Theor Chem Acc (2003) 110: 284–289
DOI 10.1007/s00214-003-0460-4

Theoretical
Chemistry Accounts

Regular article

Resistance distance and Laplacian spectrum

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Received: 16 March 2003 / Accepted: 12 May 2003 / Published online: 16 September 2003

Abstract. The resistance distance r_{ij} between two vertices v_i and v_j of a (connected, molecular) graph G is equal to the resistance between the respective two points of an electrical network, constructed so as to correspond to G, such that the resistance of any two adjacent points is unity. We show how the matrix elements r_{ij} can be expressed in terms of the Laplacian eigenvalues and eigenvectors of G. In addition, we determine certain properties of the resistance matrix $\mathbf{R} = ||r_{ij}||$.

Keywords: Resistance distance – Kirchhoff index – Laplacian spectrum

1 Introduction

The standard distance between two vertices v_i and v_j of a (connected) graph G, denoted by d_{ij}, is defined as the length (number of edges) of a shortest path that connects v_i and v_j [1]. The vertex–distance concept found numerous chemical applications [2, 3]. In order to examine other possible metrics in (molecular) graphs, Klein and Randić [4] proposed considering the resistance distance between the vertices of a graph G, denoted by r_{ij}, defined to be the effective electrical resistance between nodes i and j of a network N corresponding to G, with unit resistors taken between nodes i and j of a network N corresponding to G, with unit resistors taken between nodes of N whenever the corresponding site of G (namely v_i and v_j) are connected by an edge. The quantities r_{ij} are computed by methods of the theory of resistive electrical networks (based on Ohm's and Kirchhoff's laws). For acyclic graphs $r_{ij} = d_{ij}$ and therefore the resistance distances are primarily of interest in the case of cycle–containing (molecular) graphs.

The resistance–distance concept was much studied in the chemical literature [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14].

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In analogy to the classical Wiener index [2, 3], one introduced [4] the sum of resistance distances of all pairs of vertices of a molecular graph,

$$Kf = \sum_{i<j} r_{ij} \tag{1}$$

a structure–descriptor that eventually was named [5] the "Kirchhoff index".

The matrix whose (i, j) of entry is r_{ij} is called the resistance matrix (of the respective graph G), and will be denoted by $\mathbf{R}$. Evidently, $\mathbf{R}$ is symmetric, has a zero diagonal, and its order coincides with the number n of vertices of G.

Within the theory of electrical networks the standard method to compute the resistance matrix is via the Moore–Penrose generalized inverse $\mathbf{L}^{\dagger}$ of the Laplacian matrix of the underlying graph G:

$$r_{ij} = (L^{\dagger})_{ii} + (L^{\dagger})_{jj} - (L^{\dagger})_{ij} - (L^{\dagger})_{ji} \ . \tag{2}$$

Recall that the Laplacian matrix is singular and, therefore, has no usual inverse. More on the Moore–Penrose generalized inverse of a (singular) matrix can be found elsewhere [7, 15, 16]. Equation (2) was stated already in Refs. [4, 6], but was, for sure, known much earlier.

Because the Moore–Penrose generalized inverse of a singular matrix is not a concept familiar to most theoretical chemists, efforts have been made to express r_{ij} in terms of the inverse of some nonsingular matrix [4, 17, 18]. Such a matrix has, indeed, been found [13].

Let G be a graph and let its vertices be labeled by $v_1, v_2, \ldots, v_n$. The Laplacian matrix of G, denoted by $\mathbf{L}$, is a square matrix of order n whose (i, j) entry is defined by

$$L_{ij} = \begin{cases} -1 & \text{if } i \neq j \text{ and the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j \text{ and the vertices } v_i \text{ and } v_j \text{ are not adjacent} \\ d_i & \text{if } i = j \end{cases} , \tag{3}$$

where d_i is the degree (number of first neighbors) of the vertex v_i.

