Effective Resistances for Ladder–Like Chains

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May 29, 2014

Abstract

Here we consider a class of generalized linear chains; that is, the ladder–like chains as a perturbation of a $2n$–path by adding consecutive weighted edges between opposite vertices. This class of chains in particular includes a big family of networks that goes from the cycle, unicycle chains up to ladder networks. In this paper, we obtain the Green function, the effective resistance and the Kirchhoff index of those ladder–like chains as function of the the Green function, the effective resistance and the Kirchhoff index of a path.

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INTRODUCTION

The Kirchhoff Index was introduced in Chemistry as a better alternative to other parameters used for discriminating among different molecules with similar shapes and structures; see[?] . Since then, a new line of research with a considerable amount of production has been developed and the Kirchhoff Index has been computed for some classes of graphs with symmetries; see for instance[8?] and the references therein. This index is defined as the sum of all effective resistances between any pair of vertices of the network and it is also known as the Total Resistance;[?] .

To find the Kirchhoff index of a general network has a high degree of computational complexity. Hence, it is of interest to find closed formulae for the effective resistance and the Kirchhoff index. Some works have been published in this direction, for networks such that cycles, hexagonal chain, distance–regular graphs, see.One can also raise the problem of computing the Kirchhoff index of composite networks in terms of factors,.

In this work we deal with the computation of Green function, effective resistance and Kirchhoff Index of generalized linear chain. These networks can be obtained from a $2n$ path by adding edges between opposite vertices. Hence, they are a perturbation of the path and we can apply the result obtained in[5] to obtain the desired parameters.

Let $\Gamma = (V, E, c)$ be a *network*; this is a simple and finite connected graph with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E, where each edge (i, j) has been assigned a *conductance* $c_{ij} > 0$. Moreover, when $(i, j) \notin E$ we define $c_{ij} = 0$, in particular $c_{ii} = 0$ for any $i = 1, \ldots, n$. The *(weighted) degree* of vertex i is defined as $\delta_i = \sum_{j=1}^{n} c_{ij}$.

The *combinatorial Laplacian* of Γ is the matrix L, whose entries are $L_{ij} = -c_{ij}$ for all $i \neq j$ and $L_{ii} = \delta_i$. Therefore, for each vector $u \in \mathbb{R}^n$ and for each $i = 1, \ldots, n$

$$(Lu)_i = \delta_i u_i - \sum_{j=1}^{n} c_{ij} = \sum_{j=1}^{n} c_{ij}(u_i - u_j).$$

It is well–known that $Lu = 0$ iff $u = a\mathsf{e}$, $a \in \mathbb{R}$ and e is the all–1 vector. Moreover, the multiplicity of 0 as eigenvalue of L is equal to the number of connected components of Γ. As Γ is connected, the projector onto the trivial eigenspace is J/n, where J is the all–1 matrix,

consequently $(L + \mathsf{J}/n)$ is non–singular and we define the *Green* matrix of Γ as

$$G = (L + \mathsf{J}/n)^{-1} - \mathsf{J}/n.$$

In other words, G is the Moore–Penrose inverse of the Laplacian matrix L.

For any pair $i, j \in V$, the *effective resistance between i and j* is defined as $R_{ij} = u_i - u_j$, where $u \in \mathbb{R}^n$ is any solution of the linear system $Lu = \mathsf{e}^i - \mathsf{e}^j$, where e^i denotes the ith unit vector with 1 in the ith position and 0 elsewhere. Note that R_{ij} does not depend on the chosen solution and in addition, the following equality holds,[1]

$$R_{ij} = G_{ii} + G_{jj} - 2G_{ij}. \tag{1}$$

It is well–known that, for any $i, j, k \in V$ the triangular inequality $R_{ij} \leq R_{ik} + R_{kj}$ is an equality iff k separates vertices i and j. The *Kirchhoff index* of Γ is the value[1,2]

$$\mathsf{k} = \frac{1}{2} \sum_{i,j=1}^{n} R_{ij} = n \sum_{i=1}^{n} G_{ii}. \tag{2}$$

In order to define the objects we are going to work with, we first consider a fixed a path P on $2n$ vertices, labelled as $V = \{1, \ldots, 2n\}$. The class of *generalized linear chains* supported by the path P, denoted by $\mathbb{L}_n$, consists of all connected networks whose conductance satisfies that $c_i = c_{i\,i+1} > 0$ for $i = 1, \ldots, 2n-1$, $a_i = c_{i\,2n+1-i} \geq 0$ for any $i = 1, \ldots, n-1$ and $c_{ij} = 0$ otherwise.

We define the *link number* of Γ as $s = |\{i = 1, \ldots, n-1 : a_i > 0\}|$ which corresponds with the numbers of holes or quadrangles. So, the link number of $\Gamma \in \mathbb{L}_n$ equals 0 iff $a_1 = \cdots = a_{n-1} = 0$; 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 $1 \leq i_1 < \cdots < i_s \leq n-1$ such that $a_{i_k} > 0$ when $k = 1, \ldots, s$, whereas $a_j = 0$ otherwise, see Figure 1.

