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The tau constant and the discrete Laplacian matrix of a metrized graph

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ABSTRACT

We express the tau constant of a metrized graph in terms of the discrete Laplacian matrix and its pseudo-inverse.

1. Introduction

Metrized graphs are finite graphs equipped with a distance function on their edges. For a metrized graph Γ, the tau constant $\tau(\Gamma)$ is an invariant which plays important roles in both harmonic analysis on metrized graphs and arithmetic of curves.

Chinburg and Rumely [7] introduced a canonical measure μ_{can} of total mass 1 on a metrized graph Γ. The diagonal values of the Arakelov–Green's function $g_{\mu_{can}}(x, x)$ associated with μ_{can} are constant on Γ. Baker and Rumely called this constant "the tau constant" of a metrized graph Γ, and denoted it by $\tau(\Gamma)$. In [2, Conjecture 14.5], they posed a conjecture concerning the existence of a universal lower bound for $\tau(\Gamma)$. We call it Baker and Rumely's lower bound conjecture.

Baker and Rumely [2] introduced a measure valued Laplacian operator Δ which extends Laplacian operators studied earlier in [7,20]. This Laplacian operator combines the "discrete" Laplacian on a finite graph and the "continuous" Laplacian $-f''(x)dx$ on $\mathbb{R}$. In terms of spectral theory, the tau constant $\tau(\Gamma)$ is the trace of the inverse operator of Δ with respect to μ_{can} when Γ has total length 1.

The results in [21], [8, Chapter 4] and [9] indicate that the tau constant has important applications in arithmetic of curves such as its connection to the Effective Bogomolov Conjecture over function fields.

In the article [10], various formulas for $\tau(\Gamma)$ are given, and Baker and Rumely's lower bound conjecture is verified for a number of large families of graphs. It is shown in the article [11] that this conjecture holds for metrized graphs with edge connectivity more than 4; and that proving it for cubic graphs is sufficient to show that it holds for all graphs.

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Verifying the Baker and Rumely's lower bound conjecture in the remaining cases or showing a counter example to this conjecture, and finding metrized graphs with minimal tau constants, are interesting and subtle problems. However, except for some special cases, computing the tau constant for metrized graphs with large number of vertices is not an easy task. In this paper, we will give a formula for the tau constant of Γ in terms of the discrete Laplacian matrix L of Γ and its pseudo-inverse L^+. In particular, this formula leads to an algorithm for computing $\tau(\Gamma)$ whose complexity is at the order of matrix inversion.

In Section 2, we recall several facts about the metrized graphs, the Laplacian operator Δ, the canonical measure μ_{can} and the tau constant $\tau(\Gamma)$. In particular, we note that metrized graphs can be interpreted as electric circuits: circuit reduction theory plays an important role in this paper. At the end of Section 2, we give several formulas for the tau constant. In Section 3, we introduce the discrete Laplacian matrix L of a metrized graph. We recall some of the properties of L and L^+. We start Section 4 with a remarkable relation between the resistance on Γ and the pseudo-inverse of the discrete Laplacian on Γ [3]. We then derive several new identities by combining this relation with results from Sections 2 and 3. Finally, we express the canonical measure in terms of L and L^+, and obtain our main result which is the following theorem.

Theorem 1.1. *Let* $\mathrm{L} = (l_{pq})_{v\times v}$ *be the discrete Laplacian matrix of a metrized graph* Γ, *and let* $\mathrm{L}^+ = (l^+_{pq})_{v\times v}$ *be its pseudo-inverse. Suppose* p_i *and* q_i *are the end points of edge* e_i *of* Γ *for each* $i = 1, 2, \ldots, e$, *where* e *is the number of edges in* Γ. *Then we have*

$$\tau(\Gamma) = -\frac{1}{12}\sum_{e_i\in E(\Gamma)} l_{p_iq_i}\left(\frac{1}{l_{p_iq_i}} + l^+_{p_ip_i} - 2l^+_{p_iq_i} + l^+_{q_iq_i}\right)^2 + \frac{1}{4}\sum_{q,s\in V(\Gamma)} l_{qs}l^+_{qq}l^+_{ss} + \frac{1}{v}\,\mathrm{trace}\,(\mathrm{L}^+).$$

Up to now, the tau constant has been known for only a few graphs (see [2, pg 273] for a summary of the results from [16]). Theorem 1.1 yields a much faster algorithm for computing the tau constant as compared with the one used in [16].

We prove Theorem 1.1 at the end of Section 4. In Section 5, we give two explicit examples for the computations of $\tau(\Gamma)$ and μ_{can}, and compute the tau constant for several classes of molecular graphs. We used Mathematica [19] for these computations.

Note that there is a 1–1 correspondence between the equivalence classes of finite connected weighted graphs, the metrized graphs, and the resistive electric circuits. If an edge e_i of a metrized graph has length L_i, then we have that the resistance along e_i is L_i in the corresponding resistive electric circuit, and that the weight of e_i is $\frac{1}{L_i}$ in the corresponding weighted graph. The identities that we establish for metrized graphs in this paper are also valid for electric circuits, and they have equivalent forms for weighted graphs.

The results in this paper are improved versions of those given in [8, Sections 5.1, 5.2, 5.3 and 5.4].

2. The tau constant of a metrized graph

A metrized graph Γ is a finite connected graph whose edges are equipped with a distinguished parametrization. In particular, Γ is a one-dimensional manifold except at finitely many "branch points". One can find other definitions of metrized graphs in [17,7,2,20,1].

A metrized graph can have multiple edges and self-loops. For any given $p \in \Gamma$, the number of directions emanating from p will be called the *valence* of p, and will be denoted by $\upsilon(p)$. By definition, there can be only finitely many $p \in \Gamma$ with $\upsilon(p) \neq 2$.

A vertex set for a metrized graph Γ is a finite set of points $V(\Gamma)$ in Γ which contains all the points with $\upsilon(p) \neq 2$. It is possible to enlarge a given vertex set by adjoining additional points of valence 2 as vertices.

Given a metrized graph Γ with vertex set $V(\Gamma)$, the set of edges of Γ is the set of closed line segments with end points in $V(\Gamma)$. We will denote the set of edges of Γ by $E(\Gamma)$. However, we will denote the graph obtained from Γ by deletion of the interior points of an edge $e_i \in E(\Gamma)$ by $\Gamma - e_i$.

We denote $\#(V(\Gamma))$ and $\#(E(\Gamma))$ by v and e, respectively. We denote the length of an edge $e_i \in E(\Gamma)$ by L_i. The total length of Γ, which will be denoted by $\ell(\Gamma)$, is given by $\ell(\Gamma) = \sum_{i=1}^{e} L_i$.

Let $\mathrm{Zh}(\Gamma)$ be the set of all continuous functions $f : \Gamma \to \mathbb{C}$ such that for some vertex set $V(\Gamma)$, f is $\mathcal{C}^2$ on $\Gamma \setminus V(\Gamma)$ and $f''(x) \in L^1(\Gamma)$. Baker and Rumely [2] defined the following measure valued *Laplacian* on a given metrized graph. For a function $f \in \mathrm{Zh}(\Gamma)$,

$$\Delta_x(f(x)) = -f''(x)\mathrm{d}x - \sum_{p \in V(\Gamma)} \left[\sum_{\vec{v} \text{ at } p} d_{\vec{v}} f(p) \right] \delta_p(x). \tag{1}$$

See [2] for details and for a description of the largest class of functions for which a measure valued Laplacian can be defined.

In [7], a kernel $j_z(x, y)$ giving a fundamental solution of the Laplacian is defined and studied as a function of $x, y, z \in \Gamma$. For fixed z and y it has the following physical interpretation: when Γ is viewed as a resistive electric circuit with terminals at z and y, with the resistance in each edge given by its length, then $j_z(x, y)$ is the voltage difference between x and z, when unit current enters at y and exits at z (with reference voltage 0 at z).

For any x, y, z in Γ, the voltage function $j_z(x, y)$ on Γ is a symmetric function in x and y, which satisfies $j_x(x, y) = 0$ and $j_x(y, y) = r(x, y)$, where $r(x, y)$ is the resistance function on Γ. For each vertex set $V(\Gamma)$, $j_z(x, y)$ is continuous on Γ as a function of all three variables. As the physical interpretation suggests, $j_z(x, y) \geq 0$ for all x, y, z in Γ. For proofs of these facts, see [7], [2, sec. 1.5 and sec. 6], and [20, Appendix]. The voltage function $j_z(x, y)$ and the resistance function $r(x, y)$ on a metrized graph were also studied in [1,10].

