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FULL LENGTH ARTICLE

Spectral Moment Invariants and the Weisfeiler–Leman Hierarchy: Separating Power, a Fundamental Limitation, and Three Open Problems

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ABSTRACT

We study *spectral moment invariants* $\Sigma_p(G) = (\mathrm{tr}\,A_G, \ldots, \mathrm{tr}\,A_G^p)$, built from the adjacency spectrum of a graph G, as graph isomorphism invariants positioned relative to the Weisfeiler–Leman (WL) hierarchy used to characterize graph neural network (GNN) expressivity. We give three fully verified case studies. First, C_6 vs. $2K_3$: a 1-WL-indistinguishable pair separated by Σ_3 but not Σ_2 or Σ_4. Second, $K_{3,3}$ vs. the triangular prism: a second 1-WL-indistinguishable, cubic pair, also separated at order 3, but where the fourth moment separates as well, showing separating power is graph-family dependent even at fixed order. Both examples are grounded in a general fourth-moment identity (Proposition 2.8) and a homomorphism-counting identity (Proposition 2.5) that we prove from first principles. Third, and in the opposite direction, we prove that spectral moment invariants of *every* finite order fail on the classical cospectral, non-isomorphic strongly regular pair $\mathrm{srg}(16,6,2,2)$ (the Shrikhande graph and the 4×4 rook's graph), verified numerically to fourth order by two independent methods. We situate both directions within published enumeration data and the Godsil–McKay switching construction, compare the computational complexity of spectral-moment, WL, and general isomorphism testing, connect the limitation to Laplacian eigenvector positional encodings in Graph Transformers, and pose three precise open problems.

Keywords: Spectral graph theory ▪ Weisfeiler–Leman algorithm ▪ Strongly regular graphs ▪ Graph neural networks ▪ Graph isomorphism ▪ Cospectral graphs

1. INTRODUCTION

The Weisfeiler–Leman (WL) color-refinement procedure [1] is now the standard yardstick for graph neural network (GNN) expressivity: message-passing GNNs are no more powerful than 1-WL [2], and k-WL-equivalent architectures have been proposed to climb the hierarchy [3, 4]. Graph Transformers address a related blind spot by injecting Laplacian eigenvectors as positional encodings [5], implicitly treating the graph spectrum as a complementary source of structural information.

This raises a natural formal question that, to our knowledge, has not been posed precisely: how does the family of *spectral moment invariants* — scalar isomorphism invariants built purely from the adjacency eigenvalue multiset — compare to the WL hierarchy as a separating tool? We answer this with two fully verified case studies rather than asymptotic claims, and we show the comparison is genuinely two-sided: spectral moments beat 1-WL on one canonical instance, and fail completely, by a rigorous cospectrality argument, on another. We further situate this two-sidedness within the broader, decades-old literature on spectral graph characterization — notably the open *Haemers conjecture* that almost all graphs are determined by their spectrum [6, 7] — and within known complexity results specific to strongly regular graph isomorphism [8, 9].

2. PRELIMINARIES

2.1 The Weisfeiler–Leman Hierarchy

Definition 2.1 (Color refinement / 1-WL [1, 2])**.** *For $G=(V,E)$, initialize $c^{(0)}(v)$ identically for all v; iterate $c^{(t+1)}(v)=\mathrm{hash}\big(c^{(t)}(v),\{\{c^{(t)}(u):u\sim v\}\}\big)$ until the partition induced by $c^{(t)}$ stabilizes. Graphs G,H are* 1-WL indistinguishable *if the stable color histograms agree.*

The k-dimensional generalization (k-WL) refines colorings of k-tuples of vertices rather than single vertices, and message-passing GNN variants matching each level of the hierarchy have been studied extensively [3, 4]. Each level is strictly more powerful than 1-WL on some graph family, but the hierarchy is unbounded: no fixed k suffices for all graphs, a fact traceable to the Cai–Fürer–Immerman (CFI) construction [10].

