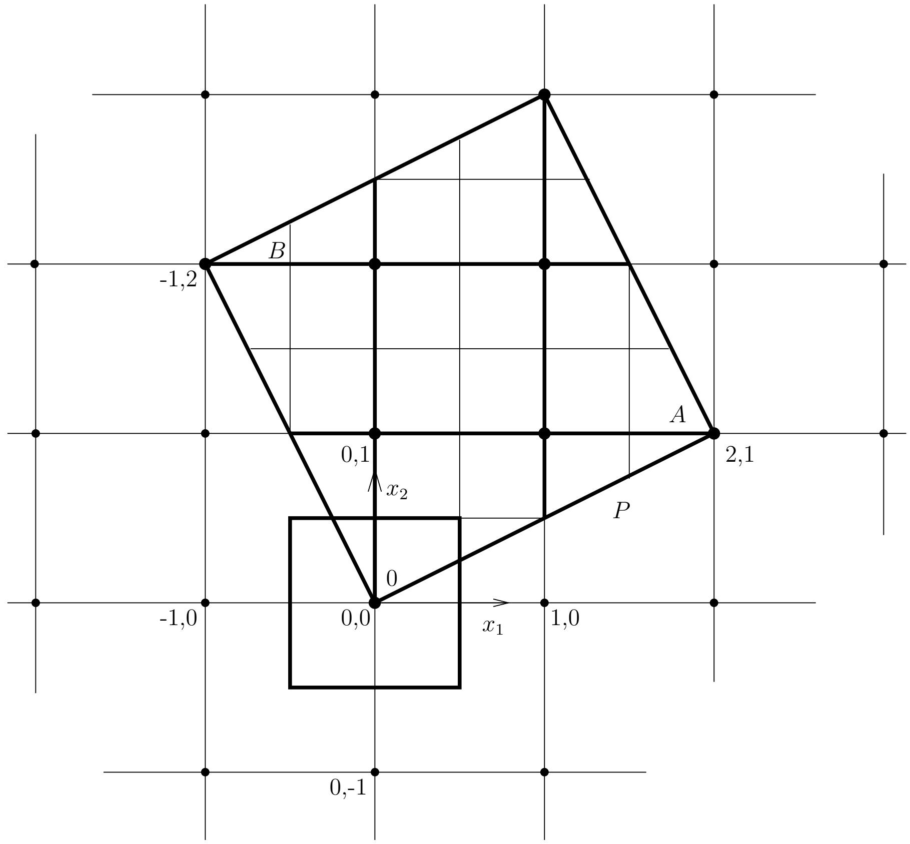


Figure 11

(4) becomes trivial, we can write down the spectrum straightaway:

$$\begin{aligned} \lambda &= \varrho_1 + \varrho_1^{-1} + \varrho_2 + \varrho_2^{-1} && \text{for } \mathfrak{F} \quad \text{and} \\ \lambda &= \varrho_1 + \varrho_1^{-1} + \varrho_2 + \varrho_2^{-1} + \varrho_1\varrho_2^{-1} + \varrho_1^{-1}\varrho_2 && \text{for } \mathfrak{T}. \end{aligned}$$

All that remains to be done is to insert the solutions of the basic equations.

Figures 11 and 12 show two respective examples for $A = \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}$, the same matrix as in the preceding example with the same solutions (ϱ_1, ϱ_2), and we obtain the following spectra.

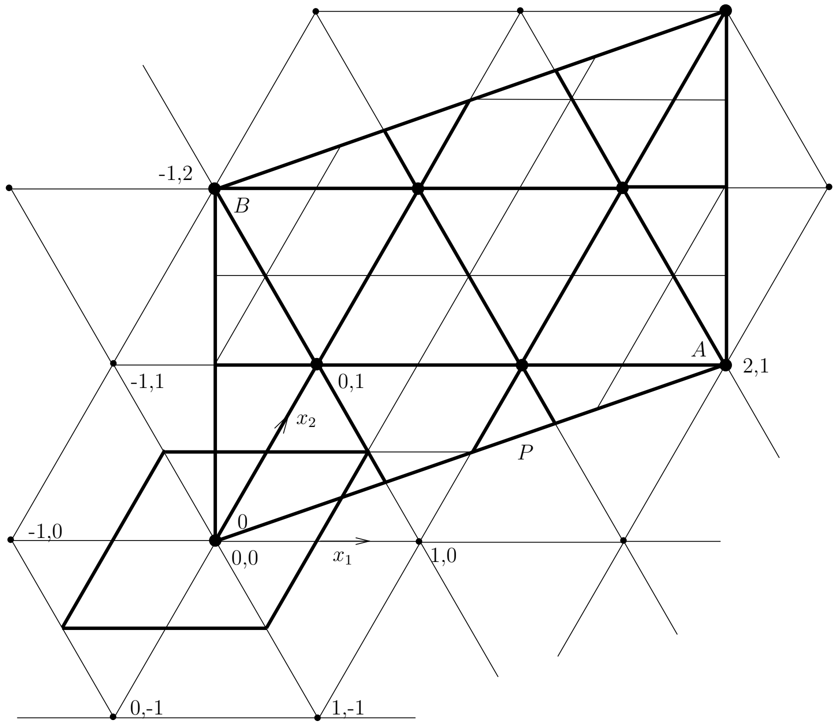


Figure 12

Spectrum of $\mathbf{F}(A)$*:*

$$\begin{aligned}\lambda_\nu &= \varepsilon^{2\nu} + \varepsilon^{-2\nu} + \varepsilon^{\nu} + \varepsilon^{-\nu} \\ &= 1 + \varepsilon^{\nu} + \varepsilon^{2\nu} + \varepsilon^{3\nu} + \varepsilon^{4\nu} - 1, \quad \nu = 0, 1, 2, 3, 4\end{aligned}$$

yielding

$$\lambda_0 = 4,\ \lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = -1$$

(note that $\mathbf{F}(A)$ is isomorphic to the complete graph on 5 vertices).

Spectrum of $\mathbf{T}(A)$:

$$\begin{aligned}\lambda_\nu &= \varepsilon^{2\nu} + \varepsilon^{-2\nu} + \varepsilon^{\nu} + \varepsilon^{-\nu} + \varepsilon^{2\nu} \cdot \varepsilon^{-\nu} + \varepsilon^{-2\nu} \cdot \varepsilon^{\nu} \\ &= 1 + \varepsilon^{\nu} + \varepsilon^{2\nu} + \varepsilon^{3\nu} + \varepsilon^{4\nu} - 1 + \varepsilon^{\nu} + \varepsilon^{-\nu}, \quad \nu = 0, 1, 2, 3, 4\end{aligned}$$

yielding

$$\lambda_0 = 6, \qquad \lambda_1{=}\lambda_4 = -1 + 2\cos\frac{2\pi}{5} = \frac{1}{2}(-3+\sqrt{5}),$$
$$\lambda_2{=}\lambda_3 = -1 + 2\cos\frac{4\pi}{5} = \frac{1}{2}(-3-\sqrt{5}).$$

Part II. Spectra and eigenvectors of toroidal 6-cages (toroidal fullerenes)

II.1 The spectrum of a toroidal fullerene

Graph **S** with corresponding parallelogram tessellation of the plane (one of three possibilities) is displayed in Figure 13 (cf. Figure 2).

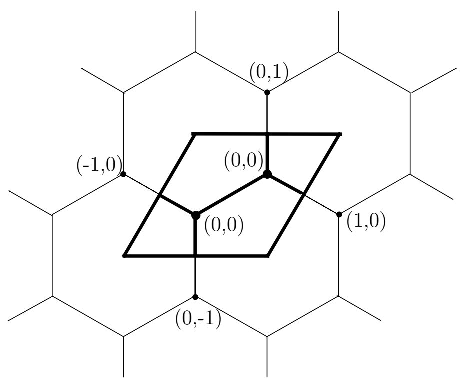


Figure 13

The neighbours of the $m = 2$ vertices v_1, v_2 in $P_{\mathbf{o}}$ are:

vertex	neighbours		
$v_1 = (0,0;1)$	$(0,0;2)$,	$(-1,0;2)$,	$(0,-1;2)$
$v_2 = (0,0;2)$	$(0,0;1)$,	$(1,0;1)$,	$(0,1;1)$.

