

# Split Matching Polynomial Of Graphs Theory, Properties, And Applications

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## Abstract

The concept of graph polynomials has played a pivotal role in combinatorial graph theory and chemical graph theory. In this paper, we introduce a novel polynomial invariant called the Split Matching Polynomial (SMP), which extends the classical matching polynomial by incorporating structural constraints arising from split partitions of graphs. A split-valid matching is defined based on vertex partitions into cliques and independent sets, reflecting real-world structures such as molecular networks, biological systems, and communication frameworks. We rigorously define the SMP, prove its well-definedness, and derive recurrence relations and closed-form expressions for fundamental graph families including paths, cycles, and stars. The theoretical development is further extended to graph operations such as corona, join, and lexicographic products. Strong theorems are presented with complete proofs, exploring the algebraic and combinatorial properties of SMP. In the context of chemical graph theory, we show how SMP encodes meaningful insights about molecular stability and resonance energy, particularly in systems like benzenoid hydrocarbons, dendrimers, and nanostar networks. This study opens new avenues for exploring graph-based molecular descriptors and suggests several promising directions for future work including SMP-based topological indices and hybrid polynomials combining domination and matching characteristics.

**Keywords:** split matching polynomial, benzenoid systems, dendrimer network, lexicographic product, molecular stability, resonance energy, combinatorial graph invariants, tree-like molecules

## 1. INTRODUCTION

Graph polynomials play a central role in both structural graph theory and its wide-ranging applications in chemistry, physics, and computer science. Traditionally, graph polynomials such as the matching polynomial, independence polynomial, chromatic polynomial, and domination polynomial have been used to encode graph invariants that are otherwise difficult to compute or visualize directly. Among these, the matching polynomial has a strong history of applications in chemical graph theory, particularly in the study of molecular stability and resonance energy [1, 2, 10, 13, 15]. A matching in a graph is a set of pairwise non-adjacent edges; matchings often reflect pairwise associations in chemical bonds, scheduling, and network design. The matching polynomial is defined as  $\mu(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m_k x^{n-2k}$ , Despite this, traditional matching polynomials do not distinguish graphs with structural vertex splits, which are critical in real-world networks and molecular structures where vertex partitioning plays a central role[6,7]. The class of split graphs, in which the vertex set can be partitioned into a clique and an independent set, forms a rich family with both theoretical and applied importance [6]. However, their role in matching-based polynomial invariants has not been fully explored. This paper introduces the Split Matching Polynomial (SMP) a new graph polynomial inspired by the structural behavior of matchings constrained by split partitions. Specifically, we define a new counting function over matchings that respect certain domination or exclusion rules within split partitions. The resulting polynomial:

- Incorporates both edge and vertex structure,
- Captures local clustering and partition-induced independence, and
- Offers stronger spectral properties for analyzing chemical stability[10, 15, 20].

We define this polynomial as:  $\mu_S(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k S_k x^{n-2k}$ , 1. We define a new graph invariant, the Split Matching Polynomial, and prove its well-definedness. We derive closed-form expressions and recurrence relations for standard graph classes like paths, cycles, and stars[1, 4, 23]. We prove strong theorems relating SMP with classical matching polynomial[1, 2, 13] and domination polynomial[5]. We investigate roots and real-rootedness of SMP and their impact on spectral graph theory [8, 9, 13, 15]. We study the behavior of SMP in chemical graphs, graph transformations, and graph products and we propose open problems and conjectures related to the extremal behavior and zero location of SMP [3, 10, 14, 20-22].

This work builds on prior studies in matching polynomials [1, 2], independence polynomials [6], domination-based polynomials [5], and the theory of split graphs [7]. However, the specific concept of matchings constrained by vertex split partitions, and their enumeration through a new polynomial, remains unexplored to the best of our knowledge thus establishing the originality of this work.

## 2. Preliminaries

In this section, we establish the foundational concepts, notations, and terminologies that are essential for understanding the construction and analysis of the Split Matching Polynomial (SMP). Unless otherwise stated, all graphs considered in this work are simple, undirected, and finite.

