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ORIGINAL PAPER

Kirchhoff index of periodic linear chains

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Abstract A periodic linear chain consists of a weighted $2n$-path where new edges have been added following a certain periodicity. In this paper, we obtain the effective resistance and the Kirchhoff index of a periodic linear chain as non trivial functions of the corresponding expressions for the path. We compute the expression of the Kirchhoff index of any homogeneous and periodic linear chain which generalizes the previously known results for ladder-like and hexagonal chains, that correspond to periods one and two respectively.

Keywords Kirchhoff index · Periodic linear chain · Effective resistance

1 Introduction

The topology of chemical compounds is conventionally represented by a molecular graph or network where edge weights correspond to bond properties. Thereby a principal question is how different graph structures can be compared. To this end, several molecular structure descriptors based in molecular networks, have been introduced.

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Among them, the Kirchhoff index is a structure-descriptor that has very nice purely mathematical and physical interpretations, see [5]. The Kirchhoff index is the sum of the effective resistance between all pair of vertices and, for a general network, it is difficult to express the index in a closed-form formulae. In view of the above, the Kirchhoff index has been studied in mathematical, physical and chemical literatures, see [1,2,6,7] and references therein.

Because the effective resistances, and hence the Kirchhoff index, can be computed from the Moore–Penrose inverse of the combinatorial Laplacian of the network, our strategy is to obtain the Moore–Penrose inverse of a periodic linear chain as a perturbation of the Moore–Penrose inverse of the underlying path after the addition of new edges. Our technique differs from the ones previously used, [6], that are based on the decomposition of the combinatorial Laplacian in structured blocks. The achievement of the goal requires solving a specific difference equation whose coefficients are closely related with the effective resistances of the path.

In [1] these authors stated the theoretical foundations for the computations of the effective resistances and the Kirchhoff index of a family of networks named generalized polyominoes. Here we give explicit formulae for the above mentioned parameters for a particular class of them which present more symmetry and can be interpreted as a model to describe the structure of some molecules. So, from now on we shall name those objects as periodic linear chains because linear chain is the common word used in Chemistry to refer to such molecular graphs.

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 $\mathsf{L_{ij}} = -\mathsf{c_{ij}}$ for all $i \neq j$ and $\mathsf{L_{ii}} = \delta_\mathsf{i}$. Therefore, for each vector $\mathsf{u} \in \mathbb{R}^n$ and for each $i = 1, \ldots, n$

$$(\mathsf{Lu})_i = \delta_i \mathsf{u}_i - \sum_{j=1}^{n} c_{ij}\mathsf{u}_j = \sum_{j=1}^{n} c_{ij}(\mathsf{u}_i - \mathsf{u}_j).$$

It is well–known that $\mathsf{Lu} = 0$ iff $\mathsf{u} = a\mathsf{e}$, $a \in \mathbb{R}$ and e is the all-1 vector.

For any pair $i, j \in V$, the *effective resistance between i and j* is defined as $R_{ij} = \mathsf{u}_i - \mathsf{u}_j$, where $\mathsf{u} \in \mathbb{R}^n$ is any solution of the linear system $\mathsf{Lu} = \mathsf{e^i} - \mathsf{e^j}$, 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, if G denotes the Moore–Penrose inverse of L, the following equality holds, [2,3]

$$R_{ij} = \mathsf{G}_{ii} + \mathsf{G}_{jj} - 2\mathsf{G}_{ij}. \tag{1}$$

Moreover, 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, see [1–3]

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

In what follows, the standard inner product on $\mathbb{R}^h$ is denoted by $\langle\cdot,\cdot\rangle$; that is, $\langle \mathsf{u},\mathsf{v}\rangle = \sum_{j=1}^{h} \mathsf{u}_j \mathsf{v}_j$ for each $\mathsf{u},\mathsf{v} \in \mathbb{R}^h$.

2 Linear periodic chains

We consider fixed a path P on $2n$ vertices, labeled as $V = \{1,\ldots,2n\}$. The class of *linear chains* supported by the path P 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 $c_{i\,j} = 0$ otherwise.