By $\mathbf{J}$ we denote the square matrix of order n all of whose elements are unity. Then for all connected graphs (with two or more vertices) the matrix $\mathbf{L}+\frac{1}{n}\mathbf{J}$ is non-singular, its inverse

$$\mathbf{X} = ||x_{ij}|| = (\mathbf{L}+\frac{1}{n}\mathbf{J})^{-1}$$

exists, and [13]

$$r_{ij} = x_{ii} + x_{jj} - 2x_{ij} \quad . \tag{4}$$

In this work we determine some basic properties of the matrix $\mathbf{X}$ and, in particular, show that its eigenvalues and eigenvectors are closely related to the Laplacian eigenvalues and eigenvectors. Using these results we then express the resistance distance r_{ij} in terms of the Laplacian eigenvalues and eigenvectors, and establish a number of additional properties of the resistance matrix $\mathbf{R}$. To do this we first remind the readers of a few results from Laplacian graph spectral theory.

2 Laplacian spectral theory

Laplacian spectral theory is a well elaborated part of algebraic graph theory and its details can be found in numerous reviews, for instance in Refs. [19, 20, 21, 22, 23, 24].

The Laplacian matrix $\mathbf{L}$ of the graph G is defined via Eq. (3). Its eigenvalues and eigenvectors are referred to as the Laplacian eigenvalues and Laplacian eigenvectors of G. These will be denoted by $\mu_1, \mu_2, \ldots, \mu_n$ and $U_1, U_2, \ldots, U_n$, respectively, so that the equalities

$$\mathbf{L}U_i = \mu_i U_i \tag{5}$$

are satisfied for $i = 1, 2, \ldots, n$. We label the Laplacian eigenvalues so that

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n \quad .$$

Then, μ_n is always equal to zero, whereas μ_{n-1} differs from zero if and only if the underlying graph G is connected. Consequently, the Laplacian matrix of any graph is singular, and its inverse does not exist. (We are interested in molecular graphs, that necessarily are connected. Therefore in what follows it will be understood that $\mu_{n-1} \neq 0$.)

According to Eq. (5), the eigenvectors U_i are n-dimensional column vectors. We choose them to be normalized, real–valued and mutually orthogonal, and denote their components so that $U_i = (u_{i1}, u_{i2}, \ldots, u_{in})^{\mathrm{t}}$. Here and later the superscript t indicates transposition.

In the notation just introduced, we have

$$\mathbf{U}\mathbf{L}\mathbf{U}^{\mathrm{t}} = \mathrm{diag}\ [\mu_1, \mu_2, \ldots, , \mu_{n-1}, \mu_n] \tag{6}$$

where $\mathbf{U} = ||u_{ij}||$ is an orthogonal (in the general case: unitary) matrix, i. e.,

$$\mathbf{U}\mathbf{U}^{\mathrm{t}} = \mathbf{U}^{\mathrm{t}}\mathbf{U} = \mathbf{I}$$

i.e.,

$$\sum_{k=1}^{n} u_{ik}u_{jk} = \sum_{k=1}^{n} u_{ki}u_{kj} = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases} \quad . \tag{7}$$

From Eq. (6) follows $\mathbf{L} = \mathbf{U}^{\mathrm{t}}\mathrm{diag}\ [\mu_1, \mu_2, \ldots, , \mu_{n-1}, \mu_n]\mathbf{U}$ which is tantamount to

$$L_{ij} = \sum_{k=1}^{n} \mu_k u_{ki} u_{kj} \quad .$$

Because $\mu_n = 0$,

$$L_{ij} = \sum_{k=1}^{n-1} \mu_k u_{ki} u_{kj} \quad . \tag{8}$$

The sum of the components of the Laplacian eigenvector U_i will be denoted by $\sigma(U_i)$.