For any real-valued, signed Borel measure μ on Γ with $\mu(\Gamma) = 1$ and $|\mu|(\Gamma) < \infty$, define the function $j_\mu(x, y) = \int_\Gamma j_\zeta(x, y)\, \mathrm{d}\mu(\zeta)$. Clearly $j_\mu(x, y)$ is symmetric, and is jointly continuous in x and y. Chinburg and Rumely [7] discovered that there is a unique real-valued, signed Borel measure $\mu = \mu_{can}$ such that $j_\mu(x, x)$ is constant on Γ. The measure μ_{can} is called the *canonical measure*. Baker and Rumely [2] called the constant $\frac{1}{2} j_\mu(x, x)$ the *tau constant* of Γ and denoted it by $\tau(\Gamma)$. The Arakelov–Green's function $g_{\mu_{can}}(x, y)$ equals $j_\mu(x, y) - \frac{1}{2} j_\mu(x, x)$, so this definition coincides with the one in the introduction.

The following theorem gives an explicit description of the canonical measure μ_{can}.

Theorem 2.1 (*[7, Theorem 2.11]*). *Let Γ be a metrized graph. Suppose that L_i is the length of edge e_i and R_i is the effective resistance between the end points of e_i in the graph $\Gamma - e_i$. Then*

$$\mu_{can}(x) = \sum_{p \in V(\Gamma)} \left(1 - \frac{1}{2} v(p)\right) \delta_p(x) + \sum_{e_i \in E(\Gamma)} \frac{\mathrm{d}x}{L_i + R_i},$$

where $\delta_p(x)$ is the Dirac measure.

Here is a function-theoretic expression for $\tau(\Gamma)$.

Lemma 2.2 (*[2, Corollary 14.3]*). *Let $\{\lambda_1, \lambda_2, \lambda_3, \ldots\}$ be the set of eigenvalues of the Laplacian Δ with respect to the canonical measure μ_{can}, that is, the set of eigenvalues of Δ acting on the space of piecewise $\mathcal{C}^2$ functions f satisfying $\int_\Gamma f \mathrm{d}\mu_{can} = 0$. Then*

$$\ell(\Gamma) \cdot \tau(\Gamma) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n}.$$

In particular, if $\ell(\Gamma) = 1$, then $\tau(\Gamma)$ is the trace of the inverse operator to Δ with respect to μ_{can}.

Here is another expression for $\tau(\Gamma)$.

Lemma 2.3 (*[16]*). *Given a metrized graph Γ, if $r(x, y)$ is its resistance function, then for each $x \in \Gamma$*

$$\tau(\Gamma) = \frac{1}{2} \int_\Gamma r(x, y) \mathrm{d}\mu_{can}(y).$$

Yet another description of $\tau(\Gamma)$ is as follows.

Lemma 2.4 (*[2, Lemma 14.4]*). *For any fixed $p \in \Gamma$, we have $\tau(\Gamma) = \frac{1}{4} \int_\Gamma (\frac{\mathrm{d}}{\mathrm{d}x} r(x, p))^2 \mathrm{d}x$.*

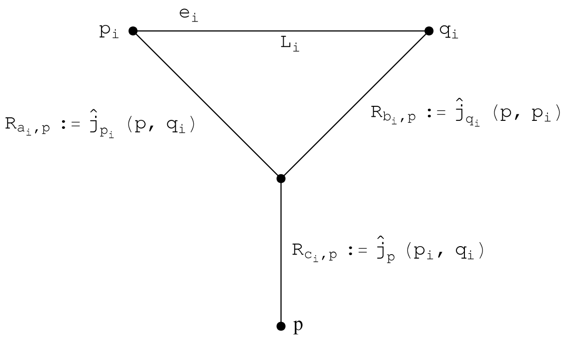

Fig. 1. Circuit reduction of $\Gamma - e_i$ with reference to p_i, q_i and p.

Remark 2.5. Let Γ be any metrized graph with resistance function $r(x, y)$. If we enlarge $V(\Gamma)$ by adjoining additional points $p \in \Gamma$ with $\upsilon(p) = 2$, the resistance function does not change, and thus $\tau(\Gamma)$ does not change by Lemma 2.4.

Note that $\tau(\Gamma)$ is an invariant of the metrized graph Γ, which depends only on the topology and the lengths of the edges of Γ.

Let $\Gamma - e_i$ be a connected graph for an edge $e_i \in E(\Gamma)$ of length L_i. Suppose p_i and q_i are the end points of e_i, and $p \in \Gamma - e_i$. By applying circuit reductions, we can transform $\Gamma - e_i$ into a Y-shaped graph with the same resistances between p_i, q_i, and p as in $\Gamma - e_i$. More details on this can be found in [10, Section 2]. Since $\Gamma - e_i$ has such a circuit reduction, Γ has the circuit reduction as illustrated in Fig. 1 with the corresponding voltage values on each segment, where $\hat{j}_x(y, z)$ is the voltage function in $\Gamma - e_i$. Throughout this paper, we will use the following notation: $R_{a_i,p} := \hat{j}_{p_i}(p, q_i)$, $R_{b_i,p} := \hat{j}_{q_i}(p_i, p)$, $R_{c_i,p} := \hat{j}_p(p_i, q_i)$, and R_i is the resistance between p_i and q_i in $\Gamma - e_i$. Note that $R_{a_i,p} + R_{b_i,p} = R_i$ for each $p \in \Gamma$. When $\Gamma - e_i$ is not connected, if p belongs to the component of $\Gamma - e_i$ containing p_i we set $R_{b_i,p} = R_i = \infty$ and $R_{a_i,p} = 0$, while if p belongs to the component of $\Gamma - e_i$ containing q_i we set $R_{a_i,p} = R_i = \infty$ and $R_{b_i,p} = 0$.

By computing the integral in Lemma 2.4, one obtains the following formula for the tau constant.

Proposition 2.6 (*[16]*)**.** *Let Γ be a metrized graph, and let L_i be the length of the edge e_i, for $i \in \{1, 2, \dots, e\}$. Using the notation above, if we fix a vertex p we have*

$$\tau(\Gamma) = \frac{1}{12} \sum_{e_i \in \Gamma} \left(\frac{L_i^3 + 3L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2} \right).$$

Here, if $\Gamma - e_i$ is not connected, i.e. R_i is infinite, the summand corresponding to e_i should be replaced by $3L_i$, its limit as $R_i \longrightarrow \infty$.

The proof of Proposition 2.6 can be found in [10, Proposition 2.9]. We will use the following remark in Section 4.

Remark 2.7. It follows from Lemma 2.4 and Proposition 2.6 that $\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2}$ is independent of the chosen vertex $p \in V(\Gamma)$.

Let p_i and q_i be the end points of the edge e_i as in Fig. 1. It follows from parallel and series circuit reductions that

$$r(p_i, p) = \frac{(L_i + R_{b_i,p})R_{a_i,p}}{L_i + R_i} + R_{c_i,p}, \quad \text{and} \quad r(q_i, p) = \frac{(L_i + R_{a_i,p})R_{b_i,p}}{L_i + R_i} + R_{c_i,p}. \tag{2}$$

Therefore, $r(p_i, p) - r(q_i, p) = \frac{L_i(R_{a_i,p} - R_{b_i,p})}{L_i+R_i}$, and so

$$\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{(r(p_i, p) - r(q_i, p))^2}{L_i}. \tag{3}$$

Proposition 2.8. *Let Γ be a metrized graph with the resistance function $r(x, y)$, and for each edge $e_i \in E(\Gamma)$, let e_i be parametrized by a segment $[0, L_i]$, under its arc-length parametrization. Then for any $p \in V(\Gamma)$,*

$$\tau(\Gamma) = -\frac{1}{4} \sum_{q \in V(\Gamma)} (\upsilon(q) - 2)r(p, q) + \frac{1}{2} \sum_{e_i \in E(\Gamma)} \frac{1}{L_i + R_i} \int_0^{L_i} r(p, x)\mathrm{d}x.$$

Proof. We have $\tau(\Gamma) = \frac{1}{2}\int_\Gamma r(p, x)\mathrm{d}\mu_{\mathrm{can}}(x)$, by Lemma 2.3. Hence by Theorem 2.1,

$$\tau(\Gamma) = \frac{1}{2} \sum_{q \in V(\Gamma)} \left(1 - \frac{1}{2}\upsilon(p)\right) \int_\Gamma r(p, x)\delta_q(x) + \sum_{e_i \in E(\Gamma)} \frac{1}{L_i + R_i} \int_0^{L_i} r(p, x)\mathrm{d}x.$$

This gives the result. □

Lemma 2.9. *Let p_i and q_i be end points of $e_i \in E(\Gamma)$. For any $p \in V(\Gamma)$,*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i + R_i}(r(p_i, p) + r(q_i, p)) - \sum_{q \in V(\Gamma)} (\upsilon(q) - 2)r(p, q).$$