Consider $h = \big|\{i = 1,\ldots,n-1 : a_i > 0\}\big|$. So, $h = 0$ 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, when $h > 0$ there exist indexes $1 \leq i_1 < \cdots < i_h \leq n-1$ such that $a_{i_k} > 0$ when $k = 1,\ldots,h$, whereas $a_j = 0$ otherwise, see Fig. 1. Therefore, h is the number of *holes* of the linear chain. Notice that in [1,2] this parameter was called *link number*.

In this work we consider *periodic linear chains*; that is, linear chains where $n = ph+1$, $p \in \mathbb{N}^*$ and $i_\ell = p(\ell-1)+1$, $\ell = 1,\ldots,h$. The number p is called the *period* of the linear chain. The class of periodic linear chains with period p and h holes is denoted by $\mathbb{L}_h^p$. In particular, $\mathbb{L}_1^{n-1}$ correspond with $2n$–cycles, whereas $\mathbb{L}_{n-1}^1$ corresponds with the *standard linear chains* on $2n$ vertices or linear chains with $n-1$ quadrangles. Moreover, $\mathbb{L}_h^2$ refers to *linear hexagonal chains* with h hexagons. When $h = 1$, it is a molecular graph called *benzene*, whereas when $h = 2$ the molecular graph is the *naphthalene*.

In this work we only treat with *homogeneous and periodic linear chains*; that means that $c_i = c > 0$ for any $i = 1,\ldots,2n-1$ and $a_{p(\ell-1)+1} = a > 0$ for any $\ell = 1,\ldots,h$, see Fig. 2 for the case of a homogeneous and hexagonal linear chain. Clearly, given $a, c > 0$ for any $h, p \in \mathbb{N}^*$ there exists a unique homogeneous and periodic linear chain with h holes and period p whose conductance is determined by the values a

Fig. 1 A linear chain

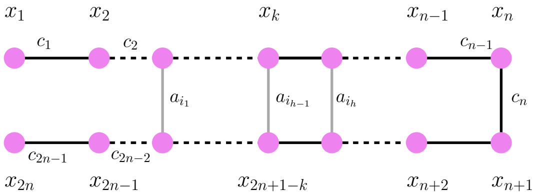
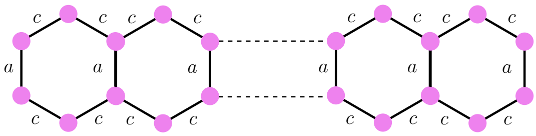


Fig. 2 Homogeneous hexagonal linear chain



and c, that we denote by $\mathbb{L}_h^p(c,a)$. When $a=c$, then this homogeneous and periodic linear chain is denoted simply as $\mathbb{L}_h^p(c)$.

If we consider G, R and k, the Moore–Penrose inverse, the effective resistance and the Kirchhoff index of the path P, it is well–known, see for instance [2], that

$$\mathsf{G}_{ij}=\frac{1}{12nc}\Big[(2n+1)(4n+1)+3\Big(i(i-2n-1)+j(j-2n-1)-2n\big|i-j\big|\Big)\Big],$$

and $R(x_i,x_j)=\dfrac{\big|i-j\big|}{c}$ for any $i,j=1,\dots,2n$ and hence $\mathsf{k}=\dfrac{n(4n^2-1)}{3c}$.

The combinatorial Laplacian of $\Gamma=\mathbb{L}_h^p(c,a)$ appears as the combinatorial Laplacian of the path perturbed by adding an edge with conductance a between vertices $x_{p(\ell-1)+1}$ and $x_{2n-p(\ell-1)}$, for all $\ell=1,\dots,h$. Since we interpret a periodic linear chain as a perturbation of the path by adding weighted edges between opposite vertices, we use the results of Section 2 of [1] to obtain the effective resistances and the Kirchhoff index of such a linear chain.