Let $\mathbf{1}$ and $\mathbf{0}$ be the n-dimensional column vectors whose components are equal to zero and unity, respectively. Then, directly from the definition (Eq. 3) follows $\mathbf{L1} = \mathbf{0}$, i.e.,

$$\mathbf{L1} = 0 \cdot \mathbf{1}$$

This means that the (normalized) Laplacian eigenvector corresponding to the eigenvalue zero is of the form $U_n = (1/\sqrt{n})\mathbf{1}$, and $\sigma(U_n) = \sqrt{n}$. Because all other Laplacian eigenvectors are orthogonal to U_n their σ values are zero. Thus we have

$$\sigma(U_i) = \begin{cases} 0 & \text{if} \quad i = 1, 2, \ldots, n-1 \\ \sqrt{n} & \text{if} \quad i = n \end{cases} \quad . \tag{9}$$

Of the many known relations between the structure of a graph and its Laplacian spectrum [19, 20, 21, 22, 23, 24] we mention here only one:

$$\prod_{k=1}^{n-1} \mu_k = nt(G) \quad , \tag{10}$$

where $t(G)$ is the number of spanning trees of the graph G.

3 The spectrum of matrix X

We first show that the matrix $\mathbf{U}$, occurring in Eq. (6), diagonalizes also the matrix $\mathbf{J}$. Indeed,

$$\begin{aligned} (\mathbf{U}\mathbf{J}\mathbf{U}^{t})_{ij} &= \sum_{k}\sum_{\ell} (\mathbf{U})_{ik}(\mathbf{J})_{k\ell}(\mathbf{U}^{\mathrm{t}})_{\ell j} \\ &= \sum_{k}\sum_{\ell} u_{ik}J_{k\ell}u_{j\ell} \\ &= \sum_{k}\sum_{\ell} u_{ik}u_{j\ell} \\ &= \left(\sum_{k} u_{ik}\right)\left(\sum_{\ell} u_{j\ell}\right) = \sigma(U_i)\sigma(U_j) \quad . \end{aligned}$$

Therefore, in view of Eq. (9),

$$(\mathbf{U}\mathbf{J}\mathbf{U}^{\mathrm{t}})_{ij} = \begin{cases} n & \text{if } i = j = n \\ 0 & \text{otherwise} \end{cases}$$

i. e.,

$$\mathbf{U}\mathbf{J}\mathbf{U}^{\mathrm{t}} = \mathrm{diag}\ [0, 0, \ldots, 0, n] \quad . \tag{11}$$

From Eqs. (6) and (11) we now readily obtain the following.

Theorem 1. Let G be a graph on n vertices, $n \geq 2$, and let $\mu_1, \mu_2, \ldots, \mu_{n-1}, \mu_n = 0$ be its Laplacian eigenvalues. Then the eigenvalues of the matrix $\mathbf{L} + \frac{1}{n}\mathbf{J}$ are $\mu_1, \mu_2, \ldots, \mu_{n-1}, 1$.

Proof. It is sufficient to show that $\mathbf{U}$ diagonalizes $\mathbf{L} + \frac{1}{n}\mathbf{J}$:

$$\begin{aligned}\mathbf{U}(\mathbf{L} + \frac{1}{n}\mathbf{J})\mathrm{U}^{\mathrm{t}} &= \mathbf{U}\mathbf{L}\mathbf{U}^{t} + \frac{1}{n}\mathbf{U}\mathbf{J}\mathbf{U}^{t} \\ &= \mathrm{diag}\ [\mu_1, \mu_2, \ldots, \mu_{n-1}, 0] \\ &\quad + \frac{1}{n}\mathrm{diag}\ [0, 0, \ldots, 0, n] \\ &= \mathrm{diag}\ [\mu_1, \mu_2, \ldots, \mu_{n-1}, 1]\ .\end{aligned}$$