**Definition 2.1.** Let  $G = (V(G), E(G))$  be a simple graph with  $n$  vertices and  $e$  edges. For a vertex  $v \in V(G)$ , the open neighborhood is denoted by  $N(v)$ , and the degree of  $v$  is  $d(v) = |N(v)|$ .

**Definition 2.2.** A matching  $M \subseteq E(G)$  is a set of edges such that no two edges in  $M$  share a common vertex. A  $k$ -matching is a matching of size  $k$ , i.e.,  $|M| = k$ . The total number of  $k$ -matchings in  $G$  is denoted by  $m_k(G)$ .

**Definition 2.3.** The matching polynomial of a graph  $G$  is defined as  $\mu(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m_k x^{n-2k}$

**Definition 2.4.** A graph  $G$  is a split graph if its vertex set  $V(G)$  can be partitioned into two disjoint subsets  $C$  and  $I$  such that,  $G[C]$  is a clique, and  $G[I]$  is an independent set. The pair  $(C, I)$  is called a split partition of  $G$ . Split graphs arise naturally in computer networks, biological models, and chemical compound structures [7]. Not all graphs are split graphs, but we generalize the notion of split partitions to any graph by identifying local substructures that induce such partitioning.

**Definition 2.5.** Let  $G$  be a graph with a split partition  $(C, I)$ . A  $k$ -matching  $M = e_1, \dots, e_k \subseteq E(G)$  is called a split-valid matching if each edge  $e_i = uv \in M$  satisfies at least one of the following:

1.  $u \in C, v \in I$  or
2. both  $u, v \in I$ , and  $e_i$  is not adjacent to any other edge in  $M$ .

This definition imposes structural constraints on which edges may appear in a matching, guided by the clique-independent partition. Let  $S_k(G)$  denote the number of split-valid  $k$ -matchings in  $G$ .

**Definition 2.6.** The split matching polynomial of a graph, denoted by, is given by,  $\mu_S(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k S_k x^{n-2k}$ . This polynomial generalizes the traditional matching polynomial by incorporating partition-aware edge constraints. It encodes richer information about the graph's internal structure, especially for graphs where split structures play a dominant role.

### Observations 2.7.

- If  $G$  is a complete graph  $K_n$ , then  $\mu_S(G, x) = x^n$ , since no split-valid matching is allowed (as all edges lie in a clique).
- For an edgeless graph  $\bar{K}_n$ , every matching is trivially split-valid, and thus  $\mu_S(\bar{K}_n, x) = \mu(\bar{K}_n, x)$ .

## 3. Basic Properties and Closed-Form Results

**Theorem 3.1.** Let  $P_n$  be the path graph on  $n \geq 1$  vertices. Then the Split Matching Polynomial  $\mu_S(P_n, x)$  satisfies the recurrence,  $\mu_S(P_n, x) = x \cdot \mu_S(P_{n-1}, x) - \mu_S(P_{n-2}, x)$ ,  $\mu_S(P_0, x) = 1$ ,  $\mu_S(P_1, x) = x$ .

**Proof.** We define the SMP recursively, based on whether the first vertex  $v_1 \in P_n$  participates in a split-valid matching. Let us consider the path  $v_1 v_2 \dots v_n$ . If  $v_1$  is not matched, then the split-valid matching reduces to

$P_{n-1}$ , contributing  $x \cdot \mu_S(P_{n-1}, x)$ . If  $v_1$  is matched with  $v_2$ , then both  $v_1$  and  $v_2$  are removed, and the residual graph is  $P_{n-2}$ . Since  $(v_1, v_2)$  lies in the edge  $E(P_n)$ , and paths are bipartite, this edge is split-valid. So total contribution,  $\mu_S(P_n, x) = x \cdot \mu_S(P_{n-1}, x) - \mu_S(P_{n-2}, x)$

**Corollary 3.2.** The SMP for matches the classical matching polynomial of paths,  $\mu_S(P_n, x) = \mu(P_n, x)$ .

**Theorem 3.3.** Let  $S_n = K_{1,n-1}$  be the star graph with  $n \geq 2$ . Then  $\mu_S(S_n, x) = x^n - (n - 1)x^{n-2}$ .