Let $q=1+c^{-1}ap$ and consider the Chebyshev equation with parameter q

$$x_{k+2}=2qx_{k+1}-x_k,\quad k\in\mathbb{Z},\tag{3}$$

whose solutions, called *Chebyshev sequences*, are all of the form $\{P_k(q)\}_{k\in\mathbb{Z}}$, where $\{P_k\}_{k\in\mathbb{Z}}$ is a sequence of Chebyshev polynomials. Due to the role played by this equation in the computation of the parameters of homogeneous and periodic linear chains, we describe some useful properties of Chebyshev sequences in "Appendix". In particular if T_k, U_k denote the kth *Chebyshev polynomials of first and second kind* respectively, then $T_k(q)>0$ for any $k\in\mathbb{Z}$ and $U_k(q)>0$ for any $k\in\mathbb{N}$. Moreover, the Chebyshev sequences defined as

$$V_k(q)=U_k(q)-U_{k-1}(q)\quad\text{and}\quad Q_k(q)=(2p+1)U_k(q)-U_{k-1}(q),\quad k\in\mathbb{Z},\tag{4}$$

play a main role to obtain the parameters of homogeneous linear periodic chains. We remark that V_k is also known as the k-th *Chebyshev polynomial of third kind.*

If we consider the $(h\times h)$-matrix $\Lambda=(\lambda_{ij})$ where

$$\begin{aligned}\lambda_{ij}&=aR_{\max\{p(i-1)+1,p(j-1)+1\}\,2n+1-\max\{p(i-1)+1,p(j-1)+1\}}\\&=\frac{a}{c}\Big(2\big(n-p\max\{j-1,i-1\}\big)-1\Big),\quad i,j=1,\dots,h,\end{aligned}$$

then the following result holds, see [1, Proposition 2.5].

Proposition 1 *The matrix* $\mathsf{I}+\Lambda$ *is invertible and its inverse* $\mathsf{M}=(b_{ij})$ *is given by*

$$b_{ij}=\delta_{ij}-\frac{aV_{\min\{i,j\}-1}(q)\,Q_{h-\max\{i,j\}}(q)}{cT_h(q)+a(p+1)U_{h-1}(q)},\quad i,j=1,\dots,h.$$

Proof According [1, Proposition 2.5], we need to obtain $\{u_j\}_{j=1}^h$ and $\{v_j\}_{j=1}^h$ the solutions of the difference equation

$$2qz_i - z_{i-1} - z_{i+1} = 0, \quad i = 2, \ldots, h-1$$

satisfying $u_1 = \dfrac{c}{2p}$, $u_2 = a + \dfrac{c}{2p}$ and $v_{h-1} = a + \dfrac{(4p+1)c}{2p(2p+1)}$, $v_h = \dfrac{c}{2p}$, respectively. Clearly $u_j = \dfrac{c}{2p} V_{j-1}(q)$, whereas $v_j = \dfrac{c}{2p(2p+1)} Q_{h-j}(q)$. □

Using the result in [1, Theorem 2.1], we can obtain an explicit expression for the Moore–Penrose inverse, effective resistances and Kirchhoff index of an homogenous and periodic linear chain. In this case, the symmetry of the chain allows us to simplify the formula in the above mentioned theorem. Specifically, according with the notations in [1], for any $j = 1, \ldots, n$ we define the vector v_j whose components are

$$\begin{aligned} \mathsf{v}_{j,m} &= R_{\max\{i_j, i_m\}\, 2n+1-\max\{i_j, i_m\}} \\ &= 2\big(n - \max\{p(m-1)+1, j\}\big) + 1, \quad m = 1, \ldots, h, \end{aligned}$$

and also the vector $\mathsf{u}_j = \mathsf{M}\mathsf{v}_j$, we have the following key result.

Theorem 1 *Given $\Gamma = \mathbb{L}_h^p(c, a)$, then for any $i, j = 1, \ldots, n$,*

$$\begin{aligned} R_{i\,j}^{\Gamma} = R_{2n+1-i\,2n+1-j}^{\Gamma} &= \frac{|i-j|}{c} - \frac{a}{4c^2}\Big[\langle \mathsf{u}_i, \mathsf{v}_i\rangle + \langle \mathsf{u}_j, \mathsf{v}_j\rangle - 2\langle \mathsf{u}_i, \mathsf{v}_j\rangle\Big], \\ R_{i\,2n+1-j}^{\Gamma} = R_{2n+1-j\,i}^{\Gamma} &= \frac{2n+1-i-j}{c} - \frac{a}{4c^2}\Big[\langle \mathsf{u}_i, \mathsf{v}_i\rangle + \langle \mathsf{u}_j, \mathsf{v}_j\rangle + 2\langle \mathsf{u}_i, \mathsf{v}_j\rangle\Big]. \end{aligned}$$

Therefore,

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

In order to apply the previous result, we only need to obtain the vectors $\mathsf{v}_j, \mathsf{u}_j$, $j = 1, \ldots, n$ and their inner products.