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

Let G and R be the Green function and the effective resistance of the path P. Since each interior vertex in a path is a cut vertex, we get

$$R_{ij} = R_{\min\{k,i\}\,\min\{k,j\}} + R_{\max\{k,i\}\,\max\{k,j\}}, \quad i, j, k = 1, \ldots, 2n. \tag{3}$$
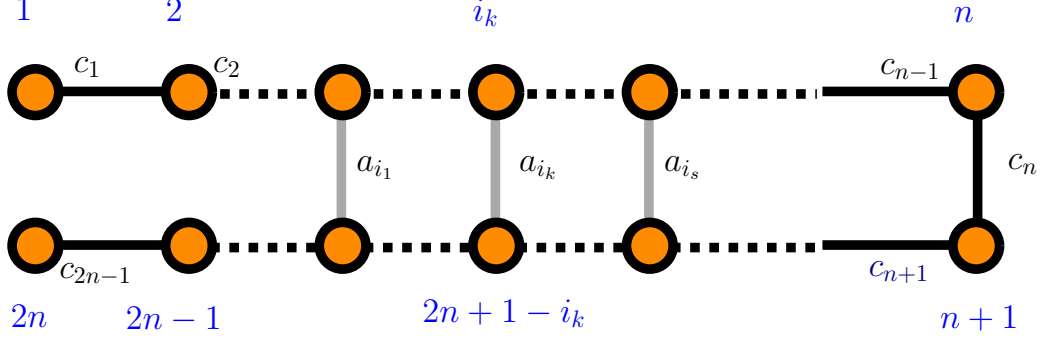
Figure 1: A Generalized Linear Chain

The authors proved in[3] that for any $i, j = 1, \ldots, 2n$, the Green function of a path is

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

where we use the usual convention that empty sums are defined as zero. Therefore, the effective resistance and the Kirchhoff index of the path are,

$$R_{ij} = \sum_{k=\min\{i,j\}}^{\max\{i,j\}-1} \frac{1}{c_k}, \quad i, j = 1, \ldots, 2n \quad \text{and} \quad \mathsf{k} = \sum_{k=1}^{2n-1} \frac{k(2n-k)}{c_k}.$$

Moreover, for a path with constant conductances, the expression of the Green function is

$$G_{ij} = \frac{1}{12nc} \left[(2n+1)(4n+1) + 3\Big(i(i - 2n - 1) + j(j - 2n - 1) - 2n|i - j| \Big) \right]$$

and hence, $\mathsf{k} = \dfrac{n}{3c}(4n^2 - 1)$ and $R_{ij} = \dfrac{|i-j|}{c}$ for any $i, j = 1, \ldots, 2n$.

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 $j = 1, \ldots, s$, an edge with conductance a_{i_j} between opposite vertices i_j and $2n + 1 - i_j$[4,5].

Since we interpret a generalized linear chain as a perturbation of the path by adding weighted edges between opposite vertices, we use[5] Theorem 2.1 to obtain the Green function, the effective resistances and the Kirchhoff index of such a chain. To this end, we consider the $(s \times s)$–matrix Λ with entries $\Lambda_{jk} = \sqrt{a_{i_j} a_{i_k}} R_{\max\{i_j, i_k\} \, 2n+1-\max\{i_j, i_k\}}$ and we take into account that $\mathsf{I} + \Lambda$ is non–singular because it is positive–definite. Let M be its inverse.

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For any $j = 1, \ldots, 2n$, we define the vector v_j whose components are

$$\mathsf{v}_{jk} = \frac{\sqrt{a_{i_k}}}{2}\left[R_{2n+1-i_k\,j} - R_{i_k\,j}\right], \quad k = 1, \ldots, s, \tag{4}$$

and also the vector $\mathsf{u}_j = \mathsf{M}\mathsf{v}_j$. Moreover, we consider the vector $\mathsf{r} = \dfrac{1}{2n}\displaystyle\sum_{j=1}^{2n}\mathsf{v}_j$.

According to the previous notation, the Green function, the effective resistance and the Kirchhoff index of a generalized linear chain, are given by the following result.

Theorem 1 *For any $i, j = 1, \ldots, 2n$, we get*

$$G_{ij}^{\Gamma} = G_{ij} - \langle \mathsf{M}(\mathsf{r} - \mathsf{v}_i), (\mathsf{r} - \mathsf{v}_j)\rangle \quad \text{and} \quad R_{ij}^{\Gamma} = R_{ij} - \langle(\mathsf{u}_i - \mathsf{u}_j), (\mathsf{v}_i - \mathsf{v}_j)\rangle.$$

In particular, the Kirchhoff index of the generalized linear chain is given by

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

Identity (3) allows us to give nice expressions for vectors v_j and r. To do this, it is useful to define for any $h = 1, \ldots, n-1$, the function $\phi_h \colon \{1, \ldots, 2n\} \longrightarrow \{h, \ldots, 2n+1-h\}$ given by

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

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

$$\Lambda_{jk} = \sqrt{a_{i_j}a_{i_k}}R_{\phi_{i_k}(i_j)\,\phi_{i_k}(2n+1-i_j)} = \sqrt{a_{i_j}a_{i_k}}R_{\phi_{i_j}(i_k)\,\phi_{i_j}(2n+1-i_k)}.$$

Lemma 2 *For any $k = 1, \ldots, s$, we have*

$$\mathsf{v}_{j,k} = \frac{\sqrt{a_{i_k}}}{2}\left[R_{i_k\,2n+1-i_k} - 2R_{i_k\,\phi_{i_k}(j)}\right], \qquad 1 \le j \le n,$$

$$\mathsf{v}_{j,k} = \frac{\sqrt{a_{i_k}}}{2}\left[2R_{\phi_{i_k}(j)\,2n+1-i_k} - R_{i_k\,2n+1-i_k}\right], \quad n+1 \le j \le 2n,$$

$$\mathsf{v}_{i,k} - \mathsf{v}_{j,k} = \frac{\sqrt{a_{i_k}}}{2}R_{\phi_{i_k}(i)\,\phi_{i_k}(j)}, \qquad\qquad\qquad 1 \le i \le j \le 2n.$$

