Explicit M-Polynomial and Degree-Based Topological Indices of Generalized Hanoi Graphs

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Abstract

The M-polynomial, introduced by Deutsch and Klavžar in 2015, provides a unifying algebraic framework for the computation of numerous degree-based topological indices such as the Zagreb, Randić, harmonic, and forgotten indices. Despite its broad applications in chemical graph theory and network analysis, closed expressions of the M-polynomial remain unknown for many important graph families.
In this work we derive, for the first time, a complete explicit expression of the M-polynomial of the generalized Hanoi graphs H_p^n for arbitrary positive p and n. Our derivation relies on a detailed combinatorial analysis of the occupancy-based structure of H_p^n, refined using Stirling and 2-associated Stirling numbers to enumerate all configurations with prescribed singleton and multiton counts. We obtain closed formulas for all diagonal and off-diagonal coefficients of the M-polynomial and show how these expressions yield exact values of the main degree-based topological indices. The correctness of the formulas is supported through numerical computation in small instances. These results provide a complete degree-based description of H_p^n and make their structural complexity fully accessible through the M-polynomial framework.

Keywords: M-polynomial; Hanoi graph; degree-based topological index; Stirling numbers; self-similar graphs; combinatorial enumeration.

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1 Introduction

Topological indices are numerical graph invariants designed to encode structural information in a compact algebraic form. Originally motivated by chemical graph theory, where molecular structures are modeled by graphs whose vertices represent atoms and edges represent bonds, these indices have found applications in quantitative structure–property and structure–activity relationships (QSPR/QSAR); see [11, 25, 26]. Among the numerous classes of such invariants, *degree-based* indices occupy a central position due to their simplicity, interpretability, and strong empirical correlations with a wide range of physicochemical properties [5].

Such indices have demonstrated strong correlations with a wide range of molecular attributes, including heat of formation, boiling point, strain energy, rigidity, and fracture toughness. As a result, topological indices play a vital role in cheminformatics, drug design, and materials science [23, 17, 6, 16, 28, 24].

The last decade has seen a growing emphasis on unifying frameworks that encode entire families of topological indices within a single polynomial. For distance-based indices, this role is played by the Hosoya and Wiener polynomials [14, 27]. A wide range of such indices can be efficiently derived from the Hosoya polynomial, as demonstrated in [7].

In the degree-based setting, Deutsch and Klavžar introduced in 2015 the *M-polynomial* [8], defined by

$$M(G; x, y) = \sum_{i \le j} m_{i,j}(G) x^i y^j,$$

where $m_{i,j}(G)$ counts the number of edges whose endpoints have degrees $\{i, j\}$. This polynomial serves as a unifying framework for expressing many degree-based topological indices in closed form, much like the Hosoya polynomial does for distance-based indices [19, 4]. Once $M(G; x, y)$ is known, a broad spectrum of classical indices—including the Zagreb, Randić, harmonic, symmetric division, forgotten, and inverse sum indegree indices—can be obtained by applying differential and integral operators to $M(G; x, y)$.

The strength of the M-polynomial lies in its comprehensive encoding of degree-related structural information. It covers data derived from the vertex degrees and the local symmetries of molecular graphs, particularly those representing 2D molecular lattices [22]. As such, the M-polynomial facilitates the computation of a broad spectrum of graph invariants that are often correlated with the physical and chemical properties of the materials under study.

Despite this unifying strength, explicit closed forms of the M-polynomial remain unknown for many important graph families, particularly those featuring self-similarity, recursive structure, or constrained dynamics. A notable example is the family of *generalized Hanoi graphs* H_p^n, which arise from the Tower of Hanoi problem with $p \ge 3$ pegs and n distinctly sized discs. Generalized Hanoi graphs occupy an important position among self-similar and recursively defined graphs; for about these graphs, see the monograph of Hinz et al. [12, Chapter 5]. Vertices correspond to legal states of the puzzle, while edges correspond to legal moves. Unlike the Sierpiński graphs S_p^n, which form a close sibling family and whose M-polynomials have been studied in [15, 9, 3] (See [12, Chapter 4] for more about Sierpiński Graphs) , the M-polynomial of H_p^n has not been computed for any $p \ge 4$ so far.

The classical case $p = 3$ (the standard Tower of Hanoi graph) has been treated in [10, 2], but the transition from three to four pegs dramatically increases combinatorial complexity. This makes the derivation of the M-polynomial for $p \ge 4$ a nontrivial problem.

This paper provides the first explicit closed-form expression of the M-polynomial of generalized Hanoi graphs H_p^n for arbitrary $p \ge 3$ and $n \ge 0$. Our main contributions are as follows:

- We develop a complete *degree-based combinatorial analysis* of the graph H_p^n, using the fact that the degree of a vertex depends solely on the number of occupied pegs in the corresponding configuration. This leads to a natural decomposition of the vertex set into *occupancy classes*.
- We provide a detailed combinatorial decomposition of the edge set of H_p^n according to occupancy transitions between pegs, leading to an exact counting of all degree pairs.
- We express all coefficients of $M(H_p^n; x, y)$ in terms of Stirling numbers of the second kind and falling factorials, ensuring computational tractability for arbitrary p and n.
- Combining these ingredients, we derive a fully explicit closed formula for $M(H_p^n; x, y)$.