Proposition 2 *For any $1 \le \ell \le h$ and any $0 \le k \le p-1$ let $i = p(\ell-1)+1+k$. Then*

$$\mathsf{v}_{i,m} = \begin{cases} 2\big(n-i\big)+1, & 1 \le m \le \ell; \\ 2\big(n-p(m-1)\big)-1, & \ell < m \le h \end{cases}$$

and hence

$$\mathsf{u}_{i,m} = \begin{cases} \dfrac{c\big[(p-k)Q_{h-\ell}(q) + kQ_{h-\ell-1}(q)\big]}{p\big[cT_h(q) + a(p+1)U_{h-1}(q)\big]} V_{m-1}(q), & 1 \le m \le \ell; \\ \dfrac{\big[2akU_{\ell-1}(q) + cV_{\ell-1}(q)\big]}{cT_h(q) + a(p+1)U_{h-1}(q)} Q_{h-m}(q), & \ell < m \le h. \end{cases}$$

Moreover, $\mathsf{v}_{n,m} = 1,\ 1 \le m \le h$ *and*

$$\mathsf{u}_{n,m} = \frac{cV_{m-1}(q)}{cT_h(q) + a(p+1)U_{h-1}(q)}, \quad 1 \le m \le h.$$

Proposition 3 *For any* $1 \le \ell_0 \le \ell_1 \le h$ *and any* $0 \le k, r \le p-1$ *consider* $i = p(\ell_0 - 1) + 1 + k$ *and* $j = p(\ell_1 - 1) + 1 + r$. *Then,*

$$\begin{aligned}\langle \mathsf{u}_i, \mathsf{v}_j \rangle = {} & \frac{c}{a}\big[2(n-j)+1\big] \\ & - \frac{c\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big]}{pa\big[cT_h(q) + a(p+1)U_{h-1}(q)\big]}\Big[(p-r)Q_{h-\ell_1}(q) + rQ_{h-\ell_1-1}(q)\Big].\end{aligned}$$

Moreover,

$$\begin{aligned}\langle \mathsf{u}_i, \mathsf{v}_n \rangle &= \frac{c}{a} - \frac{c\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big]}{a\big[cT_h(q) + a(p+1)U_{h-1}(q)\big]} \\ \langle \mathsf{u}_n, \mathsf{v}_n \rangle &= \frac{cU_{h-1}(q)}{cT_h(q) + a(p+1)U_{h-1}(q)}.\end{aligned}$$

Proof First, $\langle \mathsf{u}_i, \mathsf{v}_j \rangle = A + B + C$ where

$$A = \sum_{m=1}^{\ell_0} \mathsf{u}_{i,m}\mathsf{v}_{j,m}, \quad B = \sum_{m=\ell_0+1}^{\ell_1} \mathsf{u}_{i,m}\mathsf{v}_{j,m} \quad \text{and} \quad C = \sum_{m=\ell_1+1}^{h} \mathsf{u}_{i,m}\mathsf{v}_{j,m}.$$

