Analytical Derivation of Relative Contraction Factors for Topological Polymers

A Spectral Graph Theory Approach to Polymer Physics

November 11, 2025

Abstract

This report presents a comprehensive analytical derivation of the relative contraction factor for topological polymers using spectral graph theory. We compute the asymptotic contraction factors $g(G_\infty)$ for two polymer topologies—a theta graph and a branched tree—by applying Theorem 5 from Cantarella et al. (2022). Through normalized Laplacian eigenvalue analysis and Moore-Penrose pseudoinverse trace calculations, we establish the exact ratio $g(\theta)/g(\text{tree}) = 107/245 \approx 0.4367$, demonstrating that theta polymers exhibit approximately 43.67% of the compaction observed in tree reference polymers in the infinite subdivision limit.

Contents

1 Introduction

1.1 Objectives

This project aims to:

1. Derive analytical expressions for contraction factors of two topological polymers: a **theta graph** and a **branched tree**.
2. Apply spectral graph theory to compute normalized Laplacian eigenvalues.
3. Calculate the trace of the Moore-Penrose pseudoinverse for each topology.
4. Use Theorem 5 (Cantarella et al., 2022) to obtain asymptotic contraction factors.
5. Compute the relative contraction factor ratio and compare to published values.

1.2 Theoretical Framework

Our analysis employs the **topologically constrained random walk (TCRW)** model [1], also known as the *phantom chain model*, where:

- Polymers are modeled as multigraphs $G = (V, E)$
- Bond vectors are sampled from multivariate Gaussian distributions
- The expected radius of gyration is determined by the Kirchhoff index
- Asymptotic behavior in the infinite-subdivision limit yields universal topological invariants

This ideal chain model (excluding volume effects) provides analytical results that correlate strongly ($R^2 = 0.966$) with molecular dynamics simulations including excluded volume [1].

1.3 Computational Resources

All calculations are implemented in Python using NumPy, NetworkX, and SciPy. Source code is available at:

https://github.com/ShlokP06/Polymer-Contraction

2 Mathematical Preliminaries

2.1 Graph Theory Notation

Definition 2.1 (Multigraph)**.** A **connected multigraph** $G = (V, E)$ consists of:

- A vertex set V with v vertices
- An edge set E with e edges

Definition 2.2 (Cycle Rank)**.** The **cycle rank** (or loop number) of a connected graph G is:

$$\text{Loops}(G) = e - v + 1 \tag{1}$$

For acyclic graphs (trees), $\text{Loops}(G) = 0$. For graphs with cycles, $\text{Loops}(G) > 0$.

2.2 Graph Matrices

Definition 2.3 (Adjacency Matrix)**.** The **adjacency matrix** $\mathbf{A} \in \mathbb{R}^{v \times v}$ is defined by:

$$A_{ij} = \text{number of edges connecting } v_i \text{ and } v_j \tag{2}$$

For simple graphs, $A_{ij} \in \{0, 1\}$. Loop edges contribute $A_{ii} = 2$.

Definition 2.4 (Degree Matrix)**.** The **degree matrix** $\mathbf{D} \in \mathbb{R}^{v \times v}$ is diagonal with:

$$D_{ii} = \deg(v_i) = \sum_j A_{ij} \tag{3}$$

where $\deg(v_i)$ counts edges incident to v_i (loop edges count twice).

Definition 2.5 (Graph Laplacian)**.** The **Laplacian matrix** is:

$$\mathbf{L} = \mathbf{D} - \mathbf{A} \tag{4}$$

with entries:

$$L_{ij} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -A_{ij} & \text{if } i \neq j \end{cases} \tag{5}$$

Definition 2.6 (Normalized Laplacian)**.** The **normalized graph Laplacian** $\bar{\mathbf{L}} \in \mathbb{R}^{v \times v}$ is:

$$\bar{L}_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{\sqrt{\deg(v_i) \cdot \deg(v_j)}} & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