- We verify the correctness of our formulas through explicit enumeration for small instances and demonstrate how classical degree-based indices (Zagreb, Randić, etc.) can be directly obtained via differential operators.

The remainder of the paper is organized as follows. Section 2 recalls basic definitions and the operator formulae linking the M-polynomial to the most common degree-based indices. Section 3 introduces generalized Hanoi graphs and the occupancy-based viewpoint. Section 4 develops the degree-based combinatorial framework, culminating in a full decomposition of the edge set. Section 5 presents the explicit formula for $M(H_p^n; x, y)$. Section 5 provides numerical validation and illustrative examples. Finally, Section 6 discusses perspectives and possible extensions, including restricted Hanoi graphs and other self-similar families.

2 Preliminaries

Throughout this paper, all graphs are assumed to be finite, simple, and connected. For a graph $G = (V, E)$, we denote by $V(G)$ its vertex set and by $E(G)$ its edge set. An edge $e = \{u, v\} \in E(G)$ connects vertices $u, v \in V(G)$, and the *degree* of a vertex u is denoted by $\deg(u)$, i.e.,

$$\deg(u) = |\{v \in V(G) : \{u, v\} \in E(G)\}|.$$

The minimum and maximum degrees of G are denoted respectively by $\delta(G)$ and $\Delta(G)$.

A *molecular graph* is a graph-theoretical abstraction of a chemical compound, in which vertices correspond to non-hydrogen atoms and edges represent covalent bonds [11]. Topological indices derived from such graphs provide quantitative descriptors of molecular structure and are used in quantitative structure–property (QSPR) and structure–activity (QSAR) studies [5].

A *graph invariant* is a function I that assigns a unique value $I(G)$ to each graph G such that isomorphic graphs have equal values. When this invariant depends only on the vertex degrees, it is called a *degree-based topological index.*

Definition 1 (M-polynomial [8])**.** *The* M-polynomial *of a graph G is defined as*

$$M(G; x, y) = \sum_{i \leq j} m_{i,j}(G) x^i y^j, \tag{1}$$

where $m_{i,j}(G)$ denotes the number of edges $\{u, v\} \in E(G)$ such that $\{\deg(u), \deg(v)\} = \{i, j\}$; that is,

$$m_{i,j}(G) = \Big|\{\, \{u, v\} \in E(G) \mid \{\deg(u), \deg(v)\} = \{i, j\} \,\}\Big|.$$

The strength of the M-polynomial lies in its universality: once $M(G; x, y)$ is known, a broad class of classical indices can be obtained by applying differential or integral operators to it. Table 1 summarizes the most common degree-based indices and their operator expressions.

For completeness, we recall several widely used degree-based topological indices that can be derived from the M-polynomial:

Definition 2. *The* first Zagreb*,* second Zagreb*, and* second modified Zagreb *indices of G are* *defined respectively as:*

$$M_1(G) = \sum_{\{u,v\}\in E(G)} (\deg(u) + \deg(v)), \tag{2}$$

$$M_2(G) = \sum_{\{u,v\}\in E(G)} \deg(u) \cdot \deg(v), \tag{3}$$

$$MM_2(G) = \sum_{\{u,v\}\in E(G)} \frac{1}{\deg(u) \cdot \deg(v)}. \tag{4}$$

Definition 3. *The* generalized Randić *and* reciprocal generalized Randić *indices of G are defined, respectively, as:*

$$R_\alpha(G) = \sum_{\{u,v\}\in E(G)} (\deg(u) \cdot \deg(v))^\alpha, \tag{5}$$

$$RR_\alpha(G) = \sum_{\{u,v\}\in E(G)} \frac{1}{(\deg(u) \cdot \deg(v))^\alpha}. \tag{6}$$

Definition 4. *The* symmetric division index *of G is defined by:*

$$SSD(G) = \sum_{\{u,v\}\in E(G)} \left(\frac{\min\{\deg(u), \deg(v)\}}{\max\{\deg(u), \deg(v)\}} + \frac{\max\{\deg(u), \deg(v)\}}{\min\{\deg(u), \deg(v)\}} \right). \tag{7}$$