If $D = cT_h(q) + a(p+1)U_{h-1}(q)$, applying Lemmas 2 and 3 we get that

$$\begin{aligned}A &= \frac{c}{pD}\big[2(n-j)+1\big]\big[(p-k)Q_{h-\ell_0}(q) + kQ_{h-\ell_0-1}(q)\big]\sum_{m=1}^{\ell_0} V_{m-1}(q) \\ &= \frac{c}{pD}\big[2(n-j)+1\big]\big[(p-k)Q_{h-\ell_0}(q) + kQ_{h-\ell_0-1}(q)\big]U_{\ell_0-1}(q), \\ B &= \frac{1}{D}\big[2(n-j)+1\big]\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big]\sum_{m=\ell_0+1}^{\ell_1} Q_{h-m}(q) \\ &= \frac{c}{2paD}\big[2(n-j)+1\big]\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big] \\ &\quad \times \big[Q_{h-\ell_1-1}(q) - Q_{h-\ell_1}(q) + Q_{h-\ell_0}(q) - Q_{h-\ell_0-1}(q)\big], \\ C &= \frac{1}{D}\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big]\sum_{m=\ell_1+1}^{h}\big[2\big(n - p(m-1)\big) - 1\big]Q_{h-m}(q) \\ &= \frac{c}{2paD}\big[2akU_{\ell_0-1}(q) + cV_{\ell_0-1}(q)\big] \\ &\quad \times \Big[\big[2(n-j)+1+2r\big]\big(Q_{h-\ell_1}(q) - Q_{h-\ell_1-1}(q)\big) - 2pQ_{h-\ell_1}(q)\Big]\end{aligned}$$

and hence, we obtain that

$$\langle \mathsf{u}_i, \mathsf{v}_j \rangle = \frac{c}{a}\big[2(n-j)+1\big] - \frac{c}{paD}\Big[2akU_{\ell_0-1}(q)+cV_{\ell_0-1}(q)\Big]\Big[(p-r)Q_{h-\ell_1}(q)+rQ_{h-\ell_1-1}(q)\Big].$$

The same reasoning concludes that

$$\langle \mathsf{u}_i, \mathsf{v}_n \rangle = \sum_{m=1}^{\ell_0} \mathsf{u}_{i,m} + \sum_{m=\ell_0+1}^{h} \mathsf{u}_{i,m} = \frac{c}{a} - \frac{c}{aD}\big[2akU_{\ell_0-1}(q)+cV_{\ell_0-1}(q)\big]$$

and also that $\langle \mathsf{u}_n, \mathsf{v}_n \rangle = \dfrac{c}{D}U_{h-1}(q)$. □

Next we give the main result of this paper; that is, the expression of the Kirchhoff index of any homogeneous and periodic linear chain. We express it in two equivalent ways, either directly in terms of the Chebyshev polynomials of first and second kind, or in terms of $\alpha = q+\sqrt{q^2-1}$ and $\beta = q-\sqrt{q^2-1}$, the roots of the polynomial $x^2 - 2qx + 1$ in which Chebyshev polynomials can, in turns, be expressed, see "Appendix".

Theorem 2 *Given $p, h \in \mathbb{N}^*$ and $a, c > 0$, the Kirchhoff index of the homogeneous and periodic linear chain $\Gamma = \mathbb{L}_h^p(c,a)$ is*

$$\mathsf{k}^\Gamma = \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)\Big[F_1T_h(q)+F_2U_{h-1}(q)\Big]}{3c(ap+2c)\big[cT_h(q)+a(p+1)U_{h-1}(q)\big]}$$

where

$$\begin{aligned} F_1 &= 3c(ap+2c)+hc(p+1)(ap^2+3cp-a),\\ F_2 &= 2a(a-c)p^3+c(8a-3c)p^2+\big(a(a-c)+9c^2\big)p\\ &\quad +ac+hp(ap+2c)(ap^2+3cp-a). \end{aligned}$$

Equivalently,

$$\mathsf{k}^\Gamma = \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)\big[G_1\alpha^h+G_2\beta^h\big]}{6c(ap+2c)\big[(c\alpha+a-c)\alpha^h-(c\beta+a-c)\beta^h\big]},$$

where $G_1 = F_1(\alpha-\beta)+2F_2$ and $G_2 = F_1(\alpha-\beta)-2F_2$.

Proof If we consider $D = cT_h(q) + a(p+1)U_{h-1}(q)$ then,

$$\sum_{j=1}^{n}\langle \mathsf{u}_j, \mathsf{v}_j\rangle = \frac{c}{a}(n^2-1) + \frac{c}{D}U_{h-1}(q) - \frac{c}{paD}\sum_{\ell=1}^{h}\sum_{k=0}^{p-1}\Big[2akU_{\ell-1}(q) + cV_{\ell-1}(q)\Big]\Big[(p-k)Q_{h-\ell}(q) + kQ_{h-\ell-1}(q)\Big]$$
$$= \frac{c}{a}(n^2-1) + \frac{c}{D}U_{h-1}(q) - \frac{c(p-1)}{3D}\left[(p+1)\sum_{\ell=1}^{h}U_{\ell-1}(q)Q_{h-\ell}(q) + (2p-1)\sum_{\ell=1}^{h}U_{\ell-1}(q)Q_{h-\ell-1}(q)\right] - \frac{c^2}{2aD}\left[(p+1)\sum_{\ell=1}^{h}V_{\ell-1}(q)Q_{h-\ell}(q) + (p-1)\sum_{\ell=1}^{h}V_{\ell-1}(q)Q_{h-\ell-1}(q)\right].$$