The corresponding eigenvalue problem is

$$
\text{(10)} \qquad \left\{ \begin{array}{rcl} u_2 + \varrho_1^{-1} u_2 + \varrho_2^{-1} u_2 & = & (1 + \bar{\varrho}_1 + \bar{\varrho}_2) u_2 = \lambda u_1, \\ u_1 + \varrho_1 u_1 + \varrho_2 u_1 & = & (1 + \varrho_1 + \varrho_2) u_1 = \lambda u_2. \end{array} \right.
$$

Multiplying the right-hand sides and the left-hand sides of (10) we obtain

$$
\text{(11)} \qquad \lambda^2 = (1 + \varrho_1 + \varrho_2)(1 + \bar{\varrho}_1 + \bar{\varrho}_2) = |1 + \varrho_1 + \varrho_2|^2 \ .
$$

Thus we have proved

Theorem 2. *The characteristic polynomial of a toroidal* 6*-cage* $S = \mathbf{S}(A)$ *is*

$$
f_S(\lambda) = \prod_{\boldsymbol{\varrho} \in \mathbb{R}(A)} (\lambda^2 - |1 + \varrho_1 + \varrho_2|^2) \qquad (A \in \mathfrak{A}).
$$

An example. Let, same as above, $A = \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}$. Consider the toroidal 6-cage $\mathbf{S}(A)$ with $\triangle = 5$ hexagons (Figure 14). Equation (11), with

$$
\varrho_1 = \varepsilon^{2\nu}, \ \varrho_2 = \varepsilon^{\nu} \quad (\varepsilon = e^{\frac{2\pi i}{5}}, \quad \nu = 0, 1, 2, 3, 4),
$$

becomes

$$
\begin{array}{rcl} \lambda^2 & = & (1 + \varepsilon^{2\nu} + \varepsilon^{\nu})(1 + \varepsilon^{3\nu} + \varepsilon^{4\nu}) \\ & = & \left\{ \begin{array}{cl} 9 & \text{for } \nu = 0 \\ (\varepsilon^{2\nu} + \varepsilon^{-2\nu})^2 = (2 \cos \frac{4\pi\nu}{5})^2 & \text{for } \nu = 1, 2, 3, 4 \ , \end{array} \right. \end{array}
$$

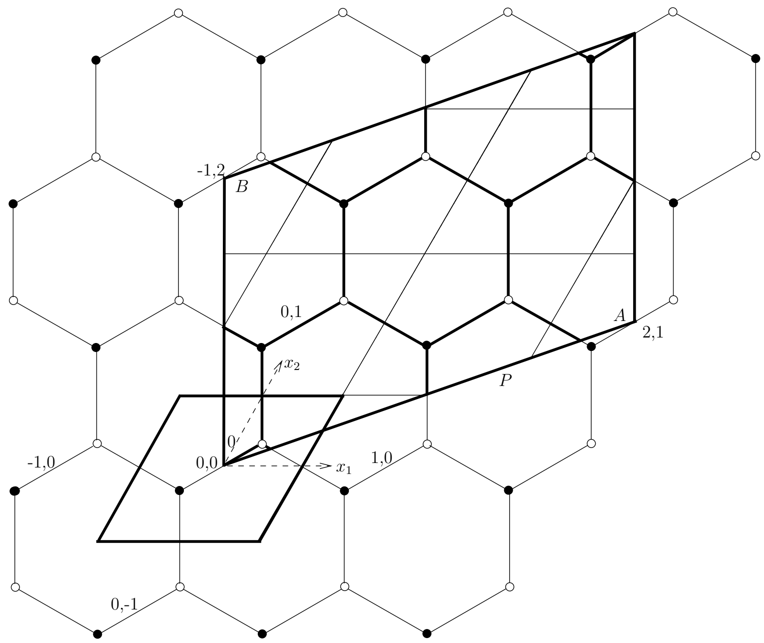


Figure 14

thus

$$
\begin{aligned}
f_S(\lambda) &= (\lambda-3)(\lambda+3)(\lambda-\frac{1}{2}(\sqrt{5}+1))^2(\lambda+\frac{1}{2}(\sqrt{5}+1))^2(\lambda-\frac{1}{2}(\sqrt{5}-1))^2(\lambda+\frac{1}{2}(\sqrt{5}-1))^2 \\
&= (\lambda-3)(\lambda+3)(\lambda^2-\lambda-1)^2(\lambda^2+\lambda-1)^2.
\end{aligned}
$$

We may fix $u_1 = 1$; by division (10) then implies

$$u_2^2 = \frac{1+\varrho_1+\varrho_2}{1+\bar{\varrho}_1+\bar{\varrho}_2} = \frac{1+\varepsilon^\nu+\varepsilon^{2\nu}}{1+\varepsilon^{3\nu}+\varepsilon^{4\nu}} = \varepsilon^{2\nu},$$

thus $u_2 = \pm\,\varepsilon^\nu$ where, by (10), the sign depends on the sign of λ.

The eigenvectors can now easily be calculated from (10): the complete result is contained in Table 1 where the components

$$e_\nu(\lambda \mid v) = e_\nu(\lambda \mid x_1, x_2; j) = \varrho_1^{x_1}\varrho_2^{x_2} \cdot u_j = \varepsilon^{(2x_1+x_2)\nu} \cdot u_j \quad (j = 1, 2)$$

of the 10 eigenvectors $\mathbf{e}_\nu(\lambda)$ ($\nu = 0, 1, 2, 3, 4$; two values of λ for each value of ν) are given only for $j = 1$, for $\lambda > 0$, and for $\nu = 0, 1, 2$, the missing entries being already determined by

$$\mathbf{e}_{5-\nu}(\lambda) = \overline{\mathbf{e}_\nu(\lambda)} \qquad (\nu \neq 0)$$

(implying that to ν and $5-\nu$ there belongs the same pair of eigenvalues) and by the relations

$$\begin{aligned} e_0(3 \mid x_1, x_2; 2) &= 1, \\ e_\nu(\lambda \mid x_1, x_2; 2) &= -(-\varepsilon)^\nu e_\nu(\lambda \mid x_1, x_2; 1) \quad (\nu = 1, 2; \lambda > 0), \\ e_\nu(-\lambda \mid x_1, x_2; j) &= (-1)^{j+1} e_\nu(\lambda \mid x_1, x_2; j) \quad (j = 1, 2;\ \nu = 0, 1, 2, 3, 4). \end{aligned}$$

		vertices $(x_1, x_2; 1)$ $(x_1, x_2) =$				
ν	λ	$(0,0)$	$(0,1)$	$(0,2)$	$(1,1)$	$(1,2)$
0	3	1	1	1	1	1
1	$\frac{1}{2}(\sqrt{5}+1)$	1	ε	ε^2	ε^3	ε^4
2	$\frac{1}{2}(\sqrt{5}-1)$	1	ε^2	ε^4	ε	ε^3

Table 1

We observe that the real part $\mathbf{e}_{\mathrm{Re}}$ and the imaginary part $\mathbf{e}_{\mathrm{Im}}$ of eigenvector $\mathbf{e} = \mathbf{e}_\nu(\lambda)$, $\nu \neq 0$, being themselves eigenvectors for λ (which has even multiplicity), satisfy

$$\mathbf{e}_{\mathrm{Re}}^2 = \mathbf{e}_{\mathrm{Im}}^2 = \frac{\triangle}{2}, \quad \mathbf{e}_{\mathrm{Re}} \cdot \mathbf{e}_{\mathrm{Im}} = 0,$$

i.e., $\mathbf{e}_{\mathrm{Re}}$ and $\mathbf{e}_{\mathrm{Im}}$ have the same norm and are orthogonal, the latter implying linear independence.

