

GREEN MATRICES ASSOCIATED WITH GENERALIZED LINEAR POLYOMINOES

A. Carmona, A.M. Encinas and M. Mitjana
Universitat Politècnica de Catalunya, BarcelonaTECH

Keywords: Polyominoes, Green functions, Effective resistance, Kirchhoff Index

Abstract

A Polyomino is an edge-connected union of cells in the planar square lattice. Here we consider generalized linear polyominoes; that is, the polyominoes supported by a $n \times 2$ lattice. In this paper, we obtain the Green function and the Kirchhoff index of a generalized linear polyomino as a perturbation of a $2n$ -path by adding weighted edges between opposite vertices. This approach deeply links generalized linear polyomino Green functions with the inverse M-matrix problem, and especially with the so-called Green matrices.

1 Introduction

A Polyomino is an edge-connected union of cells in the planar square lattice. Quoting [9], “Polyominoes have a long history, going back to the start of the 20th century, but they were popularized in the present era initially by Solomon Golomb, then by Martin Gardner in his *Scientific American* columns “Mathematical Games”. They now constitute one of the most popular subjects in mathematical recreations, and have found interest among mathematicians, physicists, biologists, and computer scientists as well.” Because the chemical constitution of a molecule is conventionally represented by a molecular graph or network, the polyominoes have attracted the attention of the Organic Chemistry community. So, several molecular structure descriptors based on network structural parameters have been introduced, see for instance [16]. In particular, in the last decade a great amount of work devoted to calculating the Kirchhoff index of linear polyominoes-like networks have been published, see [15] and references therein. In this work, we deal with this class of polyominoes, referred to here as generalized linear polyominoes, which besides including the most popular class of linear polyomino chains, also includes Cycles, Phenylenes and Hexagonal chains, to name only a few. Since the Kirchhoff index is the trace of the Green function of the network, see [3], here we obtain the Green function of such networks. To do this, we understand a polyomino as a perturbation of a path by adding weighted edges between opposite vertices. Therefore, unlike the techniques used in [15], which are based on the decomposition of the combinatorial Laplacian in structured

blocks, here we obtain the Green function of a linear polyomino from a perturbation of the combinatorial Laplacian. This approach deeply link linear polyomino Green functions with the inverse M -matrix problem, and especially with the so-called Green matrices, see [8].

This paper is organized as follows: Section 2 states the general expression of the Green function, the effective resistance and the Kirchhoff index of a generalized linear polyomino. In particular, explicit results are given for unicycle polyominoes including the cycle. The study of generalized linear polyominoes with link number greater than one, leads us to difference equations whose solution cannot always be expressed in a closed form. For this reason, we introduce self-complementary polyominoes in Section 3, for which the computation of the Green function involves the solution of a difference equation with constant coefficients. We conclude with the expression of the Kirchhoff index for a ladder network and a ladder-like polyomino.

The oldest class of symmetric, inverse M -matrices is the class of positive *type D* matrices defined by Markham [10]. A $s \times s$ matrix $\Sigma = (\sigma_{ij})$ is of type D if there exist real numbers $\{\sigma_i\}_{i=1}^s$, with $\sigma_s > \sigma_{s-1} > \dots > \sigma_1$, such that $\sigma_{ij} = \sigma_{\min\{i,j\}}$. In the same work, it was proved that if $\sigma_1 > 0$ then Σ^{-1} is a tridiagonal M -matrix. The matrix Σ is named of *weak type D* if there are no constrains on the parameters $\{\sigma_i\}_{i=1}^s$.

On the other hand, a $s \times s$ *flipped weak type D* matrix with parameters $\{\sigma_i\}_{i=1}^s$ is the matrix $\Sigma = (\sigma_{ij})$ whose entries satisfy $\sigma_{ij} = \sigma_{\max\{i,j\}}$. When, in addition, the parameters satisfy $\sigma_1 > \dots > \sigma_s$, then Σ is named a *flipped type D* matrix. In this work, we use the following result about flipped weak type D matrices, see [12].

Lemma 1.1 *Consider Σ the $s \times s$ flipped weak type D matrix with parameters $\sigma_1, \dots, \sigma_s$ and define $\sigma_{s+1} = 0$. Then Σ is invertible iff the parameters satisfy $\sigma_j \neq \sigma_{j+1}$, $j = 1, \dots, s$ and when this condition holds, then Σ^{-1} is the tridiagonal matrix*

$$\Sigma^{-1} = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 & \cdots & 0 & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & -\gamma_2 & \cdots & 0 & 0 \\ 0 & -\gamma_2 & \gamma_2 + \gamma_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \gamma_{s-2} + \gamma_{s-1} & -\gamma_{s-1} \\ 0 & 0 & 0 & \cdots & -\gamma_{s-1} & \gamma_{s-1} + \gamma_s \end{bmatrix},$$

where $\gamma_j = \frac{1}{\sigma_j - \sigma_{j+1}}$, $j = 1, \dots, s$. Moreover, Σ^{-1} is a Z -matrix iff Σ is an $s \times s$ flipped type D matrix and an M -matrix when, in addition $\sigma_s > 0$.

A *Green* matrix, G is defined as the Hadamard product $G = A \circ B$, of a weak type D matrix, A , and a flipped weak type D matrix, B , see [12]. If $A = (a_{\min\{i,j\}})$ and $B = (b_{\max\{i,j\}})$, then $G = (g_{ij})$ where

$$g_{ij} = \begin{cases} a_i b_j, & i \leq j, \\ a_j b_i, & i > j. \end{cases}$$

Therefore, \mathbf{G} looks like the Green function associated with a self-adjoint boundary value problem for an ordinary difference equation. Actually, a classical result by Gantmacher and Krein, see [8], states that \mathbf{G} is a nonsingular Green matrix iff \mathbf{G}^{-1} is an irreducible tridiagonal matrix; that is, the matrix associated with a Schrödinger operator in a path.

Let $\Gamma = (V, E, c)$ be a connected finite network on the vertex set V whose conductance is $c: V \times V \rightarrow [0, +\infty)$ such that $c(x, x) = 0$ for any $x \in V$ and moreover, x is adjacent to y iff $c(x, y) > 0$. The space of real valued functions on V is denoted by $\mathcal{C}(V)$ and for any $x \in V$, $\varepsilon_x \in \mathcal{C}(V)$ stands for the Dirac function at x . The standard inner product on $\mathcal{C}(V)$ is denoted by $\langle \cdot, \cdot \rangle$; that is, $\langle u, v \rangle = \sum_{x \in V} u(x)v(x)$ for each $u, v \in \mathcal{C}(V)$. A unitary and positive function is called a *weight* and we denote by $\Omega(V)$ the set of weights.

The *combinatorial Laplacian* or simply the *Laplacian* of the network Γ is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function

$$\mathcal{L}(u)(x) = \sum_{y \in V} c(x, y) (u(x) - u(y)), \quad x \in V. \quad (1)$$

It is well-known, that the Laplacian is a singular, self-adjoint and positive semi-definite operator on $\mathcal{C}(V)$ and moreover, $\mathcal{L}(u) = 0$ iff u is a constant function.

Given $q \in \mathcal{C}(V)$, the *Schrödinger operator* on Γ with *potential* q is the endomorphism of $\mathcal{C}(V)$ that assigns to each $u \in \mathcal{C}(V)$ the function $\mathcal{L}_q(u) = \mathcal{L}(u) + qu$.

If $\omega \in \Omega(V)$ is a *weight on* V , the function $q_\omega = -\frac{1}{\omega} \mathcal{L}(\omega)$ is named *the potential determined by* ω .

The Schrödinger operator \mathcal{L}_q is singular, self-adjoint and positive semi-definite operator iff there exist unique $\omega \in \Omega(V)$ such that $q = q_\omega$, see for instance [2]. Moreover, $\mathcal{L}_{q_\omega}(v) = 0$ iff $v = a\omega$, $a \in \mathbb{R}$. Therefore, \mathcal{L}_{q_ω} is an isomorphism on ω^\perp whose inverse extended to $\mathcal{C}(V)$ is denoted by \mathcal{G} and called *orthogonal Green operator* whose kernel G is called *orthogonal Green function*. In the sequel, we consider fixed the weight $\omega \in \Omega(V)$ and the corresponding Schrödinger operator \mathcal{L}_{q_ω} .

For any pair $x, y \in V$, we call ω -*dipole between* x and y the function $\tau_{xy} = \frac{\varepsilon_x}{\omega(x)} - \frac{\varepsilon_y}{\omega(y)}$. Clearly, $\tau_{xy} = -\tau_{yx}$ and moreover, $\tau_{xy} = 0$ iff $x = y$.