Therefore, taking into account the identities of Lemma 3,

$$\sum_{j=1}^{n}\langle \mathsf{u}_j, \mathsf{v}_j\rangle = \frac{c}{a}(n^2-1) + \frac{c}{D}U_{h-1}(q) - \frac{c}{6a(ap+2c)D}\Big[\phi_1 T_h(q) + \phi_2 U_{h-1}(q)\Big],$$

where,

$$\phi_1 = (p^2-1)p_1 + (2p^2-3p+1)p_3 + 3c(p+1)p_5 + 3(p-1)p_7,$$
$$\phi_2 = (p^2-1)p_2 + (2p^2-3p+1)p_4 + 3c(p+1)p_6 + 3(p-1)p_8.$$

Therefore,

$$\mathsf{k}^{\Gamma} = \frac{n(n^2-1)}{3c} + \frac{n}{c} - \frac{na}{cD}U_{h-1}(q) + \frac{n}{6c(ap+2c)D}\Big[\phi_1 T_h(q) + \phi_2 U_{h-1}(q)\Big]$$
$$= \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)}{6c(ap+2c)D}\Big[\big(\phi_1 + 6c(ap+2c)\big)T_h(q) + \big(\phi_2 + 6ap(ap+2c)\big)U_{h-1}(q)\Big]$$

and the result follows. □

In particular when $a = c$, we get the following result.

Corollary 1 *Given $p, h \in \mathbb{N}^*$ and $c > 0$, the Kirchhoff index of the homogeneous and periodic linear chain $\Gamma = \mathbb{L}_h^p(c)$ is*

$$\mathsf{k}^{\Gamma} = \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)}{3c(p+2)U_h(p+1)}\Big[f_1 T_h(p+1) + f_2 U_{h-1}(p+1)\Big]$$

where

$$f_1 = 3(p+2) + h(p+1)(p^2+3p-1),$$
$$f_2 = 5p^2 + 9p + 1 + hp(p+2)(p^2+3p-1).$$

Equivalently,

$$\mathsf{k}^{\Gamma} = \frac{ph(ph+1)(ph+2)}{3c} + \frac{(ph+1)\Big[g_1\Big(p+1+\sqrt{p(p+2)}\Big)^h + g_2\Big(p+1-\sqrt{p(p+2)}\Big)^h\Big]}{3c(p+2)\Big[\Big(p+1+\sqrt{p(p+2)}\Big)^{h+1} - \Big(p+1-\sqrt{p(p+2)}\Big)^{h+1}\Big]}$$

where $g_1 = f_1\sqrt{p(p+2)} + f_2$ *and* $g_2 = f_1\sqrt{p(p+2)} - f_2$.

Observe that the above result for linear chains; that is, $p = 1$ and $h = n-1$ coincides with the one obtained in [2, Corollary 12] for arbitrary a, c and with the one obtained in [6, Theorem 4.1] for $a = c$.

Next we particularize the above result to the case of some relevant molecular graphs that have been studied in the literature for some particular cases.