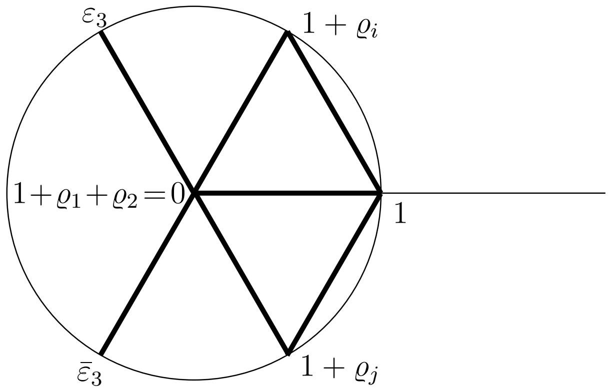


Figure 15

II.2 On the multiplicities of the eigenvalues [5]

1) Toroidal 6-cages with eigenvalue zero

By Theorem 2 zero is an eigenvalue if and only if the basic equations (3) have a solution (ϱ_1, ϱ_2) such that

$$1 + \varrho_1 + \varrho_2 = 0. \tag{12}$$

As $|\varrho_1| = |\varrho_2| = 1$, (12) holds if and only if either

$$\varrho_1 = \varepsilon_3,\ \varrho_2 = \varepsilon_3^{-1} = \bar{\varepsilon}_3 \qquad \text{or} \qquad \varrho_1 = \varepsilon_3^{-1} = \bar{\varepsilon}_3,\ \varrho_2 = \varepsilon_3^{-2} = \varepsilon_3 \qquad \text{where} \qquad \varepsilon_3 = e^{\frac{2\pi i}{3}}$$

(see Figure 15 with $(i,j) = (1,2)$ or $(2,1)$). If one of these pairs is a solution then so is the other which, in particular, implies that if zero is an eigenvalue then it is of multiplicity 4. Recall: $\varepsilon_k = e^{\frac{2\pi i}{k}}$; assume, w.l.o.g., $\varrho_1 = \varepsilon_3$, $\varrho_2 = \bar{\varepsilon}_3$. By (II), ϱ_1 is a power of $\varepsilon_\triangle$, say the r^{th} power $(0 < r < \triangle)$:

$$\varrho_1 = \varepsilon_3 = e^{\frac{2\pi i}{3}} = \varepsilon_\triangle^r = e^{\frac{r}{\triangle}2\pi i}$$

[5] Cf. [1], Sections IV and V.

which implies $\triangle = 3r$ and $\varrho_1 = \varepsilon_\triangle^r$, $\varrho_2 = \varepsilon_\triangle^{2r}$. The basic congruences (6) now yield

$$\begin{cases} a_1 r + a_2 \cdot 2r &= \sigma\triangle = \sigma \cdot 3r, \\ b_1 r + b_2 \cdot 2r &= \tau\triangle = \tau \cdot 3r \end{cases}$$

with some integers σ, τ, thus

$$\begin{cases} a_1 + 2a_2 &= 3\sigma, \\ b_1 + 2b_2 &= 3\tau \end{cases}$$

or, equivalently.

$$a_1 - a_2 \equiv b_1 - b_2 \equiv 0, \quad \bmod 3. \tag{13}$$

This necessary condition is also sufficient: from (13) we obtain

$$\triangle = |a_1 b_2 - a_2 b_1| \equiv 0, \quad \bmod 3.$$

Let $r' = \dfrac{\triangle}{3}$. (13) is equivalent to

$$\begin{cases} a_1 + 2a_2 &= 3\sigma', \\ b_1 + 2b_2 &= 3\tau' \end{cases}$$

with some integers σ', τ'; multiplication with r' yields

$$\begin{cases} a_1 r' + a_2 \cdot 2r' &= \sigma' \cdot 3r' = \sigma'\triangle, \\ b_1 r' + b_2 \cdot 2r' &= \tau' \cdot 3r' = \tau'\triangle \end{cases}$$

which means that

$$(\varepsilon_\triangle^{r'}, \varepsilon_\triangle^{2r'}) = (\varepsilon_3, \varepsilon_3^2) = (\varepsilon_3, \bar{\varepsilon}_3)$$

is a solution to the basic equations.

Thus we have proved

Theorem 3. *Let* $A = \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} \in \mathfrak{A}$. *Zero is an eigenvalue of* $\mathbf{S}(A)$, *necessarily of multiplicity* 4, *if and only if*

$$a_1 - a_2 \equiv b_1 - b_2 \equiv 0, \quad \text{mod } 3.$$

2) A general proposition on multiplicities

Case I: ϱ_1, ϱ_2 are real.

Then $\varrho_1, \varrho_2 \in \{1, -1\}$. Let $j \in \{1, 2\}$. By (II),

$$\varrho_j = \varepsilon_\triangle^k = e^{\frac{2k}{\triangle}\pi i} \quad \text{for some } k, \quad 0 \leq k < \triangle.$$

Thus $\varrho_j = -1 = e^{\pi i}$ implies $\triangle = 2k$, i.e., $\triangle$ is even.

Next we discuss the four cases $\varrho_1 = \pm 1$, $\varrho_2 = \pm 1$.

(i) $\varrho_1 = \varrho_2 = 1$ (the trivial case).

This solution is always present. We obtain $\lambda^2 = |1 + 1 + 1|^2 = 3^2$; clearly, $|1 + \varrho_1 + \varrho_2| = 3$ if and only if $\varrho_1 = \varrho_2 = 1$, and we conclude that the eigenvalues ± 3 are always present, both of multiplicity one (as is the case for *any* connected trivalent bipartite graph).

(ii) $\varrho_1 = 1$, $\varrho_2 = -1$, (iii) $\varrho_1 = -1$, $\varrho_2 = 1$, (iv) $\varrho_1 = \varrho_2 = -1$.

It can easily be verified that if $\triangle$ is even and

(A) at least one of a_1, a_2, b_1, b_2 is odd

then precisely one of (ii), (iii), (iv) is a solution, and if

(B) all of a_1, a_2, b_1, b_2 are even

then each of (ii), (iii), (iv) is a solution.

Thus for the characteristic polynomial we obtain in case (A) (at least) one, and in case (B) (at least) three factors $\lambda^2 - 1$, but it should be noted that this factor may also, in addition, result from some non-real solution (ϱ_1, ϱ_2); this happens if and only if $\varrho_1 = -1$, or $\varrho_2 = -1$, or $\varrho_2 = -\varrho_1$ (see, in particular, Section II.4, Table 2 and equations (14)).

Case II: At least one of ϱ_1, ϱ_2 is non-real.

Then the pairs (ϱ_1, ϱ_2) and $(\bar\varrho_1, \bar\varrho_2)$ are distinct but yield the same factor

$$\lambda^2 - |1 + \varrho_1 + \varrho_2|^2 = \lambda^2 - |1 + \bar\varrho_1 + \bar\varrho_2|^2.$$

Therefore, the multiplicity of the corresponding eigenvalues $\lambda \neq \pm 1$ is even.

Summarizing we have found

Theorem 4. *Let* $A = \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} \in \mathfrak{A}$, $S = \mathbf{S}(A)$, $\triangle = |\det A|$. *Then*

$$f_S(\lambda) = \lambda^{2\alpha}(\lambda^2 - 1)^{\beta}(\lambda^2 - 9)\prod_{i=1}^{\gamma}(\lambda^2 - c_i^2)^2$$

where

$$\alpha = \begin{cases} 2 & \text{if } a_1 - a_2 \equiv b_1 - b_2 \equiv 0, \mod 3, \\ 0 & \text{otherwise;} \end{cases}$$

$$\beta = \begin{cases} 3 & \text{if all of } a_1, a_2, b_1, b_2 \text{ are even (then } \triangle \text{ is a multiple of } 4), \\ 1 & \text{if } \triangle \text{ is even and at least one of } a_1, a_2, b_1, b_2 \text{ is odd,} \\ 0 & \text{if } \triangle \text{ is odd;} \end{cases}$$