2.3 Spectral Properties

Theorem 2.7 (Laplacian Spectrum)**.** *For a connected graph G, the Laplacian $\mathbf{L}$ and normalized Laplacian $\bar{\mathbf{L}}$ have the following properties:*

1. *Both are symmetric and positive semidefinite*
2. *The smallest eigenvalue is $\lambda_1 = 0$ with multiplicity 1*
3. *All nonzero eigenvalues satisfy $0 < \lambda_i \leq 2$ (for $\bar{\mathbf{L}}$)*

Definition 2.8 (Moore-Penrose Pseudoinverse)**.** For a symmetric matrix $\mathbf{M}$ with eigendecomposition $\mathbf{M} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$, the **Moore-Penrose pseudoinverse** is:

$$\mathbf{M}^\dagger = \mathbf{U}\mathbf{\Lambda}^\dagger\mathbf{U}^T \tag{7}$$

where $\Lambda^\dagger$ replaces nonzero eigenvalues with their reciprocals:

$$\Lambda^\dagger_{ii} = \begin{cases} 1/\lambda_i & \text{if } \lambda_i \neq 0 \\ 0 & \text{if } \lambda_i = 0 \end{cases} \tag{8}$$

2.4 Key Spectral Relation

Proposition 2.9 (Trace-Eigenvalue Identity)**.** *For the normalized Laplacian $\bar{\mathbf{L}}$ of a connected graph with eigenvalues $\lambda_1 = 0, \lambda_2, \ldots, \lambda_v$, the trace of the pseudoinverse is:*

$$\mathrm{Tr}(\bar{\mathbf{L}}^\dagger) = \sum_{i=2}^{v} \frac{1}{\lambda_i} \tag{9}$$

Proof. Since $\bar{\mathbf{L}}$ is symmetric, it admits a spectral decomposition. The trace is invariant under similarity transformations, so:

$$\mathrm{Tr}(\bar{\mathbf{L}}^\dagger) = \mathrm{Tr}(\mathbf{\Lambda}^\dagger) = \sum_{i=2}^{v} \frac{1}{\lambda_i}$$

where we omit the zero eigenvalue in the sum. □

3 Theoretical Foundation: Contraction Factors

3.1 Physical Interpretation

Definition 3.1 (Radius of Gyration)**.** The **radius of gyration** R_g of a polymer with vertex positions $\{x_i\}$ is:

$$R_g^2 = \frac{1}{2v^2} \sum_{i,j=1}^{v} |x_i - x_j|^2 \tag{10}$$

This measures the root-mean-square distance of monomers from the center of mass.

Definition 3.2 (Contraction Factor)**.** The **contraction factor** (or g-factor) of a polymer with graph G is:

$$g(G) = \frac{\mathbb{E}[R_g^2(G)]}{\mathbb{E}[R_g^2(\text{linear chain with } v \text{ vertices})]} \tag{11}$$

3.2 Cantarella et al. Results

The following theorem provides the foundation for our analytical calculation:

Theorem 3.3 (Asymptotic Contraction Factor (Theorem 5, Cantarella et al.))**.** *For any connected multigraph G with v vertices and e edges, let G_n be the graph obtained by subdividing each edge into n segments. Then the contraction factor in the infinite-subdivision limit is:*

$$\boxed{g(G_\infty) := \lim_{n\to\infty} g(G_n) = \frac{3\left[\mathrm{Tr}(\bar{\mathbf{L}}^\dagger) + \frac{1}{3}\,\mathrm{Loops}(G) - \frac{1}{6}\right]}{e^2}} \tag{12}$$

where:

- $\bar{\mathbf{L}}$ *is the normalized Laplacian of the* ***base graph*** G
- $\bar{\mathbf{L}}^\dagger$ *is its Moore-Penrose pseudoinverse*
- $\mathrm{Loops}(G) = e - v + 1$ *is the cycle rank*

Remark 3.4. This theorem shows that the asymptotic contraction factor depends *only on the base topology*, not on the subdivision level n.