Definition 5. *The* harmonic, inverse sum indeg, augmented Zagreb, *and* Forgotten *indices of G are defined respectively as:*

$$H(G) = \sum_{\{u,v\}\in E(G)} \frac{2}{\deg(u) + \deg(v)}, \tag{8}$$

$$ISI(G) = \sum_{\{u,v\}\in E(G)} \frac{\deg(u) \cdot \deg(v)}{\deg(u) + \deg(v)}, \tag{9}$$

$$A(G) = \sum_{\{u,v\}\in E(G)} \left(\frac{\deg(u) \cdot \deg(v)}{\deg(u) + \deg(v) - 2} \right)^3, \tag{10}$$

$$F(G) = \sum_{\{u,v\}\in E(G)} \left(\deg(u)^2 + \deg(v)^2 \right). \tag{11}$$

Let $D_x, D_y, S_x, S_y, J, Q_\alpha$ denote the operators defined by

$$\begin{aligned} D_x(g(x,y)) &= x\frac{\partial g(x,y)}{\partial x}, & D_y(g(x,y)) &= y\frac{\partial g(x,y)}{\partial y}, \\ S_x(g(x,y)) &= \int_0^x \frac{g(t,y)}{t}\, dt, & S_y(g(x,y)) &= \int_0^y \frac{g(x,t)}{t}\, dt, \\ J(g(x,y)) &= g(x,x), & Q_\alpha(g(x,y)) &= x^\alpha g(x,y). \end{aligned}$$

Then the indices above satisfy the operator identities in Table 1.

Index	Relation with $M(G;x,y)$
First Zagreb	$M_1(G) = (D_x + D_y)M(G;x,y)\big\|_{x=y=1}$
Second Zagreb	$M_2(G) = (D_xD_y)M(G;x,y)\big\|_{x=y=1}$
Modified second Zagreb	$MM_2(G) = (S_xS_y)M(G;x,y)\big\|_{x=y=1}$
Generalized Randić	$R_\alpha(G) = (D_x^\alpha D_y^\alpha)M(G;x,y)\big\|_{x=y=1}$
Reciprocal generalized Randić	$RR_\alpha(G) = (S_x^\alpha S_y^\alpha)M(G;x,y)\big\|_{x=y=1}$
Symmetric division	$SSD(G) = (D_xS_y + D_yS_x)M(G;x,y)\big\|_{x=y=1}$
Harmonic	$H(G) = 2S_xJ(M(G;x,y))\big\|_{x=1}$
Inverse sum indeg	$ISI(G) = S_xJD_xD_yM(G;x,y)\big\|_{x=1}$
Augmented Zagreb	$A(G) = S_x^3Q_{-2}JD_x^3D_y^3M(G;x,y)\big\|_{x=1}$
Forgotten	$F(G) = (D_x^2 + D_y^2)M(G;x,y)\big\|_{x=y=1}$

Table 1: Relations between degree-based indices and the M-polynomial.

3 Generalized Hanoi graphs

The Tower of Hanoi (TH) problem, invented by the French number theorist Édouard Lucas in 1883, has long served as a source of challenge and inspiration in mathematics, computer science. For more details on the mathematics related to the Tower of Hanoi, we refer the reader to the comprehensive monograph by Hinz *et al.* [12].

In its general form, the Tower of Hanoi problem is defined for $p \in \mathbb{N}$, with $p \geq 3$ pegs and $n \in \mathbb{N}_0$ discs, each of a distinct size. A *legal move* is a transfer of the topmost disc[1] from one peg to another, without ever placing a larger disc on top of a smaller one. Initially, all discs are stacked on a single peg in decreasing order of size from bottom to top—this is called a *perfect state*. The objective is to move all discs from one perfect state to another using the minimum number of legal moves.

A state (i.e., a distribution of discs across the pegs) is called *regular* if the discs on each peg are arranged in decreasing size from bottom to top. The Hanoi graphs H_p^n provide a natural mathematical model for the TH problem. In these graphs, each vertex represents a regular state, and two vertices are connected by an edge if one can be obtained from the other through a single legal move.

Numerous structural and combinatorial properties of Hanoi graphs have been explored in [12] and the references therein.

Definition 6 ([12])**.** *The Hanoi graphs H_p^n for base $p \in \mathbb{N}_3$ and exponent $n \in \mathbb{N}_0$ are defined as follows.*

$$V(H_p^n) = \{\, s_n \cdots s_1 \mid s_d \in [p]_0,\ d \in [n] \,\}$$
$$E(H_p^n) = \left\{\, \{\underline{s}i\overline{s}, \underline{s}j\overline{s}\} \mid i,j \in [p]_0, i \neq j, \underline{s} \in [p]_0^{n-d}, \overline{s} \in ([p]_0 \setminus \{i,j\})^{d-1}, d \in [n] \,\right\}$$

[1]A topmost disc is a top disc of a peg.