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In particular, $-\mathsf{v}_{2n+1-i_1} = \mathsf{v}_{i_1} = \left(\dfrac{\sqrt{a_{i_k}}}{2} R_{i_k\,2n+1-i_k}\right)^s_{k=1}$, $\mathsf{v}_j = \mathsf{v}_{i_1}$ and $\mathsf{v}_{2n+1-j} = \mathsf{v}_{2n+1-i_1}$ for

any $1 \le j \le i_1$. Moreover, $\mathsf{r}_k = \dfrac{\sqrt{a_{i_k}}}{2n} \displaystyle\sum_{j=i_k}^{2n-i_k} \dfrac{(j-n)}{c_j}$, which in turns implies

$$\mathsf{r}_k - \mathsf{v}_{j,k} = \frac{\sqrt{a_{i_k}}}{2n} \left[\sum_{m=i_k}^{2n-i_k} \frac{m}{c_m} - 2n \sum_{m=\phi_{i_k}(j)}^{2n-i_k} \frac{1}{c_m}\right], \quad 1 \le j \le 2n.$$

Unicycle linear chains

In this section we obtain the Green function, the effective resistance and the Kirchhoff index
for unicycle linear chains; that is, for those generalized linear chains whose link number
equals one. Therefore if $i_1 = h$, then we add an edge with conductance $c_{2n} = a_h > 0$ between
vertices h and $2n + 1 - h$. Since $s = 1$, the computation of M and u_j, $j = 1, \ldots, 2n$, is
straightforward. Thus,

$$\mathsf{I} + \Lambda = 1 + c_{2n} R_{h\,2n+1-h} = c_{2n} \left[\frac{1}{c_{2n}} + \sum_{j=h}^{2n-h} \frac{1}{c_j}\right]. \tag{5}$$

Moreover, for any $i, j = 1, \ldots, 2n$, we have the following useful version of Identity (3),

$$R_{ij} = R_{\min\{h,i\}\,\min\{h,j\}} + R_{\max\{2n+1-h,i\}\,\max\{2n+1-h,j\}} + R_{\phi_h(i)\,\phi_h(j)}. \tag{6}$$

Proposition 3 *For any $i, j = 1, \ldots, 2n$, we get that*

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

$$- \frac{1}{4n^2} \left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{c_k}\right]^{-1} \left[\sum_{k=h}^{2n-h} \frac{k}{c_k} - 2n \sum_{k=\phi_h(i)}^{2n-h} \frac{1}{c_k}\right] \left[\sum_{k=h}^{2n-h} \frac{k}{c_k} - 2n \sum_{k=\phi_h(j)}^{2n-h} \frac{1}{c_k}\right]$$

$$R^{\Gamma}_{ij} = \sum_{k=\min\{h,i,j\}}^{\min\{h,\max\{i,j\}\}-1} \frac{1}{c_k} + \sum_{k=\max\{2n+1-h,\min\{i,j\}\}}^{\max\{2n+1-h,i,j\}-1} \frac{1}{c_k}$$

$$+ \left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{c_k}\right]^{-1} \left[\sum_{k=\phi_h(\min\{i,j\})}^{\phi_h(\max\{i,j\})-1} \frac{1}{c_k}\right] \left[\frac{1}{c_{2n}} + \sum_{k=h}^{\phi_h(\min\{i,j\})-1} \frac{1}{c_k} + \sum_{k=\phi_h(\max\{i,j\})}^{2n-h} \frac{1}{c_k}\right].$$

In particular,

$$\mathsf{k}^{\Gamma} = \sum_{k=1}^{2n} \frac{k(2n-k)}{c_k}$$

$$+ \left[\frac{1}{c_{2n}} + \sum_{k=h}^{2n-h} \frac{1}{c_k} \right]^{-1} \left[\left[\sum_{k=h}^{2n-h} \frac{k}{c_k} \right]^2 - 2n \sum_{k=h}^{2n-h} \left[\sum_{m=k}^{2n-h} \frac{1}{c_m} \right]^2 - 2n(h-1) \left[\sum_{k=h}^{2n-h} \frac{1}{c_k} \right]^2 \right].$$

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

$$G_{ij}^{\Gamma} = G_{ij} - \mathsf{M}\,(\mathsf{r} - \mathsf{v}_i)(\mathsf{r} - \mathsf{v}_j) \text{ and } R_{ij}^{\Gamma} = R_{ij} - \mathsf{M}(\mathsf{v}_i - \mathsf{v}_j)^2.$$

The expression for the Green function is a consequence of the last identity in Lemma 2, whereas the expression for the effective resistance appears as a consequence of the mentioned Lemma and Identity (6).