Proof. We first note that $r(x, p) = \frac{(x+R_{a_i,p})(L_i-x+R_{b_i,p})}{L_i+R_i} + R_{c_i,p}$ if $x \in e_i$. By Lemma 2.4, $4\tau(\Gamma) = \int_\Gamma (\frac{\mathrm{d}}{\mathrm{d}x} r(x, y))^2 \mathrm{d}x$. Integrating by parts, we obtain

$$4\tau(\Gamma) = \sum_{e_i \in E(\Gamma)} \left(r(p, x) \cdot \frac{\mathrm{d}}{\mathrm{d}x} r(p, x) \right)\Bigg|_0^{L_i} - \sum_{e_i \in E(\Gamma)} \int_0^{L_i} r(p, x) \frac{\mathrm{d}^2}{\mathrm{d}x^2} r(p, x)\mathrm{d}x. \tag{4}$$

Since $\frac{\mathrm{d}^2}{\mathrm{d}x^2} r(p, x) = \frac{-2}{L_i+R_i}$ if $x \in e_i$, the result follows from Proposition 2.8 and Eqs. (2) and (4). □

Chinburg and Rumely [7, page 26] showed that

$$\sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i + R_i} = e - \upsilon + 1. \tag{5}$$

3. The discrete Laplacian matrix L and its pseudo-inverse L^+

Throughout this paper, all matrices will have entries in $\mathbb{R}$. To have a well-defined discrete Laplacian matrix L for a metrized graph Γ, we first choose a vertex set $V(\Gamma)$ for Γ in such a way that there are no self-loops, and no multiple edges connecting any two vertices. This can be done by enlarging the vertex set by considering additional valence 2 points as vertices whenever needed. We will call such a vertex set $V(\Gamma)$ *adequate*. If distinct vertices p and q are the end points of an edge, we call them *adjacent* vertices.

Given a matrix M, let M^T, $tr(\mathrm{M})$ and M^{-1} be the transpose, trace and inverse of M, respectively. Let I_υ be the $\upsilon \times \upsilon$ identity matrix, and let O be the zero matrix (with the appropriate size if it is not specified). Let J be the $\upsilon \times \upsilon$ matrix whose entries are all 1's.

A matrix M is called *doubly centered*, if both row and column sums are 0. That is, M is doubly centered iff $\mathrm{MY} = \mathrm{O}$ and $\mathrm{Y}^T\mathrm{M} = \mathrm{O}$, where $\mathrm{Y} = [1, 1, \ldots, 1]^T$.

Let Γ be a metrized graph with e edges and with an adequate vertex set $V(\Gamma)$ containing υ vertices. Fix an ordering of the vertices in $V(\Gamma)$. Let $\{L_1, L_2, \ldots, L_e\}$ be a labeling of the edge lengths. The matrix

$\mathrm{A} = (a_{pq})_{v\times v}$ given by

$$a_{pq} = \begin{cases} 0 & \text{if } p = q\text{, or } p \text{ and } q \text{ are not adjacent} \\ \dfrac{1}{L_k} & \text{if } p \neq q\text{, and } p \text{ and } q \text{ are connected by an edge of length } L_k \end{cases}$$

is called the *adjacency matrix* of Γ. Let $\mathrm{D} = \mathrm{diag}(d_{pp})$ be the $v \times v$ diagonal matrix given by $d_{pp} = \sum_{s\in V(\Gamma)} a_{ps}$. Then $\mathrm{L} := \mathrm{D} - \mathrm{A}$ is called the *discrete Laplacian matrix* of Γ. That is, $\mathrm{L} = (l_{pq})_{v\times v}$ where

$$l_{pq} = \begin{cases} 0 & \text{if } p \neq q\text{, and } p \text{ and } q \text{ are not adjacent} \\ -\dfrac{1}{L_k} & \text{if } p \neq q\text{, and } p \text{ and } q \text{ are connected by an edge of length } L_k \\ -\displaystyle\sum_{s\in V(\Gamma)-\{p\}} l_{ps} & \text{if } p = q. \end{cases}$$

The discrete Laplacian matrix is also known as the generalized (or the weighted) Laplacian matrix in the literature.

Example 3.1 (*[9, Remark 3.1]*)**.** For any metrized graph Γ, the discrete Laplacian matrix L is symmetric and doubly centered. That is, $\sum_{p\in V(\Gamma)} l_{pq} = 0$ for each $q \in V(\Gamma)$, and $l_{pq} = l_{qp}$ for each $p, q \in V(\Gamma)$.

In our case, Γ is connected by definition. Thus, the discrete Laplacian matrix L of Γ is a $(v \times v)$ matrix of rank $v - 1$ if the adequate vertex set $V(\Gamma)$ has v vertices. The null space of L is the one-dimensional space spanned by $[1, 1, \ldots, 1]^T$. Since L is a real symmetric matrix, it has real eigenvalues. Moreover, L is positive semi-definite. More precisely, one of the eigenvalues of L is 0 and the others are positive. Thus, L is not invertible. However, it has generalized inverses. In particular, it has the pseudo-inverse L^+, also known as the Moore–Penrose generalized inverse, which is uniquely determined by the following properties:

(i) $\mathrm{LL}^+\mathrm{L} = \mathrm{L}$, (iii) $(\mathrm{LL}^+)^T = \mathrm{LL}^+$,
(ii) $\mathrm{L}^+\mathrm{LL}^+ = \mathrm{L}^+$, (iv) $(\mathrm{L}^+\mathrm{L})^T = \mathrm{L}^+\mathrm{L}$.

A $v \times v$ matrix M is called an *EP matrix* if $\mathrm{M}^+\mathrm{M} = \mathrm{MM}^+$. A necessary and sufficient condition for M to be an EP matrix is that $\mathrm{M}u = \lambda u$ iff $\mathrm{M}^+u = \lambda^+u$, for each eigenvector u of M. Another characterization of an EP matrix M is that $\mathrm{MX} = \mathrm{O}$ iff $\mathrm{M}^T\mathrm{X} = \mathrm{O}$, where X is also $v \times v$. Any symmetric matrix is an EP matrix [6, pg 253].

The matrix L has the following properties:

(i) L and L^+ are symmetric, (iii) L and L^+ are EP matrices,
(ii) L and L^+ are doubly centered, (iv) L and L^+ are positive semi-definite.

For a discrete Laplacian matrix L of size $v \times v$, we have the following formula for L^+ (see [15, ch 10]):

$$\mathrm{L}^+ = \left(\mathrm{L} - \frac{1}{v}\mathrm{J}\right)^{-1} + \frac{1}{v}\mathrm{J} \tag{6}$$

where J is of size $v \times v$ and has all entries 1.

Remark 3.2. Since L^+ is doubly centered, $\sum_{p\in V(\Gamma)} l^+_{pq} = 0$, for each $q \in V(\Gamma)$. Also, $l^+_{pq} = l^+_{qp}$, for each $p, q \in V(\Gamma)$.

We use the following lemma and its corollary, Corollary 3.4, frequently in the rest of this article.

Lemma 3.3 ([*13*, *Equation 2.9]*)**.** *Let* J *be of size* $v \times v$ *as above and let* L *be the discrete Laplacian of a graph (not necessarily having equal edge lengths). Then* $\mathrm{LL}^+ = \mathrm{L}^+\mathrm{L} = \mathrm{I} - \frac{1}{v}\mathrm{J}$.

Lemma 3.3 was obtained by Gutman and Xiao (see [12, Lemma 3]) when L arises from a graph having edges of equal length 1.

Corollary 3.4. *Let Γ be a metrized graph and let* L *be the corresponding discrete Laplacian matrix of size $\upsilon \times \upsilon$. Then for any $p, q \in V(\Gamma)$,*

$$\sum_{s \in V(\Gamma)} l_{ps}^{+} l_{sq} = \begin{cases} -\dfrac{1}{\upsilon} & \text{if } p \neq q \\ \dfrac{\upsilon - 1}{\upsilon} & \text{if } p = q. \end{cases}$$

See [15], [6, ch 10], [4,14] for more information about L and L^{+}.

4. The discrete Laplacian, the resistance function, and the tau constant

In this section, we will obtain a formula (see Theorem 4.10) for the tau constant in terms of the entries of L and L^{+}. Our main tools will be a remarkable relation between the resistance and the pseudo-inverse L^{+} (Lemma 4.1 below), properties of L and L^{+} given in Section 3, the results from Section 1 concerning metrized graphs, and the circuit reduction theory.