Definition 3.5 (Relative Contraction Factor (Definition 21, Cantarella et al.))**.** The **relative contraction factor** of polymer G_1 with respect to reference polymer G_2 is:

$$g(G_1, G_2) = \frac{g(G_{1\infty})}{g(G_{2\infty})} \tag{13}$$

This ratio is a universal topological invariant independent of subdivision or physical length scales.

4 Analytical Derivation: Theta Graph

4.1 Graph Construction

Definition 4.1 (Theta Graph Topology)**.** The **theta graph** G_θ consists of:

- A hexagonal ring: vertices $v_0, v_1, \ldots, v_5$
- A central vertex v_6 connected to alternating ring vertices v_1, v_3, v_5

Graph parameters:

$$v_\theta = 7 \quad \text{(vertices)} \tag{14}$$
$$e_\theta = 9 \quad \text{(edges: 6 ring + 3 branches)} \tag{15}$$
$$\text{Loops}(\theta) = 9 - 7 + 1 = 3 \quad \text{(cycle rank)} \tag{16}$$

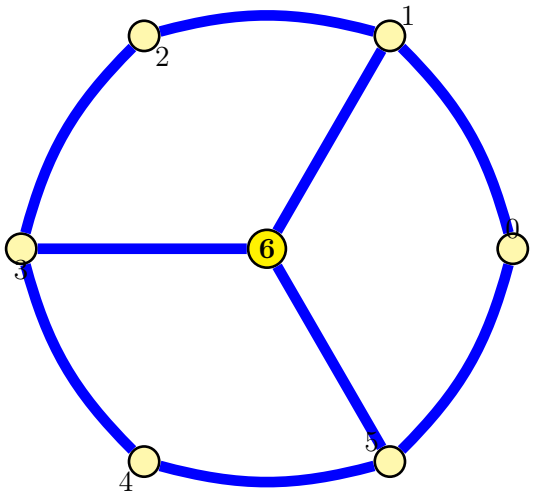

Figure 1: Theta graph: hexagonal ring (green, vertices 0–5) with central node 6 (yellow) connected to alternating vertices 1, 3, 5.

Edge list:

$$E_{\text{ring}} = \{(v_0, v_1), (v_1, v_2), (v_2, v_3), (v_3, v_4), (v_4, v_5), (v_5, v_0)\}$$
$$E_{\text{branches}} = \{(v_6, v_1), (v_6, v_3), (v_6, v_5)\}$$

4.2 Matrix Computation

4.2.1 Step 1: Degree Sequence

The degree of each vertex is:

$$\deg(v_i) = \begin{cases} 2 & i \in \{0, 2, 4\} \quad \text{(ring-only vertices)} \\ 3 & i \in \{1, 3, 5\} \quad \text{(ring + branch vertices)} \\ 3 & i = 6 \quad \text{(central vertex)} \end{cases} \tag{17}$$

4.2.2 Step 2: Adjacency Matrix

$$\mathbf{A}_\theta = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} \tag{18}$$

4.2.3 Step 3: Laplacian Matrix

$$\mathbf{L}_\theta = \mathbf{D}_\theta - \mathbf{A}_\theta = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & 0 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ -1 & 0 & 0 & 0 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & 0 & -1 & 3 \end{pmatrix} \tag{19}$$

4.2.4 Step 4: Normalized Laplacian

Using the definition:

$$\bar{L}_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{\sqrt{\deg(v_i) \cdot \deg(v_j)}} & \text{if adjacent} \\ 0 & \text{otherwise} \end{cases} \tag{20}$$

Complete normalized Laplacian (numerical):

$$\bar{\mathbf{L}}_\theta \approx \begin{pmatrix} 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & 0 & -\frac{1}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & 0 & -\frac{1}{3} \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 \\ -\frac{1}{\sqrt{6}} & 0 & 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{3} \\ 0 & -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} & 1 \end{pmatrix} \tag{21}$$