Finally, since $\mathsf{k}^{\Gamma} = 2n \sum_{j=1}^{2n} G_{jj}^{\Gamma}$, we have

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

On the other hand,

$$\sum_{j=1}^{2n} \left[\sum_{m=h}^{2n-h} \frac{m}{c_m} - 2n \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{c_m} \right]^2$$

$$= 2n \left[\sum_{m=h}^{2n-h} \frac{m}{c_m} \right]^2 - 4n \left[\sum_{m=h}^{2n-h} \frac{m}{c_m} \right] \left[\sum_{j=1}^{2n} \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{c_m} \right]$$

$$+ 4n^2 \sum_{j=1}^{2n} \left[\sum_{m=\phi_h(j)}^{2n-h} \frac{1}{c_m} \right]^2$$

$$= 4n^2(h-1) \left[\sum_{m=h}^{2n-h} \frac{1}{c_m} \right]^2 + 4n^2 \sum_{j=h}^{2n-h} \left[\sum_{m=j}^{2n-h} \frac{1}{c_m} \right]^2 - 2n \left[\sum_{m=h}^{2n-h} \frac{m}{c_m} \right]^2,$$

since

$$\sum_{j=1}^{2n} \sum_{m=\phi_h(j)}^{2n-h} \frac{1}{c_m} = h \sum_{m=h}^{2n-h} \frac{1}{c_m} + \sum_{j=h+1}^{2n-h} \sum_{m=j}^{2n-h} \frac{1}{c_m} = \sum_{m=h}^{2n-h} \frac{m}{c_m},$$

$$\sum_{j=1}^{2n} \left[\sum_{m=\phi_h(j)}^{2n-h} \frac{1}{c_m} \right]^2 = (h-1) \left[\sum_{m=h}^{2n-h} \frac{1}{c_m} \right]^2 + \sum_{j=h}^{2n-h} \left[\sum_{m=j}^{2n-h} \frac{1}{c_m} \right]^2$$

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

Corollary 4 *The Kirchhoff index of an unicycle chain with constant conductances a and c is*

$$\mathsf{k}^\Gamma = \frac{n\left[(4n^2-1)c + a(2(n-h)+1)(n(2(n-h)+1)+4h(h-1)-1)\right]}{3c(c+a(2(n-h)+1))}.$$

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 5 *The Green function and the effective resistance for the weighted $2n$–cycle are given by*

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

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

$$R^\Gamma_{ij} = \left[\sum_{k=1}^{2n}\frac{1}{c_k}\right]^{-1}\left[\sum_{k=\min\{i,j\}}^{\max\{i,j\}-1}\frac{1}{c_k}\right]\left[\sum_{k=1}^{\min\{i,j\}-1}\frac{1}{c_k} + \sum_{k=\max\{i,j\}}^{2n}\frac{1}{c_k}\right].$$

Moreover, the Kirchhoff index is given by

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

In particular, if $c_k = c$ for all $k = 1, \ldots, 2n-1$ and $c_{2n} = a$, we get

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

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

$$R^\Gamma_{ij} = \frac{|i-j|}{c\left[c+a(2n-1)\right]}\left(c+a\left(2n-1-|i-j|\right)\right),$$

and hence,

$$\mathsf{k}^\Gamma = \frac{n(4n^2-1)\left(c+a(n-1)\right)}{3c\left(c+a(2n-1)\right)}.$$

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

To end this section we rise the problem of optimizing the Kirchhoff index of an unicycle linear chain. Firstly, we assume $a = c$, then for $1 \leq h \leq n-1$,

$$k^\Gamma(h) = \frac{n(8h^3 - 12h^2n + 8hn^2 - 4n^3 - 12h^2 + 12hn - 8n^2 + 2h + n + 2)}{6a(-1 - n + h)} \qquad (7)$$

and its derivative with respect to h is

$$(k^\Gamma)'(h) = \frac{n(16h^3 - 36(n+1)h^2 + 24(n+1)^2h - 4n^3 - 12n^2 - 15n - 4)}{6a(-1 - n + h)^2}.$$

Let $\psi(h) = 16h^3 - 36(n+1)h^2 + 24(n+1)^2h - 4n^3 - 12n^2 - 15n - 4$, as

$$\psi'(h) = 48(h - (n+1))\left(h - \frac{n+1}{2}\right)$$

vanishes only at $(n+1)/2$ in the interval $[1, n-1]$. Therefore, ψ vanishes at most once in $[1, (n+1)/2]$ and once at most in $[(n+1)/2, n-1]$. Moreover, $\psi' < 0$ on $[(n+1)/2, n-1]$ and $\psi(n-1) > 0$, then ψ is positive on $[(n+1)/2, n-1]$. On the other hand, $\psi(\frac{n+2}{4}) = -3an < 0$ and $\psi(\frac{n+2}{4}) = \frac{9}{4}a(n^2 + 1) > 0$, so the $k^\Gamma(h)$ has a minimum for $h \in \left(\frac{n+1}{4}, \frac{n+2}{4}\right)$. Taking into account that $h \in \mathbb{Z}$, the minimum value of the Kirchhoff index for unicycle linear chains is attained for $h = \left\lceil \frac{n}{4} \right\rceil$. Finally, the maximum is attained for $h = n-1$ since $k^\Gamma(1) \leq k^\Gamma(n-1)$.

Let us now assume $a \neq c$, more precisely $a = \lambda c$ with $\lambda \neq 1$. Then, for $1 \leq h \leq n-1$

$$k^\Gamma(h, \lambda) = \frac{n\left(8\lambda h^3 - 12\lambda(n+1)h^2 + 2\lambda(4n^2 + 6n + 1)h - 4\lambda n^2(n+1) + \lambda(n+1) - 4n^2 + 1\right)}{3c(2h\lambda - 2\lambda n - \lambda - 1)}.$$

Let $(k^\Gamma)'(h, \lambda)$ be its derivative with respect to h.