Lemma 4.1 *([3,5], [13, Theorem A]). Suppose Γ is a graph with the discrete Laplacian* L *and the resistance function $r(x, y)$. Let* H *be a generalized inverse of* L *(i.e.,* LHL = L*). Then we have*

$$r(p, q) = \mathrm{H}_{pp} - \mathrm{H}_{pq} - \mathrm{H}_{qp} + \mathrm{H}_{qq}, \quad \text{for any } p, q \in V(\Gamma).$$

In particular, for the pseudo-inverse L^{+} we have

$$r(p, q) = l_{pp}^{+} - 2l_{pq}^{+} + l_{qq}^{+}, \quad \text{for any } p, q \in V(\Gamma).$$

Lemma 4.1 shows that the pseudo-inverses can be used to compute the resistance $r(p, q)$ between any p, q in Γ. Namely, we choose an adequate vertex set $V(\Gamma)$ containing p and q. Then we compute the corresponding pseudo-inverse, and apply Lemma 4.1. Similarly, the following lemma shows that the pseudo-inverses can be used to compute the voltage $j_p(q, s)$ for any p, q and s in Γ.

Lemma 4.2 *([9, Lemma 3.5]). Let Γ be a graph with the discrete Laplacian* L *and the voltage function $j_x(y, z)$. Then for any p, q, s in $V(\Gamma)$,*

$$j_p(q, s) = l_{pp}^{+} - l_{pq}^{+} - l_{ps}^{+} + l_{qs}^{+}.$$

Corollary 4.3. *Let Γ be a graph with the discrete Laplacian matrix* L *having the pseudo-inverse L^{+}. Then for any $p, q \in V(\Gamma)$, we have $l_{pp}^{+} \geq l_{pq}^{+}$.*

Proof. By Remark 3.2 and Lemma 4.2, $\sum_{s \in V(\Gamma)} j_p(q, s) = \upsilon \cdot (l_{pp}^{+} - l_{pq}^{+})$ for any p and q in $V(\Gamma)$. Thus the result follows from the fact that $j_p(q, s) \geq 0$ for any $p, q, s \in \Gamma$. □

Recall that we use L_i for the length of edge $e_i \in E(\Gamma)$ and R_i for the resistance between the end points of e_i in the graph $\Gamma - e_i$. The following lemma expresses an important term for computing $\tau(\Gamma)$ in terms of L and L^{+}.

Lemma 4.4. *Let* L *be the discrete Laplacian matrix of size $\upsilon \times \upsilon$ for a graph Γ. Let p_i and q_i be the end points of edge e_i for any given $e_i \in E(\Gamma)$. Then*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i R_i^2}{(L_i + R_i)^2} = \frac{4(\upsilon - 1)}{\upsilon} \operatorname{tr}(\mathrm{L}^{+}) - \sum_{p,q \in V(\Gamma)} l_{pq} l_{pp}^{+} l_{qq}^{+} - 2 \sum_{p,q \in V(\Gamma)} l_{pq} (l_{pq}^{+})^2.$$

Proof. First, we use Example 3.1 to obtain

$$\sum_{p,q\in V(\Gamma)} l_{pq}(l^+_{pp})^2 = \sum_{p\in V(\Gamma)} (l^+_{pp})^2 \left(\sum_{q\in V(\Gamma)} l_{pq}\right) = 0. \tag{7}$$

Using Corollary 3.4,

$$\sum_{p,q\in V(\Gamma)} l_{pq} l^+_{pq} l^+_{pp} = \sum_{p\in V(\Gamma)} l^+_{pp} \left(\sum_{q\in V(\Gamma)} l_{pq} l^+_{pq}\right) = \frac{\upsilon-1}{\upsilon}\cdot \mathrm{tr}\,(\mathrm{L}^+). \tag{8}$$

Then

$$\begin{aligned}
\sum_{e_i\in E(\Gamma)} \frac{L_i R_i^2}{(L_i+R_i)^2} &= \sum_{e_i\in E(\Gamma)} \frac{1}{L_i}(r(p_i,q_i))^2, \quad \text{since } r(p_i,q_i) = \frac{L_i R_i}{L_i+R_i}.\\
&= -\sum_{e_i\in E(\Gamma)} l_{p_i q_i}(l^+_{p_i p_i} + l^+_{q_i q_i} - 2 l^+_{p_i,q_i})^2, \quad \text{by Lemma 4.1}\\
&= -\frac{1}{2}\sum_{p,q\in V(\Gamma)} l_{pq}(l^+_{pp} + l^+_{qq} - 2 l^+_{pq})^2, \quad \text{as } l_{pq} = 0 \text{ if } p, q \text{ are not adjacent}\\
&= -\frac{1}{2}\sum_{p,q\in V(\Gamma)} l_{pq}(l^+_{pp} + l^+_{qq})^2 + 2\sum_{p,q\in V(\Gamma)} (l_{pq}(l^+_{pp} + l^+_{qq}) l^+_{pq} - l_{pq}(l^+_{pq})^2)\\
&= -\sum_{p,q\in V(\Gamma)} l_{pq} l^+_{pp} l^+_{qq} + \sum_{p,q\in V(\Gamma)} (4 l_{pq} l^+_{pp} l^+_{pq} - 2 l_{pq}(l^+_{pq})^2), \quad \text{by Eq. (7).}
\end{aligned}$$

Thus, the result follows from Eq. (8). □

Next, we will have several lemmas concerning identities involving the entries of L and L^+.

Lemma 4.5. *Let* L *be the discrete Laplacian matrix of a graph Γ. Then for any $p \in V(\Gamma)$,*

$$\sum_{q,s\in V(\Gamma)} l_{qs}(l^+_{qq} - l^+_{ss})(l^+_{qp} - l^+_{sp}) = -2\sum_{q,s\in V(\Gamma)} l_{qs} l^+_{qq} l^+_{sp}.$$

Proof. By using Example 3.1, for any $p \in V(\Gamma)$,

$$\sum_{q,s\in V(\Gamma)} l_{qs} l^+_{qq} l^+_{qp} = \sum_{q\in V(\Gamma)} l^+_{qq} l^+_{qp} \left(\sum_{s\in V(\Gamma)} l_{qs}\right) = 0. \tag{9}$$

Using Example 3.1 and Eq. (9) for the second equality,

$$\begin{aligned}
\sum_{q,s\in V(\Gamma)} l_{qs}(l^+_{qq} - l^+_{ss})(l^+_{qp} - l^+_{sp}) &= \sum_{q,s\in V(\Gamma)} (l_{qs} l^+_{qq} l^+_{qp} - l_{qs} l^+_{qq} l^+_{sp} - l_{qs} l^+_{ss} l^+_{qp} + l_{qs} l^+_{ss} l^+_{sp})\\
&= -\sum_{q,s\in V(\Gamma)} (l_{qs} l^+_{qq} l^+_{sp} + l_{qs} l^+_{ss} l^+_{qp}).
\end{aligned}$$

This is equivalent to what we wanted. □

Lemma 4.6. *Let* L *be the discrete Laplacian matrix of size $\upsilon \times \upsilon$ for a graph Γ, and let p_i, q_i be the end points of $e_i \in E(\Gamma)$. Then for any $p \in V(\Gamma)$,*

$$l^+_{pp} = \frac{1}{\upsilon} tr(\mathrm{L}^+) + \sum_{e_i\in E(\Gamma)} \frac{L_i}{L_i+R_i}(l^+_{pp_i} + l^+_{pq_i}) - \sum_{q\in V(\Gamma)} \upsilon(q) l^+_{pq},$$

$$l^+_{pp} = \frac{1}{\upsilon} tr(\mathrm{L}^+) - \sum_{e_i\in E(\Gamma)} \frac{R_i}{L_i+R_i}(l^+_{pp_i} + l^+_{pq_i}).$$

Proof. We use Lemma 2.9 for the first equality below and Lemma 4.1 for the second equality below. For any $p \in V(\Gamma)$,

$$\begin{aligned}
\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i+R_i)^2} &= \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i+R_i}(r(p_i,p)+r(q_i,p)) - \sum_{q \in V(\Gamma)} (\upsilon(q)-2) r(p,q) \\
&= \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i+R_i}(l^+_{p_ip_i} + l^+_{q_iq_i} - 2(l^+_{pp_i} + l^+_{pq_i} - l^+_{pp})) \\
&\quad - \sum_{q \in V(\Gamma)} (\upsilon(q)-2)(l^+_{qq} - 2l^+_{pq} + l^+_{pp}) \\
&= 2l^+_{pp} + \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i+R_i}(l^+_{p_ip_i} + l^+_{q_iq_i} - 2(l^+_{pp_i} + l^+_{pq_i})) \\
&\quad - \sum_{q \in V(\Gamma)} ((\upsilon(q)-2)l^+_{qq} + 2\upsilon(q)l^+_{pq}) \\
&\quad \text{by Eq. (5) and the fact that } \sum_{q \in V(\Gamma)} (\upsilon(q)-2) = 2e - 2v. \qquad (10)
\end{aligned}$$

If we sum equation (10) over all vertices and apply Example 3.1, we obtain

$$\begin{aligned}
\sum_{s \in V(\Gamma)} \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,s} - R_{b_i,s})^2}{(L_i+R_i)^2} &= 2 \cdot tr(\mathrm{L}^+) + v \cdot \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i+R_i}(l^+_{p_ip_i} + l^+_{q_iq_i}) \\
&\quad + v \cdot \sum_{q \in V(\Gamma)} (\upsilon(q)-2) l^+_{qq}. \qquad (11)
\end{aligned}$$