Given $x, y \in V$, we call *effective resistance between* x and y , with respect to ω , or simply effective resistance between x and y , the value

$$R(x, y) = \langle \mathcal{G}(\tau_{xy}), \tau_{xy} \rangle = \frac{G(x, x)}{\omega(x)^2} + \frac{G(y, y)}{\omega(y)^2} - \frac{2G(x, y)}{\omega(x)\omega(y)}. \quad (2)$$

In [3] the authors proved that the kernel $R: V \times V \rightarrow \mathbb{R}$ determines a metric on V . Moreover, for any $x, y, z \in V$ the triangular inequality $R(x, y) \leq R(x, z) + R(z, y)$ is an equality iff z separates x and y . Notice that when ω is the constant weight the effective resistance R coincides, up to a normalization factor, with the standard effective resistance.

The *Kirchhoff index, with respect to* ω , or simply the Kirchhoff index of Γ , is the value

$$\mathbf{k} = \sum_{x \in V} G(x, x) = \frac{1}{2} \sum_{x, y \in V} R(x, y)\omega^2(x)\omega^2(y), \quad (3)$$

see [2, 3].

2 Generalized Linear Polyominoes

We consider fixed a path P on $2n$ vertices, labeled as $V = \{x_1, \dots, x_{2n}\}$. The class of *generalized linear polyominoes* supported by the path P , denoted by \mathbb{L}_n , consists of all connected networks whose conductance satisfies that $c(x_i, x_{i+1}) > 0$ for $i = 1, \dots, 2n - 1$, $c(x_i, x_{2n+1-i}) \geq 0$ for any $i = 1, \dots, n - 1$ and $c(x_i, x_j) = 0$ otherwise. For the sake of simplicity we refer to generalized linear polyominoes simply as polyominoes.

Given $\Gamma \in \mathbb{L}_n$ and a weight ω on the vertex set V , we consider the positive numbers $\omega_j = \omega(x_j)$, $j = 1, \dots, 2n$ and $c_j = c(x_j, x_{j+1})$, $j = 1, \dots, 2n - 1$, and the non-negative numbers $a_j = c(x_j, x_{2n+1-j})$, $j = 1, \dots, n - 1$.

We define the *link number* of Γ as $s = |\{i = 1, \dots, n - 1 : a_i > 0\}|$. So, the link number of $\Gamma \in \mathbb{L}_n$ equals 0 iff $a_1 = \dots = a_{n-1} = 0$; that is, iff the underlying graph of Γ is nothing but the path P . On the other hand, if the link number of Γ is positive there exist indexes $1 \leq i_1 < \dots < i_s \leq n - 1$ such that $a_{i_k} > 0$ when $k = 1, \dots, s$, whereas $a_j = 0$ otherwise, see Figure 1.

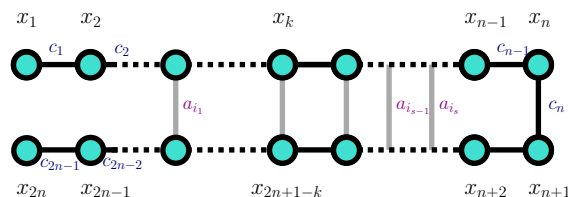


Figure 1: A Generalized Linear Polyomino

Polyominoes with link number $s = 1$ are unicycle. In particular, the $2n$ -cycle corresponds to the case $a_1 > 0$ and $a_j = 0$, $j = 2, \dots, n - 1$. A polyomino whose link number equals $n - 1$ is called a *linear polyomino chain* or *ladder* in the Graph Theory framework.

Next, we describe some examples of polyominoes with positive link number that have been considered in Organic Chemistry, see [15]. When $n = 3m$, $a_{3k-1} = 0$ for any $k = 1, \dots, m$ and $a_j > 0$, otherwise, then Γ is called *phenylene* and its link number equals $2m - 1$, see Figure 2. When $n = 2m + 1$, $a_{2k} = 0$ for any $k = 1, \dots, m$ and $a_j > 0$ otherwise, then the polyomino is called *linear hexagonal chain*, see Figure 2. When $m = 1$,

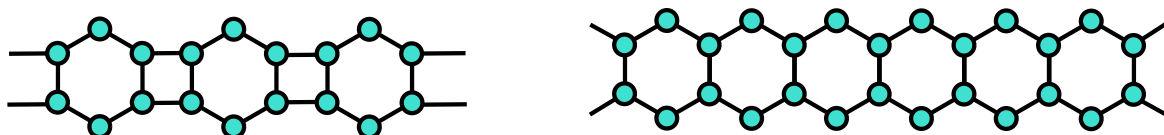


Figure 2: Phenylene (left) and hexagonal chain (right).

it is called *benzene*, whereas when $m = 2$ it is called *naphthalene*.

Given $\Gamma \in \mathbb{L}_n$, we denote its Green function as G^Γ . If Γ has positive link number s and $\{i_j\}_{j=1}^s$ is its *link sequence*, then the combinatorial Laplacian of Γ appears as the combinatorial Laplacian of the weighted path perturbed by adding for all $j = 1, \dots, s$ an edge with conductance a_{i_j} between vertices x_{i_j} and x_{2n+1-i_j} .

Consider G and R , the orthogonal Green function and the effective resistance of the path P . Since each vertex in a path is a cut vertex, we get that

$$R(x_i, x_j) = R(x_{\min\{k,i\}}, x_{\min\{k,j\}}) + R(x_{\max\{k,i\}}, x_{\max\{k,j\}}), \quad i, j, k = 1, \dots, 2n. \quad (4)$$

The authors proved in [4] that for any $i, j = 1, \dots, 2n$,

$$G(x_i, x_j) = \omega_i \omega_j \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{W_k^2}{C_k} + \sum_{k=\max\{i,j\}}^{2n-1} \frac{(1-W_k)^2}{C_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{W_k(1-W_k)}{C_k} \right],$$

where $W_j = \sum_{i=1}^j \omega_i^2$, $j = 1, \dots, 2n$, $C_k = c_k \omega_k \omega_{k+1}$, $j = 1, \dots, 2n-1$ and we use the usual convention that empty sums are defined as zero. Therefore,

$$R(x_i, x_j) = \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{C_k}, \quad i, j = 1, \dots, 2n \quad \text{and} \quad \mathbf{k} = \sum_{k=1}^{2n-1} \frac{W_k(1-W_k)}{C_k}.$$

Since we interpret a polyomino as a perturbation of the path by adding weighted edges between opposite vertices, we use [5, Theorem 3.2] to obtain the associated orthogonal Green function, the effective resistances and the Kirchhoff index of such a polyomino.

For $k = 1, \dots, s$, we consider the dipole

$$\sigma_k = \rho_k \left(\frac{\varepsilon_{x_{2n+1-i_k}}}{\omega_{2n+1-i_k}} - \frac{\varepsilon_{x_{i_k}}}{\omega_{i_k}} \right),$$

where $\rho_k = \sqrt{a_{i_k} \omega_{i_k} \omega_{2n+1-i_k}}$. Moreover, we consider the $(s \times s)$ -matrix $\Lambda = (\langle \mathcal{G}(\sigma_j), \sigma_k \rangle)$, where for any $j, k = 1, \dots, s$,

$$\begin{aligned} \langle \mathcal{G}(\sigma_j), \sigma_k \rangle &= \frac{\rho_j \rho_k}{2} \left[R(x_{2n+1-i_j}, x_{i_k}) + R(x_{i_j}, x_{2n+1-i_k}) - R(x_{2n+1-i_j}, x_{2n+1-i_k}) - R(x_{i_j}, x_{i_k}) \right] \\ &= \rho_j \rho_k R(x_{\max\{i_j, i_k\}}, x_{2n+1-\max\{i_j, i_k\}}). \end{aligned}$$

The result in [5, Theorem 3.2] establishes that matrix $\mathbf{I} + \Lambda$ is non-singular. Let \mathbf{M} be its inverse.

For any $j = 1, \dots, 2n$, we define the vector \mathbf{v}_j whose components are

$$\mathbf{v}_{jk} = \rho_k \left[R(x_{2n+1-i_k}, x_j) - R(x_{i_k}, x_j) \right], \quad k = 1, \dots, s, \quad (5)$$

and also the vector $\mathbf{u}_j = \mathbf{M} \mathbf{v}_j$. In addition, we consider the vector $\mathbf{r} = \sum_{j=1}^{2n} \omega_j^2 \mathbf{v}_j$. With this notation applying [5, Theorem 3.2], we obtain the following result.