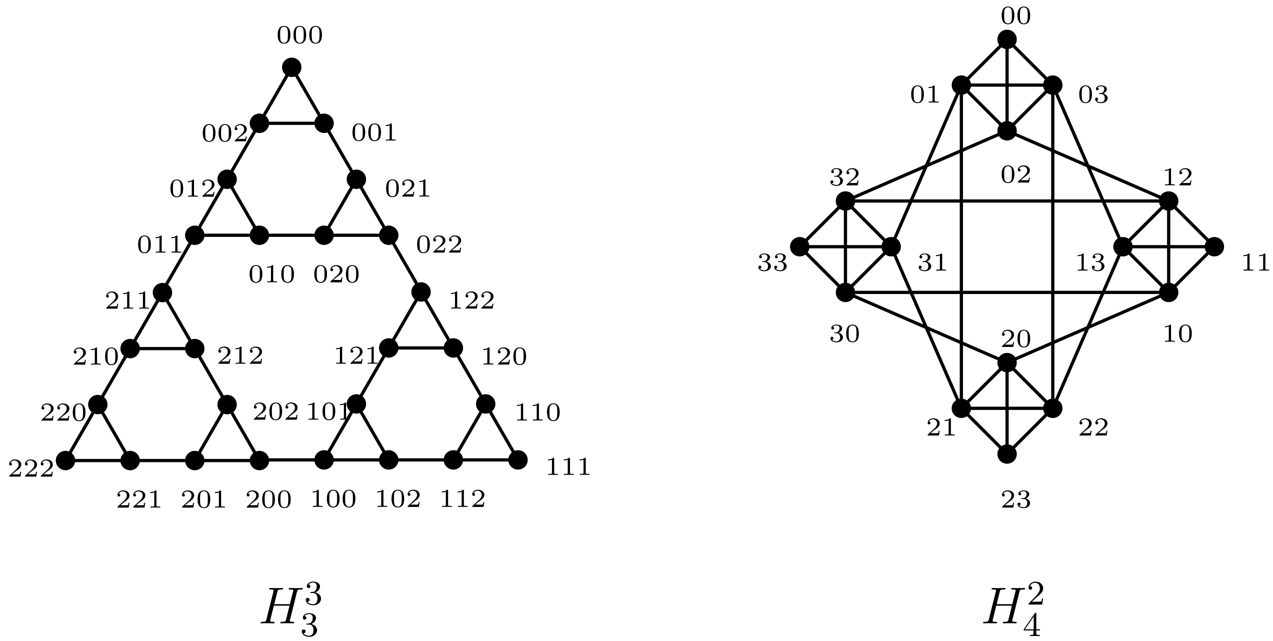

Figure 1: Examples of Hanoi graphs H_3^3 and H_4^2. Each vertex represents a regular configuration of discs, and edges represent single legal moves.

Definition 7 (Occupancy and structural parameters)**.** *For a state $s \in V(H_p^n)$, define the occupancy number $o(s) : V(H_p^n) \to [p]_0$ by*

$$o(s) = |\{i \in [p] \mid \exists\, d \in [n] : s_d = i\}|,$$

i.e., the number of pegs that contain at least one disc in state s.

Clearly, if $n = 0$, then $V(H_p^n) = \emptyset$, and the function $o(s)$ is undefined (or vacuously equal to zero). Otherwise,

$$1 \leq o(s) \leq r = \min\{n, p\}.$$

Symbol	**Meaning**
n	Number of discs
p	Number of pegs
$r = \min\{n, p\}$	Maximum possible number of occupied pegs
H_p^n	Generalized Hanoi graph with p pegs and n discs
$V(H_p^n)$, $E(H_p^n)$	Vertex set and edge set of H_p^n
$o(s)$	Occupancy of state s (number of pegs containing at least one disc)
$\Omega_p^n = \{1, \ldots, r\}$	Set of possible occupancy values, where $r = \min\{n, p\}$
$D_\mu = \{s \in V(H_p^n) : o(s) = \mu\}$	Class of configurations with exactly μ occupied pegs
$f_{p,n}(\mu)$	Degree of any vertex with occupancy μ
$\lambda_\mu = f_{p,n}(\mu)$	Degree value associated with occupancy μ
$\delta(H_p^n)$, $\Delta(H_p^n)$	Minimum and maximum vertex degrees of H_p^n
$O_p^n(\mu)$	Number of configurations with μ occupied pegs
$O_p^n(\nu \mid \mu)$	Number of configurations with μ occupied pegs, ν of which are singletons
$p^{\underline{\mu}} = p(p-1)\cdots(p-\mu+1)$	Falling factorial of order μ
$\left\{ {n \atop k} \right\}$	Stirling number of the second kind
$\left\{ {n \atop k} \right\}_{\geq 2}$	2-associated Stirling number (each block has size ≥ 2)
$A_1(H_p^n)$	Edges corresponding to moves OP $\to$ OP
$A_2(H_p^n)$	Edges corresponding to moves OP $\to$ EP
$E_1(H_p^n)$	Edges from singleton peg $\to$ empty peg
$E_2(H_p^n)$	Edges from multiton peg $\to$ occupied peg
$E_3(H_p^n)$	Edges from multiton peg $\to$ empty peg (increasing occupancy)
$M(H_p^n; x, y)$	M-polynomial of H_p^n
$m_{\lambda,\lambda'}(H_p^n)$	Number of edges joining degree classes λ and λ'
$\Gamma_p^n = \{\lambda_\mu : \mu \in \Omega_p^n\}$	Set of all realized vertex degrees in H_p^n

Table 2: Summary of notation used throughout the paper.

