

Local Formula for Topological Charge Indices and Extremal Results for Trees and Alternating Cyclics

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(Received April 26, 2026)

Abstract

Topological charge indices are distance-based molecular descriptors used in chemical graph theory. This paper gives a local, matrix-free method for computing them in connected weighted molecular graphs, including graphs with multiple bonds. This avoids dense matrix computations and leads to efficient algorithms. As consequences, we obtain simplified formulas for simple graphs and bipartite graphs, recover and extend known formulas for trees, prove sharp extremal theorems for trees, and derive a complete layer-by-layer description for alternating weighted even cycles. In the alternating cycle family, only even distance layers contribute, each nonzero layer is obtained in closed form, and the total charge index admits an explicit formula. These results describe vanishing behavior in weighted cycle families, include the benzene model and higher annulenes as examples, and show that topological charge indices detect bond-order asymmetry invisible to classical distance-count descriptors.

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1 Introduction

Topological charge indices (TCIs), introduced by Gálvez and collaborators in the molecular-topology literature [1, 2], belong to the wider class of graph-theoretical descriptors used in QSAR/QSPR, molecular design, and chemoinformatics [2, 3, 6].

To define TCIs, fix a connected multigraph $G = (V, E)$ with vertex set $V = \{1, \dots, n\}$, weighted adjacency matrix $A = (a_{ij})_{1 \leq i, j \leq n}$ where $a_{ij} \in \{0, 1, 2, \dots\}$. The weighted degree of vertex i is $\delta(i) = \sum_{j=1}^n a_{ij}$. Graph distance $d(i, j)$ is the ordinary shortest-path distance in the underlying simple graph. For $k \geq 1$, let

$$T_k = \{(i, j) : 1 \leq i < j \leq n, d(i, j) = k\}$$

be the set of vertex pairs at distance k . The k -th topological charge index is

$$G_k = \sum_{(i,j) \in T_k} |c_{ij}|. \quad (1)$$

Here $C = (c_{ij}) = AD^* - D^*A$ is the charge-transfer matrix, where the reciprocal squared distance matrix $D^* = (d_{ij}^*)$ has entries

$$d_{ij}^* = \begin{cases} 0, & i = j, \\ d(i, j)^{-2}, & i \neq j. \end{cases}$$

Recall that the diameter of a connected graph G is

$$\text{diam}(G) = \max\{d(i, j) : i, j \in V(G)\}.$$

The index G_k is evaluated only for distances that actually occur in G , namely $1 \leq k \leq \text{diam}(G)$. For $k > \text{diam}(G)$ there are no vertex pairs at distance k , so $G_k = 0$. The algebraic charge-transfer index is $\mu = \frac{1}{2} \sum_{k \geq 1} G_k$, and a graph is called *zero-TCI* if $\mu = 0$.

Two issues make the original definition unsatisfactory for structural work. First, D^* is dense, so direct multiplication by A hides the sparse graph structure and is computationally expensive. Second, the matrix

product does not reveal which local graph features actually govern the entries c_{ij} . The first systematic simplification in this direction was obtained for trees by Shahryari and Vakili-Nezhaad [5]. The present paper develops that local viewpoint for arbitrary weighted molecular graphs and exact consequences for trees and weighted cycles.

Our principal result is a local formula expressing every charge-transfer term c_{ij} through weighted degrees and layered adjacency sums. From this formula we derive explicit expressions for the first and second charge layers in simple graphs and bipartite graphs.

We then turn to the extremal theory of TCIs on trees motivated by the general program on extremal distance-based indices surveyed in [7, 8]. We give exact formulas for the algebraic index μ for paths, stars, brooms and bi-stars. We give sharp extremal inequalities for G_1 and G_2 for trees. We prove that G_1 obeys the classical path–star extremal pattern that appears for several standard indices on trees, while G_2 behaves in a genuinely different way, attaining its maximum at the balanced bi-star rather than at the path and it is closer to the Wiener polarity phenomenon.

Finally, we investigate the alternating weighted even cycles $C_{2m}(p, q)$, for which the local formula gives a complete formula for μ . In particular, this leads to a natural characterization of the zero-TCI members of this family. The alternating weighted cycles considered here show that TCIs detect weighted bond-order asymmetry invisible to descriptors based only on the underlying unweighted graph.

The flow of the paper is as follows. Section 2 proves the local distance-layer formula for TCIs for multigraphs. Section 3 derives the simple and bipartite identities. Section 4 develops the exact tree extremal theory. Section 5 treats alternating even cycles. In section 6 we record a matrix-free algorithm.

2 Local formula for TCIs

Let $G = (V, E)$ be a multigraph. We adapt the notation given in the introduction and we write $x \sim i$ to mean that x is adjacent to i . The

degree of i is

$$\delta(i) = \sum_{j=1}^n a_{ij}.$$

Fix distinct vertices $i, j \in V$ and set $k = d(i, j) \geq 1$. For a neighbor x of i , the triangle inequality gives

$$d(x, j) \in \{k-1, k, k+1\}. \quad (2)$$

For $i \neq j$ and $k = d(i, j)$, define

$$\alpha_{ij} = \sum_{\substack{x \sim i \\ d(x, j) = k-1}} a_{ix}, \quad \beta_{ij} = \sum_{\substack{x \sim i \\ d(x, j) = k}} a_{ix}.$$

Thus α_{ij} counts, with multiplicity, the incident edges of i that move one step closer to j , while β_{ij} counts the incident edges that remain in the same distance layer. The remaining incident edges go to layer $k+1$, so

$$\gamma_{ij} := \sum_{\substack{x \sim i \\ d(x, j) = k+1}} a_{ix} = \delta(i) - \alpha_{ij} - \beta_{ij}. \quad (3)$$

For convenience we write $\rho_0 := 0$ and $\rho_t := 1/t^2$ for $t \geq 1$.

Theorem 2.1 (Local formula for c_{ij}). *Let $i \neq j$ and $k = d(i, j)$. Then*

$$c_{ij} = \rho_{k+1} (\delta(i) - \delta(j)) + (\rho_{k-1} - \rho_{k+1})(\alpha_{ij} - \alpha_{ji}) + (\rho_k - \rho_{k+1})(\beta_{ij} - \beta_{ji}). \quad (4)$$

Proof. By definition,

$$M_{ij} = \sum_{x \in V} a_{ix} d_{xj}^*.$$

The only nonzero terms are for neighbors x of i , and by equation (2) such neighbors satisfy $d(x, j) \in \{k-1, k, k+1\}$. Grouping the contributions according to these three distances gives

$$\begin{aligned}
M_{ij} &= \sum_{\substack{x \sim i \\ d(x,j)=k-1}} a_{ix} \rho_{k-1} + \sum_{\substack{x \sim i \\ d(x,j)=k}} a_{ix} \rho_k + \sum_{\substack{x \sim i \\ d(x,j)=k+1}} a_{ix} \rho_{k+1} \quad (5) \\
&= \rho_{k-1} \alpha_{ij} + \rho_k \beta_{ij} + \rho_{k+1} (\delta(i) - \alpha_{ij} - \beta_{ij}) \\
&= \rho_{k+1} \delta(i) + (\rho_{k-1} - \rho_{k+1}) \alpha_{ij} + (\rho_k - \rho_{k+1}) \beta_{ij}.
\end{aligned}$$

Apply this formula to the ordered pairs (i, j) and (j, i) and subtract the two resulting expressions. Since $d(i, j) = d(j, i) = k$, the coefficients are the same in both formulas, and (4) follows. $\blacksquare$

Recall that by definition $G_k = \sum_{(i,j) \in T_k} |c_{ij}|$. Since c_{ij} depends only on weighted degrees and layered sums (4), each G_k is computable without forming D^* explicitly.