Theorem 2.1 For any $i, j = 1, \dots, 2n$, we get that

$$G^\Gamma(x_i, x_j) = G(x_i, x_j) - \frac{\omega_i \omega_j}{4} \langle \mathbf{M}(\mathbf{r} - \mathbf{v}_i), (\mathbf{r} - \mathbf{v}_j) \rangle$$

$$R^\Gamma(x_i, x_j) = R(x_i, x_j) - \frac{1}{4} \langle (\mathbf{u}_i - \mathbf{u}_j), (\mathbf{v}_i - \mathbf{v}_j) \rangle.$$

In particular, the Kirchhoff index of the polyomino is given by

$$k^\Gamma = k + \frac{1}{4} \langle \mathbf{M}\mathbf{r}, \mathbf{r} \rangle - \frac{1}{4} \sum_{j=1}^{2n} \omega_j^2 \langle \mathbf{u}_j, \mathbf{v}_j \rangle.$$

Identity (4) allows us to give nice expressions for vectors \mathbf{v}_j and \mathbf{r} . To do this, it is useful to define for any $h = 1, \dots, n-1$, the function $\phi_h: \{1, \dots, 2n\} \rightarrow \{h, \dots, 2n+1-h\}$ given by

$$\phi_h(j) = \begin{cases} h, & 1 \leq j \leq h, \\ j, & h \leq j \leq 2n+1-h, \\ 2n+1-h, & 2n+1-h \leq j \leq 2n. \end{cases}$$

Clearly, ϕ_h is nondecreasing and moreover, given $j, k = 1, \dots, s$, we have that

$$\langle \mathcal{G}(\sigma_j), \sigma_k \rangle = \rho_j \rho_k R(x_{\phi_{i_k}(i_j)}, x_{\phi_{i_k}(2n+1-i_j)}) = \rho_j \rho_k R(x_{\phi_{i_j}(i_k)}, x_{\phi_{i_j}(2n+1-i_k)}).$$

Lemma 2.2 If for any $k = 1, \dots, s$, we have that

$$\begin{aligned} \mathbf{v}_{j,k} &= \rho_k \left[R(x_{i_k}, x_{2n+1-i_k}) - 2R(x_{i_k}, x_{\phi_{i_k}(j)}) \right], & 1 \leq j \leq n, \\ \mathbf{v}_{j,k} &= \rho_k \left[2R(x_{\phi_{i_k}(j)}, x_{2n+1-i_k}) - R(x_{i_k}, x_{2n+1-i_k}) \right], & n+1 \leq j \leq 2n, \\ \mathbf{v}_{i,k} - \mathbf{v}_{j,k} &= 2\rho_k R(x_{\phi_{i_k}(i)}, x_{\phi_{i_k}(j)}), & 1 \leq i \leq j \leq 2n. \end{aligned}$$

In particular, $-\mathbf{v}_{2n+1-i_1} = \mathbf{v}_{i_1} = \left(\rho_k R(x_{i_k}, x_{2n+1-i_k}) \right)_{k=1}^s$, $\mathbf{v}_j = \mathbf{v}_{i_1}$ and $\mathbf{v}_{2n+1-j} = \mathbf{v}_{2n+1-i_1}$

for any $1 \leq j \leq i_1$. Moreover, $\mathbf{r}_k = \rho_k \left[2 \sum_{j=i_k}^{2n-i_k} \frac{W_j}{C_j} - \sum_{j=i_k}^{2n-i_k} \frac{1}{C_j} \right]$, which in turns implies that

$$\mathbf{r}_k - \mathbf{v}_{j,k} = 2\rho_k \left[\sum_{m=i_k}^{2n-i_k} \frac{W_m}{C_m} - \sum_{m=\phi_{i_k}(j)}^{2n-i_k} \frac{1}{C_m} \right], \quad 1 \leq j \leq 2n.$$

Corollary 2.3 $R^\Gamma(x_i, x_j) \leq R(x_i, x_j)$ and the equality holds iff either $1 \leq i, j \leq i_1$ or $2n+1-i_1 \leq i, j \leq 2n$.

2.1 Unicycle polyominoes

In this section we obtain the orthogonal Green function, the effective resistance and the Kirchhoff index for unicycle polyominoes; that is, for those polyominoes whose link number equals one. Therefore if $i_1 = h$, then we add an edge with conductance $a =$

$a_h > 0$ between vertices x_h and x_{2n+1-h} . Since $s = 1$, the computation of \mathbf{M} and \mathbf{u}_j , $j = 1, \dots, 2n$, is easy, since vectors and matrices are reduced to real numbers. Defining $C_{2n} = a\omega_h\omega_{2n+1-h} = \rho_1^2$, then

$$\mathbf{I} + \mathbf{\Lambda} = \mathbf{I} + C_{2n}R(x_h, x_{2n+1-h}) = C_{2n} \left[\frac{1}{C_{2n}} + \sum_{j=h}^{2n-h} \frac{1}{C_j} \right].$$

Moreover, for any $i, j = 1, \dots, 2n$, we have the following useful version of Identity (4),

$$R(x_i, x_j) = R(x_{\min\{h,i\}}, x_{\min\{h,j\}}) + R(x_{\max\{2n+1-h,i\}}, x_{\max\{2n+1-h,j\}}) + R(x_{\phi_h(i)}, x_{\phi_h(j)}). \quad (6)$$

Proposition 2.4 *For any $i, j = 1, \dots, 2n$, we get that*

$$\begin{aligned} G^\Gamma(x_i, x_j) &= \omega_i\omega_j \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{W_k^2}{C_k} + \sum_{k=\max\{i,j\}}^{2n-1} \frac{(1-W_k)^2}{C_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{W_k(1-W_k)}{C_k} \right] \\ &\quad - \omega_i\omega_j \left[\frac{1}{C_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{C_k} \right]^{-1} \left[\sum_{k=h}^{2n-h} \frac{W_k}{C_k} - \sum_{k=\phi_h(i)}^{2n-h} \frac{1}{C_k} \right] \left[\sum_{k=h}^{2n-h} \frac{W_k}{C_k} - \sum_{k=\phi_h(j)}^{2n-h} \frac{1}{C_k} \right] \\ R^\Gamma(x_i, x_j) &= \sum_{k=\min\{h,i,j\}}^{\min\{h,\max\{i,j\}\}-1} \frac{1}{C_k} + \sum_{k=\max\{2n+1-h,\min\{i,j\}\}}^{\max\{2n+1-h,i,j\}-1} \frac{1}{C_k} \\ &\quad + \left[\frac{1}{C_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{C_k} \right]^{-1} \left[\sum_{k=\phi_h(\min\{i,j\})}^{\phi_h(\max\{i,j\})-1} \frac{1}{C_k} \right] \left[\frac{1}{C_{2n}} + \sum_{k=h}^{\phi_h(\min\{i,j\})-1} \frac{1}{C_k} + \sum_{k=\phi_h(\max\{i,j\})}^{2n-h} \frac{1}{C_k} \right]. \end{aligned}$$

In particular,

$$\begin{aligned} \mathbf{k}^\Gamma &= \sum_{k=1}^{2n} \frac{W_k(1-W_k)}{C_k} \\ &\quad + \left[\frac{1}{C_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{C_k} \right]^{-1} \left[\left[\sum_{k=h}^{2n-h} \frac{W_k}{C_k} \right]^2 - \sum_{k=h}^{2n-h} \omega_k^2 \left[\sum_{m=k}^{2n-h} \frac{1}{C_m} \right]^2 - W_{h-1} \left[\sum_{k=h}^{2n-h} \frac{1}{C_k} \right]^2 \right]. \end{aligned}$$

Proof. For any $i, j = 1, \dots, 2n$, we have

$$G^\Gamma(x_i, x_j) = G(x_i, x_j) - \frac{\mathbf{M}}{4} \omega_i\omega_j(\mathbf{r} - \mathbf{v}_i)(\mathbf{r} - \mathbf{v}_j) \quad \text{and} \quad R^\Gamma(x_i, x_j) = R(x_i, x_j) - \frac{\mathbf{M}}{4} (\mathbf{v}_i - \mathbf{v}_j)^2.$$

The expression for the Green function is a consequence of the last identity in Lemma 2.2, whereas the expression for the effective resistance appears as a consequence of the mentioned Lemma and Identity (6).