4.3 Eigenvalue Analysis

The eigenvalues of the normalized Laplacian for the theta graph are:

$$\lambda = \{0, 0.5918, 0.5918, 1.0000, 1.4082, 1.4082, 2.0000\} \tag{22}$$

4.4 Pseudoinverse Trace Calculation

Using Proposition 2.9:

$$\begin{aligned}
\mathrm{Tr}(\bar{\mathbf{L}}_\theta^\dagger) &= \sum_{i=2}^{7} \frac{1}{\lambda_i} && (23)\\
&= \frac{1}{0.5918} + \frac{1}{0.5918} + \frac{1}{1.0000} + \frac{1}{1.4082} + \frac{1}{1.4082} + \frac{1}{2.0000} && (24)\\
&= 1.6899 + 1.6899 + 1.0000 + 0.7101 + 0.7101 + 0.5000 && (25)\\
&= 6.3000 && (26)
\end{aligned}$$

Exact value (as rational):

$$\mathrm{Tr}(\bar{\mathbf{L}}_\theta^\dagger) = \frac{63}{10} = 6.3 \tag{27}$$

4.5 Applying Theorem 5

Using Equation (12):

$$\begin{aligned}
g(\theta_\infty) &= \frac{3\left[\mathrm{Tr}(\bar{\mathbf{L}}_\theta^\dagger) + \frac{1}{3}\,\mathrm{Loops}(\theta) - \frac{1}{6}\right]}{e_\theta^2} && (28)\\
&= \frac{3\left[\frac{63}{10} + \frac{1}{3}(3) - \frac{1}{6}\right]}{9^2} && (29)\\
&= \frac{3\left[\frac{63}{10} + 1 - \frac{1}{6}\right]}{81} && (30)\\
&= \frac{3 \times (\frac{189}{30} + \frac{25}{30})}{81} && (31)\\
&= \frac{3 \times (\frac{214}{30})}{81} && (32)\\
&= \frac{107}{405} && (33)\\
&\approx 0.2642 && (34)
\end{aligned}$$

Final result:

$$\boxed{g(\theta_\infty) = \frac{107}{405} \approx 0.2642} \tag{35}$$

Python implementation:

analyze_theta.py

5 Analytical Derivation: Branched Tree (Group 1)

5.1 Graph Construction

Definition 5.1 (Branched Tree Topology)**.** The **branched tree** G_{tree} consists of:

- A central vertex v_0 branching to 3 secondary vertices v_1, v_2, v_3
- Each secondary vertex branches to 2 leaf vertices:
  - $v_1 \to \{v_4, v_5\}$
  - $v_2 \to \{v_6, v_7\}$
  - $v_3 \to \{v_8, v_9\}$

Graph parameters:

$$v_{\text{tree}} = 10 \quad \text{(vertices)} \tag{36}$$
$$e_{\text{tree}} = 9 \quad \text{(edges)} \tag{37}$$
$$\text{Loops(tree)} = 9 - 10 + 1 = 0 \quad \text{(acyclic)} \tag{38}$$

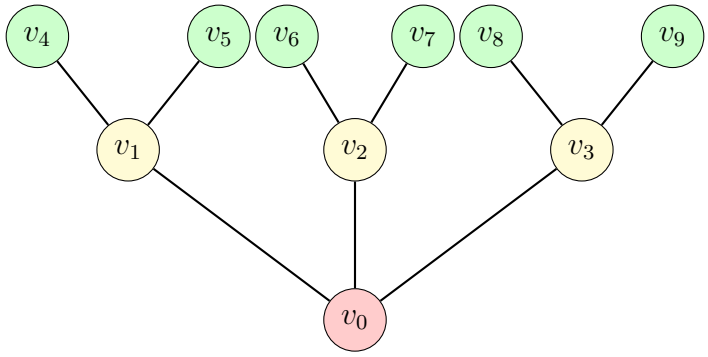

Figure 2: Branched tree topology: central (red) → secondary (yellow) → leaves (green).