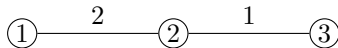
Formula (4) remains valid for $k = 1$ because the convention $\rho_0 = 0$ ensures that the formal contribution of the neighbor $x = j$ (at distance 0 from j) vanishes in M_{ij} , matching the requirement $d_{jj}^* = 0$.

Remark (Dominant terms and a large-distance approximation). For $k \geq 2$, the coefficient of the degree imbalance in (4) is $\rho_{k+1} = 1/(k+1)^2$, whereas the layer-correction coefficients satisfy

$$\rho_{k-1} - \rho_{k+1} = \frac{4k}{(k^2 - 1)^2} = O(k^{-3}), \quad \rho_k - \rho_{k+1} = \frac{2k+1}{k^2(k+1)^2} = O(k^{-3}).$$

Hence for vertices far apart (large k), the leading contribution to c_{ij} is often the degree term $\rho_{k+1}(\delta(i) - \delta(j))$, while the α - and β -terms provide finer corrections that are especially significant for small k . This suggests the approximation $c_{ij} \approx (\delta(i) - \delta(j))/(k+1)^2$ for large k , with an error controlled by the local layer imbalances $|\alpha_{ij} - \alpha_{ji}|$ and $|\beta_{ij} - \beta_{ji}|$ in (4).

Example 2.2 (A weighted tree: propene). Consider the weighted path on three vertices with a double bond between 1 and 2 and a single bond between 2 and 3:



We apply Theorem 2.1. The weighted degrees are $\delta(1) = 2$, $\delta(2) = 3$, $\delta(3) = 1$. Since the graph has no cycles $\beta_{ij} = 0$, for all $i \neq j$. For the adjacent pair $(1, 2)$ we have $k = 1$, $\alpha_{12} = a_{12} = 2$, and similarly $\alpha_{21} = a_{21} = 2$. Hence the α -term cancels in Theorem 2.1, and

$$c_{12} = \frac{\delta(1) - \delta(2)}{4} = \frac{2 - 3}{4} = -\frac{1}{4}.$$

Likewise, for the adjacent pair $(2, 3)$ we have $\alpha_{23} = \alpha_{32} = 1$, so

$$c_{23} = \frac{\delta(2) - \delta(3)}{4} = \frac{3 - 1}{4} = \frac{1}{2}.$$

Therefore

$$G_1 = |c_{12}| + |c_{23}| = \frac{1}{4} + \frac{1}{2} = \frac{3}{4}.$$

For the distance-two pair $(1, 3)$, the unique geodesic is 1-2-3, so

$$\alpha_{13} = a_{12} = 2, \quad \alpha_{31} = a_{32} = 1, \quad \beta_{13} = \beta_{31} = 0.$$

Using Theorem 2.1 with $k = 2$, we obtain

$$c_{13} = \frac{\delta(1) - \delta(3)}{9} + \left(1 - \frac{1}{9}\right) (\alpha_{13} - \alpha_{31}) = \frac{2 - 1}{9} + \frac{8}{9}(2 - 1) = 1.$$

Hence

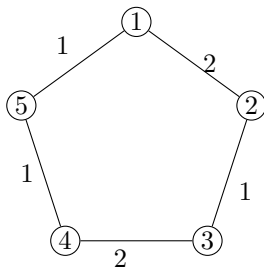
$$G_2 = |c_{13}| = 1.$$

Since $G_k = 0$ for $k > 2$, the algebraic index is

$$\mu = \frac{1}{2}(G_1 + G_2) = \frac{1}{2} \left(\frac{3}{4} + 1 \right) = \frac{7}{8}.$$

These values agree with the direct matrix computation.

Example 2.3 (1,3-Cyclopentadiene: a cycle example). Let G be the 5-cycle with edge multiplicities $(2, 1, 2, 1, 1)$ around the cycle, where the double bonds are 1-2 and 3-4:



The weighted degrees are

$$\delta(1) = 3, \quad \delta(2) = 3, \quad \delta(3) = 3, \quad \delta(4) = 3, \quad \delta(5) = 2.$$

We apply Theorem 2.1. For an adjacent pair (i, j) we have $k = 1$, so $\alpha_{ij} = a_{ij} = \alpha_{ji}$. Moreover, the graph is triangle-free, hence $\beta_{ij} = \beta_{ji} = 0$. Therefore (4) reduces to

$$c_{ij} = \frac{\delta(i) - \delta(j)}{4}.$$

Thus

$$c_{15} = \frac{\delta(1) - \delta(5)}{4} = \frac{3 - 2}{4} = \frac{1}{4}, \quad c_{45} = \frac{\delta(4) - \delta(5)}{4} = \frac{1}{4},$$

whereas all other adjacent pairs have equal weighted degrees and hence zero charge transfer. Therefore,

$$G_1 = |c_{15}| + |c_{45}| = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}.$$

To calculate G_2 , consider first the distance-two pair $(1, 3)$. Relative to $j = 3$, vertex 1 has one neighbor at distance 1 from 3 (vertex 2 with multiplicity 2) and one neighbor at distance 2 from 3 (vertex 5 with multiplicity 1). Hence

$$\alpha_{13} = 2, \quad \beta_{13} = 1.$$

Relative to $i = 1$, vertex 3 has one neighbor at distance 1 from 1 (vertex 2 with multiplicity 1) and one neighbor at distance 2 from 1 (vertex 4 with

multiplicity 2). Thus

$$\alpha_{31} = 1, \quad \beta_{31} = 2.$$

Since $\delta(1) = \delta(3)$, the degree term vanishes, and using formula (4) gives

$$c_{13} = (\rho_1 - \rho_3)(\alpha_{13} - \alpha_{31}) + (\rho_2 - \rho_3)(\beta_{13} - \beta_{31}) = \frac{8}{9} - \frac{5}{36} = \frac{3}{4}.$$

For the other distance-two pairs one obtains similarly

$$|c_{24}| = \frac{3}{4}, \quad |c_{14}| = 0, \quad |c_{25}| = 1, \quad |c_{35}| = 1.$$

Hence

$$G_2 = |c_{13}| + |c_{24}| + |c_{14}| + |c_{25}| + |c_{35}| = \frac{3}{4} + \frac{3}{4} + 0 + 1 + 1 = \frac{7}{2}.$$

Since the diameter is 2, we have $G_k = 0$ for all $k \geq 3$. Therefore

$$\mu = \frac{1}{2}(G_1 + G_2) = \frac{1}{2}\left(\frac{1}{2} + \frac{7}{2}\right) = 2.$$

These values agree with the direct matrix computation.

3 Simple and bipartite graphs

For simple graphs, the first two charge layers admit especially transparent formulas.