Corollary 2 *The Kirchhoff index of the linear hexagonal chain* $\Gamma = \mathbb{L}_h^2(c,a)$ *is*

$$\mathsf{k}^{\Gamma} = \frac{4h(h+1)(2h+1)}{3c} + \frac{(2h+1)\Big[cH_1T_h(q) + H_2U_{h-1}(q)\Big]}{2c(a+c)\big[cT_h(q) + 3aU_{h-1}(q)\big]},$$

where $H_1 = 2(a+c) + 3h(a+2c)$ *and* $H_2 = 6a^2 + 5ac + 2c^2 + 4h(a+c)(a+2c)$. *Equivalently*

$$\mathsf{k}^{\Gamma} = \frac{4h(h+1)(2h+1)}{3c} + \frac{(2h+1)\Big[h_1\big(2a+c+2\sqrt{a(a+c)}\big)^h + h_2\big(2a+c-2\sqrt{a(a+c)}\big)^h\Big]}{2c(a+c)\Big[h_3\big(2a+c+2\sqrt{a(a+c)}\big)^h - h_4\big(2a+c-2\sqrt{a(a+c)}\big)^h\Big]}$$

where

$$h_1 = 2H_1\sqrt{a(a+c)} + H_2, \quad h_2 = 2H_1\sqrt{a(a+c)} - H_2,$$
$$h_3 = 3a + 2\sqrt{a(a+c)}, \qquad h_4 = 3a - 2\sqrt{a(a+c)}.$$

In particular, if $a = c$, *then*

$$\mathsf{k}^{\Gamma} = \frac{4h(h+1)(2h+1)}{3c} + \frac{(2h+1)}{4cU_h(3)}\Big[(9h+4)T_h(3) + (24h+13)U_{h-1}(3)\Big],$$

or equivalently

$$\mathsf{k}^{\Gamma} = \frac{4h(h+1)(2h+1)}{3c} + \frac{(2h+1)\Big[\varphi_1\big(3+2\sqrt{2}\big)^h + \varphi_2\big(3-2\sqrt{2}\big)^h\Big]}{4c\Big[\big(3+2\sqrt{2}\big)^{h+1} - \big(3-2\sqrt{2}\big)^{h+1}\Big]},$$

where $\varphi_1 = 2(9h+4)\sqrt{2} + 24h + 13$ *and* $\varphi_2 = 2(9h+4)\sqrt{2} - 24h - 13$.

The above formula for the Kirchhoff index of $\mathbb{L}_h^2(c)$ basically coincides with the formula given in [6, Theorem 3.7]. We remark that there is an errata in the formula (3.10) of the mentioned paper, since the factor in the divisor must be 8 instead 4. However, the values of Table I were obtained using the correct factor.

Appendix

If for any $k \in \mathbb{Z}$, T_k and U_k are the kth Chebyshev polynomials of first and second kind respectively, see [4], it is well-known that for any sequence of Chebyshev polynomials $\{P_k\}_{k\in\mathbb{Z}}$; that is, polynomials satisfying the recurrence relation $P_{k+2}(z) = 2zP_{k+1}(z) - P_k(z)$, $k \in \mathbb{Z}$, there exist $A, B \in \mathbb{R}$ such that $P_k = AT_k + BU_{k-1}$ for any $k \in \mathbb{Z}$. Moreover, as $q = 1 + c^{-1}ap > 1$, since the values

$$\begin{aligned}\alpha &= q + \sqrt{q^2-1} = c^{-1}\big(ap + c + \sqrt{ap(ap+2c)}\big)\\ \beta &= q - \sqrt{q^2-1} = c^{-1}\big(ap + c - \sqrt{ap(ap+2c)}\big)\end{aligned} \tag{5}$$

are the roots of the polynomial $x^2 - 2qx + 1$, each Chebyshev sequence can be expressed as a linear combination of the sequences $\{\alpha^k\}_{k\in\mathbb{Z}}$ and $\{\beta^k\}_{k\in\mathbb{Z}}$. Specifically, it is also well-known, see newly [4], that

$$T_k(q) = \frac{1}{2}\big(\alpha^k + \beta^k\big) \quad \text{and} \quad U_k(q) = \frac{1}{\alpha-\beta}\big(\alpha^{k+1} - \beta^{k+1}\big), \quad k \in \mathbb{Z}, \tag{6}$$

which in particular implies that $T_k(q) > 0$ for any $k \in \mathbb{Z}$ and $U_k(q) > 0$ for any $k \in \mathbb{N}$, since $0 < \beta < 1 < \alpha$ (and $\alpha\beta = 1$).