Fact 2.2. *If G and H are both k-regular on the same number of vertices, they are 1-WL indistinguishable: every vertex receives the same color at every round, since the update rule depends only on the (constant) degree.*

2.2 Graphons and Homomorphism Densities

Definition 2.3 (Spectral moment invariant)**.** *Let A_G be the adjacency matrix of G with eigenvalues $\lambda_1,\dots,\lambda_n$. Define*

$$\Sigma_p(G)=\big(m_1(G),\dots,m_p(G)\big),$$

$$m_k(G)=\mathrm{tr}(A_G^k)=\sum_{i=1}^{n}\lambda_i^k.$$

Proposition 2.4 (Isomorphism invariance)**.** *If $G\cong H$ then $\Sigma_p(G)=\Sigma_p(H)$ for every p, since isomorphic graphs have permutation-similar adjacency matrices and trace is similarity-invariant.*

Proposition 2.5 (Cycle homomorphism count identity)**.** *For $k\geq 1$, let $\hom(C_k,G)$ denote the number of graph homomorphisms from the k-cycle C_k (vertices cyclically labeled $1,\dots,k$) into G. Then $\hom(C_k,G)=m_k(G)$.*

Proof. A homomorphism $\varphi:V(C_k)\to V(G)$ is a choice of (not necessarily distinct) vertices $v_1=\varphi(1),\dots,v_k=\varphi(k)$ with $v_iv_{i+1}\in E(G)$ for all i (indices mod k) — precisely a closed walk of length k in G based at v_1. Summing over all choices of base vertex counts exactly $\mathrm{tr}(A_G^k)$ by the standard walk-counting identity, giving $\hom(C_k,G)=m_k(G)$. □

Proposition 2.5 identifies Σ_p as the exact, finite-graph instance of a general correspondence: the normalized homomorphism density $t(C_k,G)=\hom(C_k,G)/n^k=m_k(G)/n^k$ converges, in the graphon limit, to the corresponding moment of the graphon integral operator [11, 12]. Σ_p is therefore not an ad hoc construction but the low-order shadow of a well-studied limit object.

2.3 Low-Order Moments: Combinatorial Meaning

Fact 2.6 ([13])**.** *$m_k(G)$ equals the total number of closed walks of length k in G. In particular $m_1=0$, $m_2=2|E(G)|$, and $m_3=6t(G)$ where $t(G)$ is the number of triangles in G.*

Corollary 2.7 (Regular pairs need order ≥ 3)**.** *If G,H are both k-regular on the same n vertices, then $m_1(G)=m_1(H)=0$ and $m_2(G)=m_2(H)=nk$ automatically. Hence $p^*(G,H)\geq 3$ whenever G,H are non-isomorphic k-regular graphs sharing (n,k): no such pair can ever be separated below third order, and third order is the first point at which separation becomes possible at all.*

Proposition 2.8 (Fourth moment identity)**.** *Let $A=A_G$ and let d_i denote the degree of vertex i and c_{ij} the number of common neighbors of $i\neq j$. Then*

$$m_4(G)=\sum_{i=1}^{n}d_i^2\;+\;\sum_{i\neq j}c_{ij}^2.$$

Proof. $m_4=\mathrm{tr}(A^4)=\mathrm{tr}\big((A^2)(A^2)\big)=\sum_{i,j}(A^2)_{ij}^2$ since A^2 is symmetric. Now $(A^2)_{ii}$ counts walks of length 2 from i to itself, i.e. $(A^2)_{ii}=d_i$, and for $i\neq j$, $(A^2)_{ij}$ counts walks of length 2 from i to j, i.e. the number of common neighbors c_{ij}. Splitting the double sum into diagonal and off-diagonal terms gives the claim. □