Theorem 3.1. *Let G be a simple connected graph. For every edge $(u, v) \in E(G)$,*

$$c_{uv} = \frac{\delta(u) - \delta(v)}{4}.$$

Consequently,

$$G_1(G) = \frac{1}{4} \sum_{(u,v) \in E(G)} |\delta(u) - \delta(v)|. \quad (6)$$

Proof. Let u and v be adjacent. Then $k = d(u, v) = 1$. In a simple graph, the only neighbor of u at distance 0 from v is v itself, so $\alpha_{uv} = 1$; similarly $\alpha_{vu} = 1$. Also, β_{uv} and β_{vu} both count the common neighbors of u and v ,

hence $\beta_{uv} = \beta_{vu}$. Applying Theorem 2.1 with $k = 1$ gives

$$c_{uv} = \rho_2(\delta(u) - \delta(v)) = \frac{\delta(u) - \delta(v)}{4}.$$

Summing absolute values over all edges yields (6). ■

Theorem 3.2. *Let G be a simple connected graph and let i, j be vertices with $d(i, j) = 2$. Then*

$$c_{ij} = \frac{\delta(i) - \delta(j)}{9} + \frac{5}{36}(\beta_{ij} - \beta_{ji}). \quad (7)$$

Consequently,

$$G_2(G) = \sum_{(i,j) \in T_2} \left| \frac{\delta(i) - \delta(j)}{9} + \frac{5}{36}(\beta_{ij} - \beta_{ji}) \right|. \quad (8)$$

Proof. If $d(i, j) = 2$, then α_{ij} and α_{ji} both count the common neighbors of i and j , hence $\alpha_{ij} = \alpha_{ji}$. Substituting $k = 2$ into Theorem 2.1 yields

$$\begin{aligned} c_{ij} &= \rho_3(\delta(i) - \delta(j)) + (\rho_2 - \rho_3)(\beta_{ij} - \beta_{ji}) \\ &= \frac{\delta(i) - \delta(j)}{9} + \left(\frac{1}{4} - \frac{1}{9} \right) (\beta_{ij} - \beta_{ji}) \\ &= \frac{\delta(i) - \delta(j)}{9} + \frac{5}{36}(\beta_{ij} - \beta_{ji}). \end{aligned}$$

Summing absolute values over T_2 gives (8). ■

Proposition 3.3. *If G is bipartite, then $\beta_{ij} = 0$ for all $i \neq j$.*

Proof. Let $k = d(i, j)$ and suppose that $\beta_{ij} > 0$. Then there exists a neighbor x of i such that $d(x, j) = k$. Take shortest paths $P_i : j \rightsquigarrow i$ and $P_x : j \rightsquigarrow x$. Let u be their last common vertex. Then the subpath of P_i from u to i , the edge ix , and the subpath of P_x from x to u form a cycle. Its length is

$$(k - d(j, u)) + 1 + (k - d(j, u)) = 2(k - d(j, u)) + 1,$$

which is odd. This contradicts the fact that a bipartite graph has no odd

cycle [4]. Therefore $\beta_{ij} = 0$. ■

Many chemically relevant graph families are bipartite. In particular, benzenoid (polyhex) graphs have no odd cycles and therefore satisfy Proposition 3.3.

Corollary 3.4 (Simplified local formula in the bipartite case). *If G is bipartite and $d(i, j) = k$, then*

$$c_{ij} = \rho_{k+1} (\delta(i) - \delta(j)) + (\rho_{k-1} - \rho_{k+1})(\alpha_{ij} - \alpha_{ji}). \quad (9)$$

Proof. By Proposition 3.3, $\beta_{ij} = \beta_{ji} = 0$. Substituting into (4) yields (9). ■

Theorem 3.5. *Let G be a simple connected bipartite graph. Then*

$$G_2(G) = \frac{1}{9} \sum_{(i,j) \in T_2} |\delta(i) - \delta(j)|. \quad (10)$$

Proof. Since G is bipartite, Proposition 3.3 gives $\beta_{ij} = \beta_{ji} = 0$. Substituting into Theorem 3.2, formula (7) becomes

$$c_{ij} = \frac{\delta(i) - \delta(j)}{9}.$$

Taking absolute values and summing over T_2 yields (10). ■

Graphs with vanishing charge–transfer matrix are absolute minimizers of every topological charge index. This leads to a natural classification problem. Recall that a connected graph G is called *distance-regular* if, for any two vertices $x, y \in V(G)$ with $d(x, y) = i$, the numbers of neighbors of y at distances $i - 1$, i , and $i + 1$ from x depend only on i , and not on the particular choice of x and y .

Theorem 3.6. *Every simple distance-regular graph is zero-TCI. In particular, unweighted cycles, complete graphs, and hypercubes are zero-TCI graphs.*

Proof. We use the matrix definition of G_k given in the introduction. Let G be a simple distance-regular graph with adjacency matrix A and diameter

d . For each $k = 0, 1, \dots, d$, let A_k denote the distance- k matrix of G , defined by

$$(A_k)_{ij} = \begin{cases} 1, & \text{if } d(i, j) = k, \\ 0, & \text{otherwise.} \end{cases}$$

Thus $A_0 = I$ and $A_1 = A$. By definition of D^* , we have $(D^*)_{ij} = d(i, j)^{-2}$ and $(D^*)_{ii} = 0$. Therefore

$$D^* = \sum_{k=1}^d \frac{1}{k^2} A_k.$$

A standard property of distance-regular graphs is that each distance matrix A_k is a polynomial in the adjacency matrix A [4]. Hence $D^* = P(A)$ for some polynomial P and $AD^* = AP(A) = P(A)A = D^*A$. Thus $C = AD^* - D^*A = 0$ and by Definition (1),

$$G_k = 0 \quad \text{for all } k.$$

■

Theorem 2.1 gives a simple necessary condition in the simple-graph case.

Corollary 3.7. *For a simple connected graph G , the following are equivalent:*

1. $G_1(G) = 0$;
2. every edge of G joins vertices of equal degree;
3. G is regular.

In particular, every zero-TCI graph satisfies $G_1 = 0$ by definition, hence is regular.

Proof. By Theorem 3.1, the identity $G_1(G) = 0$ holds if and only if $|\delta(u) - \delta(v)| = 0$ for every edge uv . This proves the equivalence of (1) and (2). Since G is connected, condition (2) propagates along paths and is therefore equivalent to regularity. ■

4 Trees and extremal problem

Extremal problems ask for the graphs in a prescribed class that maximize or minimize a chosen graph invariant. For distance-based topological indices, this “extremal program” has become a central line of research in chemical graph theory [7, 8]. The survey [8] emphasizes that, beyond the classical Wiener-type indices, much less is known for other distance-based descriptors. The formulas derived in Corollary 4.2 below make analogous questions accessible for TCIs.

Definition 4.1. Let $\mathcal{C}$ be a class of connected graphs and let I be a graph invariant. The *extremal problem* for I on $\mathcal{C}$ is to characterize the graphs in $\mathcal{C}$ that minimize or maximize I . For TCIs in the present paper the natural choices are $I = G_k$ and $I = \mu$.

For trees, Theorem 2.1 simplifies further because between any two vertices there is a unique geodesic.