We denote by $\Omega_p^n = [r]$ the set of possible occupancy values. Pegs may therefore be classified as follows:

- *Empty peg* (EP): contains no disc.
- *Occupied Peg* (OP): contains at least one disc.
- *Singleton peg* (SP): is an OP that contains exactly one disc.
- *Multiton peg* (MP): is an OP that contains two or more discs.

Table 2 summarizes the notation used throughout the paper for ease of reference.

4 Degree-based combinatorial analysis

In this section, we develop a detailed combinatorial characterization of vertex degrees and edge structures in the generalized Hanoi graphs H_p^n. We begin by analyzing how vertex degrees depend on the occupancy number of the configuration, then enumerate all vertices according to their occupancy composition, and finally derive explicit formulas for the number of edges of different structural types. This analysis constitutes the combinatorial foundation of the M-polynomial derivation that follows.

4.1 Dependence of vertex degree on occupancy

Lemma 1 (Degree as a function of occupancy [13, 1])**.** *For a vertex s with occupancy $o(s) = \mu$, its degree in H_p^n is given by*

$$\deg(s) = f_{p,n}(\mu) = \sum_{\ell=1}^{\mu}(p-\ell) = \binom{p}{2} - \binom{p-\mu}{2}. \tag{12}$$

Proof. Consider a configuration s in which μ pegs are occupied. Each of the μ pegs contains a stack of discs, and the smallest (topmost) disc on each peg can be moved to another peg, provided that the destination peg either is empty or has a larger top disc.

Let us enumerate all possible target pegs for each of these μ possible moves. For the peg containing the smallest top disc overall, all the remaining $p-1$ pegs are available destinations. For the peg containing the next smallest top disc, one of these destinations is forbidden (the peg holding the globally smallest top disc), leaving $p-2$ options. Proceeding in this manner, the total number of legal moves (hence, the degree of s) equals

$$(p-1) + (p-2) + \cdots + (p-\mu) = \sum_{\ell=1}^{\mu}(p-\ell) = \binom{p}{2} - \binom{p-\mu}{2}.$$

This argument relies on the symmetry and legality constraints of the Tower of Hanoi rules and holds for any valid configuration with occupancy μ. □

Corollary 1 (Degree bounds)**.**

$$\delta(H_p^n) = f_{p,n}(1) = p-1, \qquad \Delta(H_p^n) = f_{p,n}(r) = \binom{p}{2} - \binom{p-r}{2}.$$

Proof. The smallest degree arises when only one peg is occupied ($\mu = 1$), since only that single peg provides possible moves to the other $p-1$ pegs. Conversely, the largest degree occurs when all $r = \min\{n, p\}$ pegs are occupied, producing the maximum number of active move pairs. □

Corollary 2 (Characterization of the degree set of H_p^n)**.** *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, the set of all possible vertex degrees in the graph H_p^n is given by*

$$\Gamma_p^n = \left\{ \sum_{\ell=1}^{\mu}(p-\ell) \;\middle|\; \mu \in \Omega_p^n \right\} = \left\{ p-1,\ 2p-3,\ \ldots,\ \sum_{\ell=1}^{\min\{n,p\}}(p-\ell) \right\}. \tag{13}$$

Proof. The result follows directly from the proof of Lemma 1. □

Proposition 1 (Non-injectivity and surjectivity of the mapping $f_{p,n}$)**.** *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, the function*

$$f_{p,n} : \Omega_p^n \longrightarrow \Gamma_p^n$$

is surjective but not injective. Consequently, $f_{p,n}$ is not bijective.

Proof. From Lemma 2, we know that

$$f_{p,n}(p) = f_{p,n}(p-1) = \Delta(H_p^n),$$

while clearly $p \neq p-1$. Hence, $f_{p,n}$ maps two distinct elements of Ω_p^n to the same value, and is therefore not injective.

To show surjectivity, let $\gamma \in \Gamma_p^n$ and consider the equation $f_{p,n}(\mu) = \gamma$.

- If $\gamma \in \Gamma_p^n \setminus \{\Delta(H_p^n)\}$, then

$$\mu = p - \frac{1 + \sqrt{1 + 4\big(p(p-1) - 2\gamma\big)}}{2}$$

  yields a unique $\mu \in \Omega_p^n$ such that $f_{p,n}(\mu) = \gamma$.

- If $\gamma = \Delta(H_p^n)$, there exist exactly two values $\mu_1, \mu_2 \in \Omega_p^n$ satisfying

$$\mu_1 = p - \frac{1 + \sqrt{1 + 4\big(p(p-1) - 2\gamma\big)}}{2}, \qquad \mu_2 = p - \frac{1 - \sqrt{1 + 4\big(p(p-1) - 2\gamma\big)}}{2},$$

  and both verify $f_{p,n}(\mu_1) = f_{p,n}(\mu_2) = \gamma$.