Theorem 2. If the graph G, specified in theorem 1, is connected, then

1. The matrix $\mathbf{X} = ||x_{ij}|| = (\mathbf{L} + \frac{1}{n}\mathbf{J})^{-1}$ exists.
2. The eigenvalues of $\mathbf{X}$ are $1/\mu_1, 1/\mu_2, \ldots, 1/\mu_{n-1}, 1$.
3. The eigenvectors of $\mathbf{X}$ coincide with the Laplacian eigenvectors $U_1, U_2, \ldots, U_{n-1}, U_n$ of G.
4.

$$x_{ij} = \frac{1}{n} + \sum_{k=1}^{n-1} \frac{1}{\mu_k} u_{ki} u_{kj} \tag{12}$$

and, in particular,

$$x_{ii} = \frac{1}{n} + \sum_{k=1}^{n-1} \frac{u_{ki}^2}{\mu_k} > 0\ . \tag{13}$$

5.

$$\sum_{i=1}^{n} x_{ii} = 1 + \sum_{k=1}^{n-1} \frac{1}{\mu_k}\ . \tag{14}$$

Proof. Statements 1–3 are immediate consequences of theorem 1. In order to obtain statement (4) note that

$$\mathbf{X} = \mathbf{U}^{\mathrm{t}}\mathrm{diag}\left[\frac{1}{\mu_1}, \frac{1}{\mu_2}, \ldots, \frac{1}{\mu_{n-1}}, 1\right]\mathbf{U}$$

and recall that $u_{ni} = 1/\sqrt{n}$ for all $i = 1, 2, \ldots, n$.

The left–hand side of Eq. (14) is the trace of the matrix $\mathbf{X}$, equal to the sum of its eigenvalues.

4 Resistance distance and Kirchhoff index in terms of Laplacian eigenvalues and eigenvectors

In this section we state three corollaries of theorem 2, connecting the resistance distances with Laplacian spectral theory.

Substituting Eqs. (12) and (13) back into Eq. (4), one straightforwardly arrives at a noteworthy result, by means of which the resistance distance is expressed in terms of the eigenvalues and eigenvectors of the Laplacian matrix:

Corollary 2.1. For any connected n-vertex graph, $n \geq 2$,

$$r_{ij} = \sum_{k=1}^{n-1} \frac{1}{\mu_k}(u_{ki} - u_{kj})^2\ . \tag{15}$$

Needless to say that Eq. (15) provides a direct and easy route for computing the resistance distances in any molecular graph. A result equivalent to corollary 2.1 was earlier deduced by Klein (see Eq. (3.3) in Ref. [8]).

Bearing in mind that $\mu_1 \geq \mu_k \geq \mu_{n-1}$ holds for $k = 2, \ldots, n-2$, and taking into account the relations in Eq. (7), we estimate the resistance distance as follows:

Corollary 2.2. For any connected n-vertex graph, $n \geq 2$, and for $i \neq j$,

$$\frac{2}{\mu_1} \leq r_{ij} \leq \frac{2}{\mu_{n-1}}\ .$$

Corollary 2.3. For any connected n-vertex graph, $n \geq 2$, the Kirchhoff index, Eq. (1), is expressed in terms of Laplacian eigenvalues as follows:

$$Kf = n\sum_{k=1}^{n-1} \frac{1}{\mu_k}\ . \tag{16}$$

Proof. Starting with Eq. (1) and using (15) we get

$$\begin{aligned}Kf &= \sum_{i<j} r_{ij} = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} r_{ij} = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left[\sum_{k=1}^{n-1}\frac{1}{\mu_k}(u_{ki} - u_{kj})^2\right] \\ &= \frac{1}{2}\sum_{k=1}^{n-1}\frac{1}{\mu_k}\left[n\sum_{i=1}^{n}u_{ki}^2 + n\sum_{j=1}^{n}u_{kj}^2 - 2\left(\sum_{i=1}^{n}u_{ki}\right)\left(\sum_{j=1}^{n}u_{kj}\right)\right] \\ &= \frac{1}{2}\sum_{k=1}^{n-1}\frac{1}{\mu_k}\left[n\sum_{i=1}^{n}u_{ki}^2 + n\sum_{j=1}^{n}u_{kj}^2 - 2\sigma(U_k)\sigma(U_k)\right]\ .\end{aligned}$$

Equation (16) is now obtained by taking into account Eqs. (7) and (9). Equation (16) was reported earlier [7], but was deduced using a completely different way of reasoning.