Lemma 1 *For any* $k \in \mathbb{Z}$ *the following identities hold:*

$$T_{k\pm1}(q) = qT_k(q) \pm (q^2-1)U_{k-1}(q) \qquad \textit{and} \qquad U_k(q) = T_k(q) + qU_{k-1}(q).$$

Moreover

$$U_k(q)U_m(q) = \frac{1}{2(q^2-1)}\Big[T_{k+m+2}(q) - T_{k-m}(q)\Big], \quad k, m \in \mathbb{Z}$$

and given $m \geq 1$,

$$\sum_{k=1}^{m} T_{m-2k}(q) = \sum_{k=1}^{m} T_{m+2-2k}(q) = qU_{m-1}(q),$$
$$\sum_{k=1}^{m} T_{m+1-2k}(q) = U_{m-1}(q)$$
$$\sum_{k=1}^{m} T_{m-1-2k}(q) = \big(2(q^2-1)+1\big)U_{m-1}(q).$$

Lemma 2 *If* $\{P_k(q)\}_{k\in\mathbb{Z}}$ *is a Chebyshev sequence, then for any* $A, B \in \mathbb{R}$, *and* $r, t \in \mathbb{N}^*$ *such that* $t \leq r$

$$\sum_{k=t}^{r}(Ak+B)P_k(q) = \frac{c}{2pa}(Ar+B)\big(P_{r+1}(q) - P_r(q)\big) - \frac{c}{2pa}(At+B)\big(P_t(q) - P_{t-1}(q)\big) + \frac{cA}{2pa}\big(P_t(q) - P_r(q)\big).$$

The following relations between the polynomials defined in (4), are very useful throughout the paper. All of them are consequence of Lemma 1.

Lemma 3 *For any* $m \in \mathbb{Z}$ *we have*

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

In addition,

$$\sum_{\ell=1}^{h} U_{\ell-1}(q)Q_{h-\ell}(q) = \frac{1}{2a(ap+2c)}\big[p_1T_h(q) + p_2U_{h-1}(q)\big],$$
$$\sum_{\ell=1}^{h} U_{\ell-1}(q)Q_{h-\ell-1}(q) = \frac{1}{2a(ap+2c)}\big[p_3T_h(q) + p_4U_{h-1}(q)\big]$$
$$\sum_{\ell=1}^{h} V_{\ell-1}(q)Q_{h-\ell}(q) = \frac{1}{(ap+2c)}\big[p_5T_h(q) + p_6U_{h-1}(q)\big],$$
$$\sum_{\ell=1}^{h} V_{\ell-1}(q)Q_{h-\ell-1}(q) = \frac{1}{c(ap+2c)}\big[p_7T_h(q) + p_8U_{h-1}(q)\big]$$

where,

$$p_1 = ch(2ap + a + 2c), \qquad p_2 = ah(2p + 1)(ap + 2c) + c(a - 2c),$$
$$p_3 = hc(2c - a), \qquad p_4 = ha(ap + 2c) + 2(a - c)(ap + c) + ac,$$
$$p_5 = hc(p + 1), \qquad p_6 = hp(ap + 2c) + c(p + 1),$$
$$p_7 = hc\big((a - c)p + c\big), \qquad p_8 = c^2 - p(a - c)(h(ap + 2c) - c).$$

References

1. A. Carmona, A.M. Encinas, M. Mitjana, Green matrices associated with generalized linear polyominoes. Linear Algebra Appl. **468**, 38–47 (2015)
2. A. Carmona, A.M. Encinas, M. Mitjana, Effective resistances for ladder-like chains. Int. J. Quantum Chem. **114**, 1670–1677 (2014)
3. D.J. Klein, M. Randiĉ, Resistance distance. J. Math. Chem. **12**, 81–95 (1993)
4. J.C. Mason, D.C. Handscomb, *Chebyshev Polynomials* (Chapman and Hall/CRC, London, 2003)
5. W. Xiao, I. Gutman, Resistance distance and Laplacian spectrum. Theor. Chem. Acc. **110**, 284–289 (2003)
6. Y. Yang, H. Zhang, Kirchhoff index of linear hexagonal chains. Int. J. Quantum Chem. **108**, 503–512 (2008)
7. H. Zhang, Y. Yang, C. Li, Kirchhoff index of composite graphs. Discrete Appl. Math. **157**, 2918–2927 (2009)