Corollary 4.2 (Simple trees). *Let $\mathcal{T}$ be a simple tree. For $k \geq 1$,*

$$G_k(\mathcal{T}) = \frac{1}{(k+1)^2} \sum_{(i,j) \in T_k} |\delta(i) - \delta(j)|. \quad (11)$$

Proof. Let $i \neq j$ with $k = d(i, j)$. In a tree there is a unique i - j geodesic, hence i has exactly one neighbor in the layer $k-1$ with respect to j , and similarly for j . Therefore $\alpha_{ij} = \alpha_{ji} = 1$. Trees are bipartite, so $\beta_{ij} = \beta_{ji} = 0$ by Proposition 3.3. Substituting into (4) gives $c_{ij} = \rho_{k+1}(\delta(i) - \delta(j)) = (\delta(i) - \delta(j))/(k+1)^2$. Taking absolute values and summing over T_k yields (11). ■

For simple trees, Corollary 4.2 recovers the compact formula proved by Shahryari and Vakili-Nezhaad [5].

The tree case already yields sharp results.

Theorem 4.3. *Let $\mathcal{T}$ be a simple tree of order $n \geq 3$. Then*

$$\frac{1}{2} \leq G_1(\mathcal{T}) \leq \frac{(n-1)(n-2)}{4}. \quad (12)$$

The lower bound is attained if and only if $\mathcal{T} \cong P_n$, while the upper bound is attained if and only if $\mathcal{T} \cong S_n$.

Proof. By Corollary 4.2,

$$G_1(\mathcal{T}) = \frac{1}{4} \sum_{uv \in E(\mathcal{T})} |\delta(u) - \delta(v)|.$$

For the lower bound, let L be the number of leaves of $\mathcal{T}$. Every edge incident with a leaf contributes at least 1 to the sum, and these leaf-edges are distinct. Hence

$$4G_1(\mathcal{T}) \geq L \geq 2,$$

so $G_1(\mathcal{T}) \geq 1/2$.

Assume equality holds. Then necessarily $L = 2$, because otherwise the leaf-edges alone would contribute more than 2 to the sum. A tree with exactly two leaves is a path, so $\mathcal{T} \cong P_n$. Conversely, in P_n the only edges with unequal endpoint degrees are the two end edges, and each contributes 1, so $G_1(P_n) = 1/2$.

For the upper bound, we use the inequality $|a - b| \leq a + b - 2$ for positive integers a, b and $|E(\mathcal{T})| = n - 1$. We get

$$4G_1 \leq \sum_{uv \in E(\mathcal{T})} (\delta(u) + \delta(v) - 2) = \sum_{v \in V(\mathcal{T})} \delta(v)^2 - 2(n - 1).$$

Now write $\delta(v) = 1 + x_v$ with $x_v \geq 0$. Since $\sum_v \delta(v) = 2(n - 1)$, we have $\sum_v x_v = n - 2$ and $\sum_v x_v^2 \leq (n - 2)^2$. Hence

$$\begin{aligned} \sum_v \delta(v)^2 &= \sum_v (1 + 2x_v + x_v^2) = n + 2(n - 2) + \sum_v x_v^2 \\ &\leq n + 2(n - 2) + (n - 2)^2 = n(n - 1). \end{aligned}$$

Consequently,

$$4G_1 \leq n(n - 1) - 2(n - 1) = (n - 1)(n - 2),$$

which proves the upper bound in (12).

Assume equality holds. Then all the inequalities above must be equal-

ities. In particular, $\sum_v x_v^2 = (n-2)^2$, which forces one x_v to equal $n-2$ and all the others to be 0. Equivalently, one vertex has degree $n-1$ and every other vertex has degree 1, so $\mathcal{T} \cong S_n$. The converse is immediate because each edge of S_n contributes $n-2$. ■

Proposition 4.4. *For the path P_n with $n \geq 2$,*

$$G_k(P_n) = \begin{cases} \frac{2}{(k+1)^2}, & 1 \leq k \leq n-2, \\ 0, & k \geq n-1, \end{cases} \quad (13)$$

and therefore

$$\mu(P_n) = \sum_{t=2}^{n-1} \frac{1}{t^2}. \quad (14)$$

For the star S_n ,

$$G_1(S_n) = \frac{(n-1)(n-2)}{4}, \quad G_k(S_n) = 0 \quad (k \geq 2), \quad (15)$$

and therefore

$$\mu(S_n) = \frac{(n-1)(n-2)}{8}. \quad (16)$$

Proof. In P_n , only the two end vertices have degree 1, while every internal vertex has degree 2. Fix k with $1 \leq k \leq n-2$. Among the pairs at distance k , exactly two have unequal endpoint degrees, and each contributes $1/(k+1)^2$ by Corollary 4.2. Hence $G_k(P_n) = 2/(k+1)^2$. For $k = n-1$, there is unique pair and it has equal endpoint degrees, so $G_{n-1}(P_n) = 0$. Formula (14) follows by summing $G_k/2$.

For S_n , the center has degree $n-1$ and every leaf has degree 1. By Corollary 4.2, each edge contributes $(n-2)/4$, giving $G_1(S_n) = \frac{1}{4}(n-1)(n-2)$. Any pair at distance at least 2 consists of two leaves and therefore has equal degrees, so $G_k(S_n) = 0$ for $k \geq 2$. Formula (16) is immediate. ■

Remark. Formula (14) shows that $\mu(P_n)$ increases to

$$\sum_{t=2}^{\infty} \frac{1}{t^2} = \frac{\pi^2}{6} - 1,$$

whereas (16) gives $\mu(S_n) \sim n^2/8$. Thus the algebraic charge-transfer index stays bounded on paths but grows quadratically on stars.

Remark (Comparison with classical distance-based tree extremals). The path–star pattern in Theorem 4.3 is consistent with the classical extremal behavior of several standard distance-based indices on trees. Indeed, Xu, Liu, Das, Gutman, and Furtula list in their survey [8, Theorem 3.1] that, among trees of fixed order, the Wiener index and hyper-Wiener index are minimized by the star and maximized by the path, whereas the Harary index and reciprocal complementary Wiener index have the reverse extremal order. Thus the first charge layer G_1 fits the same broad path–star extremal paradigm that governs these better-known indices.

A broom $B_{n,\ell}$ is the tree obtained by attaching $\ell - 1$ pendent vertices to one pendent vertex of the path $P_{n-\ell+1}$, where $2 \leq \ell \leq n - 1$. Since a broom is obtained by attaching a collection of pendent edges to one end of a path, its TCI behavior combines the star-like contribution coming from the branching end with the path-like contribution coming from the handle. The next proposition makes this interaction explicit.

Proposition 4.5 (Brooms). *Let $B_{n,\ell}$ be a broom. Then*

$$G_1(B_{n,\ell}) = \frac{\ell(\ell - 1)}{4}, \quad (17)$$

for every $2 \leq k \leq n - \ell$,

$$G_k(B_{n,\ell}) = \frac{2(\ell - 1)}{(k + 1)^2}, \quad (18)$$

and $G_{n-\ell+1}(B_{n,\ell}) = 0$. Consequently,

$$\mu(B_{n,\ell}) = \frac{\ell(\ell - 1)}{8} + (\ell - 1) \sum_{t=3}^{n-\ell+1} \frac{1}{t^2}. \quad (19)$$

Proof. Label the broom so that $u_0 u_1 \dots u_{n-\ell}$ is the path and $\ell_1, \dots, \ell_{\ell-1}$ are the pendent vertices attached to u_0 . Then

$$\delta(u_0) = \ell, \quad \delta(u_{n-\ell}) = 1, \quad \delta(\ell_i) = 1,$$

and every remaining path vertex has degree 2.