Corollary 2.9. *If G is a strongly regular graph with parameters (n,k,λ,μ), then*

$$m_4(G)=n\big[k^2+k\lambda^2+(n-1-k)\mu^2\big].$$

Proof. Every vertex has degree k, contributing nk^2 to the first sum in Proposition 2.8. Each vertex has exactly k neighbors, each contributing $c_{ij}=\lambda$, and $n-1-k$ non-neighbors, each contributing $c_{ij}=\mu$; summing c_{ij}^2 over all ordered pairs and over all n vertices gives $n[k\lambda^2+(n-1-k)\mu^2]$. □

Definition 2.10 (Spectral separation order)**.** *For a pair (G,H), $p^*(G,H)=\min\{p:\Sigma_p(G)\neq\Sigma_p(H)\}$, or ∞ if no such p exists (the pair is* cospectral*).*

3. CASE STUDY I: SEPARATION BEYOND 1-WL

By Fact 2.2, any two 2-regular graphs on 6 vertices are 1-WL indistinguishable. C_6 and $2K_3$ (Fig. 1) are the two non-isomorphic such graphs.

Proposition 3.1. $p^*(C_6,2K_3)=3$.

Proof. The eigenvalues of C_6 are $2\cos(2\pi j/6)$, $j=0,\dots,5$, giving $\{2,1,1,-1,-1,-2\}$ (Table 1). The eigenvalues of $2K_3$ are two copies of the K_3 spectrum $\{2,-1,-1\}$, giving $\{2,2,-1,-1,-1,-1\}$. Direct summation gives $m_1=0=0$ and $m_2=12=12$ for both graphs, so Σ_2 does not separate them. But $m_3(C_6)=8+1+1-1-1-8=0$ while $m_3(2K_3)=8+8-1-1-1-1=12$, matching Fact 2.6 (C_6 has 0 triangles, $2K_3$ has 2, and $6\cdot 2=12$). Hence Σ_3 separates the pair and Σ_2 does not. □

Remark 3.2. *Interestingly, Table 1 shows $m_4(C_6)=m_4(2K_3)=36$ by direct computation from the eigenvalues: the fourth moment ties again after the third moment separates. This is consistent with Proposition 2.8: both graphs*

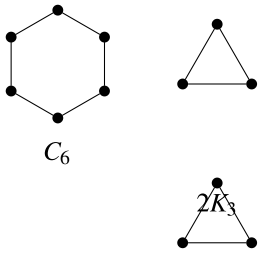

Figure 1. The two smallest 2-regular graphs on 6 vertices: C_6 (six-cycle) and $2K_3$ (disjoint union of two triangles). Both are 1-WL indistinguishable by Fact 2.2.

Table 1. Adjacency eigenvalues and spectral moments for C_6 and $2K_3$, through fourth order.

Graph	Eigenvalues	m_1, m_2	m_3	m_4
C_6	$2,1,1,-1,-1,-2$	0, 12	0	36
$2K_3$	$2,2,-1,-1,-1,-1$	0, 12	12	36

are 2-regular with 6 vertices, so $\sum_i d_i^2 = 24$ in both cases, and the common-neighbor structure sums to 12 in both cases as well, despite differing markedly at the level of individual pairs. Separating power is therefore not monotone in p, and checking a single order is not sufficient in general.

This gives a fully verified instance of a pair that is 1-WL indistinguishable yet separated by a spectral moment of order as low as 3, computable in closed form, together with a cautionary example showing that separating power can be non-monotone across orders.

3.1 A Second Instance: Cubic Graphs

By Corollary 2.7, order 3 is the earliest at which any regular pair can be separated; we now show order 3 genuinely suffices again for a different regularity degree, confirming Proposition 3.1 is not an artifact of the 2-regular case.