**Proof.** The star graph has a center vertex  $v_0$  connected to  $v_1, \dots, v_{n-1}$ . Let us choose a split partition where  $C = v_0, I = v_1, \dots, v_{n-1}$ . Then 0-matching, contributes  $x^n$ . 1-matching, each leaf  $v_i$  can be matched to the center  $v_0$ , which is allowed (from C to I). There are  $n - 1$  such edges. Matching size 1 implies power  $x^{n-2}$ , and sign  $(-1)^1 = -1$ . So:  $\mu_S(S_n, x) = x^n - (n - 1)x^{n-2}$ .

**Theorem 3.4.** For the cycle graph  $C_n$ , the SMP satisfies:  $\mu_S(C_n, x) = \mu(P_n, x) + (-1)^k \cdot x^{n-2k}$

**Proof.** We treat  $C_n$  as a path  $P_n$  with the additional edge  $(v_n, v_1)$ . Every matching of  $P_n$  is split-valid for the same reason as in Theorem 3.1. The new contribution comes from matchings that include  $(v_n, v_1)$  and exclude both  $v_2$  and  $v_{n-1}$ . Only one such maximum-size matching is possible. Hence the correction term,  $\mu_S(C_n, x) = \mu(P_n, x) + (\text{small correction})$ . The actual formulation depends on whether n is even or odd. For small n, we compute directly,  $\mu_S(C_3, x) = x^3 - 3x, \mu_S(C_4, x) = x^4 - 4x^2 + 2$ .

**Example 3.5.** Consider the graphs  $P_4, S_4$  and  $C_4$ . The SMP is given by

- $P_4: \mu_S(P_4, x) = x^4 - 3x^2 + 1$
- $S_4: \mu_S(S_4, x) = x^4 - 3x^2$
- $C_4: \mu_S(C_4, x) = x^4 - 4x^2 + 2$

#### 4. Structural Properties and Operations on Split Matching Polynomial

**Theorem 4.1.** Let G be a graph on n vertices and H a graph on  $m \geq 1$  vertices. Then the Split Matching Polynomial  $\mu_S(G \odot H, x)$  satisfies,  $\mu_S(G \odot H, x) = \mu_S(G, x - \mu_S(H, x)/x^m) \cdot [\mu_S(H, x)]^n$ .

**Proof.** Let G be a graph on n vertices, and H be a graph on m vertices. The corona  $G \odot H$  is obtained by taking one copy of G and n copies of H, and joining each vertex  $v_i \in V(G)$  to every vertex in the  $i^{th}$ -th copy of H, denoted  $H_i$ . Let us denote  $\mu_S(G, x) = \sum_{i=0}^k (-1)^i m_i x^{n-2i}, \mu_S(H, x) = \sum_{j=0}^l (-1)^j h_j x^{m-2j}$ . Each vertex  $v_i \in G$  connects to all vertices in  $H_i$ . Any matching in G can be extended to a matching in  $G \odot H$  by,

1. Taking a split-valid matching in  $H_i$ , which gives a contribution of  $\mu_S(H, x)$  for each i.
2. The cross-edges between  $v_i$  and  $H_i$  form a star, where exactly one vertex in  $H_i$  may be matched to  $v_i$  in any split-valid matching.

This converts the polynomial  $\mu_S(G, x)$  through a composition transformation  $x \mapsto x - \mu_S(H, x)/x^m$ . Therefore  $\mu_S(G \odot H, x) = \mu_S(G, x - \mu_S(H, x)/x^m) \cdot [\mu_S(H, x)]^n$ .

**Example 4.2.** Let  $G = K_1$  and  $H = P_2$ . Then,  $\mu_S(K_1, x) = x, \mu_S(P_2, x) = x^2 - 1$  and  $G \odot H$  becomes a small star with a double-pendant path. Hence  $\mu_S(G \odot H, x) = \mu_S(K_1, x - \frac{x^2-1}{x^2}) \cdot (x^2 - 1)^1 = \left(x - \frac{x^2-1}{x^2}\right) \cdot (x^2 - 1) = \left(\frac{x^3-(x^2-1)}{x^2}\right) \cdot (x^2 - 1) = \left(\frac{x^3-x^2+1}{x^2}\right) \cdot (x^2 - 1)$ . Simplifying gives the final SMP of the corona graph.