On the other hand, by Remark 2.7,

$$\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i+R_i)^2} = \frac{1}{v} \sum_{s \in V(\Gamma)} \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,s} - R_{b_i,s})^2}{(L_i+R_i)^2}. \qquad (12)$$

Hence the first equality in the lemma follows from Eqs. (10)–(12). Then the second equality in the lemma follows from the first equality and the fact that

$$\sum_{q \in V(\Gamma)} \upsilon(q) l^+_{pq} = \sum_{e_i \in E(\Gamma)} (l^+_{pp_i} + l^+_{pq_i}). \qquad \square$$

Lemma 4.7. *Let* L *be the discrete Laplacian matrix of a graph* Γ. *Let* p_i *and* q_i *be end points of* $e_i \in E(\Gamma)$. *Then*

$$\sum_{q,s \in V(\Gamma)} l_{qs} l^+_{qq} l^+_{ss} = -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs}(l^+_{qq} - l^+_{ss})^2 = \sum_{e_i \in E(\Gamma)} \frac{1}{L_i}(l^+_{p_ip_i} - l^+_{q_iq_i})^2 \geq 0.$$

Proof. By Eq. (7), $\sum_{q,s \in V(\Gamma)} l_{qs}(l^+_{qq} - l^+_{ss})^2 = -2 \sum_{q,s \in V(\Gamma)} l_{qs} l^+_{qq} l^+_{ss}$. This gives the first equality in the lemma. Then the second equality is obtained by using the definition of L. $\square$

Theorem 4.8 below expresses the first term in the formula for $\tau(\Gamma)$ from Proposition 2.6 in terms of the entries of L and L^+. This theorem combines the technical lemmas above, and it will be used in the proof of Theorem 4.10.

Theorem 4.8. *Let* L *be the discrete Laplacian matrix of size* $v \times v$ *for a metrized graph* Γ. *Let* p_i *and* q_i *be end points of edge* $e_i \in E(\Gamma)$, *and let* R_i, $R_{a_i,p}$, $R_{b_i,p}$ *and* L_i *be as defined before. Then*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{b_i,p} - R_{a_i,p})^2}{(L_i+R_i)^2} = \frac{4}{v} tr(\mathrm{L}^+) - \frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs}(l^+_{qq} - l^+_{ss})^2.$$

Proof. Note that for each $p \in V(\Gamma)$, the following equality follows from Example 3.1:

$$\sum_{q,s \in V(\Gamma)} l_{qs} (l_{qp}^+)^2 = \sum_{q \in V(\Gamma)} (l_{qp}^+)^2 \sum_{s \in V(\Gamma)} l_{qs} = 0. \tag{13}$$

By Corollary 3.4, for each $p \in V(\Gamma)$,

$$\sum_{q,s \in V(\Gamma)} l_{qs} l_{qq}^+ l_{sp}^+ = l_{pp}^+ - \frac{1}{v} tr(\mathrm{L}^+). \tag{14}$$

Similarly, by Corollary 3.4 and Remark 3.2, for any $p \in V(\Gamma)$ we have

$$\sum_{q,s \in V(\Gamma)} l_{qs} l_{qp}^+ l_{sp}^+ = l_{pp}^+. \tag{15}$$

Hence for each $p \in V(\Gamma)$,

$$\begin{aligned}
\sum_{e_i \in E(\Gamma)} \frac{L_i (R_{b_i,p} - R_{a_i,p})^2}{(L_i + R_i)^2} &= \sum_{e_i \in E(\Gamma)} \frac{1}{L_i} (r(p_i, p) - r(q_i, p))^2, \quad \text{by Eq. (3)} \\
&= -\sum_{e_i \in E(\Gamma)} l_{p_i q_i} (-2 l_{pp_i}^+ + l_{p_i p_i}^+ + 2 l_{pq_i}^+ - l_{q_i q_i}^+)^2, \quad \text{by Lemma 4.1} \\
&= -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs} (-2 l_{pq}^+ + l_{qq}^+ + 2 l_{ps}^+ - l_{ss}^+)^2 \\
&= -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs} (l_{qq}^+ - l_{ss}^+)^2 + 2 \sum_{q,s \in V(\Gamma)} l_{qs} (l_{qq}^+ - l_{ss}^+)(l_{pq}^+ - l_{ps}^+) \\
&\quad - 2 \sum_{q,s \in V(\Gamma)} l_{qs} (l_{pq}^+ - l_{ps}^+)^2 \\
&= -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs} (l_{qq}^+ - l_{ss}^+)^2 - 4 \sum_{q,s \in V(\Gamma)} l_{qs} l_{qq}^+ l_{sp}^+ \\
&\quad - 2 \sum_{q,s \in V(\Gamma)} l_{qs} (l_{pq}^+ - l_{ps}^+)^2, \quad \text{by Lemma 4.5} \\
&= -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs} (l_{qq}^+ - l_{ss}^+)^2 - 4 \sum_{q,s \in V(\Gamma)} l_{qs} l_{qq}^+ l_{sp}^+ \\
&\quad + 4 \sum_{q,s \in V(\Gamma)} l_{qs} l_{pq}^+ l_{ps}^+, \quad \text{by Eq. (13).} \\
&= -\frac{1}{2} \sum_{q,s \in V(\Gamma)} l_{qs} (l_{qq}^+ - l_{ss}^+)^2 - 4 \left(l_{pp}^+ - \frac{1}{v} tr(\mathrm{L}^+) \right) + 4 (l_{pp}^+), \\
&\quad \text{by Eqs. (14) and (15).}
\end{aligned}$$

This gives the result. □

Lemma 4.9 below expresses the second term in the formula for $\tau(\Gamma)$ from Proposition 2.6 in terms of the entries of L and L^+.

Lemma 4.9. *Let* L *be the discrete Laplacian matrix of a metrized graph Γ. Suppose p_i and q_i are end points of edge e_i. Then*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i^3}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{1}{L_i} (L_i - l_{p_i p_i}^+ + 2 l_{p_i q_i}^+ - l_{q_i q_i}^+)^2.$$

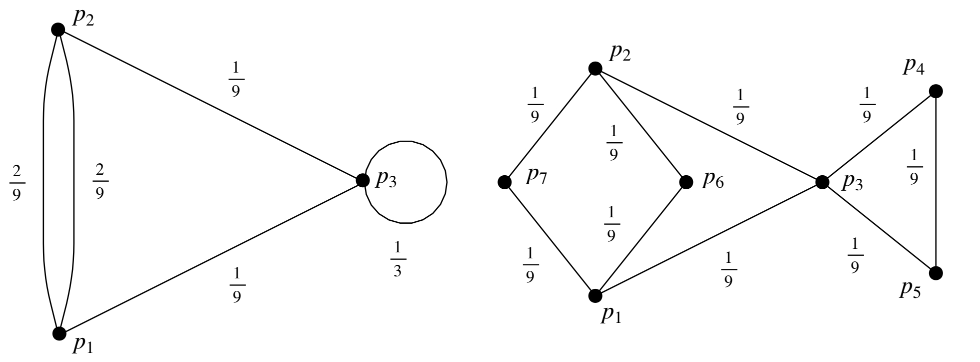

Fig. 2. Γ with $V(\Gamma) = \{1, 2, 3\}$ and with an adequate vertex set $\{1, 2, 3, 4, 5, 6, 7\}$.

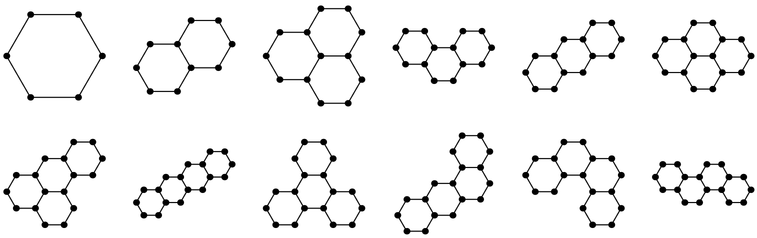

Fig. 3. Fusene graphs.

Proof. Since $\frac{L_i R_i}{L_i + R_i} = r(p_i, q_i)$ for each $e_i \in E(\Gamma)$, we have

$$\sum_{e_i \in E(\Gamma)} \frac{L_i^3}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{1}{L_i} \left(L_i - \frac{L_i R_i}{L_i + R_i} \right)^2 = \sum_{e_i \in E(\Gamma)} \frac{1}{L_i} (L_i - r(p_i, q_i))^2.$$

Then the result follows from Lemma 4.1. $\square$

Our main result is the following formula for $\tau(\Gamma)$.