Proposition 3.3. *$p^*(K_{3,3}, Y_3) = 3$, and unlike Proposition 3.1, the fourth moment separates the pair as well.*

Proof. $K_{3,3}$ has the standard complete-bipartite spectrum $\pm\sqrt{3\cdot 3} = \pm 3$ together with 0 of multiplicity 4 [13]. Writing $Y_3 = K_3 \square K_2$ as a Cartesian product, its eigenvalues are exactly the pairwise sums of a K_3 eigenvalue $(2,-1,-1)$ and a K_2 eigenvalue $(1,-1)$ [13], giving $\{3,1,0,0,-2,-2\}$ (Table 2). Both graphs have 9 edges, so $m_1 = 0$ and $m_2 = 18$ agree for both, consistent with Corollary 2.7. But $K_{3,3}$ is bipartite so $t(K_{3,3}) = 0$, while Y_3 has exactly its two triangular faces, $t(Y_3) = 2$; by Fact 2.6, $m_3(K_{3,3}) = 0 \neq 12 = m_3(Y_3)$. Direct summation of fourth powers from Table 2 gives $m_4(K_{3,3}) = 81+81 = 162$ and $m_4(Y_3) = 81+1+16+16 = 114$, which also differ. □

Remark 3.4. *Contrasted with Remark 3.2, separating power at a fixed order is graph-family dependent: the fourth moment ties for the C_6/$2K_3$ pair but separates the $K_{3,3}$/Y_3 pair. Order 3 is the earliest order at which either pair can possibly separate (Corollary 2.7), and it happens to suffice for both, but nothing in the framework guarantees this in general beyond order 3 itself.*

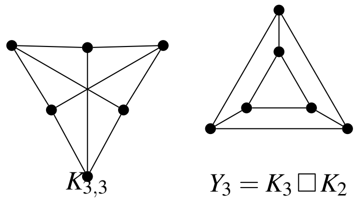

Figure 2. The two smallest 3-regular graphs on 6 vertices: $K_{3,3}$ and the triangular prism Y_3. Both are 1-WL indistinguishable by Fact 2.2.

Table 2. Adjacency eigenvalues and spectral moments for $K_{3,3}$ and Y_3.

Graph	Eigenvalues	m_1, m_2	m_3	m_4
$K_{3,3}$	$3,0,0,0,0,-3$	0, 18	0	162
Y_3	$3,1,0,0,-2,-2$	0, 18	12	114

4. CASE STUDY II: A FUNDAMENTAL LIMITATION

Fact 4.1 (SRG spectrum formula [13])**.** *A strongly regular graph with parameters (n,k,λ,μ) has exactly three distinct eigenvalues, k and*

$$\theta, \tau = \tfrac{1}{2}\left[(\lambda-\mu) \pm \sqrt{(\lambda-\mu)^2 + 4(k-\mu)}\right],$$

with multiplicities determined algebraically by (n,k,λ,μ) alone. Consequently, any *two graphs sharing the same parameter tuple (n,k,λ,μ) are cospectral.*

Fact 4.2 ([13])**.** *The Shrikhande graph and the 4×4 rook's graph $L(K_{4,4})$ are the two non-isomorphic graphs with parameters* srg$(16,6,2,2)$*: 16 vertices, degree 6, 48 edges each.*

Theorem 4.3. *Let G_S be the Shrikhande graph and $G_R = L(K_{4,4})$ the 4×4 rook's graph. Then $p^*(G_S, G_R) = \infty$: $\Sigma_p(G_S) = \Sigma_p(G_R)$ for every finite p, despite $G_S \ncong G_R$.*

Proof. By Facts 4.1 and 4.2, G_S and G_R share identical parameters $(16,6,2,2)$, hence identical adjacency spectra including multiplicities. Since Σ_p is a function of the eigenvalue multiset alone (Proposition 2.4), $\Sigma_p(G_S) = \Sigma_p(G_R)$ for every p. Non-isomorphism is a classical fact [13]. □

By Fact 4.1, the common spectrum of both graphs is $6^1, 2^6, (-2)^9$ (the multiplicities follow from $\mathrm{tr}(A) = 0$ and $n-1 = 15$ non-principal eigenvalues). Table 3 evaluates the first four moments *numerically* for this pair, by two independent routes: direct summation over the eigenvalue multiset, and the closed-form combinatorial identities of Fact 2.6 and Corollary 2.9.