$$\gamma = \tfrac{1}{2}(\triangle - \alpha - \beta - 1),$$

and

$$0 < c_i < 3 \quad \text{for} \quad i = 1, 2, \ldots, \gamma.$$

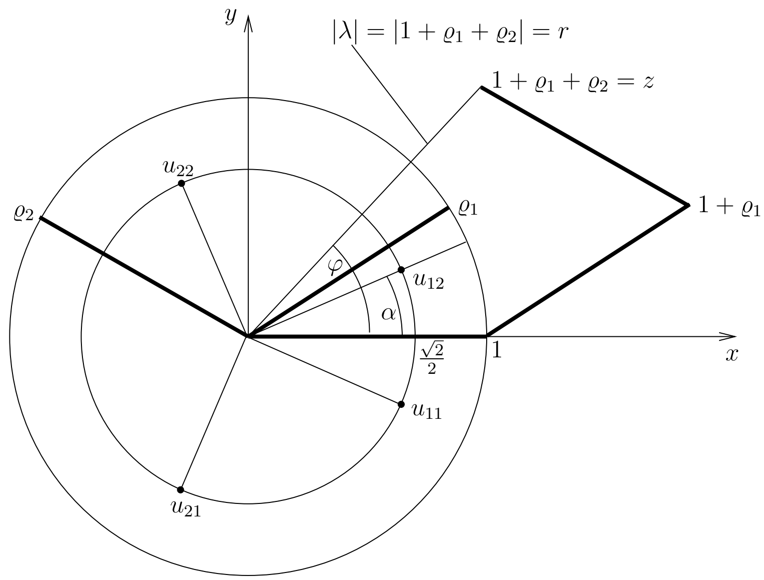


Figure 16

II.3 The eigenvectors of a toroidal fullerene

To set up a system of eigenvalues and corresponding pairwise orthogonal eigenvectors according to Theorem 1 we need, for every $\boldsymbol{\varrho} \in \mathbb{R}(A)$, a pair of eigenvalues $\lambda = \lambda(\mu; \boldsymbol{\varrho})$ and corresponding orthonormal eigenvectors $\mathbf{u} = \mathbf{u}(\mu; \boldsymbol{\varrho})$ $(\mu = 1, 2)$ satisfying equations (10) which may be rewritten as

$$(10') \qquad \begin{cases} \bar{z}u_2 &= \lambda u_1, \\ z u_1 &= \lambda u_2, \end{cases} \quad z = 1 + \varrho_1 + \varrho_2.$$

Setting

$$z = re^{i\varphi} \ (r = r(\boldsymbol{\varrho}) \geq 0,\ 0 \leq \varphi = \varphi(\boldsymbol{\varrho}) < 2\pi;\ \varphi \text{ arbitrary if } r = 0), \varphi = 2\alpha,$$

such a pair is

$$\lambda(\mu; \boldsymbol{\varrho}) = (-1)^{\mu-1} r, \quad \mathbf{u}(\mu; \boldsymbol{\varrho}) = \tfrac{1}{\sqrt{2}}(i^{1-\mu}e^{-i\alpha},\ i^{\mu-1}e^{i\alpha}) \qquad (\mu = 1, 2) \text{ (Figure 16)}.$$

The set of real parts and imaginary parts of the complex eigenvectors $\mathbf{e}$ so found is again a complete system of eigenvectors for $S = \mathbf{S}(A)$; it is a straightforward procedure to

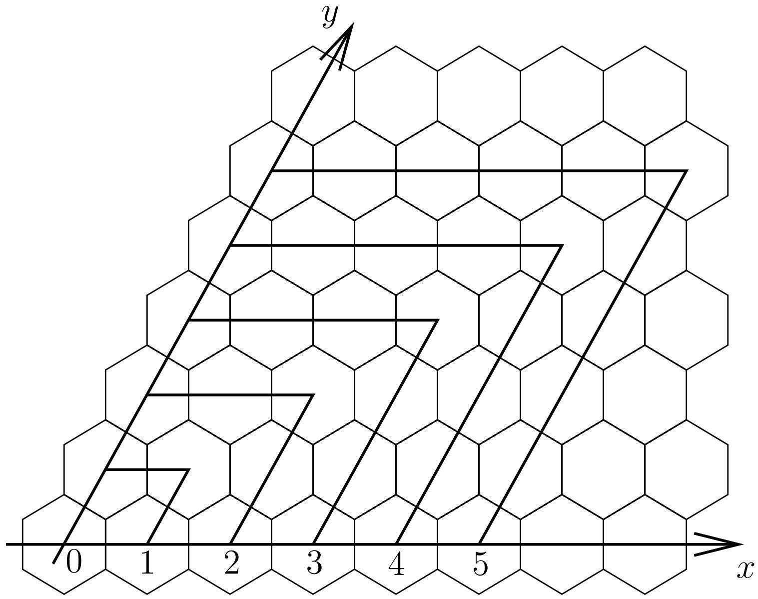


Figure 17

prove that these real eigenvectors are pairwise orthogonal, too.

II.4 A special sequence of toroidal fullerenes

Consider the sequence of fullerenes $S_n = \mathbf{S}(A_n)$ where $A_n = \begin{pmatrix} n & 0 \\ 0 & n \end{pmatrix}$, $n = 1, 2, 3, \ldots$ (Figure 17). The basic equations for S_n are $\varrho_1^n = \varrho_2^n = 1$ with the n^2 solutions

$$\varrho_1 = \varepsilon_n^\mu,\ \varrho_2 = \varepsilon_n^\nu \quad (\varepsilon_n = e^{\frac{2\pi i}{n}};\ \mu, \nu = 0, 1, \ldots, n-1),$$

so the spectrum of S_n is $\{\pm|1+\varepsilon_n^\mu+\varepsilon_n^\nu| \mid \mu, \nu = 0, 1, \ldots, n-1\}$ (for $n = 8$, see Table 2).

Let g, p, q be positive integers. Because of

$$\varepsilon_{gpq}^{gqj} = \varepsilon_p^j, \quad \varepsilon_{gpq}^{gpk} = \varepsilon_q^k \quad (0 \le j < p,\ 0 \le k < q),$$

the numbers $\pm|1+\varepsilon_p^j+\varepsilon_q^k|$ are eigenvalues for S_{gpq}. This means that, given any two roots of unity ϱ_1, ϱ_2, the numbers $\pm|1+\varrho_1+\varrho_2|$ are eigenvalues for infinitely many toroidal fullerenes. Note that the set of these numbers is dense in the interval $-3 \le \lambda \le 3$.

Let $\boldsymbol{\varrho} \in \mathbf{R}(A_n)$, $|1+\varrho_1+\varrho_2| = \lambda_0$. Then for the 12 ordered pairs

$$\begin{aligned}(\sigma_1,\sigma_2) \;=\; & (\varrho_1,\varrho_2), \quad (\varrho_2,\varrho_1), \quad (\bar\varrho_1,\bar\varrho_2), \quad (\bar\varrho_2,\bar\varrho_1),\\ & (\bar\varrho_1\varrho_2,\bar\varrho_1), \quad (\bar\varrho_1,\bar\varrho_1\varrho_2), \quad (\varrho_1\bar\varrho_2,\varrho_1), \quad (\varrho_1,\varrho_1\bar\varrho_2),\\ & (\bar\varrho_2,\varrho_1\bar\varrho_2), \quad (\varrho_1\bar\varrho_2,\bar\varrho_2), \quad (\varrho_2,\bar\varrho_1\varrho_2), \quad (\bar\varrho_1\varrho_2,\varrho_2)\end{aligned}$$

also $|1+\sigma_1+\sigma_2| = \lambda_0$. We conclude that, generically, the multiplicity $m_n(\lambda)$ of an (unspecified) eigenvalue λ of a toroidal fullerene S_n is 12.

The case $n = 8$.