Theorem 4.10. *Let* L *be the discrete Laplacian matrix of size $v \times v$ for a metrized graph Γ, and let* L^+ *be its Moore–Penrose pseudo-inverse. Suppose p_i and q_i are end points of $e_i \in E(\Gamma)$. Then we have*

$$\tau(\Gamma) = -\frac{1}{12} \sum_{e_i \in E(\Gamma)} l_{p_i q_i} \left(\frac{1}{l_{p_i q_i}} + l^+_{p_i p_i} - 2 l^+_{p_i q_i} + l^+_{q_i q_i} \right)^2 + \frac{1}{4} \sum_{q,s \in V(\Gamma)} l_{qs} l^+_{qq} l^+_{ss} + \frac{1}{v} tr(\mathrm{L}^+),$$

$$\tau(\Gamma) = -\frac{1}{12} \sum_{e_i \in E(\Gamma)} l_{p_i q_i} \left(\frac{1}{l_{p_i q_i}} + l^+_{p_i p_i} - 2 l^+_{p_i q_i} + l^+_{q_i q_i} \right)^2 - \frac{1}{4} \sum_{e_i \in E(\Gamma)} l_{p_i q_i} (l^+_{p_i p_i} - l^+_{q_i q_i})^2 + \frac{1}{v} tr(\mathrm{L}^+).$$

Proof. By Proposition 2.6, for any $p \in V(\Gamma)$

$$\tau(\Gamma) = \frac{1}{12} \sum_{e_i \in E(\Gamma)} \frac{L_i^3}{(L_i + R_i)^2} + \frac{1}{4} \sum_{e_i \in E(\Gamma)} \frac{L_i (R_{b_i,p} - R_{a_i,p})^2}{(L_i + R_i)^2}.$$

Thus the first equality in the theorem follows from Lemma 4.9, Theorem 4.8 and Lemma 4.7. Then the second equality follows from Lemma 4.7. $\square$

Corollary 4.11. *Let* L *be the discrete Laplacian matrix of size $v \times v$ for a graph Γ. Then we have* $\tau(\Gamma) \geq \frac{1}{v} tr(\mathrm{L}^+)$.

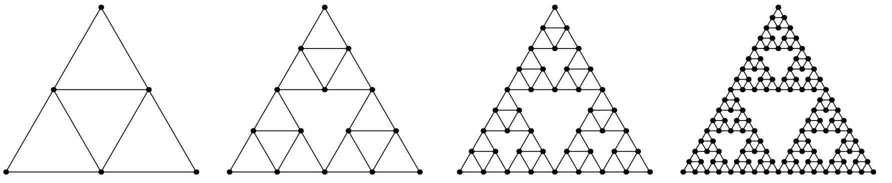

Fig. 4. Sierpinski graphs.

Table 1
The tau constants for the fusene graphs listed in Fig. 3.

Mathematica name	Vertex	Edge	Genus	Tau constant
{Cycle, 6}	6	6	1	$\frac{1}{12} \cong 0.0833333$
{Fusene, {2, 1}}	10	11	2	$\frac{67}{924} \cong 0.0725108$
{Fusene, {3, 1}}	13	15	3	$\frac{179}{2940} \cong 0.0608844$
{Fusene, {3, 2}}	14	16	3	$\frac{671}{9792} \cong 0.0685253$
{Fusene, {3, 3}}	14	16	3	$\frac{671}{9792} \cong 0.0685253$
{Fusene, {4, 1}}	16	19	4	$\frac{485}{8892} \cong 0.0545434$
{Fusene, {4, 3}}	17	20	4	$\frac{277}{4564} \cong 0.0606924$
{Fusene, {4, 2}}	18	21	4	$\frac{19907}{299628} \cong 0.0664391$
{Fusene, {4, 4}}	18	21	4	$\frac{79}{1188} \cong 0.0664983$
{Fusene, {4, 5}}	18	21	4	$\frac{19907}{299628} \cong 0.0664391$
{Fusene, {4, 6}}	18	21	4	$\frac{19907}{299628} \cong 0.0664391$
{Fusene, {4, 7}}	18	21	4	$\frac{19907}{299628} \cong 0.0664391$

Table 2
The tau constants for the Sierpinski graphs listed in Fig. 4.

Mathematica name	Vertex	Edge	Genus	Tau constant
{Sierpinski, 2}	6	9	4	$\frac{19}{324} \cong 0.058642$
{Sierpinski, 3}	15	27	13	$\frac{125}{2916} \cong 0.0428669$
{Sierpinski, 4}	42	81	40	$\frac{110273}{3280500} \cong 0.0336147$
{Sierpinski, 5}	123	243	121	$\frac{20903107}{738112500} \cong 0.0283197$

Next, we will express μ_{can} in terms of the discrete Laplacian matrix and its pseudo-inverse.

Proposition 4.12. *For a given metrized graph Γ, let* L *be its discrete Laplacian, and let* L^+ *be the corresponding pseudo-inverse. Suppose p_i and q_i denote the end points of $e_i \in E(\Gamma)$. Then we have*

$$\mu_{can}(x) = \sum_{p \in V(\Gamma)} \left(1 - \frac{1}{2}v(p)\right) \delta_p(x) - \sum_{e_i \in E(\Gamma)} (l_{p_i q_i} + l_{p_i q_i}^2 (l_{p_i p_i}^+ - 2l_{p_i q_i}^+ + l_{q_i q_i}^+)) \mathrm{d}x.$$

Proof. The result follows from Theorem 2.1, Lemma 4.1, and the fact that $r(p_i, q_i) = \frac{L_i R_i}{L_i + R_i}$ for each $e_i \in E(\Gamma)$. $\square$

Theorem 1.1 (equivalently Theorem 4.10) and Eq. (6) yield an algorithm for computing $\tau(\Gamma)$ and μ_{can} whose computational complexity and memory consumption are at the level of a matrix inversion.

Table 3
The tau constants for the fullerene graphs listed in Fig. 5.

Mathematica name	Vertex	Edge	Genus	Tau constant
{Fullerene, {26, 1}}	26	39	14	$\frac{7355009}{310441950} \cong 0.0236921$
{Fullerene, {30, 1}}	30	45	16	$\frac{8469668299}{376900322940} \cong 0.0224719$
{Fullerene, {36, 1}}	36	54	19	$\frac{9458767}{457228800} \cong 0.0206872$
{Fullerene, {36, 5}}	36	54	19	$\frac{1870203361309}{89834777091072} \cong 0.0208183$
{Fullerene, {40, 19}}	40	60	21	$\frac{51201373387}{2580599234400} \cong 0.0198409$
{Fullerene, {42, 29}}	42	63	22	$\frac{90912940434424}{4612386087287433} \cong 0.0197106$
{Fullerene, {42, 39}}	42	63	22	$\frac{4125154143737}{212106260089332} \cong 0.0194485$
{Fullerene, {44, 37}}	44	66	23	$\frac{21405369093991}{1114465134182400} \cong 0.0192069$
{Fullerene, {44, 62}}	44	66	23	$\frac{884769233189201}{44890049931959232} \cong 0.0197097$
{Fullerene, {44, 63}}	44	66	23	$\frac{312505972215103}{16243272520993287} \cong 0.0192391$
{Fullerene, {44, 66}}	44	66	23	$\frac{11494830502198}{596035416363453} \cong 0.0192855$
{Fullerene, {44, 75}}	44	66	23	$\frac{3799664631422701}{198451222848853128} \cong 0.0191466$
{Fullerene, {60, 1}}	60	90	31	$\frac{206820207359384351}{1125487374488870140} \cong 0.0183761$
{Fullerene, {70, 4085}}	70	105	36	$\frac{577119823897247737}{35801159217650251425} \cong 0.0161201$
{Fullerene, {80, 6877}}	80	120	41	$\frac{3160741321}{204906240000} \cong 0.0154253$

Table 4
The tau constants for the Archimedean graphs listed in Fig. 6.

Mathematica name	Vertex	Edge	Genus	Tau constant
CuboctahedralGraph	12	24	13	$\frac{9}{256} \cong 0.0351563$
SmallRhombicuboctahedralGraph	24	48	25	$\frac{665041}{22579200} \cong 0.0294537$
SnubCubicalGraph	24	60	37	$\frac{155391917}{4335648768} \cong 0.0358405$
TruncatedCubicalGraph	24	36	13	$\frac{97}{3456} \cong 0.0280671$
TruncatedOctahedralGraph	24	36	13	$\frac{50735}{2032128} \cong 0.0249664$
IcosidodecahedralGraph	30	60	31	$\frac{6101}{216000} \cong 0.0282454$
SmallRhombicosidodecahedralGraph	60	120	61	$\frac{9956707537}{395646768000} \cong 0.0251656$
TruncatedDodecahedralGraph	60	90	31	$\frac{16211}{810000} \cong 0.0200136$
TruncatedIcosahedralGraph	60	90	31	$\frac{960971207}{56610576000} \cong 0.0169751$

5. Examples

In this section, we compute the tau constant and the canonical measure for some metrized graphs. First we give two explicit examples.