Finally, since $\mathbf{k}^\Gamma = \sum_{j=1}^{2n} G^\Gamma(x_j, x_j)$, we have

$$\mathbf{k}^\Gamma = \mathbf{k} - \left[\frac{1}{C_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{C_k} \right]^{-1} \sum_{j=1}^{2n} \omega_j^2 \left[\sum_{m=h}^{2n-h} \frac{W_m}{C_m} - \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} \right]^2.$$

On the other hand,

$$\begin{aligned}
\sum_{j=1}^{2n} \omega_j^2 \left[\sum_{m=h}^{2n-h} \frac{W_m}{C_m} - \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} \right]^2 &= \left[\sum_{m=h}^{2n-h} \frac{W_m}{C_m} \right]^2 - 2 \left[\sum_{m=h}^{2n-h} \frac{W_m}{C_m} \right] \left[\sum_{j=1}^{2n} \omega_j^2 \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} \right] \\
&\quad + \sum_{j=1}^{2n} \omega_j^2 \left[\sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} \right]^2 \\
&= W_{h-1} \left[\sum_{m=h}^{2n-h} \frac{1}{C_m} \right]^2 + \sum_{j=h}^{2n-h} \omega_j^2 \left[\sum_{m=j}^{2n-h} \frac{1}{C_m} \right]^2 - \left[\sum_{m=h}^{2n-h} \frac{W_m}{C_m} \right]^2,
\end{aligned}$$

since

$$\begin{aligned}
\sum_{j=1}^{2n} \omega_j^2 \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} &= W_h \sum_{m=h}^{2n-h} \frac{1}{C_m} + \sum_{j=h+1}^{2n-h} \omega_j^2 \sum_{m=j}^{2n-h} \frac{1}{C_m} \\
&= W_h \sum_{m=h}^{2n-h} \frac{1}{C_m} + \sum_{m=h+1}^{2n-h} \frac{1}{C_m} \sum_{j=h+1}^m \omega_j^2 = \sum_{m=h}^{2n-h} \frac{W_m}{C_m}, \\
\sum_{j=1}^{2n} \omega_j^2 \left[\sum_{m=\phi_h(j)}^{2n-h} \frac{1}{C_m} \right]^2 &= W_{h-1} \left[\sum_{m=h}^{2n-h} \frac{1}{C_m} \right]^2 + \sum_{j=h}^{2n-h} \omega_j^2 \left[\sum_{m=j}^{2n-h} \frac{1}{C_m} \right]^2
\end{aligned}$$

and hence, the expression for the Kirchhoff index follows. \square

Next, we particularize the above theorem to $h = 1$ that corresponds to the $2n$ -cycle. Although the case of cycles with constant weight and conductances is well-known, see for instance [6], as far as authors' knowledge, this is the first time that the orthogonal Green function for a weighted cycle is obtained.

Corollary 2.5 *The Green function and the effective resistance with respect to the weight ω for the weighted $2n$ -cycle are given by*

$$\begin{aligned}
G^\Gamma(x_i, x_j) &= \omega_i \omega_j \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{W_k^2}{C_k} + \sum_{k=\max\{i,j\}}^{2n} \frac{(1-W_k)^2}{C_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{W_k(1-W_k)}{C_k} \right] \\
&\quad - \omega_i \omega_j \left[\sum_{k=1}^{2n} \frac{1}{C_k} \right]^{-1} \left[\sum_{k=1}^{2n} \frac{W_k}{C_k} - \sum_{k=i}^{2n} \frac{1}{C_k} \right] \left[\sum_{k=1}^{2n} \frac{W_k}{C_k} - \sum_{k=j}^{2n} \frac{1}{C_k} \right], \\
R^\Gamma(x_i, x_j) &= \left[\sum_{k=1}^{2n} \frac{1}{C_k} \right]^{-1} \left[\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{C_k} \right] \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{1}{C_k} + \sum_{k=\max\{i,j\}}^{2n} \frac{1}{C_k} \right].
\end{aligned}$$

Moreover the Kirchhoff index is given by

$$\kappa^\Gamma = \sum_{k=1}^{2n} \frac{W_k(1-W_k)}{C_k} + \left[\sum_{k=1}^{2n} \frac{1}{C_k} \right]^{-1} \left[\left[\sum_{k=1}^{2n-1} \frac{W_k}{C_k} \right]^2 - \sum_{j=1}^{2n-1} \omega_j^2 \left[\sum_{k=j}^{2n-1} \frac{1}{C_k} \right]^2 \right].$$

The case in which the weight ω is constant; that is, $\omega_j = \sqrt{\frac{1}{2n}}$ is given in the following result.

Corollary 2.6 *The Green function and the effective resistance with respect to the constant weight for the weighted $2n$ -cycle are given by*

$$G^\Gamma(x_i, x_j) = \frac{1}{4n^2} \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{k^2}{c_k} + \sum_{k=\max\{i,j\}}^{2n} \frac{(2n-k)^2}{c_k} - \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{k(2n-k)}{c_k} \right]$$

$$- \frac{1}{4n^2} \left[\sum_{k=1}^{2n} \frac{1}{c_k} \right]^{-1} \left[\sum_{k=1}^{2n} \frac{k}{c_k} - \sum_{k=i}^{2n} \frac{2n}{c_k} \right] \left[\sum_{k=1}^{2n} \frac{k}{c_k} - \sum_{k=j}^{2n} \frac{2n}{c_k} \right],$$

$$R^\Gamma(x_i, x_j) = 2n \left[\sum_{k=1}^{2n} \frac{1}{c_k} \right]^{-1} \left[\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_k} \right] \left[\sum_{k=1}^{\min\{i,j\}-1} \frac{1}{c_k} + \sum_{k=\max\{i,j\}}^{2n} \frac{1}{c_k} \right].$$

Moreover, the Kirchhoff index is

$$k^\Gamma = \frac{1}{2n} \sum_{k=1}^{2n} \frac{k(2n-k)}{c_k} + \frac{1}{2n} \left[\sum_{k=1}^{2n} \frac{1}{c_k} \right]^{-1} \left[\left(\sum_{k=1}^{2n-1} \frac{k}{c_k} \right)^2 - 2n \sum_{j=1}^{2n-1} \left(\sum_{k=j}^{2n-1} \frac{1}{c_k} \right)^2 \right].$$

In particular, if $c_k = c$ for all $k = 1, \dots, 2n-1$ we get that

$$G^\Gamma(x_i, x_j) = \frac{1}{12nc} \left[(2n+1)(4n+1) + 3(i(i-2n-1) + j(j-2n-1) - 2n|i-j|) \right]$$

$$- \frac{a}{4c[c+a(2n-1)]} [2(n-i)+1][2(n-j)+1],$$

$$R^\Gamma(x_i, x_j) = \frac{2n|i-j|}{[c+a(2n-1)]} (c+a(2n-1-|i-j|)),$$

and hence,

$$k^\Gamma = \frac{(4n^2-1)(c+a(n-1))}{6c(c+a(2n-1))}.$$

The last expression, when $a = c$, coincides with the one obtained in [6].

2.2 Polyominoes with link number greater than one

Assume now that $s \geq 2$. If D is the $(s \times s)$ -diagonal matrix whose entries are given by ρ_1, \dots, ρ_s , then $D^{-1}MD^{-1} = D^{-2} + R$, where

$$R = \begin{bmatrix} R(x_{i_1}, x_{2n+1-i_1}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ R(x_{i_2}, x_{2n+1-i_2}) & R(x_{i_2}, x_{2n+1-i_2}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \\ \vdots & \vdots & \ddots & \vdots \\ R(x_{i_s}, x_{2n+1-i_s}) & R(x_{i_s}, x_{2n+1-i_s}) & \cdots & R(x_{i_s}, x_{2n+1-i_s}) \end{bmatrix}.$$

Thus, R is a $s \times s$ flipped type D matrix with parameters $\{R(x_{i_k}, x_{2n+1-i_k})\}_{k=1}^s$, since $R(x_1, x_{2n+1-1}) > \dots > R(x_{n-1}, x_{n+1})$. Therefore, from Lemma 1.1, R^{-1} is a tridiagonal M -matrix; that is, a positive definite Schrödinger operator on a path with s vertices, where

$$\gamma_k = \frac{1}{R(x_{i_k}, x_{i_{k+1}}) + R(x_{2n+1-i_{k+1}}, x_{2n+1-i_k})}, \quad k = 1, \dots, s-1 \quad \text{and} \quad \gamma_s = \frac{1}{R(x_{i_s}, x_{2n+1-i_s})}.$$

In consequence, $R^{-1}D^{-1}MD^{-1} = R^{-1}D^{-2} + I$ and hence $R^{-1}D^{-1}MD = R^{-1} + D^2$. So, $R^{-1} + D^2$ is an strictly diagonally dominant tridiagonal M -matrix and hence it is invertible and moreover $(R^{-1} + D^2)^{-1} > 0$. In addition,

$$M^{-1} = D[R^{-1} + D^2]^{-1}R^{-1}D^{-1} = D[I - (R^{-1} + D^2)^{-1}D^2]D^{-1} = I - D(R^{-1} + D^2)^{-1}D$$

and we only need to calculate $(R^{-1} + D^2)^{-1}$.