$\mu\backslash\nu$	0	1	2	3	4	5	6	7
0	9	a^+	5	a^-	**1**	a^-	5	a^+
1	a^+	a^+	b^+	3	**1**	**1**	3	b^+
2	5	b^+	5	3	**1**	b^-	**1**	3
3	a^-	3	3	a^-	**1**	b^-	b^-	**1**
4	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**
5	a^-	**1**	b^-	b^-	**1**	a^-	3	3
6	5	3	**1**	b^-	**1**	3	5	b^+
7	a^+	b^+	3	**1**	**1**	3	b^+	a^+

the entries are

$c_{\mu\nu} = |1+\varepsilon_8^\mu+\varepsilon_8^\nu|^2$,

$\varepsilon_8 = e^{\frac{2\pi i}{8}} = \frac{1}{\sqrt2}(1+i)$;

$a^\pm = 5 \pm 2\sqrt2 = 5 \pm \sqrt8$,

$b^\pm = (1\pm\sqrt2)^2 = 3\pm\sqrt8$

The spectrum of S_8 is $\{\pm\sqrt{c_{\mu\nu}} \mid \mu,\nu = 0,1,\dots,7\}$;

$f_{S_8}(\lambda) = (\lambda^2-9)(\lambda^2-5)^6(\lambda^2-3)^{12}(\lambda^2-1)^{21}(\lambda^4-10\lambda^2+17)^6(\lambda^4-6\lambda^2+1)^6$.

Table 2

There are exceptions. The multiplicity reduces if there occur coincidences among the 12 pairs listed above, so, e.g.,

$$m_n(3) = m_n(-3) = 1, \qquad m_n(0) = \begin{cases} 4 & \text{if } n \text{ is a multiple of 3,}\\ 0 & \text{otherwise.}\end{cases}$$

There are also eigenvalues with multiplicity greater than 12:

$$m_n(1) = m_n(-1) = \begin{cases} 3(n-1) & \text{if } n \text{ is even,} \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

(cf. Table 2); checking for n up to 300 we found only one eigenvalue $\lambda \geq 0,\ \lambda \neq 1$ with $m_n(\lambda) > 12$, namely, $\lambda = \sqrt{3}$: the numbers $\pm\sqrt{3}$ are eigenvalues for $n = 3$ as well as for $n = 8$ with multiplicities 6 and 12, respectively, entailing that, for $n = 3 \cdot 8 = 24$ and all multiples of 24, $m_n(\sqrt{3}) = m_n(-\sqrt{3}) \geq 6 + 12 = 18$; in fact, $m_n(\sqrt{3}) = m_n(-\sqrt{3}) = 18$ $(n = 24k,\ 1 \leq k \leq 12)$.[6]

Part III. Spectrum and eigenvectors of a $(3,6)$–cage

III.1 Preliminaries

A $(3,6)$–*cage* is a trivalent polyhedron each face of which is either a hexagon or a triangle; by Euler's formula the number of triangles is four. The structure of the $(3,6)$–cages is well known [4],[5]; in [3] the interrelations between the spectra of (generalized) $(3,6)$–cages and toroidal 6–cages are discussed in some detail. In a quantum–chemical context, A. Ceulemans et al. [2] developed methods based on solid–state (crystal) physics which allow the spectra and eigenspaces of $(3,6)$-cages explicitly to be calculated.

$(3,6)$–cages C depend on three parameters r, s, t [3][7] (Figures 18, 19)

r is the **r**adius (number of **r**ings),

s is the **s**ize (number of **s**teps = half the number of **s**pokes),

t is the **t**wist (**t**orsion) $\quad (-s < t \leq s; \quad t \equiv r, \bmod 2)$.

[6]The authors thank W. Rausch for carrying out the calculations.

[7]The notation used here differs from that in [3]: the new s equals the old S and is half the old s. Note also that t may be negative.

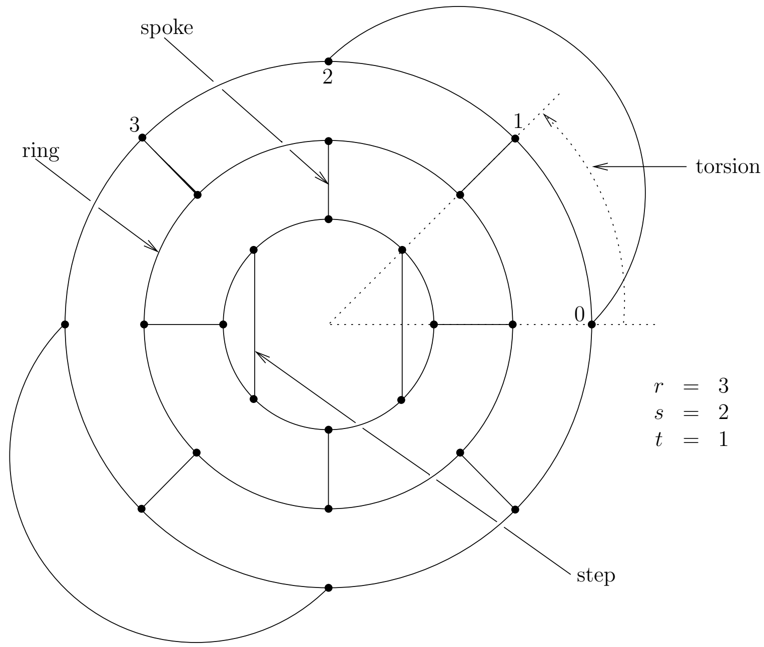
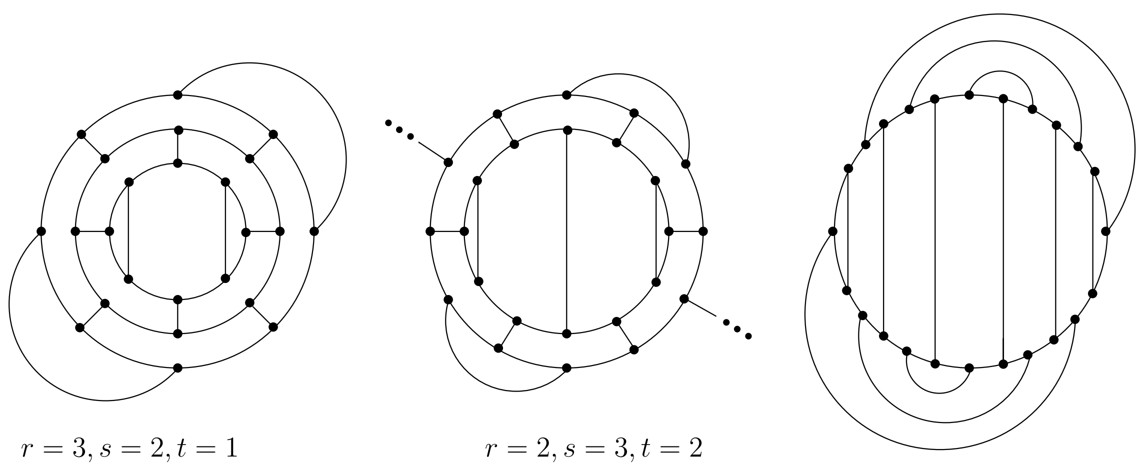


Figure 18



$r = 3, s = 2, t = 1$ $r = 2, s = 3, t = 2$ $r = 1, s = 6, t = 5$

Figure 19

We shall briefly write $C = [r, s, t]$. This representation is, in general, not unique [3]: there may be up to three different tripels determining the same $(3, 6)$–cage (Figure 19); the product rs is the same in all of them. Given C, we shall arbitrarily fix some triple r, s, t such that $C = [r, s, t]$. The numbers v of vertices, e of edges and h of hexagons are $v = 4rs$, $e = 6rs$ and $h = 2(rs - 1)$.

In 1995 P.W. Fowler [3] formulated the

Conjecture. *The spectrum of any* $(3, 6)$*–cage* C *has the form*

$$\{3, -1, -1-1; \lambda_1, \lambda_2, \ldots, \lambda_{2(\nu-1)}; -\lambda_1, -\lambda_2, \ldots, -\lambda_{2(\nu-1)}\}$$

where $\nu = \frac{1}{4}v(C) = rs$*; equivalently,*

$$f_C(\lambda) = (\lambda - 3)(\lambda + 1)^3\, g_C(\lambda^2)$$

where g_C *is a polynomial of degree* $\frac{1}{2}(v(C) - 4)$.

Using the results of Part II we shall now explicitly determine the eigenvalues and a system of pairwise orthogonal real eigenvectors for any $(3, 6)$–cage $[r, s, t]$ thus, in particular, prove Fowler's conjecture.