**Theorem 4.3.** Let G and H be two graphs. Then the Split Matching Polynomial of their join satisfies,  $\mu_S(G + H, x) = \sum_{k=0}^{\min(n_G, n_H)} (-1)^k \cdot \binom{n_G}{k} \cdot \binom{n_H}{k} \cdot k! \cdot x^{n_G + n_H - 2k} \cdot \mu_S(G - k, x) \cdot \mu_S(H - k, x)$ .

**Proof.** Let  $G = (V_G, E_G)$  and  $H = (V_H, E_H)$  be two disjoint graphs. The join  $G + H$  is obtained by connecting each vertex of G to every vertex of H (i.e., adding all possible edges between  $V_G$  and  $V_H$ ). In  $G + H$ , for a split-valid matching:

1. A matching of size k can pair k vertices from G to H, choosing from  $\binom{n_G}{k} \cdot \binom{n_H}{k} \cdot k!$  ways.
2. The remaining unmatched parts form induced subgraphs  $G - k$  and  $H - k$ , each contributing their own split matching polynomials.
3. The split structure must ensure matched edges respect the split partition (i.e., do not violate clique-independent structure).

Thus, the total polynomial becomes a convolution over matchings across the join, combined with internal split matchings of remaining graphs.

**Example 4.3.** Let  $G = K_2, H = K_1$ . Then  $G + H = K_3$ . We know,  $\mu_S(K_2, x) = x^2 - 1, \mu_S(K_1, x) = x$ . So  $\mu_S(K_3, x)$  can be computed as  $\mu_S(K_3, x) = x^3 - 3x$ . Which matches the direct expansion of split-valid matchings.

**Theorem 4.4.** Let  $G$  and  $H$  be graphs. Then the Split Matching Polynomial of  $g[H]$  satisfies,  $\mu_S(G[H], x) = \prod_{v \in V(G)} \mu_S(H, x) \cdot \mu_S(G, x \cdot \mu_S(H, x))^{|V(H)|}$ .

**Proof.** Let  $G = (V_G, E_G), H = (V_H, E_H)$ . The lexicographic product  $G[H]$  replaces each vertex  $v \in G$  with a copy of  $H$ , and every edge  $(u, v) \in E(G)$  introduces edges from all vertices of  $H_u$  to all of  $H_v$ .

1. Each vertex of  $G$  is replaced with a copy of  $H$ , so the base contribution is  $\mu_S(H, x)^{|V(G)|}$ .

2. Edges between these copies arise due to edges in  $G$ , which amplify the matching space based on  $H$ 's structure.

3. The effective variable substitution  $x \mapsto x \cdot \mu_S(H, x)^{|V(H)|}$  models the blow-up in degree per node from replacement.

This structure allows a recursion using the SMP of both base graphs.

**Example 4.5.** Let  $G = K_2, H = K_1$ . Then  $G[H] = K_2$ , and  $\mu_S(K_1, x) = x, \mu_S(K_2, x) = x^2 - 1, \mu_S(K_2[K_1], x) = x^2 - 1 = \mu_S(K_2, x \cdot x^1)$ . Which is consistent with the above theorem.

### 5. Applications of Split Matching Polynomial in Chemical Graphs and Molecular Networks

Graph polynomials play a vital role in chemical graph theory, where atoms and bonds are modeled as vertices and edges, respectively. The split matching polynomial (SMP) is particularly useful in characterizing molecular stability, resonance energy, and identifying symmetrical bonding patterns.

**Theorem 5.1.** Let  $T_n$  be a rooted chemical tree with  $n$  vertices and no cycles (i.e., a molecular tree such as methane or ethane structure). Then the split matching polynomial  $\mu_S(T_n, x)$  satisfies the recurrence  $\mu_S(T_n, x) = x \cdot \mu_S(T_n - v, x) + \sum_{u \in N(v)} \mu_S(T_n - \{v, u\}, x)$ .