For $k = 1$, the edges with unequal endpoint degrees are the $\ell - 1$ edges $u_0\ell_i$, the edge u_0u_1 , and the terminal edge $u_{n-\ell-1}u_{n-\ell}$. Their total degree imbalance is

$$(\ell - 1)(\ell - 1) + (\ell - 2) + 1 = \ell(\ell - 1),$$

so (17) follows from Corollary 4.2. When $\ell = n - 1$, the path reduces to the edge u_0u_1 with u_1 a leaf, and the three edge categories merge; the count $\ell(\ell - 1)$ remains correct.

Now let $2 \leq k \leq n - \ell$. The distance- k pairs with unequal degrees are exactly the following: the $\ell - 1$ pairs (ℓ_i, u_{k-1}) , the pair (u_0, u_k) , and the pair $(u_{n-\ell-k}, u_{n-\ell})$ when $k \leq n - \ell - 1$; when $k = n - \ell$, the last two types collapse to $(u_0, u_{n-\ell})$ together with the $\ell - 1$ pairs $(\ell_i, u_{n-\ell-1})$. In either case the total degree imbalance is $2(\ell - 1)$, and (18) follows from Corollary 4.2. The last statement and (19) are immediate. ■

A bi-star $BS(n_1, n_2)$ is a tree obtained by joining the centers of the stars S_{n_1+1} and S_{n_2+1} . We will need the following formulas for the G_2 extremal problem on trees.

Proposition 4.6 (Bi-stars). *Let $BS(n_1, n_2)$ be a bi-star. Then*

$$G_1(BS(n_1, n_2)) = \frac{n_1^2 + n_2^2 + |n_1 - n_2|}{4}, \quad (20)$$

$$G_2(BS(n_1, n_2)) = \frac{2n_1n_2}{9}, \quad (21)$$

$G_k(BS(n_1, n_2)) = 0$ for $k \geq 3$, and therefore

$$\mu(BS(n_1, n_2)) = \frac{n_1^2 + n_2^2 + |n_1 - n_2|}{8} + \frac{n_1n_2}{9}. \quad (22)$$

Proof. Let u and v be the two adjacent non-pendent vertices of $BS(n_1, n_2)$, where u is adjacent to n_1 pendent vertices

$$x_1, \dots, x_{n_1},$$

and v is adjacent to n_2 pendent vertices

$$y_1, \dots, y_{n_2}.$$

Thus

$$\delta(u) = n_1 + 1, \quad \delta(v) = n_2 + 1,$$

and every other vertex has degree 1. We apply Corollary 4.2. For G_1 , there are three kinds of edges: the n_1 edges ux_i , the n_2 edges vy_j and the central edge uv . Their contributions lead to

$$4G_1(BS(n_1, n_2)) = n_1 \cdot n_1 + n_2 \cdot n_2 + |n_1 - n_2|.$$

This gives formula (20).

For G_2 , the distance-2 pairs are of the following types:

- two pendent vertices adjacent to u or v , namely $\{x_r, x_s\}$ or $\{y_r, y_s\}$; these contribute 0 because vertices degrees are 1;
- pairs $\{x_i, v\}$, of which there are n_1 , each contributing

$$|\delta(x_i) - \delta(v)| = |1 - (n_2 + 1)| = n_2;$$

- likewise, pairs $\{u, y_j\}$, of which there are n_2 , each contributing

$$|\delta(u) - \delta(y_j)| = |(n_1 + 1) - 1| = n_1.$$

Hence

$$9G_2(BS(n_1, n_2)) = n_1n_2 + n_2n_1 = 2n_1n_2,$$

and so

$$G_2(BS(n_1, n_2)) = \frac{2n_1n_2}{9}.$$

Now $G_3 = 0$ since every distance-3 pair $\{x_i, y_j\}$ consists of two leaves. Also, $G_k = 0$ for all $k \geq 3$ since $\text{diam}(BS) = 3$. Then direct substitution gives μ . This proves (22). ■

Theorem 4.7 (Exact extrema of G_2 on trees). *Let $\mathcal{T}$ be a simple tree of order $n \geq 4$. Then*

$$0 \leq G_2(\mathcal{T}) \leq \frac{2}{9} \left\lfloor \frac{(n-2)^2}{4} \right\rfloor.$$

The lower bound is attained if and only if $\mathcal{T} \cong S_n$. The upper bound is attained if and only if

$$\mathcal{T} \cong BS\left(\left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil\right).$$

Proof. Since $\mathcal{T}$ is a tree, every pair of vertices at distance 2 has a unique common neighbor. Because T_2 is defined with the convention $i < j$, each distance-two pair is represented exactly once by some $(i, j) \in T_2$. For such a pair, the vertices i and j can be written uniquely as an unordered pair $\{i, j\} \subseteq N(w)$, where w is the middle vertex on the unique i - j path and

$$N(w) := \{u \in V(\mathcal{T}) : u \sim w\}.$$

Hence, by Corollary 4.2,

$$9G_2(\mathcal{T}) = \sum_{w \in V(\mathcal{T})} \sum_{\{u,v\} \subseteq N(w)} |\delta(u) - \delta(v)|. \quad (23)$$

For $u \in V(\mathcal{T})$ define $x_u := \delta(u) - 1$. Fix $w \in V(\mathcal{T})$. Then we have

$$\sum_{\{u,v\} \subseteq N(w)} |\delta(u) - \delta(v)| = \sum_{\{u,v\} \subseteq N(w)} |x_u - x_v| \leq \sum_{\{u,v\} \subseteq N(w)} (x_u + x_v).$$

Now each term x_u appears exactly $\delta(w) - 1$ times in the last sum, so

$$\sum_{\{u,v\} \subseteq N(w)} (x_u + x_v) = (\delta(w) - 1) \sum_{u \sim w} x_u = (\delta(w) - 1) \sum_{u \sim w} (\delta(u) - 1).$$

Substituting into (23), we obtain

$$9G_2(\mathcal{T}) \leq \sum_{w \in V(\mathcal{T})} (\delta(w) - 1) \sum_{u \sim w} (\delta(u) - 1).$$

Finally, each edge $uw \in E(\mathcal{T})$ contributes the term

$$(\delta(w) - 1)(\delta(u) - 1)$$

twice in this double sum, once from the vertex w and once from the vertex u . Hence

$$9G_2(\mathcal{T}) \leq 2 \sum_{uw \in E(\mathcal{T})} (\delta(u) - 1)(\delta(w) - 1) = 2 \sum_{uw \in E(\mathcal{T})} x_u x_w. \quad (24)$$

Let $A \cup B$ be the bipartition of the tree $\mathcal{T}$. Then

$$\sum_{uw \in E(\mathcal{T})} x_u x_w \leq \left(\sum_{u \in A} x_u \right) \left(\sum_{w \in B} x_w \right) \leq \left\lfloor \frac{\left(\sum_{u \in V(\mathcal{T})} x_u \right)^2}{4} \right\rfloor.$$