It can be easily proved that for $\lambda > 1$, $(k^\Gamma)'(h, \lambda)$ vanishes at the interval $[\frac{n+1}{4}, \frac{n+2}{4}]$ and the minimum of the function is attained again for $h = \left\lceil \frac{n}{4} \right\rceil$. On the other hand, for $\lambda < 1$ this is $a < c$, there is a zero of $(k^\Gamma)'(h, \lambda)$ in the interval $[\frac{n - \frac{1}{\lambda}}{4}, \frac{n+2}{4}]$. Consequently, when the conductance a is very small compared with c, the Kirchhoff index of the unicycle chain is minimum for $h = 1$. In any case, the Kirchhoff index of the unicycle chain with conductances a and c, reaches its maximum for $h = n-1$.

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Ladder–like chains

A *ladder–like chain* is a generalized linear chain obtained by adding s consecutive edges, $1 \leq s \leq n - h$, from vertex h with the same conductance $a > 0$, to the path with constant conductance $c > 0$, (see Figure 2), so $i_k = h + k - 1$ and $a_{i_k} = a > 0$, $k = 1, \ldots, s$. In particular, when $s = n - 1$ the corresponding generalized linear chain is nothing else but a ladder network. In this section, we aim to compute the Green function, the effective resistance and the Kirchhoff index for the ladder–like chain.
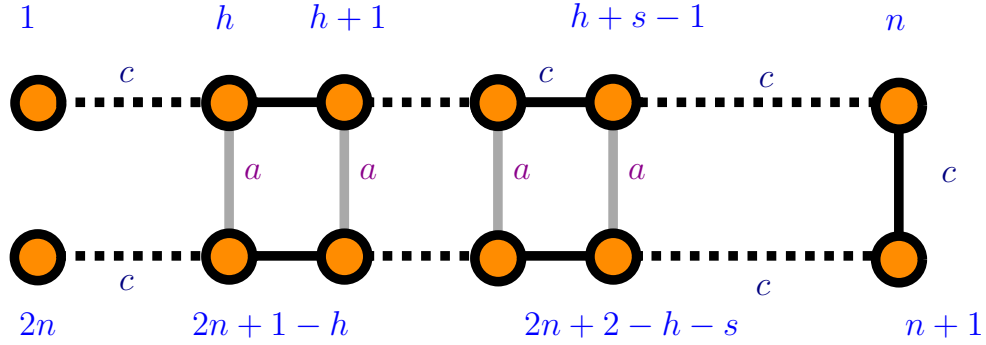

Figure 2: A ladder–like chain

Associated with the ladder–like chain, we consider $q = 1 + \dfrac{a}{c}$ and we define the following auxiliary function in terms of Chebyshev polynomials

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

where $V_k(q) = U_k(q) - U_{k-1}(q)$ and $U_k(q)$ is the k–th Chebyshev polynomials of second kind, see[7] and Annex A. 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

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

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

From Lemma 2 we get $\mathsf{v}_{2n+1-j} = -\mathsf{v}_j$ which leads to $\mathsf{u}_{2n+1-j} = -\mathsf{u}_j$, for any $j = 1, \ldots, n$ and moreover, $\mathsf{r} = 0$. Therefore, for ladder–like chains, Theorem 1 reads as follows.

Corollary 6 *For any $i, j = 1, \ldots, n$, we get*

$$G_{ij}^{\Gamma} = G_{2n+1-i\,2n+1-j}^{\Gamma} = G_{ij} - \langle u_i, v_j \rangle,$$

$$G_{i\,2n+1-j}^{\Gamma} = G_{2n+1-i\,j}^{\Gamma} = G_{i\,2n+1-j} + \langle u_i, v_j \rangle,$$

$$R_{ij}^{\Gamma} = R_{2n+1-i\,2n+1-j}^{\Gamma} = R_{ij} - \langle u_i, v_i \rangle - \langle u_j, v_j \rangle + 2\langle u_i, v_j \rangle,$$

$$R_{i\,2n+1-j}^{\Gamma} = R_{2n+1-i\,j}^{\Gamma} = R_{i\,2n+1-j} - \langle u_i, v_i \rangle - \langle u_j, v_j \rangle - 2\langle u_i, v_j \rangle.$$

Moreover, $k^{\Gamma} = \dfrac{n}{3c}(4n^2 - 1) - 4n \sum_{j=1}^{n} \langle u_j, v_j \rangle.$

Notice that in order to compute the Green function and the effective resistance for a ladder–like chain, it suffices to obtain the values $\langle u_i, v_j \rangle$ for any $i, j = 1, \ldots, n$. Therefore, the key is to compute M. Applying the results of[5] Proposition 2.5 we get the following expression for M.

Lemma 7 *If $\mathsf{M} = (b_{ij})$, then*

$$b_{ij} = \delta_{ij} - \frac{a V_{\min\{i,j\}-1}(q) Q_{s-\max\{i,j\}}(q)}{c V_s(q) + a\big(2(n - s - h) + 1\big) U_{s-1}(q)}$$

Notice that when $s = 1$, the above formula gives $b_{11} = \dfrac{c}{c + a(2(n - h) + 1)}$, that coincides with the inverse of (5) for constant conductances.

Next results are devoted to obtain the vectors $v_j, u_j, j = 1, \ldots, n$ and their inner product.