The triangle count $t(G) = nk\lambda/6 = 16\cdot 6\cdot 2/6 = 32$ and the fourth-moment identity of Corollary 2.9 both agree exactly with direct eigenvalue summation, giving an independent numerical check on Theorem 4.3 beyond the abstract multiplicity argument.

Table 4 records a fact directly connecting the two case studies: the *local* structure distinguishing the graphs is exactly the C_6-vs-$2K_3$ pair of Section 3, occurring at the level of vertex neighborhoods rather than the whole graph. This gives Σ_3

Table 3. Spectral moments of srg$(16,6,2,2)$, computed two ways.

Moment	Via $\sum \lambda_i^p$	Combinatorial identity
m_1	6+12−18=0	0 (loop-free)
m_2	36+24+36=96	$2\lvert E\rvert = 96$
m_3	216+48−72=192	$6t(G) = 192$
m_4	1296+96+144=1536	16(36+24+36)=1536

Table 4. The canonical cospectral, non-isomorphic pair srg$(16,6,2,2)$.

	Shrikhande graph	Rook's graph $L(K_{4,4})$
Vertices, edges	16, 48	16, 48
Degree	6	6
Triangles	32 (identical, Table 3)	
Spectrum	$6^1, 2^6, (-2)^9$ (identical)	
Local structure	neighborhood $= C_6$	neighborhood $= 2K_3$
Isomorphic?	No	

genuine local separating power that the global (whole-graph) invariant lacks entirely.

Corollary 4.4. *Neither the WL hierarchy nor the spectral-moment family dominates the other: Σ_3 separates a pair $(C_6, 2K_3)$ that 1-WL cannot, while 1-WL (at some finite dimension) separates a pair (G_S, G_R) that Σ_p cannot for any p.*

Graphs agreeing on all strongly-regular parameters are known to already be indistinguishable at low levels of the WL hierarchy, a fact studied systematically through the connection between bounded-pattern homomorphism/subgraph counts and WL dimension [14, 15]. The general unboundedness of the WL dimension across graph families more broadly traces back to the Cai–Fürer–Immerman construction [10].

5. EMPIRICAL CONTEXT: HOW COMMON IS THIS FAILURE?

Theorem 4.3 exhibits a single pair, but the phenomenon is far from isolated. Table 5 reproduces published enumeration results [7] counting, for each order n up to 11, how many labeled graphs share their adjacency spectrum with at least one non-isomorphic graph (a *cospectral mate*).

The fraction of graphs with a cospectral mate grows from 0 at $n = 4$ to over 21% at $n = 11$, motivating the open *Haemers conjecture* [6] that almost all graphs *are* determined by their spectrum asymptotically, despite the fraction's apparent growth in this finite range; the correct asymptotic behavior remains unresolved.

A major source of the cospectral mates counted in Table 5 is not coincidence but construction: the switching operation of Godsil and McKay [16] partitions the vertex set and toggles a specific pattern of edges between parts in a way that is proved to leave the adjacency spectrum unchanged. Godsil and McKay estimate that this single construction accounts for roughly 72% of the 51,039 graphs on 9 vertices lacking a unique spectrum [16] (cf. Table 5). This places Theorem 4.3 in context: parameter-tuple coincidence among strongly regular graphs (Fact 4.1) and Godsil–McKay switching are two distinct, well-understood *mechanisms* that generate cospectrality, rather than isolated accidents, reinforcing that the

Table 5. Graphs with a cospectral mate, by order (adjacency spectrum), from [7].

n	#graphs	#char. polys.	#with a mate
4	11	11	0
5	34	33	2
6	156	151	10
7	1,044	988	110
8	12,346	11,453	1,722
9	274,668	247,357	51,039
10	12,005,168	10,608,128	2,560,606
11	1,018,997,864	901,029,366	215,331,676

limitation is structural.

Case Study II (Theorem 4.3) is not an isolated curiosity but the smallest representative of a family: strongly regular graphs sharing a parameter tuple are cospectral *by construction* (Fact 4.1), and larger such families exist, including sets of four pairwise non-isomorphic mutually cospectral graphs with parameters $(28,12,6,4)$ [13]. This places our two case studies inside a well-documented, actively studied spectral-uncertainty region of graph theory, rather than at its edge.