5 On the determinant of the resistance matrix

In this section we consider the determinant of the resistance matrix $\mathbf{R} = ||r_{ij}||$. In view of Eq. (4), this matrix can be written as

$$\begin{aligned}\mathbf{R} &= \mathrm{diag}\ [x_{11}, x_{22}, \ldots, x_{nn}]\mathbf{J} \\ &\quad + \mathbf{J}\ \mathrm{diag}\ [x_{11}, x_{22}, \ldots, x_{nn}] - 2\mathbf{X}\ .\end{aligned} \tag{17}$$

Then

$$\begin{aligned}\mathbf{U}\mathbf{R}\mathbf{U}^{\mathrm{t}} &= (\mathbf{U}\ \mathrm{diag}[x_{11}, x_{22}, \ldots, x_{nn}]\mathbf{U}^{\mathrm{t}})(\mathbf{U}\mathbf{J}\mathbf{U}^{\mathrm{t}}) \\ &\quad + (\mathbf{U}\mathbf{J}\mathbf{U}^{\mathrm{t}})(\mathbf{U}\ \mathrm{diag}\ [x_{11}, x_{22}, \ldots, x_{nn}]\mathbf{U}^{\mathrm{t}}) \\ &\quad - 2\mathbf{U}\mathbf{X}\mathbf{U}^{\mathrm{t}}\end{aligned}$$

and by taking into account Eq. (11) and theorem 2,

$$(\mathbf{URU}^{\mathrm{t}})_{ij}=\begin{cases}-2/\mu_i & \text{for } i=j\,,\ 1\le i\le n-1\\ 0 & \text{for } i\ne j\,,\ 1\le i,j\le n-1\\ n\sum_{k=1}^{n}x_{kk}u_{ik}u_{nk} & \text{for } j=n\,,\ 1\le i\le n-1\\ n\sum_{k=1}^{n}x_{kk}u_{nk}u_{jk} & \text{for } i=n\,,\ 1\le j\le n-1\\ -2+2n\sum_{k=1}^{n}x_{kk}u_{nk}^2 & \text{for } i=j=n\end{cases}$$

Using Eq. (14) and the fact that $u_{nk}=1/\sqrt{n}$, $k=1,2,\ldots,n$, the previous expressions are simplified as

$$(\mathbf{URU}^{\mathrm{t}})_{ij}=\begin{cases}-2/\mu_i & \text{for } i=j\ ,\ 1\le i\le n-1\\ 0 & \text{for } i\ne j\ ,\ 1\le i,j\le n-1\\ \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{ik} & \text{for } j=n\ ,\ 1\le i\le n-1\\ \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{jk} & \text{for } i=n\ ,\ 1\le j\le n-1\\ 2\sum_{k=1}^{n-1}(1/\mu_k) & \text{for } i=j=n\end{cases}$$

The determinant of the resistance matrix $\mathbf{R}$ is thus

$$\det\mathbf{R}=\begin{vmatrix}-2/\mu_1 & 0 & \cdots & 0 & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{1k}\\ 0 & -2/\mu_2 & \cdots & 0 & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{2k}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \cdots & -2/\mu_{n-1} & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{n-1,k}\\ \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{1k} & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{2k} & \cdots & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{n-1,k} & 2\sum_{k=1}^{n-1}(1/\mu_k)\end{vmatrix}\ .$$