III.2 Calculation of spectrum and eigenvectors

An intuitive spatial representation of C is depicted in Figure 20. Take two copies C_1, C_2 of C, cut the edges representing the steps and glue the two copies together as indicated in Figure 21: the result is a toroidal 6–cage $S(C)$ where the adjacency relation in C is retained in $S(C)$: if in $S(C)$ vertices labelled p and q are adjacent then so are vertices labelled p and q in C. That means that C is a divisor of $S(C)$ (or, $S(C)$ is cover of C; for the divisor concept, see [3, Section 2]).

A third representation of C is obtained by flattening out the labelled toroidal 6–cage $S(C)$ in the plane, i.e., by representing $S(C)$ by a parallelogram P, spanned by vectors

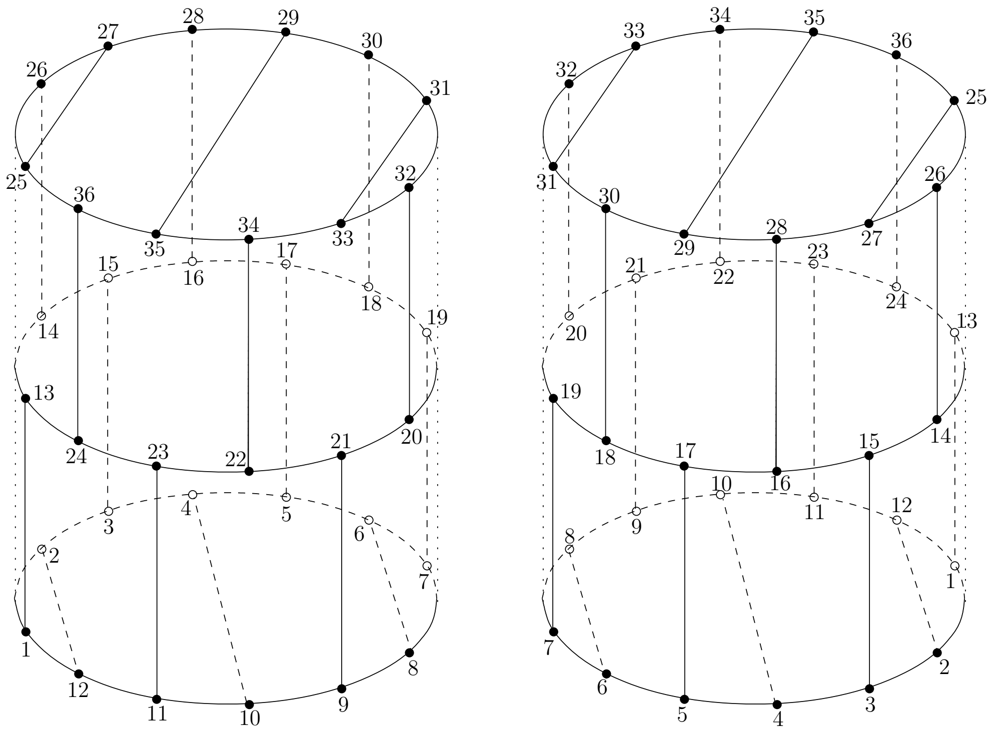


Figure 20

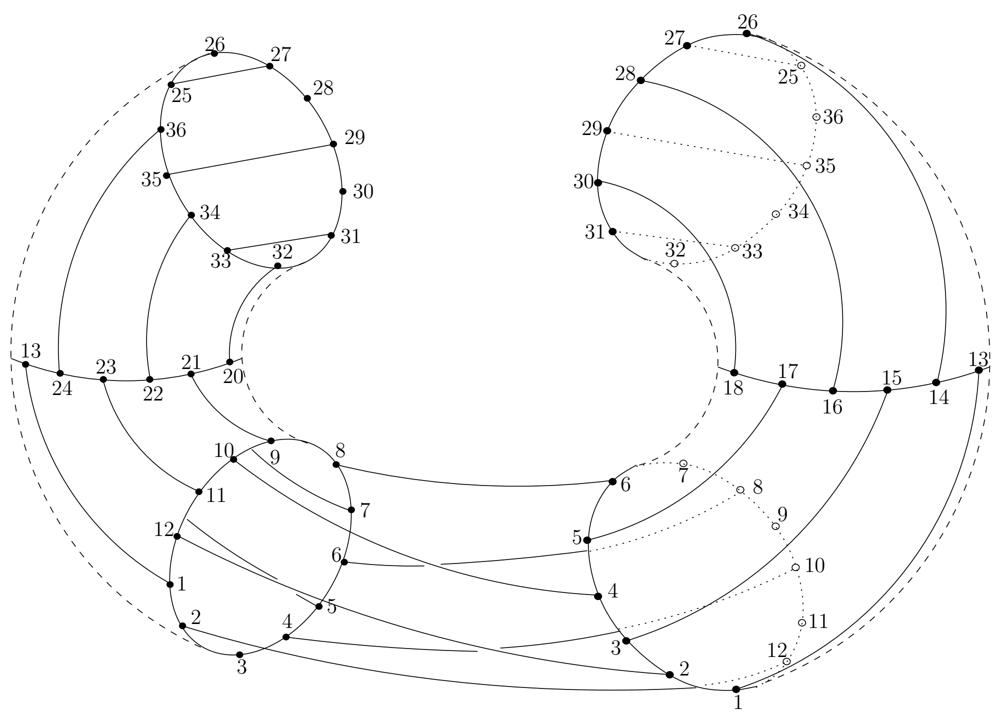


Figure 21

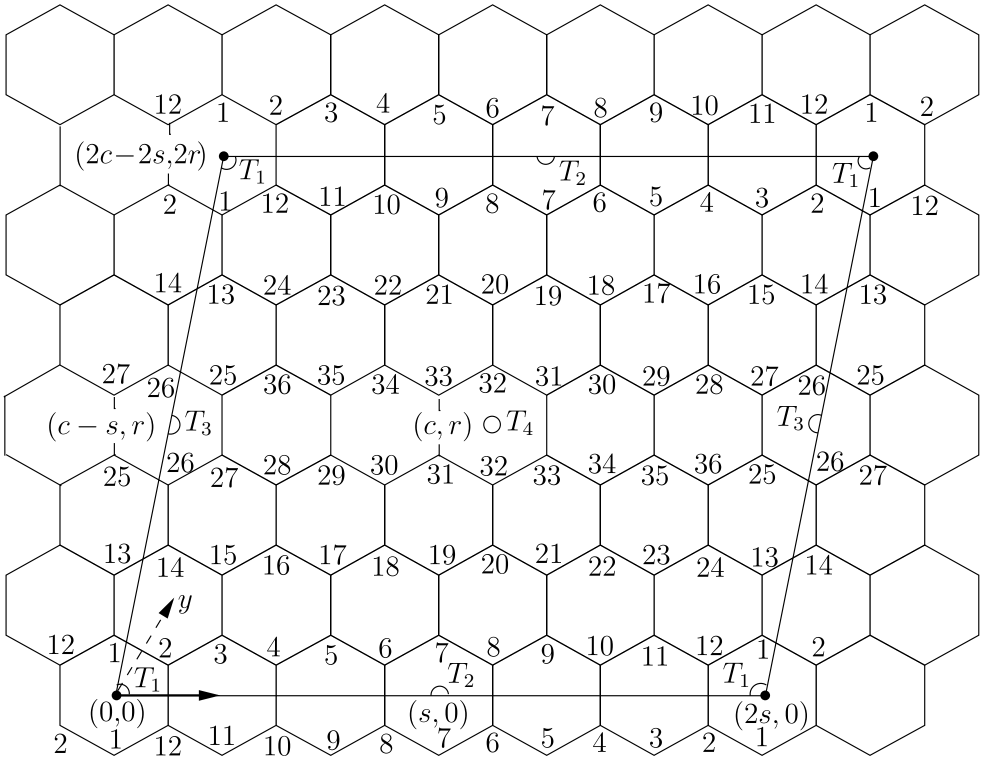


Figure 22

$\mathbf{a} = (a_1, a_2), \mathbf{b} = (b_1, b_2)$, over the hexagonal tessellation, as described in II.1; the triangles of C, marked by small circles, correspond to those hexagons whose vertices carry only three different labels (Figure 22). C is retrieved by identifying all vertices having the same label.