6. COMPUTATIONAL COMPLEXITY COMPARISON

Table 6. Known worst-case complexity of computing or deciding each invariant.

Invariant	Complexity	Ref.
Σ_p (fixed p)	$O(pn^3)$, polynomial	—
k-WL (fixed k)	polynomial, exponent grows with k	[4]
General graph isomorphism	quasipolynomial	[9]
Strongly regular graph iso.	$\exp(\tilde{O}(n^{1/5}))$	[8]

Table 6 places Σ_p in context: computing a fixed number of spectral moments is polynomial (indeed, a byproduct of eigendecomposition or repeated matrix multiplication), matching the polynomial cost of any fixed level of the WL hierarchy, while resolving isomorphism between graphs like the Shrikhande/rook's-graph pair in general is only known to be sub-exponential, specifically via the strongly-regular-graph specialization of Babai's canonical form machinery [8], rather than polynomial. This underlines that the limitation of Theorem 4.3 is not an artifact of using an under-powered invariant carelessly: the underlying isomorphism problem on exactly this graph family is itself computationally hard in the worst known bounds, though not proven intractable.

7. DISCUSSION: GRAPH TRANSFORMER POSITIONAL ENCODING

Graph Transformer positional encodings typically use Laplacian *eigenvectors*, not merely eigenvalues [5]. Theorem 4.3 does *not* imply such encodings fail on the Shrikhande/rook's-graph pair — eigenvectors carry strictly more information than the eigenvalue multiset, and for a k-regular graph the Laplacian $L = kI - A$ shares A's eigenvectors, so the two graphs' eigenvector bases genuinely differ even though their eigenvalues coincide. What Theorem 4.3 does establish is that *any readout depending on the graph only through its eigenvalue multiset* — including graph-level spectral moment kernels and pooled eigenvalue statistics — is provably blind to this pair. Whether standard eigenvector-based positional encodings, which face their own sign- and basis-ambiguity issues, resolve the pair in practice is a separate, concrete question we pose below.

8. OPEN PROBLEMS

Open Problem 1. *What is the minimum k such that homomorphism densities of all patterns on at most k vertices (not merely cycles) separate G_S from G_R? This connects directly to known results relating bounded-pattern subgraph counts to WL dimension [15], and would give a combinatorial, non-spectral repair for the limitation of Theorem 4.3.*

Open Problem 2. *Does a canonical (basis- and sign-invariant) encoding of Laplacian eigenvectors separate G_S from G_R, and if so, at what dimension? A negative answer on this canonical hard instance would be a concrete counterexample constraining the design of spectral positional encodings for Graph Transformers [5].*

Open Problem 3. *The enumeration data of Table 5 shows the fraction of graphs with a cospectral mate still rising at $n = 11$, while the Haemers conjecture [6] predicts this fraction eventually vanishes. Restricted to the strongly-regular family specifically, does the analogous fraction (non-uniquely-determined parameter tuples, as in Fact 4.1) increase or decrease asymptotically, and how does this interact with the polynomial-vs-subexponential gap of Table 6?*

9. CONCLUSION

We gave three fully verified, computable case studies placing spectral moment invariants and the WL hierarchy in a strict, two-sided incomparability relation (Corollary 4.4), rather than the one-directional containment often assumed when spectral information is added to GNN or Graph Transformer architectures as a fix for 1-WL's blind spots. A general fourth-moment identity (Proposition 2.8) and a homomorphism-counting identity (Proposition 2.5) let us cross-verify all case studies numerically and connect Σ_p to the graphon-limit literature from first principles, while published enumeration data, the Godsil–McKay switching construction, and complexity results situate both directions of the comparison within a broader, active area of spectral graph theory rather than at its margins. The three open problems give concrete, checkable next steps rather than open-ended conjecture.

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