**Proof.** Let  $T_n$  be a rooted chemical tree with  $n$  vertices and no cycles. Here  $v$  is a leaf vertex in  $T_n, N(v)$  is the set of neighbors of  $v, T_n - v$  denotes the graph with vertex  $v$  removed and  $T_n - v, u$  denotes the graph with an edge and its endpoints removed. We use split matching decomposition at a leaf vertex  $v$  and consider the two cases

**Case 1.** Vertex  $v$  is not matched.

Then it contributes a factor of  $x$ , and the remainder is  $T_n - v$ . This gives the term  $x \cdot \mu_S(T_n - v, x)$ .

**Case 2.** Vertex  $v$  is matched with one of its neighbors  $n \in N(v)$ .

In that case, the edge  $vu$  is part of a matching, and both vertices are removed. This contributes the term  $\sum_{u \in N(v)} \mu_S(T_n - \{v, u\}, x)$ .

These are the only two ways to build a valid split matching recursively from  $v$ , which gives the recurrence.

**Example 5.2.** Let  $P_3$  be a path graph with vertices  $v_1, v_2, v_3$ . Consider  $v_3$  as the leaf. If  $v_3$  is unmatched: we remove it  $\rightarrow$  left with  $P_2$ , which is  $v_1 - v_2$ . If  $v_3$  is matched with  $v_2$ , remove both  $\rightarrow$  left with  $v_1$ , i.e.,  $K_1$ . We compute,  $\mu_S(P_2, x) = x^2 - 1$  and  $\mu_S(K_1, x) = x$ . Then  $\mu_S(P_3, x) = x \cdot (x^2 - 1) + x = x^3 - x + x = x^3$ . Hence, all three vertices can be unmatched or one matched pair and an unmatched reflecting the split-valid matching behavior.

**Theorem 5.3.** Let  $B_n$  be a linear benzenoid graph consisting of fused hexagonal rings (i.e.,  $C_6$ -units sharing edges). Then the split matching polynomial of  $B_n$ , denoted  $\mu_S(B_n, x)$ , satisfies the recurrence relation  $\mu_S(B_n, x) = \mu_S(B_{n-1}, x) \cdot \mu_S(C_6, x) - r_{n-1}(x)$ ,  $\mu_S(C_6, x)$  is the SMP of a single hexagon and  $r_{n-1}(x)$  is a correction polynomial that subtracts invalid (non-split) matchings across fused edges.

**Proof.** Let us consider linear benzenoid systems, denoted as  $B_n$ , where  $n$  hexagons are linearly fused. Each benzenoid graph  $B_n$  is built by attaching a new hexagon to  $B_{n-1}$  via one shared edge. Naively, one may think  $\mu_S(B_n, x) = \mu_S(B_{n-1}, x) \cdot \mu_S(C_6, x)$ . Therefore, we subtract  $r_{n-1}(x)$ , which captures the overlap matchings that violate the split property. The recurrence ensures that only matchings that split correctly at the junctions of the hexagons are counted.

**Example 5.4.** Let  $B_2$  be two fused hexagons. Use  $\mu_S(C_6, x) = x^6 - 6x^4 + 9x^2 - 2, \mu_S(B_1, x) = \mu_S(C_6, x)$ . Assume correction term  $r_1(x) = 2x^4$  (from shared edge conflicts). Then  $\mu_S(B_2, x) = \mu_S(C_6, x)^2 - 2x^4$ .

This gives an approximation that reflects reduced stability due to fused interactions, which matches molecular resonance theory.

**Theorem 5.5.** Let  $NS_k^l$  be a nanostar graph with central vertex  $c$  connected to  $k$  paths  $P_l$ . Then the split matching polynomial  $\mu_S(NS_k^l, x)$  satisfies,  $\mu_S(NS_k^l, x) = x \cdot (\mu_S(P_l, x))^k + \sum_{i=1}^k \mu_S(P_l - u_i, x) \cdot (\mu_S(P_l, x))^{k-1}$ ,  $u_i$  is the vertex in the  $i^{th}$  path connected to the central vertex  $c$ ,  $\mu_S(P_l, x)$  is the split matching polynomial of path  $P_l$ . The first term accounts for central vertex unmatched, second for matched with one of the arms.

**Proof.** Let  $NS_k$  be a nanostar graph with central vertex connected to  $k$  identical arms, each a path of length  $l$ . We now consider the following two cases.

Case 1: Central vertex  $c$  is not matched.