When $s = 2$, then

$$(R^{-1} + D^2)^{-1} = \frac{1}{(\rho_1^2 + \gamma_1)(\rho_2^2 + \gamma_2) + \rho_1^2\gamma_1} \begin{bmatrix} \rho_2^2 + \gamma_1 + \gamma_2 & \gamma_1 \\ \gamma_1 & \rho_1^2 + \gamma_1 \end{bmatrix}. \quad (7)$$

When $s \geq 3$, $R^{-1} + D^2$ is a tridiagonal matrix and hence we could compute its inverse by applying the specific techniques for this class of matrices, see for instance [13, 14]. Alternatively, we apply the usual techniques for discrete boundary value problems, see [1, 7]. Specifically, we have the following result expressing the entries of $R^{-1} + D^2$ in terms of two solutions of a difference equations. In particular, we obtain that $R^{-1} + D^2$ is a Green matrix as Gantmacher & Krein's theorem assures.

First, observe that the invertibility of $R^{-1} + D^2$ implies that if a sequence $\{z_i\}_{i=1}^s$ satisfies

$$(\rho_i^2 + \gamma_{i-1} + \gamma_i)z_i - \gamma_{i-1}z_{i-1} - \gamma_i z_{i+1} = 0, \quad i = 2, \dots, s-1, \quad (8)$$

and $(\rho_1^2 + \gamma_1)z_1 - \gamma_1 z_2 = (\rho_s^2 + \gamma_s + \gamma_{s-1})z_s - \gamma_{s-1}z_{s-1} = 0$, then $z_i = 0$, for any $i = 1, \dots, s$. Moreover, we have the following result about linearly independent solutions of the above difference equation.

Lemma 2.7 *If two sequences $\{z_i^k\}_{i=1}^s$, $k = 1, 2$, satisfy*

$$(\rho_i^2 + \gamma_{i-1} + \gamma_i)z_i^k - \gamma_{i-1}z_{i-1}^k - \gamma_i z_{i+1}^k = 0, \quad i = 2, \dots, s-1,$$

then $\gamma_j[z_j^1 z_{j+1}^2 - z_{j+1}^1 z_j^2]$ is constant for $j = 1, \dots, s-1$. In addition, the constant is null iff there exist $\alpha, \beta \in \mathbb{R}$ such that $|\alpha| + |\beta| > 0$ and $\alpha z_j^1 + \beta z_j^2 = 0$ for any $j = 1, \dots, s$.

Proposition 2.8 *Consider $\{u_j\}_{j=1}^s$ and $\{v_j\}_{j=1}^s$ the solutions of (8) characterized by satisfying the initial conditions*

$$u_1 = \gamma_1, \quad u_2 = \rho_1^2 + \gamma_1$$

and the final conditions

$$v_{s-1} = \rho_s^2 + \gamma_s + \gamma_{s-1}, \quad v_s = \gamma_{s-1},$$

respectively. Then,

$$\gamma_{s-1}u_{s-1} - (\rho_s^2 + \gamma_s + \gamma_{s-1})u_s = \frac{\gamma_1}{\gamma_{s-1}}[\gamma_1v_2 - (\rho_1^2 + \gamma_1)v_1] \neq 0,$$

and moreover,

$$b_{ij} = \delta_{ij} - \frac{\rho_i\rho_j}{\gamma_1((\rho_1^2 + \gamma_1)v_1 - \gamma_1v_2)} u_{\min\{i,j\}}v_{\max\{i,j\}}, \quad i, j = 1, \dots, s,$$

where $\mathbf{M} = (b_{ij})$.

Proof. From Lemma (2.7) we know that $\gamma_j[u_jv_{j+1} - u_{j+1}v_j]$ is constant, which implies that

$$\gamma_1[\gamma_1v_2 - (\rho_1^2 + \gamma_1)v_1] = \gamma_{s-1}[\gamma_{s-1}u_{s-1} - (\rho_s^2 + \gamma_s + \gamma_{s-1})u_s].$$

To obtain the entries of $(\mathbf{R}^{-1} + \mathbf{D}^2)^{-1}$, first observe that given $f_1, \dots, f_s \in \mathbb{R}$, a sequence $\{z_i\}_{i=1}^s$ is a solution of the difference equation

$$(\rho_i^2 + \gamma_{i-1} + \gamma_i)z_i - \gamma_{i-1}z_{i-1} - \gamma_iz_{i+1} = f_i, \quad i = 2, \dots, s-1,$$

iff there exists $\alpha, \beta \in \mathbb{R}$ such that

$$z_i = \alpha u_i + \beta v_i + \frac{1}{\gamma_1(\gamma_1v_2 - (\rho_1^2 + \gamma_1)v_1)} \sum_{k=2}^i [u_iv_k - v_iu_k]f_k, \quad i = 1, \dots, s.$$

In addition, the sequence verifies that

$$(\rho_1^2 + \gamma_1)z_1 - \gamma_1z_2 = f_1 \quad \text{and} \quad (\rho_s^2 + \gamma_s + \gamma_{s-1})z_s - \gamma_{s-1}z_{s-1} = f_s,$$

iff

$$\alpha = \frac{-1}{\gamma_1(\gamma_1v_2 - (\rho_1^2 + \gamma_1)v_1)} \left[\gamma_{s-1}f_s + \sum_{k=2}^{s-1} v_k f_k \right] \quad \text{and} \quad \beta = \frac{f_1}{(\rho_1^2 + \gamma_1)v_1 - \gamma_1v_2}.$$

Therefore, the entries of $(\mathbf{R}^{-1} + \mathbf{D}^2)^{-1}$ are easily obtained choosing for any $j = 1, \dots, s$ the values $f_k = 0$ when $k \neq j$ and $f_j = 1$. \square

Observe that when $s = 2$, if we consider u_1, u_2, v_1, v_2 defined as

$$u_1 = \gamma_1, \quad u_2 = \rho_1^2 + \gamma_1, \quad v_1 = \rho_2^2 + \gamma_2 + \gamma_1, \quad v_2 = \gamma_1,$$

then

$$(\rho_1^2 + \gamma_1)v_1 - \gamma_1v_2 = (\rho_1^2 + \gamma_1)(\rho_2^2 + \gamma_2) + \rho_1^2\gamma_1$$

which, in view of Identity (7), implies that the entries of $(\mathbf{R}^{-1} + \mathbf{D}^2)^{-1}$ are given by

$$\frac{1}{\gamma_1((\rho_1^2 + \gamma_1)v_1 - \gamma_1v_2)} u_{\min\{i,j\}}v_{\max\{i,j\}}, \quad i, j = 1, 2.$$

Therefore, the result of the above proposition is also true for $s = 2$.

The above proposition shows that the computation of the Green function, the effective resistances and the Kirchhoff index for a polyomino with link number greater than two, involves the solution of a difference equation whose coefficients are completely determined by the effective resistances of the path. However, it is not always possible to find a closed form for the solutions of such a linear difference equation. In addition, the computation of vectors u_j , $j = 1, \dots, 2n$ is, in general, very involved.

3 Self-complementary Polyominoes

In this section, we introduce a family of polyominoes for which the above-mentioned computation can be carried out in a simple way, since we impose some symmetry constraints.

Observe that from Lemma (2.2) when $1 \leq j \leq i_1$, we have that $\mathbf{v}_{j,k} + \mathbf{v}_{2n+1-j,k} = 0$, whereas when $i_1 \leq j \leq n$ we have

$$\mathbf{v}_{j,k} + \mathbf{v}_{2n+1-j,k} = 2\rho_k \left[R(x_{2n+1-i_k}, x_{2n+1-j}) - R(x_{i_k}, x_j) \right].$$

So, if the path satisfies that $R(x_{2n+1-i}, x_{2n+1-j}) = R(x_i, x_j)$ for any $i, j = 1, \dots, n$, then for any polyomino supported by the path, we have that $\mathbf{v}_{2n+1-j} = -\mathbf{v}_j$, $j = 1, \dots, n$, which implies that $\mathbf{u}_{2n+1-j} = -\mathbf{u}_j$, $j = 1, \dots, n$.

The underlying weighted path is called *symmetric* if it satisfies that $c_{2n-j} = c_j$ and moreover $\omega_{2n+1-j} = \omega_j$ for any $j = 1, \dots, n$. In this case, for any $k = 1, \dots, 2n-1$ we have

$$\begin{aligned} C_{2n-k} &= c_{2n-k} \omega_{2n+1-k} \omega_{2n-k} = c_k \omega_k \omega_{k+1} = C_k, \\ W_{2n-k} &= \sum_{j=1}^{2n-k} \omega_j^2 = \sum_{j=1}^{2n-k} \omega_{2n+1-j}^2 = \sum_{j=k+1}^{2n} \omega_j^2 = 1 - W_k, \end{aligned}$$

which, in particular, implies that $W_n = \frac{1}{2}$.