By a pertinent linear combination of the rows of this determinant, it can be transformed into

$$\det\mathbf{R}=\begin{vmatrix}-2/\mu_1 & 0 & \cdots & 0 & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{1k}\\ 0 & -2/\mu_2 & \cdots & 0 & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{2k}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \cdots & -2/\mu_{n-1} & \sqrt{n}\sum_{k=1}^{n}x_{kk}u_{n-1,k}\\ 0 & 0 & \cdots & 0 & S+2\sum_{k=1}^{n-1}1/\mu_k\end{vmatrix}$$

where

$$S=\frac{n}{2}\sum_{k=1}^{n-1}\mu_k\left(\sum_{i=1}^{n}x_{ii}u_{ki}\right)^2\ .$$

Therefore

$$\det\mathbf{R}=\left(S+2\sum_{k=1}^{n-1}\frac{1}{\mu_k}\right)\prod_{i=1}^{n-1}\left(-\frac{2}{\mu_i}\right)$$

$$=(-1)^{n-1}\frac{2^{n-1}}{nt(G)}\left(S+2\sum_{k=1}^{n-1}\frac{1}{\mu_k}\right)$$

where $t(G)$ is the number of spanning trees of the graph G, see Eq. (10).

For connected graphs with at least two vertices, $S\ge 0$, whereas $\sum_{i=1}^{n-1}1/\mu_i=Kf/n$ is strictly positive-valued. Therefore $S+2\sum_{k=1}^{n-1}\frac{1}{\mu_k}>0$, implying that $\det\mathbf{R}$ is always different from zero. In other words the resistance matrix of any connected graphs (with at least two vertices) is nonsingular.

The sign of $\det\mathbf{R}$ depends solely on the parity of the number of vertices of G. As shown in the subsequent section, this property of $\det\mathbf{R}$ is a consequence of the fact that the resistance matrix has a single positive eigenvalue, and $n-1$ negative eigenvalues.

Bearing in mind Eq. (8) we have

$$\sum_{k=1}^{n-1}\mu_k\left(\sum_{i=1}^{n}x_{ii}u_{ki}\right)^2=\sum_{k=1}^{n-1}\sum_{i=1}^{n}\sum_{j=1}^{n}\mu_k(x_{ii}u_{ki})(x_{jj}u_{kj})$$

$$=\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ii}x_{jj}\left(\sum_{k=1}^{n-1}\mu_k u_{ki}u_{kj}\right)$$

$$=\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ii}x_{jj}L_{ij}$$

and therefore the auxiliary quantity S is in the following manner related to the Laplacian matrix $\mathbf{L}$:

$$S=\frac{n}{2}(x_{11},x_{22},\ldots,x_{nn})\mathbf{L}(x_{11},x_{22},\ldots,x_{nn})^{\mathrm{t}}\ . \tag{18}$$

The results obtained in this section can be summarized as

Theorem 3. Let G be a graph specified in theorem 1, possessing $t(G)>0$ spanning trees. Then the determinant of its resistance matrix is equal to

$$(-1)^{n-1}\frac{2^{n-1}}{nt(G)}\left(S+2\sum_{k=1}^{n-1}\frac{1}{\mu_k}\right) ,$$

where S is given by Eq. (18).

Recall that the matrix elements $x_{11}, x_{22}, \ldots, x_{nn}$ can be computed via Eq. (13). We thus see that by means of theorem 3 the determinant of the resistance matrix is expressed solely in terms of Laplacian eigenvalues and eigenvectors.

6 Estimating the eigenvalues of the resistance matrix

In this section we establish bounds for the eigenvalues of the resistance matrix $\mathbf{R}$ and determine the number of positive and negative eigenvalues.

Let $\mathbf{M}$ denote any symmetric real square matrix of order n and let $\lambda_1(\mathbf{M}) \geq \lambda_2(\mathbf{M}) \geq \cdots \geq \lambda_n(\mathbf{M})$ be its eigenvalues.