Proposition 8 *It is satisfied that $v_j = v_h$ and hence $u_j = u_h$, $j = 1, \ldots, h$. Moreover, for any $j = 1, \ldots, n$ and any $m = 1, \ldots, s$, we get*

$$v_{j,m} = \frac{\sqrt{a}}{2c}\Big(2\big(n - \phi_{h+m-1}(j)\big) + 1\Big),$$

$$u_{j,m} = \frac{\sqrt{a}}{2} \frac{V_{\min\{\phi_h(j)-h,m-1\}}(q) Q_{s-1-\max\{\phi_h(j)-h,m-1\}}(q)}{c V_s(q) + a\big(2(n - s - h) + 1\big) U_{s-1}(q)}.$$

Proof. Given $j = 1, \ldots, n$ and $m = 1, \ldots, s$, from Lemma 2 we have

$$v_{j,m} = \frac{\sqrt{a}}{2c}\Big[2n + 1 - 2i_m - 2\big[\phi_{i_m}(j) - i_m\big]\Big] = \frac{\sqrt{a}}{2c}\Big[2\big(n - \phi_{i_m}(j)\big) + 1\Big],$$

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

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Since $u_j = Mv_j$, if we consider $\alpha = cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)$, then for $m = 1, \ldots, s$, we have

$$u_{j,m} = \frac{\sqrt{a}}{2c}\Big(2\big(n - \phi_{h+m-1}(j)\big) + 1\Big) - \frac{a}{\alpha}\frac{\sqrt{a}}{2c}Q_{s-m}(q)\sum_{k=1}^{m}V_{k-1}(q)\Big(2\big(n - \phi_{h+k-1}(j)\big) + 1\Big)$$

$$- \frac{a}{\alpha}\frac{\sqrt{a}}{2c}V_{m-1}(q)\sum_{k=m+1}^{s}Q_{s-k}(q)\Big(2\big(n - \phi_{h+k-1}(j)\big) + 1\Big).$$

The result follows after carefully considering each of the cases $1 \leq j \leq h; h \leq j \leq h + s - 1; h + s - 1 \leq j \leq n$ and applying Lemma 13 in Annex A.

Corollary 9 *Given* $1 \leq i, j \leq n$, *then*

$$\langle u_i, v_j \rangle = \frac{a\big(2(n - i) + 1\big)\big(2(n - j) + 1\big)U_{s-1}(q)}{4c\big[cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)\big]}$$

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

$$\langle u_i, v_j \rangle = \frac{1}{4c}\left[\Big(2(n - \phi_h(\max\{i, j\})) + 1\Big) - \frac{cV_{\phi_h(\min\{i,j\})-h}(q)Q_{s-1+h-\phi_h(\max\{i,j\})}(q)}{cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)}\right],$$

otherwise.

Once we have obtained the inner product, the expression for the Green function of a ladder–like chain is straightforward. Next we compute the effective resistance of a ladder–like chain according to the position in the path of the involved vertices.

Corollary 10 *For any* $i, j = 1, \ldots, n$, *we get*

$$R_{ij}^{\Gamma} = R_{2n+1-i\,2n+1-j}^{\Gamma} = \frac{|i - j|\Big[cV_s(q) + a\big(2(n - s - h) + 1 - |i - j|\big)U_{s-1}(q)\Big]}{c\big[cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)\big]},$$

$$R_{i\,2n+1-j}^{\Gamma} = R_{2n+1-i\,j}^{\Gamma} = \frac{(2n + 1 - i - j)\Big[cV_s(q) + a\big(i + j - 2(s + h)\big)U_{s-1}(q)\Big]}{c\big[cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)\big]}.$$

for $h + s \leq i, j \leq n$ *and*

$$R_{ij}^{\Gamma} = R_{2n+1-i\,2n+1-j}^{\Gamma} = \frac{|i - j|}{2c}$$

$$+ \frac{V_{\min\{i,j\}-h}(q)\Big(Q_{s+h-1-\min\{i,j\}}(q) - Q_{s+h-1-\max\{i,j\}}(q)\Big)}{4\big[cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)\big]}$$

$$+ \frac{Q_{s+h-1-\max\{i,j\}}(q)\Big(V_{\max\{i,j\}-h}(q) - V_{\min\{i,j\}-h}(q)\Big)}{4\big[cV_s(q) + a\big(2(n - s - h) + 1\big)U_{s-1}(q)\big]}$$

$$R^{\Gamma}_{i\,2n+1-j} = R^{\Gamma}_{2n+1-i\,j} = \frac{2n+1-\max\{i,j\}}{2c}$$

$$+\frac{V_{\min\{i,j\}-h}(q)\Big(Q_{s+h-1-\min\{i,j\}}(q) + Q_{s+h-1-\max\{i,j\}}(q)\Big)}{4\big[cV_s(q) + a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}$$

$$+\frac{Q_{s+h-1-\max\{i,j\}}(q)\Big(V_{\max\{i,j\}-h}(q) + V_{\min\{i,j\}-h}(q)\Big)}{4\big[cV_s(q) + a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}$$

for $h \leq i,j \leq h+s$.