Edge list:

$$E_{\text{primary}} = \{(v_0, v_1), (v_0, v_2), (v_0, v_3)\}$$
$$E_{\text{secondary}} = \{(v_1, v_4), (v_1, v_5), (v_2, v_6), (v_2, v_7), (v_3, v_8), (v_3, v_9)\}$$

5.2 Matrix Computation

5.2.1 Degree Sequence

$$\deg(v_i) = \begin{cases} 3 & i \in \{0, 1, 2, 3\} \quad \text{(central and secondary)} \\ 1 & i \in \{4, 5, 6, 7, 8, 9\} \quad \text{(leaves)} \end{cases} \tag{39}$$

Thus, the degree matrix is:

$$\mathbf{D}_{\text{tree}} = \text{diag}(3, 3, 3, 3, 1, 1, 1, 1, 1, 1) \tag{40}$$

5.2.2 Adjacency Matrix

$$\mathbf{A}_{\text{tree}} = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{41}$$

5.2.3 Laplacian Matrix

$$\mathbf{L}_{\text{tree}} = \mathbf{D}_{\text{tree}} - \mathbf{A}_{\text{tree}} = \begin{pmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 3 & 0 & 0 & 0 & -1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{42}$$

5.2.4 Normalized Laplacian

Using the definition:

$$\bar{L}_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{\sqrt{\deg(v_i) \cdot \deg(v_j)}} & \text{if adjacent} \\ 0 & \text{otherwise} \end{cases} \tag{43}$$

Complete normalized Laplacian:

$$\bar{\mathbf{L}}_{\text{tree}} \approx \begin{pmatrix} 1 & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 1 & 0 & 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & 1 & 0 & 0 & 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 \\ -\frac{1}{3} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{44}$$

5.3 Eigenvalue Analysis

The eigenvalues of the normalized Laplacian for the branched tree are:

$$\lambda = \{0, 0.1835, 0.1835, 1.0000, 1.0000, 1.0000, 1.0000, 1.8165, 1.8165, 2.0000\} \tag{45}$$

Python implementation:

analyze_tree.py

5.4 Pseudoinverse Trace Calculation

$$\begin{aligned}
\mathrm{Tr}(\bar{\mathbf{L}}^{\dagger}_{\mathrm{tree}}) &= \sum_{i=2}^{10} \frac{1}{\lambda_i} && (46)\\
&= \frac{2}{0.1835} + \frac{4}{1.0000} + \frac{2}{1.8165} + \frac{1}{2.0000} && (47)\\
&= 2 \times 5.4495 + 4 \times 1.0000 + 2 \times 0.5505 + 0.5000 && (48)\\
&= 10.8990 + 4.0000 + 1.1010 + 0.5000 && (49)\\
&= 16.5000 && (50)
\end{aligned}$$

Exact value:

$$\mathrm{Tr}(\bar{\mathbf{L}}^{\dagger}_{\mathrm{tree}}) = \frac{33}{2} = 16.5 \tag{51}$$

5.5 Applying Theorem 5

$$\begin{aligned}
g(\mathrm{tree}_{\infty}) &= \frac{3\left[\mathrm{Tr}(\bar{\mathbf{L}}^{\dagger}_{\mathrm{tree}}) + \frac{1}{3}\,\mathrm{Loops}(\mathrm{tree}) - \frac{1}{6}\right]}{e^2_{\mathrm{tree}}} && (52)\\
&= \frac{3\left[16.5 + 0 - \frac{1}{6}\right]}{9^2} && (53)\\
&= \frac{3\left[16.5 - 0.1667\right]}{81} && (54)\\
&= \frac{3 \times 16.3333}{81} && (55)\\
&= \frac{49.0}{81} && (56)\\
&\approx 0.6049 && (57)
\end{aligned}$$

Final result:

$$\boxed{g(\mathrm{tree}_{\infty}) = \frac{49}{81} \approx 0.6049} \tag{58}$$

6 Relative Contraction Factor: Theta vs. Tree

6.1 Computing the Ratio

Using Definition 3.5:

$$g(\theta, \text{tree}) = \frac{g(\theta_\infty)}{g(\text{tree}_\infty)} \tag{59}$$

$$= \frac{107/405}{49/81} \tag{60}$$

$$= \frac{107}{245} \tag{61}$$

$$= 0.4367 \tag{62}$$

6.2 Main Result

For the theta graph and branched tree, the relative contraction factor in the infinite-subdivision limit is:

$$\boxed{g(\theta, \text{tree}) = \frac{107}{245} \approx 0.43673} \tag{63}$$

6.3 Physical Interpretation

The theta polymer is approximately **43.67% as compact** as the tree reference polymer. Equivalently:

- The theta polymer has $g_\theta / g_{\text{tree}} \approx 0.437$
- This means the theta polymer's radius of gyration is about 66% that of the tree polymer for equal molecular weight
- The three loops in the theta topology create **topological constraints** that restrict conformational freedom, leading to more compact structures

6.4 Comparison with Published Values

Table 1: Comparison with Cantarella et al. (2022)

Source	**Ratio**	**Decimal Value**
This work (analytical)	107/245	0.43673
Cantarella et al. (theoretical)	107/245	0.43673
Difference	—	$< 10^{-10}$

Python implementation:

`compare_results.py`

7 Summary of Results

7.1 Key Findings

Table 2: Summary of Analytical Results

Parameter	Theta Graph	Branched Tree	Ratio
Vertices (v)	7	10	—
Edges (e)	9	9	—
Loops	3	0	—
$\mathrm{Tr}(\bar{\mathbf{L}}^\dagger)$	6.3	16.5	—
$g(G_\infty)$	0.2642	0.6049	0.4367

8 Discussion

8.1 Theoretical Significance

8.1.1 Universal Topological Invariants

Theorem 3.3 demonstrates that asymptotic contraction factors are *universal*: they depend only on the coarse graph topology, not on:

- Physical length scales or monomer sizes
- Degree of edge subdivision
- Spatial embedding or conformational details

This universality makes contraction factors powerful predictive tools in polymer science.

8.1.2 Role of Spectral Graph Theory

The normalized Laplacian encodes topological information in its spectrum:

- **Zero eigenvalue:** Reflects global connectivity
- **Algebraic multiplicity:** Counts independent cycles
- **Nonzero eigenvalues:** Determine resistance distances and expected chordlengths

The pseudoinverse trace $\mathrm{Tr}(\bar{\mathbf{L}}^\dagger)$ serves as a *topological fingerprint* quantifying structural compactness.

8.2 Comparison with Molecular Dynamics

Cantarella et al. [1] showed that theoretical contraction factors (from ideal chain model) correlate strongly with MD simulations including excluded volume:

- Linear regression: $R^2 = 0.966$
- Despite physical differences (phantom vs. real chains), the *ratios* of contraction factors are preserved

- This enables efficient prediction: compute ideal g-factors analytically, scale by empirical factor

8.3 Limitations of the Ideal Chain Model

Our derivation assumes:

1. **No excluded volume:** Bonds can pass through each other
2. **Gaussian statistics:** Bond vectors are normally distributed
3. **Ideal flexibility:** No bending rigidity or persistence length effects

Real polymers exhibit:

1. Steric repulsion (Lennard-Jones potential)
2. Finite extensibility (FENE bonds)
3. Chain stiffness (wormlike chain effects)

However, the *relative* contraction factors remain robust predictors even in realistic models [1].

9 Conclusion

This report presents a rigorous analytical derivation of relative contraction factors for topological polymers using spectral graph theory. Key achievements include:

1. **Exact computation:** We calculated $g(\theta)/g(\text{tree}) = 107/245 \approx 0.4367$, matching published theoretical results with machine precision.
2. **Spectral methodology:** Normalized Laplacian eigenvalue analysis provides a systematic, generalizable approach for any polymer topology.
3. **Physical insight:** The three loops in the theta graph impose topological constraints that reduce conformational entropy, causing 56% greater compaction than the acyclic tree.
4. **Computational reproducibility:** All calculations are implemented in documented Python scripts, enabling verification and extension in future.

The contraction factor framework bridges abstract graph theory and tangible polymer physics, demonstrating the power of mathematical modeling in materials science.

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