Proposition 3.1 *If the path is symmetric, then*

$$G(x_i, x_{2n+1-j}) = G(x_{2n+1-i}, x_j) \quad \text{and} \quad R(x_i, x_{2n+1-j}) = R(x_{2n+1-i}, x_j), \quad i, j = 1, \dots, 2n.$$

In addition, $\mathbf{k} = 2 \sum_{k=1}^{n-1} \frac{W_k W_{2n-k}}{C_k} + \frac{1}{4C_n}$.

Corollary 3.2 *If the path is symmetric, then $\mathbf{v}_{2n+1-j} = -\mathbf{v}_j$, $\mathbf{u}_{2n+1-j} = -\mathbf{u}_j$, for any $j = 1, \dots, n$ and hence, $\mathbf{r} = \mathbf{0}$. Therefore for any $i, j = 1, \dots, n$,*

$$G^\Gamma(x_i, x_j) = G^\Gamma(x_{2n+1-i}, x_{2n+1-j}) = G(x_i, x_j) - \frac{\omega_i \omega_j}{4} \langle \mathbf{u}_i, \mathbf{v}_j \rangle,$$

$$G^\Gamma(x_i, x_{2n+1-j}) = G^\Gamma(x_{2n+1-i}, x_j) = G(x_i, x_{2n+1-j}) + \frac{\omega_i \omega_j}{4} \langle \mathbf{u}_i, \mathbf{v}_j \rangle,$$

$$R^\Gamma(x_i, x_j) = R^\Gamma(x_{2n+1-i}, x_{2n+1-j}) = R(x_i, x_j) - \frac{1}{4} \left[\langle \mathbf{u}_i, \mathbf{v}_i \rangle + \langle \mathbf{u}_j, \mathbf{v}_j \rangle - 2\langle \mathbf{u}_i, \mathbf{v}_j \rangle \right],$$

$$R^\Gamma(x_i, x_{2n+1-j}) = R^\Gamma(x_{2n+1-i}, x_j) = R(x_i, x_{2n+1-j}) - \frac{1}{4} \left[\langle \mathbf{u}_i, \mathbf{v}_i \rangle + \langle \mathbf{u}_j, \mathbf{v}_j \rangle + 2\langle \mathbf{u}_i, \mathbf{v}_j \rangle \right].$$

Moreover, $\mathbf{k}^\Gamma = 2 \sum_{k=1}^{n-1} \frac{W_k W_{2n-k}}{C_k} + \frac{1}{4C_n} - \frac{1}{2} \sum_{j=1}^n \omega_j^2 \langle \mathbf{u}_j, \mathbf{v}_j \rangle$.

Notice that to compute the Green function and the effective resistance for a polyomino supported by a symmetric path it suffices to obtain the values $\langle \mathbf{u}_i, \mathbf{v}_j \rangle$ for any $i, j = 1, \dots, n$. Therefore, the key is to solve the difference equation (8). Observe that the symmetry of the path implies that $\gamma_k = \frac{1}{2R(x_{i_k}, x_{i_{k+1}})}$ for any $k = 1, \dots, s-1$, but in general it remains very hard to obtain a closed expression for the solution of the difference equation. Next, we introduce a family of polyominoes whose associated difference equation has constant coefficients.

A polyomino is called *self-complementary* if it is supported by a symmetric path and there exists $d > 0$ and $\mu > 0$ such that

- (i) $d = a_{i_k} \omega_{i_k}^2$, for any $k = 2, \dots, s$.
- (ii) $\mu = \sum_{j=i_k}^{i_{k+1}-1} \frac{1}{C_j}$, for any $k = 1, \dots, s-1$.

Clearly, any polyomino supported by a symmetric path and with link number $s \leq 2$ is self-complementary, so this definition is relevant for polyominoes with link number $s \geq 3$. In this case, $\rho_k = \sqrt{d}$, $k = 1, \dots, s$, $\gamma_k = \frac{1}{2\mu}$, $k = 1, \dots, s-1$ and hence the difference equation (8) is

$$\left(d + \frac{1}{\mu}\right) z_i - \frac{1}{2\mu} z_{i+1} - \frac{1}{2\mu} z_{i-1} = 0, \quad i = 2, \dots, s-1,$$

or, in an equivalent manner, if $q = 1 + d\mu$,

$$z_{i+1} = 2qz_i - z_{i-1}, \quad i = 2, \dots, s-1,$$

which is a *Chebyshev recurrence*. Therefore, its solutions can be expressed in the form $z_i = \alpha U_{i-2}(q) + \beta U_{i-1}(q)$, or alternatively of the form $z_i = \alpha U_{s-1-i}(q) + \beta U_{s-i}(q)$, where U_i is the i -th Chebyshev polynomial of second kind, see [1]. Therefore, if V_i denotes the i -th Chebyshev polynomial of third kind; that is, $V_i = U_i - U_{i-1}$, with the notations of Proposition 2.8, we get that

$$u_i = \gamma_1 V_{i-1}(q) + (\rho_1^2 - d) U_{i-2}(q) \quad \text{and} \quad v_i = \gamma_1 V_{s-i}(q) + \gamma_s U_{s-i-1}(q), \quad i = 1, \dots, s$$

and hence, for any $i, j = 1, \dots, s$,

$$b_{11} = 1 - \frac{\rho_1^2 \left[V_{s-1}(q) + 2\mu\gamma_s U_{s-2}(q) \right]}{\rho_1^2 U_{s-1}(q) + \gamma_s V_{s-1}(q) + (\rho_1^2 - d)(2\mu\gamma_s - 1) U_{s-2}(q)}$$

$$b_{1j} = b_{j1} = - \frac{\rho_1 \sqrt{d} \left[V_{s-j}(q) + 2\mu\gamma_s U_{s-1-j}(q) \right]}{\rho_1^2 U_{s-1}(q) + \gamma_s V_{s-1}(q) + (\rho_1^2 - d)(2\mu\gamma_s - 1) U_{s-2}(q)}$$

for any $j = 2, \dots, s$ and

$$b_{ij} = \delta_{ij} - \frac{d \left[V_{\min\{i,j\}-1}(q) + 2\mu(\rho_1^2 - d) U_{\min\{i,j\}-2}(q) \right] \left[V_{s-\max\{i,j\}}(q) + 2\mu\gamma_s U_{s-1-\max\{i,j\}}(q) \right]}{\rho_1^2 U_{s-1}(q) + \gamma_s V_{s-1}(q) + (\rho_1^2 - d)(2\mu\gamma_s - 1) U_{s-2}(q)}$$

for any $i, j = 2, \dots, s$.

Notice that if we take $s = 1$ in the above formulae, then taking into account that $U_{-1}(q) = 0$ and $U_0(q) = V_0(q) = 1$, we obtain

$$b_{11} = 1 - \frac{\rho_1^2}{\rho_1^2 + \gamma_1} = \frac{\gamma_1}{\rho_1^2 + \gamma_1} = \frac{1}{1 + \rho_1^2 \gamma_1^{-1}} = \frac{1}{1 + \rho_1^2 R(x_h, x_{2n+1-h})}$$

and hence, the above expression for the entries of \mathbf{M} is valid for all $1 \leq s \leq n - 1$.

We finish this paper by studying a very particular family of self-complementary polyominoes.

3.1 Ladder-like Polyominoes

In this section we compute the Green function, the effective resistance and the Kirchhoff index for those polyominoes built by adding $1 \leq s \leq n - h$ consecutive edges from vertex x_h with the same conductance $a > 0$, to the path with constant conductance $c > 0$. Specifically, assume that $\omega_j = \sqrt{\frac{1}{2n}}$, $j = 1, \dots, 2n$ and $c_j = c > 0$, $j = 1, \dots, 2n - 1$, which implies that the path is symmetric,

$$G(x_i, x_j) = \frac{1}{12nc} \left[(2n+1)(4n+1) + 3 \left(i(i-2n-1) + j(j-2n-1) - 2n|i-j| \right) \right]$$

and hence, $k = \frac{1}{6c}(4n^2 - 1)$ and $R(x_i, x_j) = \frac{2n}{c} |i - j|$ for any $i, j = 1, \dots, 2n$. Moreover, $i_k = h + k - 1$, $a_{i_k} = a > 0$ and $\rho_k = \sqrt{\frac{a}{2n}}$, $k = 1, \dots, s$.