Thus, every $\gamma \in \Gamma_p^n$ admits at least one preimage in Ω_p^n, which proves that $f_{p,n}$ is surjective. □

Remark 1. *The degree of a vertex depends exclusively on its occupancy $\mu = o(s)$; the exact arrangement of discs among the μ pegs is irrelevant. Therefore, all vertices can be partitioned into* degree classes

$$D_\mu = \{\, s \in V(H_p^n) \mid o(s) = \mu \,\},$$

and each vertex in D_μ has degree $f_{p,n}(\mu)$.

4.2 Adjacency relations between degree classes

We next determine which degree classes are connected by edges in H_p^n.

Proposition 2 (Adjacency of occupancy classes)**.** *If $u, v \in V(H_p^n)$ are adjacent, then*

$$|o(u) - o(v)| \in \{0, 1\}.$$

Proof. A legal move transfers one disc from a source peg to a target peg.

Case 1. If the target peg already contains one or more discs, the total number of occupied pegs does not increase. If the source peg still contains other discs after the move, the total occupancy remains unchanged; if it becomes empty, the number of occupied pegs decreases by one.

Case 2. If the target peg was empty, then after the move it becomes occupied, possibly increasing the number of occupied pegs by one (unless the source peg was a singleton, in which case the occupancy remains constant).

Hence the occupancy can only remain the same or differ by one between adjacent vertices. □

Corollary 3 (Difference of degrees between adjacent vertices). *If $u, v \in V(H_p^n)$ are adjacent and $o(u) \le o(v)$, then*

$$\deg(u) = \begin{cases} \deg(v), & \text{if } o(u) = o(v), \\ \deg(v) - (p - o(v)), & \text{if } o(v) = o(u) + 1. \end{cases} \tag{14}$$

Proof. When $o(u) = o(v)$, both vertices belong to the same degree class and therefore share the same degree $f_{p,n}(o(u))$. If $o(v) = o(u) + 1$, then from (12),

$$\deg(v) - \deg(u) = f_{p,n}(o(u) + 1) - f_{p,n}(o(u)) = (p - o(v)),$$

yielding the claimed difference. □

Corollary 4. *If $u, v \in V(H_p^n)$ are adjacent and either $o(u) = p$ or $o(v) = p$, then* $\deg(u) = \deg(v)$.

Proof. The result follows directly from Corollary 3. □

Lemma 2 (Characterization of vertices of maximal degree). *For all $p \in \mathbb{N}_3$, $n \in \mathbb{N}_0$, and $s \in V(H_p^n)$, we have*

$$\deg(s) = \Delta(H_p^n) \quad \Longleftrightarrow \quad o(s) \in \{p,\, p-1\}. \tag{15}$$

Lemma 3 (Monotonicity between occupancy and degree). *For all $p \in \mathbb{N}_3$, $n \in \mathbb{N}_0$, and $\{u, v\} \in E(H_p^n)$, the following implication holds:*

$$o(u) \le o(v) \implies \deg(u) \le \deg(v). \tag{16}$$

Proof. If $o(u) = o(v)$, then by Lemma 1, we have $\deg(u) = \deg(v)$, since the degree of a state depends solely on the number of occupied pegs.

Now assume, without loss of generality, that $o(u) = o(v) - 1$ and $o(u) < p$. Let the $o(v)$ topmost discs in state v be indexed in increasing order of size as $d_1, d_2, \dots, d_{o(v)}$. Consider removing the largest disc $d_{o(v)}$; the remaining $o(v) - 1 = o(u)$ discs then generate exactly $\deg(u)$ legal moves. The additional disc $d_{o(v)}$ contributes $p - o(v)$ further legal moves, since it can move to all pegs not already occupied by one of the smaller discs.

Hence,

$$\deg(v) = \deg(u) + (p - o(v)) \ge \deg(u),$$

which proves the claim. □

Proposition 3 (Difference of degrees between adjacent vertices). *Let $p \in \mathbb{N}_3$, $n \in \mathbb{N}_0$, and $\{u, v\} \in E(H_p^n)$. Then*

$$|\deg(u) - \deg(v)| \in \{\, 0,\; p - \max\{o(u),\, o(v)\}\,\}\,. \tag{17}$$

Proof. If $o(u) = o(v)$, the difference is zero. If $o(v) = o(u) + 1$, then from the proof of Lemma 3, $\deg(v) - \deg(u) = p - o(v)$, which equals $p - \max\{o(u), o(v)\}$. The same holds symmetrically when $o(u) = o(v) + 1$. $\square$

4.3 Enumeration of configurations by occupancy

Let $O_p^n(\mu)$ denote the number of vertices in H_p^n having exactly μ occupied pegs. We derive a closed formula for this quantity.