Example 5.1. Let Γ be a complete graph on five vertices where each edge length is equal to $\frac{1}{10}$, and so $\ell(\Gamma) = 1$. Then Γ has the following discrete Laplacian matrix and pseudo-inverse:

$$\mathrm{L} = \begin{bmatrix} 40 & -10 & -10 & -10 & -10 \\ -10 & 40 & -10 & -10 & -10 \\ -10 & -10 & 40 & -10 & -10 \\ -10 & -10 & -10 & 40 & -10 \\ -10 & -10 & -10 & -10 & 40 \end{bmatrix} \quad \text{and}$$

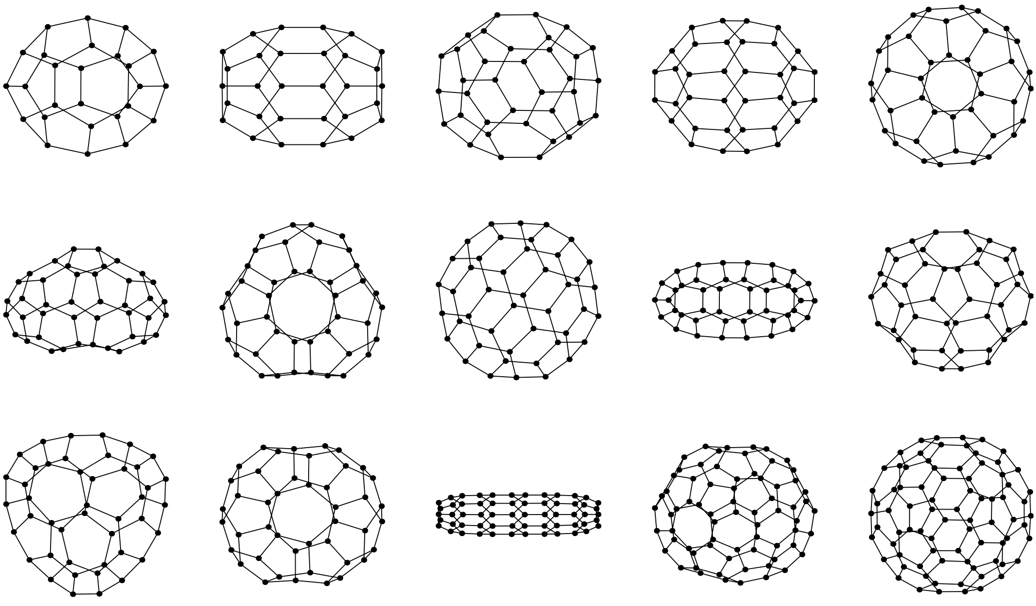

Fig. 5. Fullerene graphs.

Table 5
The tau constants for the zero-symmetric graphs listed in Fig. 7.

Mathematica name	Vertex	Edge	Genus	Tau constant
{CubicTransitive, 41}	24	36	13	$\frac{28849}{1168128} \cong 0.0246968$
{CubicTransitive, 47}	26	39	14	$\frac{575018035}{24613480476} \cong 0.0233619$
{CubicTransitive, 51}	28	42	15	$\frac{1601541769}{72592693992} \cong 0.022062$
{CubicTransitive, 52}	28	42	15	$\frac{27228427}{1194965352} \cong 0.022786$
GreatRhombicuboctahedralGraph	48	72	25	$\frac{2434001017}{127209139200} \cong 0.0191339$
GreatRhombicosidodecahedralGraph	120	180	61	$\frac{123570761111647883}{8587673220814128000} \cong 0.0143893$

$$\mathrm{L}^+ = \begin{bmatrix} \frac{2}{125} & -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} \\ -\frac{1}{250} & \frac{2}{125} & -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} \\ -\frac{1}{250} & -\frac{1}{250} & \frac{2}{125} & -\frac{1}{250} & -\frac{1}{250} \\ -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} & \frac{2}{125} & -\frac{1}{250} \\ -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} & -\frac{1}{250} & \frac{2}{125} \end{bmatrix}.$$

Thus, we obtain $\tau(\Gamma) = \frac{23}{500}$ by applying Theorem 4.10. Moreover, by Proposition 4.12,

$$\mu_{can}(x) = -\sum_{p \in V(\Gamma)} \delta_p(x) + 6 \sum_{e_i \in E(\Gamma)} \mathrm{d}x.$$

Example 5.2. Let Γ be a metrized graph illustrated as the first graph in Fig. 2, where the edge lengths are also shown. Note that $\ell(\Gamma) = 1$. Since Γ with the set of vertices $V(\Gamma) = \{1, 2, 3\}$ has a

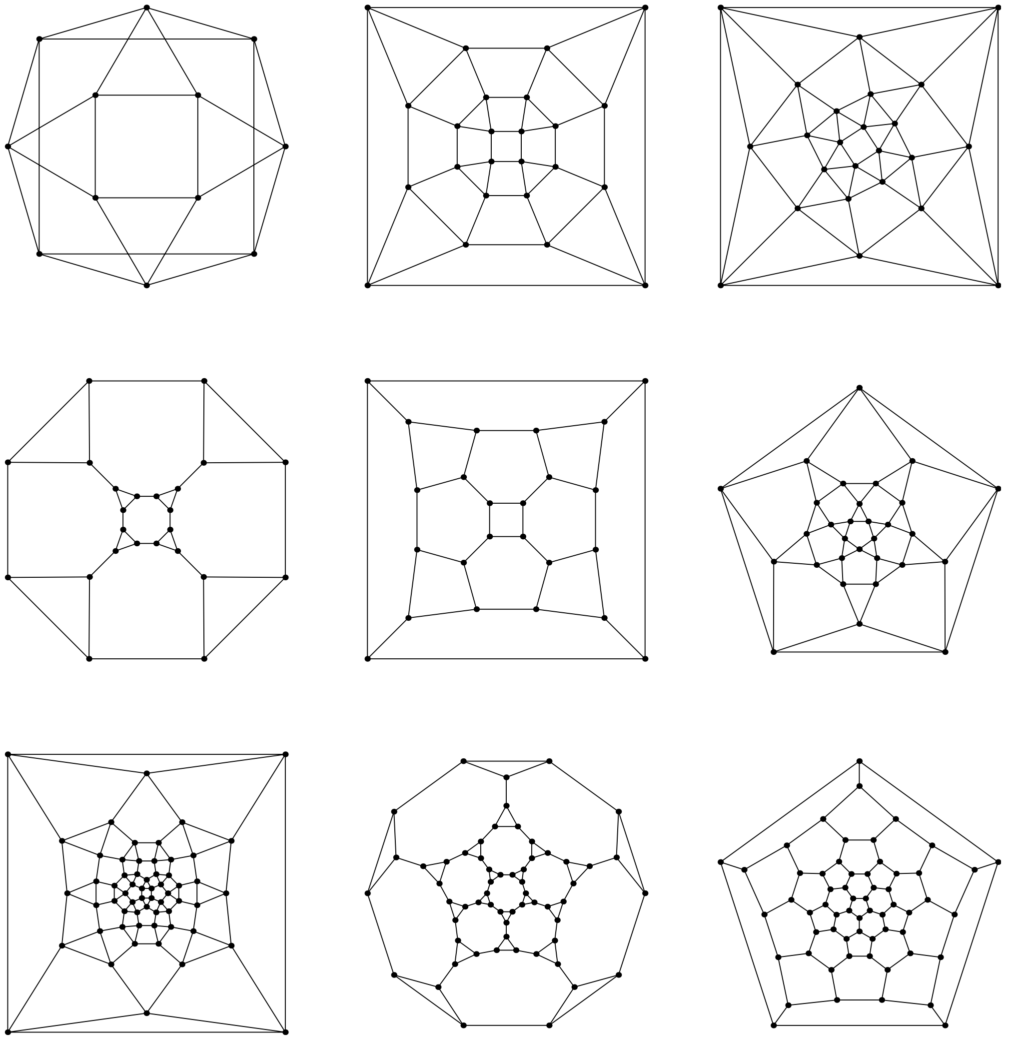

Fig. 6. Archimedean graphs.