We call this class of self-complementary polyominoes *ladder-like polyominoes* (see Figure 3) since when $s = n - 1$ the corresponding polyomino is nothing else but a ladder

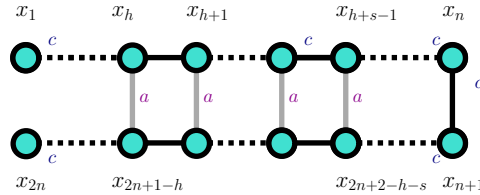


Figure 3: A Ladder-like Polyomino

network. Associated with the ladder-like polyomino located at vertex x_h and with link number $1 \leq s \leq n - h$, we define

$$Q_k(q) = \begin{cases} (2(n-h-s)+1)V_k(q) + 2U_k(q), & k \geq 0, \\ 2(n-h-s+k) + 3 & k \leq 0. \end{cases}$$

Observe that $Q_0(q)$ is defined unambiguously, since $V_0(q) = U_0(q) = 1$. Moreover, it is clear that $\{Q_k(q)\}_{k \geq 0}$ is a Chebyshev sequence. In addition, taking into account that $V_k(1) = 1$ and $U_k(1) = k + 1$ for any $k \in \mathbb{Z}$, then

$$Q_k(q) = (2(n-h-s)+1)V_k(1) + 2U_k(1), \quad \text{for any } k \leq 0,$$

which implies that $\{Q_k(q)\}_{k \leq 0}$ is also a Chebyshev sequence.

From the expression for products of Chebyshev polynomials, see [11, Chapter 2], we deduce the following useful results.

Lemma 3.3 *For any $1 \leq m \leq s+1$ we have*

$$aQ_{s-m}(q)U_{m-1}(q) + \frac{c}{2}V_{m-1}(q) \left[Q_{s-m}(q) - Q_{s-m-1}(q) \right] = cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q).$$

Moreover, if for any $k \in \mathbb{Z}$, T_k and W_k denote the k -th Chebyshev polynomial of first and fourth kind, respectively; that is $W_k(q) = U_k(q) + U_{k-1}(q)$, then

$$\sum_{m=1}^s V_{m-1}(q)Q_{s-m}(q) = \frac{c}{a+2c} \left[s(2(n-h-s)+1)T_s(q) + sW_s(q) + 2(n-h-s+1)U_{s-1}(q) \right].$$

The parameters of the ladder-like polyomino are $\rho_1^2 = d = \frac{a}{2n}$, $\mu = \frac{2n}{c}$, $q = 1 + \frac{a}{c}$, $\gamma_s = \frac{c}{2n[2(n-s-h)+3]}$ and moreover $\gamma_1 = \frac{c}{4n}$ when $s \geq 2$. Therefore, when $s \geq 2$, applying Proposition 2.8

$$u_i = \frac{c}{4n} V_{i-1}(q) \quad \text{and} \quad v_i = \frac{c}{4n(2(n-s-h)+3)} Q_{s-i}(q), \quad \text{for any } i = 1, \dots, s.$$

Moreover, since $2aU_{s-1}(q) + cV_{s-1}(q) = cV_s(q)$, we get that

$$\rho_1^2 U_{s-1}(q) + \gamma_s V_{s-1}(q) = \frac{1}{2n(2(n-s-h)+3)} \left[cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q) \right]$$

and hence,

$$b_{ij} = \delta_{ij} - \frac{aV_{\min\{i,j\}-1}(q)Q_{s-\max\{i,j\}}(q)}{cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q)} \quad (9)$$

for any $i, j = 1, \dots, s$. Recall that Formula (9), is also valid when $s = 1$.

To obtain the Green function, the effective resistances and the Kirchhoff index of a ladder-like polyomino, we only need to obtain the vectors $\mathbf{v}_j, \mathbf{u}_j$, $j = 1, \dots, n$ and their inner products. To do this we use the following property for the sum of Chebyshev polynomials, see for instance [11].

Lemma 3.4 *If $\{P_k\}_{k=0}^\infty$ is a Chebyshev sequence, given $S(k) = \alpha k + \beta$, where $\alpha, \beta \in \mathbb{R}$, and $r, t \in \mathbb{N}^*$ such that $t \leq r$ then,*

$$\sum_{k=t}^r S(k)P_k(q) = \frac{c}{2a} \left[S(r)(P_{r+1}(q) - P_r(q)) - S(t)(P_t(q) - P_{t-1}(q)) + \alpha(P_t(q) - P_r(q)) \right].$$

Proposition 3.5 *It is satisfied that $\mathbf{v}_j = \mathbf{v}_h$ and hence $\mathbf{u}_j = \mathbf{u}_h$, $j = 1, \dots, h$. Moreover, for any $j = 1, \dots, n$ and any $m = 1, \dots, s$, we get that*

$$\begin{aligned} \mathbf{v}_{j,m} &= \frac{\sqrt{2na}}{c} \left(2(n - \phi_{h+m-1}(j)) + 1 \right), \\ \mathbf{u}_{j,m} &= \frac{\sqrt{2na}V_{\min\{\phi_h(j)-h,m-1\}}(q)Q_{s-1-\max\{\phi_h(j)-h,m-1\}}(q)}{cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q)}. \end{aligned}$$

Proof. Given $j = 1, \dots, n$ and $m = 1, \dots, s$, from Lemma 2.2 we have

$$\mathbf{v}_{j,m} = \frac{\sqrt{2na}}{c} \left[2n + 1 - 2i_m - 2[\phi_{i_m}(j) - i_m] \right] = \frac{\sqrt{2na}}{c} \left[2(n - \phi_{i_m}(j)) + 1 \right],$$

and the expression for $\mathbf{v}_{j,m}$ follows bearing in mind that $i_m = h + m - 1$.

Since $\mathbf{u}_j = M\mathbf{v}_j$, if we consider $K = \frac{\sqrt{2na}}{c[cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q)]}$, then for $m = 1, \dots, s$, we have that

$$\begin{aligned} \mathbf{u}_{j,m} &= \frac{\sqrt{2na}}{c} \left(2(n - \phi_{h+m-1}(j)) + 1 \right) - aKQ_{s-m}(q) \sum_{k=1}^m V_{k-1}(q) \left(2(n - \phi_{h+k-1}(j)) + 1 \right) \\ &\quad - aKV_{m-1}(q) \sum_{k=m+1}^s Q_{s-k}(q) \left(2(n - \phi_{h+k-1}(j)) + 1 \right). \end{aligned}$$

When $h \leq j \leq h + s - 1$, then $\phi_{h+k-1}(j) = j$ if $1 \leq k \leq j + 1 - h$, whereas $\phi_{h+k-1}(j) = h + k - 1$ if $j + 1 - h < k \leq s$. Therefore, when $1 \leq m \leq j + 1 - h$, we get

$$\begin{aligned} \mathbf{u}_{j,m} &= \frac{\sqrt{2na}}{c} (2(n - j) + 1) - aK(2(n - j) + 1)Q_{s-m}(q) \sum_{k=1}^m V_{k-1}(q) \\ &\quad - aKV_{m-1}(q) \left[(2(n - j) + 1) \sum_{k=m+1}^{j+1-h} Q_{s-k}(q) + \sum_{k=j+2-h}^s Q_{s-k}(q) (2(n - h - k) + 3) \right]. \end{aligned}$$

Applying Lemma 3.4, we get that

$$\begin{aligned} \sum_{k=1}^m V_{k-1}(q) &= U_{m-1}(q), \\ \sum_{k=m+1}^{j+1-h} Q_{s-k}(q) &= \frac{c}{2a} \left[Q_{s+h-2-j}(q) - Q_{s+h-1-j}(q) + Q_{s-m} - Q_{s-1-m} \right], \\ \sum_{k=j+2-h}^s Q_{s-k}(q) (2(n - h - k) + 3) &= \frac{c}{2a} (2(n - j) + 1) \left[Q_{s+h-1-j}(q) - Q_{s+h-2-j}(q) \right] \\ &\quad - \frac{c}{a} Q_{s+h-1-j}(q) \end{aligned}$$

In addition, applying Lemma 3.3, we obtain that

$$\mathbf{u}_{j,m} = cKV_{m-1}(q)Q_{s+h-1-j}(q).$$

The remaining cases follow by similar reasonings. □

Corollary 3.6 *Given $1 \leq i, j \leq n$, then*

$$\langle \mathbf{u}_i, \mathbf{v}_j \rangle = \frac{2na(2(n-i)+1)(2(n-j)+1)U_{s-1}(q)}{c[cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q)]}$$

when $h + s \leq i, j \leq n$, whereas

$$\langle \mathbf{u}_i, \mathbf{v}_j \rangle = \frac{2n}{c} \left[(2(n - \phi_h(\max\{i, j\})) + 1) - \frac{cV_{\phi_h(\min\{i, j\})-h}(q)Q_{s-1+h-\phi_h(\max\{i, j\})}(q)}{cV_s(q) + a(2(n-s-h)+1)U_{s-1}(q)} \right],$$

otherwise.

The expression for the Green function and the effective resistance for a ladder-like polyomino can be easily obtained from Corollary 3.2 by substituting the value of $\langle \mathbf{u}_i, \mathbf{v}_j \rangle$ just obtained.