Theorem 1 (Number of configurations by occupancy [18, 1])**.** *For all $p \geq 3$ and $n \geq 0$,*

$$O_p^n(\mu) = \left\{ {n \atop \mu} \right\} p^{\underline{\mu}}, \qquad 1 \leq \mu \leq r, \tag{18}$$

where $\left\{ {n \atop \mu} \right\}$ is the Stirling number of the second kind and $p^{\underline{\mu}} = p(p-1)\cdots(p-\mu+1)$ the falling factorial.

Proof. We must count all distinct distributions of n labeled discs among p labeled pegs such that exactly μ pegs are nonempty.

First, we partition the n discs into μ nonempty groups, each corresponding to a stack on one peg. The number of such partitions is $\left\{ {n \atop \mu} \right\}$. Then, we assign each group to a distinct peg. Since the pegs are labeled, this can be done in $p^{\underline{\mu}} = p!/(p-\mu)!$ ways.

Each assignment yields a distinct configuration because the order of discs within a stack is determined by their sizes. Multiplying both factors gives the result (18). $\square$

Lemma 4 ([18])**.** *For all $p \geq 3$ and $n \geq 0$, let $r = \min\{n, p\}$, then*

$$\sum_{\mu=1}^{r} O_p^n(\mu) = p^n. \tag{19}$$

Proof. This follows from the classical identity $\sum_{\mu=0}^{n} \left\{ {n \atop \mu} \right\} x^{\underline{\mu}} = x^n$ with $x = p$. $\square$

We refine the counting by distinguishing the number of singleton pegs within a configuration. Let $O_p^n(\nu \mid \mu)$ denote the number of configurations with μ occupied pegs, among which ν pegs are singletons (contain exactly one disc).

Theorem 2 (Configurations with μ occupied and ν singletons)**.** *For all $1 \leq \nu \leq \mu \leq r$,*

$$O_p^n(\nu \mid \mu) = \binom{n}{\nu} \left\{ {n-\nu \atop \mu-\nu} \right\}_{\geq 2} p^{\underline{\mu}}, \tag{20}$$

where $\left\{ {n-\nu \atop \mu-\nu} \right\}_{\geq 2}$ denotes the 2-associated Stirling number of the second kind.

Proof. We first choose ν discs to serve as singletons, in $\binom{n}{\nu}$ ways. The remaining $n-\nu$ discs must be arranged on the remaining $\mu-\nu$ pegs, each receiving at least two discs. The number of such partitions is $\left\{ {n-\nu \atop \mu-\nu} \right\}_{\geq 2}$. Finally, we assign these μ stacks to distinct pegs in $p^{\underline{\mu}}$ ways. The product of these three factors yields (20). □

Lemma 5. *Summing over all admissible values of ν,*

$$O_p^n(\mu) = \sum_{\nu=0}^{\mu} O_p^n(\nu \mid \mu) = \sum_{\nu=0}^{\mu} \binom{n}{\nu} \left\{ {n-\nu \atop \mu-\nu} \right\}_{\geq 2} p^{\underline{\mu}}. \tag{21}$$

with the convention that

$$\left\{ {n-\mu \atop 0} \right\}_{\geq 2} = \begin{cases} 1, & \text{if } n = \mu; \\ 0, & \text{otherwise.} \end{cases}$$

4.4 Edge decomposition and degree-based classification

In this section, we refine the combinatorial structure of the edge set of the generalized Hanoi graph H_p^n by decomposing it into several disjoint subsets according to the nature of the moves between states. We begin by recalling that each edge $\{u, v\} \in E(H_p^n)$ corresponds to a legal move of a disc between two pegs under the standard Tower of Hanoi rules. Depending on whether this move increases, decreases, or preserves the number of occupied pegs, the edges can be classified into different categories.

The following Proposition establishes a first-level partition of the edge set into two fundamental blocks.

Proposition 4. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, the edge set of the Hanoi graph H_p^n can be expressed as*

$$E(H_p^n) = A_1(H_p^n) \cup A_2(H_p^n), \tag{22}$$

where $A_1(H_p^n) \cap A_2(H_p^n) = \emptyset$, and

$$A_1(H_p^n) = \Big\{ \{u, v\} \in E(H_p^n) \mid \{u,v\} \textit{ corresponds to a move from an OP to another OP} \Big\}, \tag{23}$$

$$A_2(H_p^n) = \Big\{ \{u, v\} \in E(H_p^n) \mid \{u,v\} \textit{ corresponds to a move from an OP to an EP} \Big\}. \tag{24}$$

The next result provides closed expressions for the cardinalities of these two classes.