self-loop and two multiple edges, we need to work with an adequate vertex set to have the associated discrete Laplacian matrix. This can be done by adjoining two additional points on each self-loop, and one additional point on each multiple edge, to the vertex set. The new metrized graph is illustrated by the second graph in Fig. 2. As we know by Remark 2.5 that the new length distribution for the self-loop and the multiple edges will not change $\tau(\Gamma)$. Now, Γ has the following discrete Laplacian matrix L and pseudo-inverse L^{+} respectively:

$$\begin{bmatrix} 27 & 0 & -9 & 0 & 0 & -9 & -9 \\ 0 & 27 & -9 & 0 & 0 & -9 & -9 \\ -9 & -9 & 36 & -9 & -9 & 0 & 0 \\ 0 & 0 & -9 & 18 & -9 & 0 & 0 \\ 0 & 0 & -9 & -9 & 18 & 0 & 0 \\ -9 & -9 & 0 & 0 & 0 & 18 & 0 \\ -9 & -9 & 0 & 0 & 0 & 0 & 18 \end{bmatrix} \quad \text{and}$$

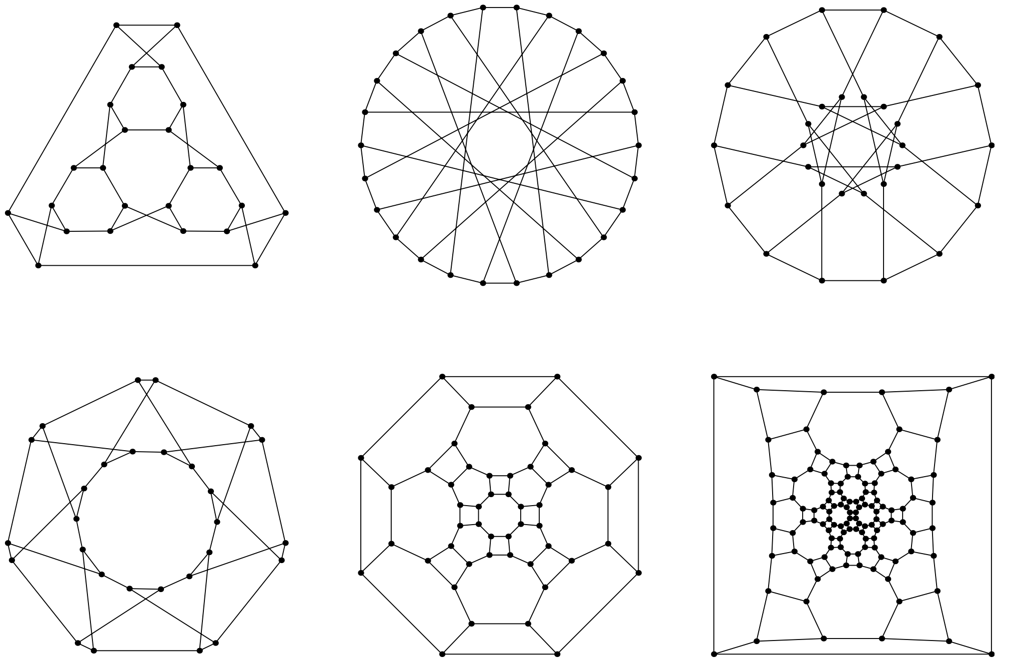

Fig. 7. Zero-symmetric graphs.

$$\begin{bmatrix} \frac{47}{1323} & -\frac{2}{1323} & -\frac{1}{147} & -\frac{10}{441} & -\frac{10}{441} & \frac{4}{441} & \frac{4}{441} \\ -\frac{2}{1323} & \frac{47}{1323} & -\frac{1}{147} & -\frac{10}{441} & -\frac{10}{441} & \frac{4}{441} & \frac{4}{441} \\ -\frac{1}{147} & -\frac{1}{147} & \frac{11}{441} & \frac{4}{441} & \frac{4}{441} & -\frac{13}{882} & -\frac{13}{882} \\ -\frac{10}{441} & -\frac{10}{441} & \frac{4}{441} & \frac{89}{1323} & \frac{40}{1323} & -\frac{3}{98} & -\frac{3}{98} \\ -\frac{10}{441} & -\frac{10}{441} & \frac{4}{441} & \frac{40}{1323} & \frac{89}{1323} & -\frac{3}{98} & -\frac{3}{98} \\ \frac{4}{441} & \frac{4}{441} & -\frac{13}{882} & -\frac{3}{98} & -\frac{3}{98} & \frac{25}{441} & \frac{1}{882} \\ \frac{4}{441} & \frac{4}{441} & -\frac{13}{882} & -\frac{3}{98} & -\frac{3}{98} & \frac{1}{882} & \frac{25}{441} \end{bmatrix}.$$

Finally, applying Theorem 4.10 gives $\tau(\Gamma) = \frac{23}{324}$. By Proposition 4.12, we have the following canonical measure for Γ: $\mu_{can}(x) = -\frac{1}{2}\delta_{p_1}(x) - \frac{1}{2}\delta_{p_2}(x) - \delta_{p_3}(x) + 3\sum_{e_i \in E(\Gamma)} dx$.

In the rest of this section, we use Mathematica's GraphData function [18] to obtain the plots and adjacency matrix of several classes of graphs having various topologies and symmetries. We compute the tau constant by implementing Theorem 1.1 in Mathematica [19]. From now on, we consider metrized graphs with total length 1, and we assume that each graph has equal edge lengths.

Some fusene graphs, planar 2-connected graphs whose bounded faces are hexagons, are considered in Table 1 and Fig. 3.

Some Sierpinski graphs are considered in Table 2 and in Fig. 4.

Some fullerene graphs, planar cubic graphs whose bounded faces pentagons or hexagons, are considered in Table 3 and in Fig. 5.

Some Archimedean graphs, skeletons of one of the 13 Archimedean solids, are considered in Table 4 and Fig. 6.

Some zero-symmetric graphs, vertex-transitive cubic graphs with edges partitioned into three orbits, are considered in Table 5 and in Fig. 7.

Since the tau constant is an invariant of metrized graphs, it becomes an invariant of molecular graphs. It would be interesting to understand the relation between the tau constant and other graph invariants.

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References

[1] M. Baker, X. Faber, Metrized graphs, Laplacian operators, and electrical networks, in: G. Berkolaiko, R. Carlson, S.A. Fulling, P. Kuchment (Eds.), Proceedings of the Joint Summer Research Conference on Quantum Graphs and Their Applications, in: Contemporary Mathematics, vol. 415, Snowbird Utah, 2006, pp. 15–33.
[2] M. Baker, R. Rumely, Harmonic analysis on metrized graphs, Canad. J. Math. 59 (2) (2007) 225–275.
[3] R.B. Bapat, Resistance matrix of a weighted graph, MATCH Commun. Math. Comput. Chem. 50 (2004) 73–82.
[4] R.B. Bapat, The Laplacian matrix of a graph, Math. Student 65 (1996) 214–223.
[5] R.B. Bapat, Resistance distance in graphs, The Mathematics Student 68 (1999) 87–98.
[6] S. Barnett, Matrices Methods and Applications, Clarendon Press, Oxford, 1990.
[7] T. Chinburg, R. Rumely, The capacity pairing, J. Reine Angew. Math. 434 (1993) 1–44.
[8] Z. Cinkir, The Tau Constant of Metrized Graphs, Thesis at University of Georgia, Athens, GA. 2007.
[9] Z. Cinkir, Generalized Foster's identities, Int. J. Quantum Chem., published online March 2010 doi:10.1002/qua.22521.
[10] Z. Cinkir, The tau constant of a metrized graph and its behavior under graph operations, Available at http://arxiv.org/abs/0901.0407v3 (submitted for publication).
[11] Z. Cinkir, The tau constant and the edge connectivity of a metrized graph, Available at http://arxiv.org/abs/0901.1481v2 (submitted for publication).
[12] I. Gutman, W. Xiao, Bulletin T.CXXIX de l'Académie serbe des sciences et des arts — 2004 Classe des sciences mathématiques et naturelles sciences mathématiques, No. 29, 2004.
[13] D.J. Klein, M. Randić, Resistance distance, J. Math. Chem. 12 (1993) 81–95.
[14] R. Merris, Laplacian matrices of graphs: a survey, Linear Algebra Appl. 197, 198 (1994) 143–176.
[15] C. Rao, S. Mitra, Generalized Inverse of Matrices and its Applications, John Wiley and Sons, 1971.
[16] Summer 2003 Research Experience for Undergraduates (REU) on metrized graphs at the University of Georgia.
[17] R. Rumely, Capacity Theory on Algebraic Curves, in: Lecture Notes in Mathematics, vol. 1378, Springer-Verlag, Berlin, Heidelberg, New York, 1989.
[18] Wolfram Research, Inc., Mathematica Documentation Center, Version 7.0, Champaign, IL, 2008, Available at http://reference.wolfram.com/mathematica/ref/GraphData.html.
[19] Wolfram Research, Inc., Mathematica, Version 7.0, Champaign, IL, 2008.
[20] S. Zhang, Admissible pairing on a curve, Invent. Math. 112 (1993) 171–193.
[21] S. Zhang, Gross–Schoen cycles and dualising sheaves, Invent. Math. 179 (2010) 1–73.