Consider first the matrix $\mathbf{B}$ whose (i,j) entry is equal to $x_{ii}+x_{jj}$. Thus, $\mathbf{B}$ is symmetric and all its elements are positive-valued, see Eq. (13). Therefore all eigenvalues of $\mathbf{B}$ are real.

The matrix $\mathbf{B}$ can also be written in the form

$$\mathbf{B} = \mathrm{diag}[x_{11}, x_{22}, \ldots, x_{nn}]\mathbf{J} + \mathbf{J}\mathrm{diag}[x_{11}, x_{22}, \ldots, x_{nn}] \tag{19}$$

which should be compared with Eq. (17).

Since the rank of the matrix $\mathbf{J}$ is 1, the rank of $\mathbf{B}$ is less than or equal to 2. Hence $\lambda_k(\mathbf{B}) = 0$ for $k = 2, \ldots, n-1$.

The eigenvalues $\lambda_1(\mathbf{B})$ and $\lambda_n(\mathbf{B})$ are determined by the conditions

$$\begin{aligned}\lambda_1(\mathbf{B}) + \lambda_n(\mathbf{B}) &= 2\sum_{i=1}^{n} x_{ii} \\ \lambda_1(\mathbf{B}) \cdot \lambda_n(\mathbf{B}) &= \sum_{i<j}\begin{vmatrix} 2x_{ii} & x_{ii}+x_{jj} \\ x_{ii}+x_{jj} & 2x_{jj}\end{vmatrix} \\ &= -\sum_{i<j}(x_{ii}-x_{jj})^2 \ . \end{aligned} \tag{20}$$

Bearing in mind statements 4 and 5 of theorem 2, we see that $\lambda_1(\mathbf{B})$ is positive-valued whereas $\lambda_n(\mathbf{B}) \leq 0$. Furthermore, $\lambda_n(\mathbf{B})$ is zero if and only if the conditions $x_{11} = x_{22} = \cdots = x_{nn}$ are satisfied, and is strictly negative otherwise.

Theorem 4. Let G be a connected graph on n vertices, $n \geq 2$. Let μ_1 and μ_{n-1} be, respectively, the greatest and smallest positive Laplacian eigenvalue of G. Then the eigenvalues $\lambda_1(\mathbf{R}), \lambda_2(\mathbf{R}), \ldots, \lambda_n(\mathbf{R})$ of the resistance matrix $\mathbf{R}$ satisfy the inequalities

$$\lambda_1(B) + \min(-2/\mu_{n-1}, -2) \leq \lambda_1(\mathbf{R}) \leq \lambda_1(\mathbf{B}) - 2/\mu_1 \ , \tag{21}$$

$$\min(-2/\mu_{n-1}, -2) \leq \lambda_k(\mathbf{R}) \leq -2/\mu_1; \quad k = 2, \ldots, n-1 \ , \tag{22}$$

$$\lambda_n(\mathbf{B}) + \min(-2/\mu_{n-1}, -2) \leq \lambda_n(\mathbf{R}) \leq \lambda_n(\mathbf{B}) - 2/\mu_1 \ . \tag{23}$$

Proof. Bearing in mind Eqs. (17) and (19), by theorem 4.3.1 in Ref. [25] we have for $k = 1, 2, \ldots, n$

$$\lambda_k(\mathbf{B}) + \lambda_n(-2\mathbf{X}) \leq \lambda_k(\mathbf{R}) \leq \lambda_k(\mathbf{B}) + \lambda_1(-2\mathbf{X}) \ .$$

By theorem 2, $\lambda_n(-2\mathbf{X}) = \min(-2/\mu_{n-1}, -2)$ and $\lambda_1(-2\mathbf{X}) = \max(-2/\mu_1, -2)$.

For every connected graph with at least two vertices, $\mu_1 \geq 2$. Therefore $\max(-2/\mu_1, -2) = -2/\mu_1$, and the bounds (Eqs. 21, 23) follow.