We may choose P such that the origin of the coordinate system coincides with the centre of a hexagon representing a triangle, T_1 say, and the x–axis follows a row of hexagons cutting those edges that correspond to the steps of the ladder connecting T_1 with another triangle, T_2 say (Figure 22).

This configuration (including the labels) is invariant under a rotation of 180° around the centre of P which interchanges the images of C_1, C_2. As a consequence: if distinct vertices $(x_1, x_2; j)$ and $(x_1', x_2'; j')$ in P $((x_1, x_2), (x_1', x_2') \in \mathbf{X}(A); j, j' \in \{1, 2\})$ have the

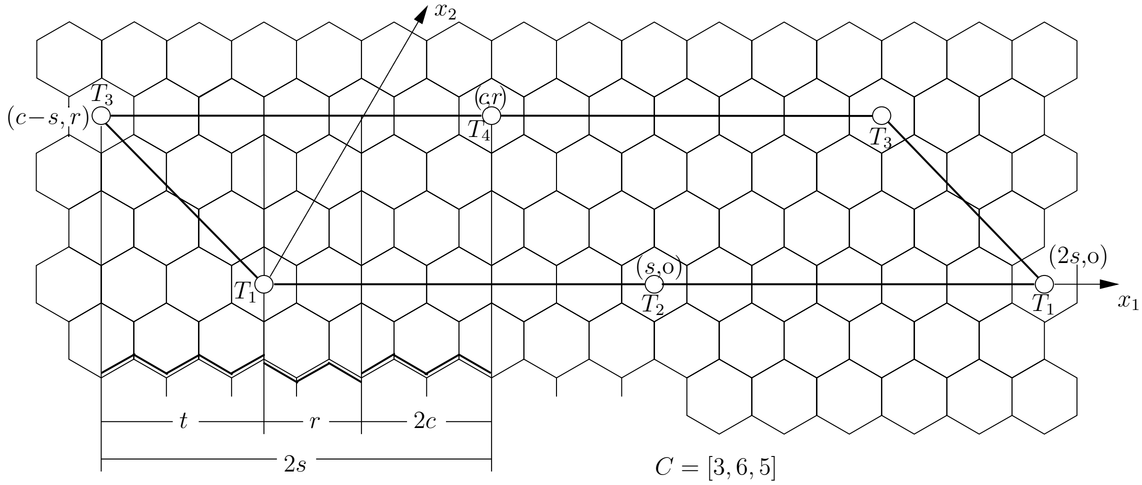


Figure 23

same label then

$$(x_1', x_2') = (a_1 + b_1 - 1 - x_1, a_2 + b_2 - 1 - x_2)$$

$$\equiv (-x_1 - 1, -x_2 - 1), \quad \text{mod } (\mathbf{a}, \mathbf{b}) \tag{15}$$

$$\text{and } j' = 3 - j.$$

Let the centre of P have coordinates (c, r); note that c depends on the twist t: we have $r + 2c + t = 2s$ or $r + t = 2(s - c)$ (Figure 23, note that t may be negative). The vectors spanning P are

$$\mathbf{a} = (2s, 0), \qquad \mathbf{b} = (2(c - s), 2r) = (-r - t, 2r),$$

the corresponding matrix A is

$$A = \begin{pmatrix} 2s & 0 \\ -r - t & 2r \end{pmatrix}; \quad \triangle = |\det A| = 4rs.$$

Note that all entries of A are even, therefore, the basic equations for A have precisely four real solutions, namely,

$$(\varrho_1, \varrho_2) = (1,1), (1,-1), (-1,1), (-1,-1)$$

(see II.2, 2, case I(B)); as a further consequence, the congruences (15) are, in particular, valid modulo 2.

All the solutions of the basic congruences and equations are

$$(16) \qquad \begin{array}{l} \left.\begin{array}{l} k_1 \equiv 2r\mu \qquad , \\ k_2 \equiv (r+t)\mu + 2s\nu, \end{array}\right\} \text{ mod } 4rs \quad ; \\ \varrho_1 = \varepsilon_\triangle^{k_1}, \quad \varrho_2 = \varepsilon_\triangle^{k_2}, \\ \mu = 0,1,\ldots,2s-1 \quad , \quad \nu = 0,1,\ldots,2r-1 \end{array}$$

where $\varepsilon_\triangle = e^{\frac{2\pi i}{\triangle}}$ (cf. I.3).

Next we shall explicitly write down a system of $4rs$ eigenvalues and corresponding pairwise orthogonal real eigenvectors for C. The simple idea is this: for every real solution $\boldsymbol{\varrho}$ and for every pair of non-real solutions $\boldsymbol{\varrho}, \bar{\boldsymbol{\varrho}}$ of the basic equations we shall construct an eigenvector $\mathbf{e}^*$ for $S(C)$ whose components for any two vertices $(x_1, x_2; j), (x_1', x_2'; j')$ in P with the same label are equal: then the restriction $\mathbf{e}^*_C$ of $\mathbf{e}^*$ to the vertex set of C is an eigenvector for C.

Let V_C and V_S be the vertex sets of C and $S(C)$, respectively; if $\mathbf{v}$ is a vector on V_S, let $\mathbf{v}_C$ denote its restriction to V_C.

We refer to I.2, Theorem 1 and II.3 and begin with the real solutions of the basic equations.

1) $\boldsymbol{\varrho} = (1,1)$ (trivial). Choose $\mu = 1$, then $\alpha = 0$, $e^{i\alpha} = 1$, $\lambda = 3$, $\mathbf{e}(1;1,1) = \frac{1}{\sqrt{2}}(1,1,\ldots,1)$ implying that $\mathbf{e}_C(1;1,1)$ is an eigenvector for C, $\lambda = 3$.

For what follows suppose that the distinct vertices $(x_1, x_2; j)$ and $(x_1', x_2'; j')$ in P have the same label: then (15) holds.

2) $\boldsymbol{\varrho} = (1,-1)$. Choose $\mu = 2$, then $\alpha = 0$, $e^{i\alpha} = 1$, $\lambda = -1$. Let $\mathbf{e} = \mathbf{e}(2;1,-1)$. By

Theorem 1 and (15) we have

$$\begin{aligned}\sqrt{2}\, e(x_1', x_2'; j') &= (-1)^{x_2'} \cdot (-1)^{j'} \cdot i \\ &= (-1)^{-x_2-1} \cdot (-1)^{3-j} \cdot i \\ &= (-1)^{x_2} \cdot (-1)^{j} \cdot i = \sqrt{2}\, e(x_1, x_2; j)\end{aligned}$$

implying that the restriction $\mathbf{e}_C(2; 1, -1)$ of $\mathbf{e}$ to V_C is an eigenvector for C, and so is the real vector $-i\mathbf{e}_C(2; 1, -1)$; $\lambda = -1$.

3) $\boldsymbol{\varrho} = (-1, 1)$. Analogously, $-i\mathbf{e}_C(2; -1, 1)$ is a real eigenvector for C, $\lambda = -1$.

4) $\boldsymbol{\varrho} = (-1, -1)$. Choose $\mu = 2$, then $\alpha = \frac{\pi}{2}$, $e^{i\alpha} = i$, $\lambda = -1$.

Let $\mathbf{e} = \mathbf{e}(2; -1, -1)$. For $j' = 1, 2$ we have

$$\begin{aligned}\sqrt{2}\, e(x_1', x_2'; j') &= (-1)^{x_1'} \cdot (-1)^{x_2'} (\mp i)^2 \\ &= (-1)^{-x_1-1} \cdot (-1)^{-x_2-1} \cdot (-1) = (-1)^{x_1} \cdot (-1)^{x_2} \cdot (\pm i)^2 \\ &= \sqrt{2}\, e(x_1, x_2; j) \quad \text{where } j = 3 - j' :\end{aligned}$$

$\mathbf{e}_C(2; -1, -1)$ is a real eigenvector for C, $\lambda = -1$.