Using these inequalities with $\sum_{u \in V(\mathcal{T})} x_u = n - 2$ in (24), we get

$$G_2(\mathcal{T}) \leq \frac{2}{9} \left\lfloor \frac{(n-2)^2}{4} \right\rfloor.$$

The lower bound $G_2(\mathcal{T}) \geq 0$ is obvious. Suppose now that $G_2(\mathcal{T}) = 0$. If $\text{diam}(\mathcal{T}) \geq 3$, let

$$v_0 v_1 v_2 \cdots v_D$$

be a diametral path in $\mathcal{T}$. Then $d(v_0, v_2) = 2$, while

$$\delta(v_0) = 1, \quad \delta(v_2) \geq 2.$$

Therefore the pair $\{v_0, v_2\}$ contributes positively to

$$\sum_{\{i,j\} \in T_2} |\delta(i) - \delta(j)|,$$

contrary to $G_2(\mathcal{T}) = 0$. Hence $\text{diam}(\mathcal{T}) \leq 2$, and therefore $\mathcal{T} \cong S_n$. Conversely, if $\mathcal{T} \cong S_n$, then every distance-2 pair consists of two pendent vertices, so their degrees are equal and $G_2(S_n) = 0$.

It remains to characterize the equality case in the upper bound. Sup-

pose that

$$G_2(\mathcal{T}) = \frac{2}{9} \left\lfloor \frac{(n-2)^2}{4} \right\rfloor.$$

Then equality must hold in every inequality above. In particular, for each fixed $w \in V(\mathcal{T})$,

$$\sum_{\{u,v\} \subseteq N(w)} |x_u - x_v| = \sum_{\{u,v\} \subseteq N(w)} (x_u + x_v).$$

Since

$$0 \leq (x_u + x_v) - |x_u - x_v| \quad (\{u, v\} \subseteq N(w)),$$

the sum of these nonnegative terms is equal to 0. Hence each term is 0, and therefore

$$|x_u - x_v| = x_u + x_v \quad \text{for every } \{u, v\} \subseteq N(w).$$

Because $x_u, x_v \geq 0$, this is equivalent to

$$x_u x_v = 0 \quad \text{for every } \{u, v\} \subseteq N(w).$$

Thus, for every vertex w , at most one neighbor of w can be non-pendent.

Since the upper bound is positive for $n \geq 4$, the extremal tree is not a star, so $\mathcal{T}$ has at least two non-pendent vertices. Let a and b be two such vertices, and let

$$a = v_0, v_1, \dots, v_m = b$$

be the unique a - b path in $\mathcal{T}$. Every internal vertex of this path is non-pendent. If $m \geq 2$, then v_1 has two non-pendent neighbors, namely v_0 and v_2 , a contradiction. Hence $m = 1$, so any two non-pendent vertices are adjacent.

It follows that $\mathcal{T}$ has exactly two non-pendent vertices. Indeed, if there were three, then one of them would be adjacent to two non-pendent vertices, again a contradiction. Therefore $\mathcal{T}$ has exactly two adjacent non-pendent vertices, and all remaining vertices are pendent and attached to

one of them. Hence

$$\mathcal{T} \cong BS(n_1, n_2) \quad \text{for some } n_1, n_2 \geq 1 \text{ with } n_1 + n_2 = n - 2.$$

By Proposition 4.6,

$$G_2(BS(n_1, n_2)) = \frac{2n_1n_2}{9}.$$

For fixed $n_1 + n_2 = n - 2$, the product n_1n_2 is maximal exactly when

$$\{n_1, n_2\} = \left\{ \left\lfloor \frac{n-2}{2} \right\rfloor, \left\lceil \frac{n-2}{2} \right\rceil \right\}.$$

Since

$$\left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-2}{2} \right\rceil = \left\lfloor \frac{(n-2)^2}{4} \right\rfloor,$$

the balanced bi-star satisfies

$$G_2(BS(n_1, n_2)) = \frac{2n_1n_2}{9} = \frac{2}{9} \left\lfloor \frac{(n-2)^2}{4} \right\rfloor.$$

This gives the stated extremal tree and completes the proof. ■

Remark (Comparison with the Wiener polarity phenomenon). Theorem 4.7 shows that the second charge layer does *not* follow the classical path–star pattern: its minimum is attained by the star, but its maximum is attained by the balanced bi-star rather than by the path. This behavior is closer in spirit to the Wiener polarity index than to the Wiener or Harary indices. Indeed, Xu *et al.* record in [8, Theorem 3.2] that, among trees of fixed order, the Wiener polarity index is minimized by the star and maximized by the balanced bi-star, or by a related diameter-4 family. They also note that the Wiener polarity index is therefore not a branching measure in the usual path–star sense. In this respect, G_2 exhibits a similar departure from the standard extremal scheme.

Remark. The first two layers already show that the sequence (G_k) does not satisfy a uniform extremal pattern on trees. The star S_n is extremal

for G_1 , but

$$G_k(S_n) = 0 \quad (k \geq 2),$$

because $\text{diam}(S_n) = 2$. On the other hand, the balanced bi-star is extremal for G_2 , yet

$$G_3(BS(n_1, n_2)) = 0,$$

since the only pairs of vertices at distance 3 in a bi-star are pairs of pendent vertices from opposite sides, and these have equal degrees. Hence even the trees that are extremal for G_1 and G_2 need not contribute at the next layer. This suggests that the higher charge indices G_k should be studied layer by layer.

Corollary 4.8. *A simple connected tree is zero-TCI if and only if it is K_2 .*

Proof. If a simple connected tree is zero-TCI, then it is regular by Corollary 3.7. A tree of order at least 3 has a leaf, hence cannot be regular. Therefore the only possibility is K_2 . Conversely, K_2 has just one edge, its endpoints have equal degree, and hence all TCIs vanish. ■

5 Alternating even cycles

We now illustrate how the local distance-layer formula yields a complete layer-by-layer description for a natural family of weighted even cycles.

Definition 5.1. Let $m \geq 2$ and let $p, q \in \{1, 2, 3, \dots\}$. The *alternating weighted cycle* $C_{2m}(p, q)$ is the cycle on vertices $0, 1, \dots, 2m - 1$ in which the edge $\{t, t + 1\}$ (indices mod $2m$) has multiplicity p for even t and multiplicity q for odd t .

Thus every vertex has weighted degree $p + q$, and benzene is modeled by $C_6(2, 1)$.

Theorem 5.2 (All charge layers of $C_{2m}(p, q)$). *Let $G = C_{2m}(p, q)$ with*

$m \geq 2$. Then, for each k with $1 \leq k \leq m$,

$$G_k = \begin{cases} \frac{8mk}{(k^2 - 1)^2} |p - q|, & \text{if } k \text{ is even and } 2 \leq k \leq m - 1, \\ 0, & \text{otherwise.} \end{cases} \quad (25)$$

Consequently,

$$\mu(C_{2m}(p, q)) = \begin{cases} m|p - q| \left(1 - \frac{1}{(m - 1)^2}\right), & \text{if } m \text{ is even,} \\ m|p - q| \left(1 - \frac{1}{m^2}\right), & \text{if } m \text{ is odd.} \end{cases} \quad (26)$$

Proof. For $t \in \{0, 1, \dots, 2m - 1\}$, write

$$w_t := a_{t, t+1},$$

so that $w_t = p$ if t is even and $w_t = q$ if t is odd (indices modulo $2m$).