Proposition 11 *The Kirchhoff index of the ladder–like chain is*

$$k^{\Gamma} = \frac{n(4n^2-1)}{3c} - \frac{n}{c}\Big[(h+s-1)\big(2(n-h)+1\big) - s(s-1)\Big]$$

$$+\frac{n\big[(h-1)Q_{s-1}(q) - f(n,h,s)U_{s-1}(q) + g(n,h,s)U_s(q)\big]}{\big[cV_s(q) + a\big(2(n-h-s)+1\big)U_{s-1}(q)\big]},$$

where

$$f(n,h,s) = \frac{\big(2(n-h-s)+1\big)\big((c+a)s - c\big) - c(s+1)}{(2c+a)}$$

$$+\frac{a(n-h-s+1)\big(2(n-h-s)+1\big)\big(2(n-h-s)+3\big)}{3c}$$

$$g(n,h,s) = \frac{2cs(n-h-s+1)}{(2c+a)}.$$

Proof. First, we have

$$\sum_{j=h+s}^{n} \langle \mathsf{u}_j, \mathsf{v}_j \rangle = \frac{a}{4c\alpha}U_{s-1}(q)\sum_{j=h+s}^{n}\big(2(n-j)+1\big)^2$$

$$= \frac{a}{12c\alpha}U_{s-1}(q)\big(n-h-s+1\big)\big(2(n-h-s)+1\big)\big(2(n-h-s)+3\big),$$

in addition,

$$\sum_{j=1}^{h+s-1} \langle \mathsf{u}_j, \mathsf{v}_j \rangle = \frac{1}{4c}\sum_{j=1}^{h+s-1}\left[\big(2(n-\phi_h(j))\big)+1\big) - \frac{cV_{\phi_h(j)-h}(q)Q_{s-1+h-\phi_h(j)}(q)}{cV_s(q) + a\big(2(n-s-h)+1\big)U_{s-1}(q)}\right].$$

Moreover,

$$\sum_{j=1}^{h+s-1}\big(2(n-\phi_h(j))+1\big) = (h-1)\big(2(n-h)+1\big) + \sum_{j=h}^{h+s-1}\big(2(n-j)+1\big)$$

$$= (h+s-1)\big(2(n-h)+1\big) - s(s-1),$$

whereas taking into account the last identity in Lemma 14,

$$\sum_{j=1}^{h+s-1} V_{\phi_h(j)-h}(q)Q_{s-1+h-\phi_h(j)}(q) = (h-1)Q_{s-1}(q) + \sum_{j=1}^{s} V_{j-1}(q)Q_{s-j}(q)$$

$$= (h-1)Q_{s-1}(q) + \frac{2sc(n-h-s+1)}{2c+a}U_s(q)$$

$$- \frac{\big(2(n-h-s)+1\big)\big((c+a)s-c\big)-c(s+1)}{2c+a}U_{s-1}(q),$$

Thus,

$$\mathsf{k}^{\Gamma} = \frac{n(4n^2-1)}{3c} - 4n\sum_{j=1}^{h+s-1}\langle \mathsf{u}_j, \mathsf{v}_j\rangle - 4n\sum_{j=h+s}^{n}\langle \mathsf{u}_j, \mathsf{v}_j\rangle$$

$$= \frac{n(4n^2-1)}{3c} - \frac{n}{c}\sum_{j=1}^{h+s-1}\left[\big(2(n-\phi_h(j))\big)+1\big) - \frac{cV_{\phi_h(j)-h}(q)Q_{s-1+h-\phi_h(j)}(q)}{cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)}\right]$$

$$- \frac{na}{c}\sum_{j=h+s}^{n}\frac{\big(2(n-j)+1\big)^2 U_{s-1}(q)}{4c\big[cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}$$

$$= \frac{n(4n^2-1)}{3c} - \frac{n}{c}\Big((h+s-1)\big(2(n-h)+1\big)-s(s-1)\Big)$$

$$+ \frac{n(h-1)Q_{s-1}(q)}{\big[cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]} + \frac{2scn(n-h-s+1)\,U_s(q)}{(2c+a)\big[cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}$$

$$- \frac{n\Big(\big(2(n-h-s)+1\big)\big((c+a)s-c\big)-c(s+1)\Big)U_{s-1}(q)}{(2c+a)\big[cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}\Bigg]$$

$$- \frac{na(n-h-s+1)\big(2(n-h-s)+1\big)\big(2(n-h-s)+3\big)U_{s-1}(q)}{3c\big[cV_s(q)+a\big(2(n-s-h)+1\big)U_{s-1}(q)\big]}.$$

□

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

Corollary 12 *The Kirchhoff index of the standard ladder is*

$$\mathsf{k}^{\Gamma} = \frac{n(n^2+2)}{3c} + \frac{n\big[2c^2(n-1)U_{n-1}(q)-\big(c(a(n+1)-c)+a^2-c^2\big)U_{n-2}(q)\big]}{c(2c+a)\big[cV_{n-1}(q)+aU_{n-2}(q)\big]}.$$

In particular, when $a = c$, then

$$\mathsf{k}^{\Gamma} = \frac{n(n^2-1)}{3c} + \frac{n}{c}\sum_{k=0}^{n-1}\frac{1}{1+2\sin^2(\frac{k\pi}{2n})}.$$

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Proof. The first Identity follows substituting $s = n - 1$ and $h = 1$ in Proposition 11. On the other hand, when $a = c$, then $q = 2$ and

$$\frac{n\big[2(n-1)U_{n-1}(2) - nU_{n-2}(2)\big]}{3cU_{n-1}(2)} = \frac{nU'_{n-1}(2)}{cU_{n-1}(2)} = \frac{n}{c} \sum_{k=1}^{n-1} \frac{1}{2 - \cos(\frac{k\pi}{n})}$$

since $\big\{\cos(\frac{k\pi}{n})\big\}_{k=1}^{n-1}$ are the zeroes of the Chebyshev polynomial U_{n-1}, see[7]. $\qquad\square$

In the Chemistry community, standard ladders are known as linear polyomino chains. Then, the last formula coincides with that obtained in[8] Theorem 4.1 for a linear polyomino chain with $n - 1$ squares.