Proposition 3.7 *The Kirchhoff index of the ladder-like polyomino is*

$$\begin{aligned} k^\Gamma &= \frac{(4n^2 - 1)}{6c} - \frac{1}{2c} [(h + s - 1)(2(n - h) + 1) - s(s - 1)] \\ &+ \frac{(n - h - s + 1) \left[6c^2 - a(a + 2c)(2(n - h - s) + 1)(2(n - h - s) + 3) \right]}{6c(a + 2c) [cV_s(q) + a(2(n - h - s) + 1)U_{s-1}(q)]} U_{s-1}(q) \\ &+ \frac{\left[(h - 1)(a + 2c)Q_{s-1}(q) + cs[(2(n - h - s) + 1)T_s(q) + W_s(q)] \right]}{2(a + 2c) [cV_s(q) + a(2(n - h - s) + 1)U_{s-1}(q)]} \end{aligned}$$

Proof. First, we have

$$\begin{aligned} \sum_{j=h+s}^n \langle \mathbf{u}_j, \mathbf{v}_j \rangle &= \frac{2na}{c\alpha} U_{s-1}(q) \sum_{j=h+s}^n (2(n - j) + 1)^2 \\ &= \frac{2na}{3c\alpha} U_{s-1}(q) (n - h - s + 1)(2(n - h - s) + 1)(2(n - h - s) + 3), \end{aligned}$$

whereas

$$\sum_{j=1}^{h+s-1} \langle \mathbf{u}_j, \mathbf{v}_j \rangle = \frac{2n}{c} \sum_{j=1}^{h+s-1} \left[(2(n - \phi_h(j)) + 1) - \frac{cV_{\phi_h(j)-h}(q)Q_{s-1+h-\phi_h(j)}(q)}{cV_s(q) + a(2(n - s - h) + 1)U_{s-1}(q)} \right].$$

Moreover,

$$\begin{aligned} \sum_{j=1}^{h+s-1} (2(n - \phi_h(j)) + 1) &= (h - 1)(2(n - h) + 1) + \sum_{j=h}^{h+s-1} (2(n - j) + 1) \\ &= (h + s - 1)(2(n - h) + 1) - s(s - 1), \end{aligned}$$

whereas taking into account the last identity in Lemma 3.3,

$$\begin{aligned} \sum_{j=1}^{h+s-1} V_{\phi_h(j)-h}(q)Q_{s-1+h-\phi_h(j)}(q) &= (h - 1)Q_{s-1}(q) + \sum_{j=h}^{h+s-1} V_{j-h}(q)Q_{h+s-1-j}(q) \\ &= (h - 1)Q_{s-1}(q) + \sum_{j=1}^s V_{j-1}(q)Q_{s-j}(q) \\ &= (h - 1)Q_{s-1}(q) + \frac{2c}{a + 2c} (n - h - s + 1)U_{s-1}(q) \\ &+ \frac{cs}{a + 2c} \left[(2(n - h - s) + 1)T_s(q) + W_s(q) \right], \end{aligned}$$

and the result follows. \square

When $s = 1$ we recover the unicycle case and the following formula coincides with that in Proposition 2.4 for constant weight and constant conductance in the path. When, in addition, $h = 1$, then we get the obtained formula for the cycle.

Corollary 3.8 *The Kirchhoff index of the unicycle ladder-like polyomino is*

$$k^\Gamma = \frac{(4n^2 - 1)[c + a(n - 1)] - 4ah(h - 1)(n - 1)}{6c[c + a(2(n - h) + 1)]}.$$

When the polyomino is the standard ladder; that is, when $s = n - 1$ and hence $h = 1$, we have the following result.

Corollary 3.9 *The Kirchhoff index of the standard ladder is*

$$k^\Gamma = \frac{n^2 + 2}{6c} + \frac{[2c^2 - a(a + 2c)]U_{n-2}(q) + c^2(n - 1)[T_{n-1}(q) + W_{n-1}(q)]}{2c(a + 2c)[cV_{n-1}(q) + aU_{n-2}(q)]}.$$

In particular, when $a = c$, then

$$k^\Gamma = \frac{n^2 - 1}{6c} + \frac{1}{2c} \sum_{k=0}^{n-1} \frac{1}{1 + \sin^2\left(\frac{k\pi}{2n}\right)}.$$

Proof. The first Identity follows substituting $s = n - 1$ and $h = 1$ in Proposition 3.7. On the other hand, when $a = c$, then $q = 2$ and $T_{n-1}(2) + W_{n-1}(2) = T_n(2)$. Therefore, we have

$$k^\Gamma = \frac{n^2 + 2}{6c} + \frac{(n - 1)T_n(2) - U_{n-2}(2)}{6cU_{n-1}(2)}$$

Taking into account that $U'_{n-1}(2) = \frac{1}{3}[(n - 1)T_n(2) - U_{n-2}(2)]$, see [11], we get

$$\frac{(n - 1)T_n(2) - U_{n-2}(2)}{6cU_{n-1}(2)} = \frac{U'_{n-1}(2)}{2cU_{n-1}(2)} = \frac{1}{2c} \sum_{k=1}^{n-1} \frac{1}{2 - \cos\left(\frac{k\pi}{n}\right)}$$

since $\left\{\cos\left(\frac{k\pi}{n}\right)\right\}_{k=1}^{n-1}$ are the zeroes of the Chebyshev polynomial U_{n-1} . □

In the Chemistry community, standard ladders are known as linear polyomino chains. Then, the last formula coincides with that obtained in [15, Theorem 4.1] for a linear polyomino chain with $n - 1$ squares.

Acknowledgments. This work has been partly supported by the Spanish Research Council (Comisión Interministerial de Ciencia y Tecnología,) under projects MTM2010-19660 and MTM2011-28800-C02-01/MTM.

4 References

- [1] E. Bendito, A. Carmona, A.M. Encinas. Eigenvalues, eigenfunctions and Greens functions on a path via Chebyshev polynomials. *Appl. Anal. Discrete Math.*, **3** (2009), 282–302.

- [2] E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto. Characterization of symmetric M -matrices as resistive inverses, *Linear Algebra Appl.*, **430** (2009), 1336–1349.
- [3] E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto, M. Mitjana. Kirchhoff indexes of a network. *Linear Algebra Appl.*, **432** (2010), 2278–2292.
- [4] E. Bendito, A. Carmona, A.M. Encinas, and M. Mitjana. The M -matrix inverse problem for singular and symmetric Jacobi matrices. *Linear Algebra Appl.*, **436** (2012), 1090–1098.
- [5] A. Carmona, A.M. Encinas, M. Mitjana. Discrete Elliptic Operators and their Green Operators, to appear in *Linear Algebra Appl.*, (2013), <http://dx.doi.org/10.1016/j.laa.2013.07017>.
- [6] Ellis, Robert Byron, III. Chip-firing games with Dirichlet eigenvalues and discrete Green's functions, Ph.D. University of California, San Diego. 2002.
- [7] C.M. da Fonseca and J. Petronilho. Explicit inverses of some tridiagonal matrices. *Linear Algebra Appl.*, **325** (2001), 7–21.
- [8] F.P. Gantmacher and M.G. Krein. *Oscillation matrices and kernels and small vibrations of mechanical systems*. AMS Chelsea Publishing, Providence, RI, 2002 (Translation based on the 1941 Russian original)
- [9] S.W. Golomb and D.A. Klarner. Polyominoes, in *Handbook of Discrete and Computational Geometry, 2d edition*, J.E. Goodman and J.O'Rourke (eds.) Chapman & Hall/CRC, 2004, Chapter 15.
- [10] Markham, T.L.. Nonnegative Matrices whose Inverses are M -Matrices, *Proc. Amer. Math. Soc.*, **36** (1972), 326–330.
- [11] J.C. Mason and D.C. Handscomb, *Chebyshev Polynomials*, Chapman & Hall/CRC, 2003.
- [12] McDonald, J.J., Nabben, R., Neumann, M., Schenieder, H., Tsatsomeros, M.J. Inverse Tridiagonal Z -Matrices, *Linear Multilinear Algebra*, **45** (1998), 75–97.
- [13] Usmani, R. Inversion of a Jacobi's tridiagonal matrix, *Linear Algebra Appl.*, **212/213** (1994), 413–414.
- [14] Usmani, R. Inversion of Jacobi's tridiagonal matrix, *Computers Math. Appl.*, **27** (1994), 59–66.
- [15] Yang, Y., Zhang, H. Kirchhoff index of Linear Hexagonal Chains, *Int. J. Quantum Chem.*, **108** (2008), 503–512.
- [16] Z. Yarahmadi, A.R. Ashrafi and S. Moradi. Extremal Polyomino chains with respect to Zagreb indices. *App. Math. Letters*, **25** (2012), 166–171.