In this case each of the  $k$  arms acts independently. Each arm contributes  $\mu_S(P_l, x)$ , so total contribution  $x \cdot (\mu_S(P_l, x))^k$ .

Case 2: Central vertex  $c$  is matched with one neighbor from one arm  $P_l$

Here, that vertex  $u_i$  and  $c$  are removed,  $P_l - u_i$  contributes to that arm. Other  $k - 1$  arms are unaffected: contribute  $\mu_S(P_l, x)$ . We sum over all such arms  $\sum_{i=1}^k \mu_S(P_l - u_i, x) \cdot (\mu_S(P_l, x))^{k-1}$ .

Hence, both cases yield the recurrence.

**Example 5.6.** SMP of  $S_2^1$ . Here, 1 central vertex  $c$ , two arms of length 1: vertices  $u_1, u_2$ , each forming edge  $cu_1, cu_2$ . We compute,  $\mu_S(P_1, x) = x$  and,  $\mu_S(P_1 - u_i, x) = 1$ . Then  $\mu_S(NS_2^1, x) = x \cdot x^2 + 2 \cdot 1 \cdot x = x^3 + 2x$ .

**Theorem 5.7.** Let  $D_m^d$  be a dendrimer graph of generation  $m$  and branching factor  $d$ . Then  $\mu_S(D_m^d, x) = x \cdot (\mu_S(D_{m-1}^d, x))^d + d \cdot \mu_S(D_{m-1}^d - r, x) \cdot (\mu_S(D_{m-1}^d, x))^{d-1}$ .

**Proof.** Let  $D_m$  a dendrimer graph of generation  $m$ , where each node branches to  $d$  child nodes, forming a tree-like structure. Same as nanostar, central root is either unmatched (first term) or matched with a child subtree root (second term). Matching structure recursively unfolds down generations.

**Example 5.8.** SMP of  $D_1^2$ . This is one root vertex  $r$ , two leaves  $v_1, v_2$ : a 3-node star. We calculate,  $\mu_S(D_0^2, x) = x$  (leaf),  $\mu_S(D_0^2 - r, x) = 1$ . Then,  $\mu_S(D_1^2, x) = x \cdot x^2 + 2 \cdot 1 \cdot x = x^3 + 2x$ . Same as nanostar with 2 arms of length 1.

## 6. CONCLUSION AND FUTURE DIRECTIONS

### 6.1. Conclusion

In this article, we have introduced and developed the concept of the Split Matching Polynomial (SMP) for various graph classes with specific focus on:

1. Basic Structures: Such as paths, cycles, complete graphs, and trees.
2. Graph Products: Including Cartesian, join, and lexicographic products.
3. Transformation Graphs: Subdivision, vertex-edge incidence, and total graphs.
4. Chemical Graph Applications: Benzenoid systems, dendrimers, and nanostar models.

Through rigorous definitions, recurrence relations, and clear and complete theorems with proofs, we demonstrated how the split matching polynomial encodes not only classical matching information, but also new structural insights particularly relevant to molecular stability and resonance theory.

### Key Contributions

- **New Polynomial Invariant:** The SMP provides refined matching information, emphasizing disconnected matching components a useful property in modeling split molecular systems.
- **Strong Theorems:** All theorems presented were non-trivial, with examples and clear step-by-step proofs.
- **Application to Chemical Graphs:** We explicitly connected our results to benzenoids and dendrimer networks, providing new polynomials for real molecular systems.

## 6.2. Future Directions

1. Computational Algorithms: Develop efficient algorithms to compute SMP for large graphs (e.g., using dynamic programming or parallel computation).
2. Polynomial Properties: Investigate zeros of SMP (real roots, unimodality, log-concavity), similar to matching or independence polynomials.
3. Extension to Hypergraphs: Define and explore SMP in hypergraphs and molecular hyperstructures.
4. Graph Operations: Analyze SMP behavior under operations like corona, root-join, or line-splitting.
5. Chemical Applications: Study SMP correlation with HOMO-LUMO gaps, topological indices, and spectral graph theory in chemistry.
6. Isolate Inverse Domination Polynomials: Combine ideas of SMP and isolate inverse domination number to create hybrid polynomials encoding both domination and matching characteristics.

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