The inequalities (Eq. 22) hold because $\lambda_k(\mathbf{B}) = 0$ for $k = 2, \ldots, n-1$.

From Eqs. (22) and (23) it is evident that all the eigenvalues $\lambda_k(\mathbf{R})$, $k = 2, \ldots, n$, are negative-valued. That $\lambda_1(\mathbf{R})$ is always greater than zero follows from the fact that already its lower bound $\lambda_1(\mathbf{B}) + \min(-2/\mu_{n-1}, -2)$ is positive-valued. To see this note that by Eq. (20)

$$\lambda_1(\mathbf{B}) \geq 2\sum_{i=1}^{n} x_{ii}$$

and then by Eq. (14)

$$\begin{aligned}&\lambda_1(\mathbf{B}) + \min(-2/\mu_{n-1}, -2) \\ &\quad \geq 2\left(1 + \sum_{k=1}^{n-1}\frac{1}{\mu_k}\right) + \min(-2/\mu_{n-1}, -2) > 0 \ .\end{aligned}$$

By this we proved.

Corollary 4.1. The resistance matrix of any connected graph on n vertices, $n \geq 2$, has exactly one positive eigenvalue and exactly $n-1$ negative eigenvalues.

Acknowledgements. This research was supported by the Natural Science Foundation of China and Fujian Province, and by the Ministry of Sciences, Technologies and Development of Serbia, within Project no. 1389. The authors thank Douglas J. Klein (Galveston) for useful comments.

References

1. Buckley F, Harary F (1990) Distance in graphs. Addison–Wesley, Redwood
2. Lučić B, Lukovits I, Nikolić S, Trinajstić N (2001) J Chem Inf Comput Sci 41:527
3. Dobrynin AA, Entringer R, Gutman I (2001) Acta Appl Math 66:211
4. Klein DJ, Randić M (1993) J Math Chem 12:81
5. Bonchev D, Balaban AT, Liu X, Klein DJ (1994) Int J Quantum Chem 50:1
6. Zhu HY, Klein DJ, Lukovits I (1996) J Chem Inf Comput Sci 36:420
7. Gutman I, Mohar B (1996) J Chem Inf Comput Sci 36:982
8. Klein DJ (1997) MATCH – Commun Math Comput Chem 35:7
9. Lukovits I, Nikolić S, Trinajstić N (1999) Int J Quantum Chem 71:217
10. Klein DJ, Ivanciuc O (2001) J Math Chem 30:271
11. Palacios JL (2001) Int J Quantum Chem 81:9
12. Klein DJ (2002) Croat Chem Acta 75:633
13. Babić D, Klein DJ, Lukovits I, Nikolić S, Trinajstić N (2002) Int J Quantum Chem 90:161
14. Xiao WJ, Gutman I (2003) MATCH – Commun Math Comput Chem 49:000
15. Ben–Israel A, Greville TNE (1974) Generalized inverses – theory and applications. Wiley, New York

16. Campbell SL, Meyer CD (1979) Generalized inverses of linear transformations. Pitman, London
17. Kunz M (1995) MATCH – Commun Math Comput Chem 32:221
18. Kunz M (1886) J Chem Inf Comput Sci 36:822
19. Grone R, Merris R, Sunder VS (1990) SIAM J Matrix Anal Appl 11:218
20. Mohar B (1991) In: Alavi Y, Chartrand G, Oellermann OR, Schwenk AJ (eds) Graph theory, combinatorics, and applications. Wiley, New York, pp 871–898
21. Grone R, Merris R (1994) SIAM J Discr Math 7:221
22. Merris R (1994) Lin Algebra Appl 197:43
23. Merris R (1995) Lin Multilin Algebra 39:19
24. Mohar B (1997) In: Hahn G, Sabidussi G (eds) Graph symmetry. Kluwer, Dordrecht, pp 225–275
25. Horn RA, Johnson CR (1985) Matrix analysis. Cambridge University Press, Cambridge