Since C_{2m} is an even cycle, it is bipartite. Hence Proposition 3.3 gives

$$\beta_{ij} = 0 \quad (i \neq j).$$

Also every vertex has the same weighted degree,

$$\delta(i) = p + q.$$

Therefore the degree term in Theorem 2.1 vanishes, and for every pair of distinct vertices with $d(i, j) = k$ we have

$$c_{ij} = (\rho_{k-1} - \rho_{k+1})(\alpha_{ij} - \alpha_{ji}). \quad (27)$$

We now determine $\alpha_{ij} - \alpha_{ji}$.

Case 1: $k = m$. Let $j = i + m$. Then i and j are opposite vertices of the cycle. Both neighbors of i lie at distance $m - 1$ from j , so both incident edges of i contribute to α_{ij} . Hence

$$\alpha_{ij} = w_{i-1} + w_i = p + q.$$

Similarly,

$$\alpha_{ji} = p + q.$$

Thus (27) gives $c_{ij} = 0$ for every diametral pair, and therefore

$$G_m = 0.$$

Case 2: $1 \leq k \leq m - 1$. Fix a pair at distance k , and choose the cyclic orientation so that

$$j = i + k \pmod{2m}$$

along the unique shortest arc from i to j . Then the only neighbor of i lying one step closer to j is $i + 1$, so

$$\alpha_{ij} = a_{i, i+1} = w_i.$$

Likewise, the unique neighbor of j lying one step closer to i is $j - 1 = i + k - 1$, so

$$\alpha_{ji} = a_{j, j-1} = w_{i+k-1}.$$

If k is odd, then i and $i + k - 1$ have the same parity, hence

$$w_i = w_{i+k-1},$$

so $\alpha_{ij} = \alpha_{ji}$ and therefore

$$c_{ij} = 0.$$

Thus

$$G_k = 0 \quad \text{for all odd } k.$$

If k is even, then i and $i + k - 1$ have opposite parity, hence one of w_i, w_{i+k-1} equals p and the other equals q . Therefore

$$|\alpha_{ij} - \alpha_{ji}| = |p - q|.$$

Using (27),

$$|c_{ij}| = (\rho_{k-1} - \rho_{k+1})|p - q| = \frac{4k}{(k^2 - 1)^2}|p - q|.$$

For each $k < m$, the cycle C_{2m} has exactly $2m$ unordered pairs of vertices at distance k . Hence, for even k with $2 \leq k \leq m - 1$,

$$G_k = 2m \cdot \frac{4k}{(k^2 - 1)^2}|p - q| = \frac{8mk}{(k^2 - 1)^2}|p - q|.$$

This proves (25).

Finally,

$$\mu = \frac{1}{2} \sum_{k=1}^m G_k,$$

and only the even layers $2, 4, \dots, m - 1$ contribute. Hence

$$\begin{aligned} \mu(C_{2m}(p, q)) &= 4m|p - q| \sum_{\substack{k=2 \\ k \text{ even}}}^{m-1} \frac{k}{(k^2 - 1)^2} \\ &= m|p - q| \sum_{\substack{k=2 \\ k \text{ even}}}^{m-1} \left(\frac{1}{(k-1)^2} - \frac{1}{(k+1)^2} \right). \end{aligned} \tag{28}$$

This is a telescoping sum over the odd integers. Hence

$$\mu(C_{2m}(p, q)) = m|p - q| \left(1 - \frac{1}{(2\lfloor (m-1)/2 \rfloor + 1)^2} \right).$$

The parity form (26) is immediate. ■

Corollary 5.3 (Extremal weighted alternation at fixed weighted degree).

Fix integers $m \geq 2$ and $s \geq 2$, and consider the family

$$\mathcal{C}_{m,s} := \{ C_{2m}(p, q) : p, q \in \mathbb{N}, p + q = s \}.$$

For each even k with $2 \leq k \leq m - 1$, the quantity G_k and the total index μ are increasing functions of $|p - q|$ on $\mathcal{C}_{m,s}$. Consequently:

1. The maximum of every nonzero layer G_k and of μ on $\mathcal{C}_{m,s}$ is attained exactly at the extreme pairs

$$(p, q) = (1, s-1) \quad \text{or} \quad (s-1, 1).$$

2. The minimum is attained at the most balanced pairs:

$$(p, q) = \begin{cases} \left(\frac{s}{2}, \frac{s}{2}\right), & \text{if } s \text{ is even,} \\ \left(\frac{s-1}{2}, \frac{s+1}{2}\right) \text{ or } \left(\frac{s+1}{2}, \frac{s-1}{2}\right), & \text{if } s \text{ is odd.} \end{cases}$$

In particular, if s is even, then the minimum value is 0 for every charge layer and for μ .

Proof. By Theorem 5.2, every nonzero G_k and μ is a positive constant depending only on m and k , multiplied by $|p - q|$. Thus the extremal problem reduces to maximizing or minimizing $|p - q|$ subject to $p, q \in \mathbb{N}$ and $p + q = s$. The maximum is $s - 2$, attained only at $(1, s - 1)$ and $(s - 1, 1)$, and the minimum is 0 when s is even and 1 when s is odd, attained exactly at the most balanced pairs. ■

Corollary 5.4 (Zero-TCI criterion in the alternating family). *In the family $\mathcal{C}_{2m}(p, q)$, the following hold:*

1. every 4-cycle $\mathcal{C}_4(p, q)$ is zero-TCI;
2. for $m \geq 3$, the graph $\mathcal{C}_{2m}(p, q)$ is zero-TCI if and only if $p = q$.

Proof. If $m = 2$, then the interval $2 \leq k \leq m - 1$ is empty, so Theorem 5.2 gives $G_k = 0$ for all k . If $p = q$, then every nonzero formula in (25) vanishes, so $G_k = 0$ for all k and the graph is zero-TCI. Alternatively, when $p = q$, the graph $\mathcal{C}_{2m}(p, p)$ satisfies $A = p A(\mathcal{C}_{2m})$ and has unchanged distances, so

$$C(\mathcal{C}_{2m}(p, p)) = p C(\mathcal{C}_{2m}) = 0$$

by Theorem 3.6. Assume now that $m \geq 3$. Conversely, if $p \neq q$, then Theorem 5.2 gives

$$G_2 = \frac{16m}{9}|p - q| > 0,$$

so the graph cannot be zero-TCI. ■

Remark (Distance-count versus charge-transfer behavior). Xu *et al.* emphasize in Section 1 of [8] that the classical distance-based indices W , WW , H , and RCW are determined by the numbers $d(G, k)$ of vertex pairs at distance k . Hence, for the simple cycle C_{2m} , they depend only on m . Theorem 5.2 shows that the topological charge indices behave differently on $C_{2m}(p, q)$: they detect the weighted alternation through $|p - q|$, and only the even distance layers contribute. This provides a simple family in which TCIs distinguish bond-order asymmetry invisible to classical distance-count descriptors.