Note that in these four cases the absolute value of all components of the eigenvectors found is the same, namely, $\frac{1}{\sqrt{2}}$.

Now assume $\boldsymbol{\varrho}$ to be non-real. Fix $\mu \in \{1, 2\}$ and consider the pair $\boldsymbol{\varrho}, \bar{\boldsymbol{\varrho}}$: for both, $\lambda = (-1)^{\mu-1} \mid 1 + \varrho_1 + \varrho_2 \mid$. By Theorem 1,

$$\mathbf{e}(\mu; \boldsymbol{\varrho}) = \{\varrho_1^{x_1} \varrho_2^{x_2} u_j(\mu; \boldsymbol{\varrho}) \mid (x_1, x_2) \in \mathbf{X}(A), j \in \{1, 2\}\}.$$

Recall from II.3: $\mathbf{u}(\mu; \boldsymbol{\varrho}) = \frac{1}{\sqrt{2}}(i^{1-\mu} e^{-i\alpha}, i^{\mu-1} e^{i\alpha})$ where $\alpha = \frac{1}{2}\varphi(\boldsymbol{\varrho}) = \frac{1}{2}\arg(1 + \varrho_1 + \varrho_2)$.

This implies
$$\begin{aligned}\overline{u_j(\mu; \boldsymbol{\varrho})} &= u_{3-j}(\mu; \boldsymbol{\varrho}) = (-1)^{\mu-1} u_j(\mu; \bar{\boldsymbol{\varrho}}), \\ \overline{\mathbf{u}(\mu; \boldsymbol{\varrho})} &= (-1)^{\mu-1} \mathbf{u}(\mu; \bar{\boldsymbol{\varrho}}), \quad \text{thus} \\ \mathbf{e}(\mu; \bar{\boldsymbol{\varrho}}) &= (-1)^{\mu-1} \overline{\mathbf{e}(\mu; \boldsymbol{\varrho})}.\end{aligned}$$

Let $c = \frac{1}{\sqrt{2}} e^{\frac{2\pi i}{\triangle} \cdot \frac{k_1+k_2}{2}}$, then $c/\bar{c} = 2c^2 = e^{\frac{2\pi i}{\triangle}(k_1+k_2)} = \varrho_1\varrho_2$, $c = \bar{c}\varrho_1\varrho_2$, $\bar{c} = c\bar{\varrho}_1\bar{\varrho}_2$. The linear combination

$$\mathbf{e}^* = c\,\mathbf{e}(\mu;\boldsymbol{\varrho}) + (-1)^{\mu-1}\bar{c}\,\mathbf{e}(\mu;\bar{\boldsymbol{\varrho}}) = c\,\mathbf{e}(\mu;\boldsymbol{\varrho}) + \bar{c}\,\overline{\mathbf{e}(\mu;\boldsymbol{\varrho})}$$

is a real eigenvector for λ, its norm is $||\mathbf{e}^*|| = ||\mathbf{e}|| = \triangle = 4rs$.

We have

$$\begin{aligned}
e^*(x_1', x_2'; j') &= c\,\varrho_1^{x_1'}\varrho_2^{x_2'} u_{j'}(\mu;\boldsymbol{\varrho}) + (-1)^{\mu-1}\bar{c}\bar{\varrho}_1{}^{x_1'}\bar{\varrho}_2{}^{x_2'} u_{j'}(\mu;\bar{\boldsymbol{\varrho}}) \\
&= c\,\varrho_1^{-x_1-1}\varrho_2^{-x_2-1}(-1)^{\mu-1}u_{3-j'}(\mu;\bar{\boldsymbol{\varrho}}) + \bar{c}\bar{\varrho}_1{}^{-x_1-1}\bar{\varrho}_2{}^{-x_2-1}u_{3-j'}(\mu;\boldsymbol{\varrho}) \\
&= c\bar{\varrho}_1\bar{\varrho}_2 \cdot \bar{\varrho}_1{}^{x_1}\bar{\varrho}_2{}^{x_2}(-1)^{\mu-1}u_j(\mu;\bar{\boldsymbol{\varrho}}) + \bar{c}\varrho_1\varrho_2 \cdot \varrho_1^{x_1}\varrho_2^{x_2}u_j(\mu;\boldsymbol{\varrho}) \\
&= (-1)^{\mu-1}\bar{c} \cdot \bar{\varrho}_1{}^{x_1}\bar{\varrho}_2{}^{x_2}u_j(\mu;\bar{\boldsymbol{\varrho}}) + c \cdot \varrho_1^{x_1}\varrho_2^{x_2}u_j(\mu;\boldsymbol{\varrho}) \\
&= e^*(x_1, x_2; j).
\end{aligned}$$

This implies that $\mathbf{e}^*_C$ is an eigenvector for C, $\lambda = (-1)^{\mu-1} \mid 1 + \varrho_1 + \varrho_2 \mid$, $\mu = 1, 2$.

Every component of the $4rs$ eigenvectors of C so found occurs exactly twice as a component of its parent; as a consequence, as the eigenvectors $\mathbf{e}, \mathbf{e}^*$ of $S(C)$ used are pairwise orthogonal, so are their offsprings $\mathbf{e}_C, \mathbf{e}^*_C$ whose common norm is half the norm of their parents, i.e., equal to $2rs$. The result:

Theorem 5. *Given the parameters r,s,t of a* $(3,6)$*–cage* C*, equations* (16) *and the procedure described above allow to write down explicitly the spectrum and a complete system of orthonormal real eigenvectors for* C*.*
In particular, the characteristic polynomial of C *is*

$$f_C(\lambda) = (\lambda - 3)(\lambda + 1)^3 \prod_{\boldsymbol{\varrho} \in \mathbb{R}^*(C)} (\lambda^2 - |1 + \varrho_1 + \varrho_2|^2)$$

where $\mathbb{R}^*(C)$ *is a complete set of non-real solutions of the basic equations for* C (see equations (16)) *such that if* $\boldsymbol{\varrho} \in \mathbb{R}^*(C)$ *then* $\bar{\boldsymbol{\varrho}} \notin \mathbb{R}^*(C)$*.*

Zero is an eigenvalue of C if and only if it is an eigenvalue of $S(C)$ (its multiplicity is $m_C(0) = \frac{1}{2}m_{S(C)}(0)$); this is the case if and only if $a_1 - a_2 = 2s \equiv 0$ and $b_1 - b_2 = -t - 3r \equiv 0, \bmod 3$ (Theorem 4). This yields

Theorem 6. *Zero is an eigenvalue of a* $(3,6)$*–cage* $[r,s,t]$*, necessarily of multiplicity 2, if and only if* $s \equiv t \equiv 0, \bmod 3$*.*

III.3 Generalization

The toroidal 6–cages having a $(3,6)$–cage as a divisor are all of a special kind: the entries of the matrices A defining them are all even. However, in [3] the concept of a $(0,3,6)$–cage, generalizing that of a $(3,6)$–cage, is defined, and it turns out that every $(0,3,6)$–cage has some toroidal 6–cage on twice as many vertices as a cover, and, conversely, every toroidal 6-cage has some $(0,3,6)$–cage on half as many vertices as a divisor. This completes and thus rounds off the investigations. The whole theory developed in the preceding sections carries over to $(0,3,6)$–cages; in particular, Fowler's conjecture generalized for $(0,3,6)$–cages (Conjecture 7.1 in [3]) can so be proved.

Concluding Remark

The methods developed in Part I immediately generalize to weighted and/or directed periodic graphs and toroidal graphs in the euclidean space of any dimension. In the case of directed graphs, the coefficients matrix of the reduced eigenvalue problem (4) need no longer be Hermitean, thus the geometric multiplicity of an eigenvalue may be smaller than its algebraic multiplicity.

Mutatis mutandis, the results also hold for the spectra and eigenvectors of graph matrices other than the adjacency matrix $\mathbb{A}$, e.g., the Laplacean $\mathbb{L} = \mathbb{D} - \mathbb{A}$ where $\mathbb{D}$ is the degree matrix.

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