Annex A

In this section we write the results related with the Chebyshev sequences that we need across the paper.

The following Lemma shows a useful property for the sum of Chebyshev polynomials, see for instance[7].

Lemma 13 *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,*

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

From the expression for products of Chebyshev polynomials, see[7] Chapter 2, we deduce the following equalities.

Lemma 14 *For any $1 \leq m \leq s + 1$ we have*

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

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

$$\sum_{j=1}^{s} V_{j-1}(q)Q_{s-j}(q) = \frac{c}{a+2c}\Big[s\big(2(n-h-s) + 1\big)T_s(q) + sW_s(q) + 2(n - h - s + 1)U_{s-1}(q)\Big],$$

which is equivalent to

$$\sum_{j=1}^{s} V_{j-1}(q)Q_{s-j}(q) = \frac{2s(n-h-s+1)}{q+1}U_s(q) - \frac{\big(2(n-h-s)+1\big)\big(qs-1\big)-s-1}{q+1}U_{s-1}(q)$$

Proof.

$$\sum_{j=1}^{s} V_{j-1}(q)Q_{s-j}(q) = \sum_{j=1}^{s}\Big(U_{j-1}(q)-U_{j-2}(q)\Big)\Big(\big(2(n-h-s)+1\big)\big(U_{s-j}(q)-U_{s-j-1}(q)\big)+2U_{s-j}(q)\Big)$$

$$= \sum_{j=1}^{s}\Big(U_{j-1}(q)-U_{j-2}(q)\Big)\Big(\big(2(n-h-s)+3\big)U_{s-j}(q)-\big(2(n-h-s)+1\big)U_{s-j-1}(q)\Big)$$

$$= \big(2(n-h-s)+3\big)\sum_{j=1}^{s}\Big(U_{s-j}(q)U_{j-1}(q)-U_{s-j}(q)U_{j-2}(q)\Big)$$

$$- \big(2(n-h-s)+1\big)\sum_{j=1}^{s}\Big(U_{s-j-1}(q)U_{j-1}(q)-U_{s-j-1}(q)U_{j-2}(q)\Big)$$

$$= \frac{\big(2(n-h-s)+3\big)}{2(q^2-1)}\Big[sT_{s+1}(q)-\sum_{j=1}^{s}T_{s-2j+1}(q)-sT_s(q)+\sum_{j=1}^{s}T_{s-2j+2}(q)\Big]$$

$$- \frac{\big(2(n-h-s)+1\big)}{2(q^2-1)}\Big[sT_s(q)-\sum_{j=1}^{s}T_{s-2j}(q)-sT_{s-1}(q)+\sum_{j=1}^{s}T_{s-2j+1}(q)\Big]$$

$$= \frac{\big(2(n-h-s)+1\big)s}{2(q^2-1)}\Big[T_{s+1}(q)-2T_s(q)+T_{s-1}(q)\Big]+\frac{2s}{2(q^2-1)}\Big[T_{s+1}(q)-T_s(q)\Big]+$$

$$+ \frac{\big(2(n-h-s)+1\big)}{2(q^2-1)}\Big[-2\sum_{j=1}^{s}T_{s-2j+1}(q)+\sum_{j=1}^{s}T_{s-2j+2}(q)+\sum_{j=1}^{s}T_{s-2j}(q)\Big]+$$

$$+ \frac{2}{2(q^2-1)}\Big[-\sum_{j=1}^{s}T_{s-2j+1}(q)+\sum_{j=1}^{s}T_{s-2j+2}(q)\Big]$$

$$= \frac{\big(2(n-h-s)+1\big)s(q-1)}{(q^2-1)}T_s(q)+\frac{s\Big(T_{s+1}(q)-T_s(q)\Big)}{q^2-1}$$

$$+ \frac{\big(2(n-h-s)+2\big)}{(q+1)}U_{s-1}(q)$$

$$= \frac{2s(n-h-s+1)}{q+1}U_s(q) - \frac{\big(2(n-h-s)+1\big)\big(qs-1\big)-s-1}{q+1}U_{s-1}(q)$$

taking into account

$$\sum_{\ell=1}^{s}T_{s-2\ell}(q)=\sum_{\ell=1}^{s}T_{s+2-2\ell}(q)=U_s(q)-T_s(q)=qU_{s-1}(q),\quad \sum_{\ell=1}^{s}T_{s+1-2\ell}(q)=U_{s-1}(q).$$

$\square$

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CONCLUSIONS

We have obtained the Green function, the effective resistance, and the Kirchhoff index of a class of generalized linear chains that includes cycles, unicycle chains and ladder chains also known as polyomino chains in the Chemistry community. The starting point is a path with arbitrary conductances on their edges, then we interpret each generalized chain as a convenient perturbation of the mentioned path. Therefore, we obtain the expressions of the Green function, the effective resistance, and the Kirchhoff index as function of its corresponding in the path. In particular we obtain, as far as we know for the first time, the Green function of a weighted cycle. We explicitly give the Kirchhoff index for unicycle chains with two different conductances and we discuss when the Kirchhoff index is optimum according to the size of the cycle. The last section is devoted to the study of ladder–like chains again as a perturbation of the path. For them we have also find the desired results. In order to achieve the last goal, we have had to deal with Chebyshev polynomials'tools that are included in Annex A.

ACKNOWLEDGMENTS

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