Example 5.5. For annulene modeled by $C_{14}(2, 1)$, we have $m = 7$ and $|p - q| = 1$. The active layers are $k = 2, 4, 6$, and

$$G_2 = \frac{112}{9}, \quad G_4 = \frac{224}{225}, \quad G_6 = \frac{48}{175}, \quad G_k = 0 \text{ otherwise.}$$

Therefore

$$\mu = \frac{1}{2}(G_2 + G_4 + G_6) = \frac{48}{7}.$$

6 A matrix-free algorithm

Theorem 2.1 reduces the computation of TCIs to shortest-path distances together with the layered adjacency sums α_{ij} and β_{ij} . Thus the dense reciprocal-distance matrix D^* never needs to be formed explicitly. Instead, one may compute the charge-transfer terms c_{ij} directly from local data obtained by repeated breadth-first searches.

6.1 Pseudocode

Algorithm 1 (Matrix-free evaluation of TCIs).

1. **Input:** a connected weighted graph G on n vertices, given in adjacency-list form with multiplicities a_{uv} .

2. Compute the weighted degrees

$$\delta(v) = \sum_{x \sim v} a_{vx} \quad (v \in V(G)).$$

3. Initialize $D := 0$.

4. For each source vertex $s \in V(G)$:

- (a) run a breadth-first search (BFS) on the underlying simple graph to obtain

$$d_s[v] = d(v, s) \quad (v \in V(G));$$

- (b) update

$$D := \max\{D, \max_{v \in V(G)} d_s[v]\};$$

thus, after all BFS runs, $D = \text{diam}(G)$;

- (c) scan each adjacency list once and compute the layered sums

$$\alpha_{vs} = \sum_{x \sim v, d_s[x]=d_s[v]-1} a_{vx}, \quad \beta_{vs} = \sum_{x \sim v, d_s[x]=d_s[v]} a_{vx};$$

- (d) store the values $d_s[v]$, α_{vs} , and β_{vs} for all $v \in V(G)$.

5. Initialize $G_k := 0$ for $1 \leq k \leq D$.

6. For each unordered pair $i < j$:

- (a) let $k = d(i, j)$;

- (b) evaluate c_{ij} from Theorem 2.1 using the stored values $\delta(i)$, $\delta(j)$, α_{ij} , α_{ji} , β_{ij} , and β_{ji} ;

- (c) add $|c_{ij}|$ to G_k .

7. **Output:** the charge layers $\{G_k\}_{1 \leq k \leq D}$, where $D = \text{diam}(G)$, and hence

$$\mu = \frac{1}{2} \sum_{k=1}^D G_k.$$

6.2 Complexity and storage

The cost of Algorithm 1 is governed by the repeated breadth-first searches and the final aggregation over unordered vertex pairs.

Proposition 6.1. *Algorithm 1 runs in $O(n(m+n))$ time for the distance-layer preprocessing and in $\Theta(n^2)$ time for the final pair aggregation. In particular, for sparse molecular graphs with $m = O(n)$, the total running time is quadratic up to constants.*

Proof. For each source vertex $s \in V(G)$, one breadth-first search on the underlying simple graph computes the distances $d_s[v]$ for all $v \in V(G)$ in $O(m+n)$ time. The same pass also yields $\max_v d_s[v]$, so the diameter is obtained as

$$\text{diam}(G) = \max_{s \in V(G)} \max_{v \in V(G)} d_s[v]$$

without additional asymptotic cost.

After the BFS from a fixed source s , one scan of all adjacency lists computes the layered sums α_{vs} and β_{vs} for all vertices v . This costs $O(m)$. Repeating these two steps over all n choices of s gives a total preprocessing time of

$$O(n(m+n)).$$

Once the distances and layered sums have been stored, the algorithm loops over all unordered pairs $i < j$. There are exactly $\binom{n}{2} = \Theta(n^2)$ such pairs, and the value of c_{ij} is then obtained in constant time from Theorem 2.1. Hence the final aggregation costs $\Theta(n^2)$.

Therefore the total running time is

$$O(n(m+n)) + \Theta(n^2).$$

In particular, if $m = O(n)$, then the whole algorithm is quadratic. ■

The storage requirement is $O(n^2)$ if one keeps the arrays $d_s[v]$, α_{vs} , and β_{vs} for all ordered pairs (v, s) . This is convenient for the final pair aggregation. If memory is an issue, the same method can also be implemented in streaming form, processing one source vertex at a time and updating the relevant pair contributions without storing all layers simultaneously.

6.3 Computational considerations

The main point of Algorithm 1 is not merely to avoid dense matrix multiplication, but to align computation with the local structure of Theorem 2.1. The quantities α_{ij} and β_{ij} are precisely the data that appear in the formula for c_{ij} , so the algorithm translates the matrix definition of TCIs into a layer-by-layer evaluation scheme.

For sparse molecular graphs this is computationally favorable, since the dense matrix D^* is never formed. Even when a direct matrix product may be competitive for moderate sizes on optimized numerical platforms, the present scheme has two structural advantages:

1. it provides an interpretable local decomposition of each c_{ij} in terms of degree imbalance and directional layer couplings;
2. it allows partial or targeted evaluation, for example when one is interested only in layers up to a prescribed distance or only in pairs involving a selected set of vertices.

Thus the matrix-free algorithm should be viewed as a computational corollary of the local theory rather than as a benchmarking claim.

7 Conclusion

We established a local distance-layer formula for the charge-transfer entries c_{ij} of the topological charge matrix in connected weighted molecular graphs. This formula expresses each c_{ij} in terms of weighted vertex degrees together with the layered adjacency sums α_{ij} and β_{ij} , thereby replacing the dense matrix product AD^* by explicitly local graph data. As a result, the first two charge layers become transparent in simple and bipartite graphs, and the tree case admits an exact all-layer description.

The extremal consequences already show that TCIs behave differently from many classical distance-based indices. For trees of fixed order, the first charge layer G_1 follows the classical path-star pattern: it is minimized by the path and maximized by the star. In contrast, the second layer G_2 is minimized by the star but maximized by the balanced bi-star. Thus

the charge-transfer viewpoint departs from the usual path–star paradigm already at distance two.

For the alternating weighted cycle family $C_{2m}(p, q)$, the local formula yields a complete layer-by-layer description. Only even distance layers contribute, each nonzero layer is obtained in closed form, the total index μ is explicit, and the zero-TCI members of the family are completely characterized. In particular, this family provides a simple model in which TCIs detect bond-order asymmetry that is invisible to classical distance-count descriptors based only on the underlying unweighted cycle.

From the computational side, the same formulas lead to a matrix-free breadth-first search procedure that avoids constructing the dense reciprocal-distance matrix. Structurally, they identify a part of the TCI theory that is both mathematically complete and chemically interpretable. Broader cyclic classes, including unicyclic, bicyclic, and benzenoid families, will be treated separately.

Acknowledgment: The authors are grateful to M. Shahryari for providing a copy of his paper on topological charge indices during their study of chemical graphs. Yassir Dinar acknowledges Sultan Qaboos University for the financial support received under Internal Grant IG/SCI/M/25/075.

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