Proposition 5. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$. Then we have*

$$|A_1(H_p^n)| = \frac{1}{2} \sum_{\mu=1}^{r} \binom{\mu}{2} O_p^n(\mu), \tag{25}$$

$$|A_2(H_p^n)| = \frac{1}{2} \sum_{\mu=1}^{r} \mu(p-\mu) O_p^n(\mu). \tag{26}$$

From these two disjoint families, one can recover the total number of edges of H_p^n. This value has been previously obtained by Klavžar and Milutinović [18] and Arett [1] through a different reasoning based on the degree distribution of the vertices. Their approach consisted in summing, for each possible number of occupied pegs μ, the product of the number of corresponding states $O_p^n(\mu)$ and the degree $f_{p,n}(\mu)$ of each state, giving:

$$E(H_p^n) = \frac{1}{2}\sum_{\mu=1}^{r} O_p^n(\mu) f_{p,n}(\mu) = \frac{1}{2}\sum_{\mu=1}^{r} \left\{ {n \atop \mu} \right\} p^{\underline{\mu}} \left[\binom{p}{2} - \binom{p-\mu}{2} \right]. \tag{27}$$

A similar method was later extended to restricted Hanoi graphs in [20], a result that can also be applied to the classical family H_p^n.

However, by exploiting the disjoint decomposition introduced in Proposition 4, we can recover the same result more structurally, as shown below.

Theorem 3 ([18, 1])**.** *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$. Then we have*

$$E(H_p^n) = \frac{1}{4}\sum_{\mu=1}^{r} \mu\,(2p - \mu - 1)\, O_p^n(\mu). \tag{28}$$

Proof. From Propositions 4 and 5, we have

$$\begin{aligned} E(H_p^n) &= |A_1(H_p^n)| + |A_2(H_p^n)| \\ &= \frac{1}{2}\sum_{\mu=1}^{r} \binom{\mu}{2} O_p^n(\mu) + \frac{1}{2}\sum_{\mu=1}^{r} \mu(p-\mu) O_p^n(\mu) \\ &= \frac{1}{2}\sum_{\mu=1}^{r} \left(\frac{\mu(\mu-1)}{2} + \mu(p-\mu) \right) O_p^n(\mu) \\ &= \frac{1}{4}\sum_{\mu=1}^{r} \mu\,(2p-\mu-1)\, O_p^n(\mu). \end{aligned}$$

□

We now refine the above dichotomy by examining more closely the nature of the move that generates each edge. Depending on whether the source and target configurations differ by one in the number of occupied pegs, or whether the moved disc comes from a singleton or multiton peg, we distinguish three mutually exclusive situations.

Theorem 4. *Let $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$. For every edge $\{u, v\} \in E(H_p^n)$ with $o(u) \le o(v)$. Then the edge $\{u, v\}$ corresponds to exactly one of the following three disjoint cases:*

(c_1) *A disc is moved from a singleton peg to an empty peg (occurs only if $o(u) = o(v)$);*

(c_2) *A disc is moved from a multiton peg to an occupied peg (also only if $o(u) = o(v)$);*

(c_3) *A disc is moved from a multiton peg to an empty peg (occurs only if $o(u) = o(v) - 1$).*

Hence, the edge set of H_p^n admits the following disjoint decomposition:

$$E(H_p^n) = E_1(H_p^n) \cup E_2(H_p^n) \cup E_3(H_p^n), \tag{29}$$

where

$$E_i(H_p^n) = \{\{u, v\} \in E(H_p^n) \mid \{u, v\} \text{ satisfies } (\mathsf{c}_i)\}, \quad i = 1, 2, 3, \tag{30}$$

and these subsets are pairwise disjoint, i.e., $E_i(H_p^n) \cap E_j(H_p^n) = \emptyset$ for all $i \neq j$.

Proof. This result follows directly from the case analysis presented in the proof of Proposition 2. □

Note that the reverse situations of `(c₂)` and `(c₃)` cannot occur under the assumption $o(u) \leq o(v)$, as they would imply a decrease in the number of occupied pegs. Consequently, only case `(c₁)` is symmetric. This observation will be taken into account in ulterior enumerations.

The following theorem enumerates the number of edges belonging to each of these three categories.
Theorem 5. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$. Then we have*

$$|E_1(H_p^n)| = \frac{1}{2}\sum_{\mu=1}^{r}(p-\mu)\sum_{\nu=0}^{\mu}\nu\, O_p^n(\nu \mid \mu), \tag{31}$$

$$|E_2(H_p^n)| = \frac{1}{2}\binom{p}{2}p^n - \frac{1}{4}\sum_{\mu=1}^{r}(p-\mu)\sum_{\nu=0}^{\mu}(p+3\mu-2\nu-1)\, O_p^n(\nu \mid \mu), \tag{32}$$

$$|E_3(H_p^n)| = \sum_{\mu=1}^{r}(p-\mu)\sum_{\nu=0}^{\mu}(\mu-\nu)\, O_p^n(\nu \mid \mu). \tag{33}$$

Proof. The term $|E_1(H_p^n)|$ counts edges $\{u, v\} \in E(H_p^n)$ such that $o(u) = o(v) \leq p-1$, where the move is from a singleton peg to an empty peg. The number of such states u is given by $O_p^n(\nu \mid \mu)$, where $\mu \in [p-1]$ and $\nu \in [\mu]$. For each such state u (or equivalently v), there are ν singleton pegs from which a disc can be chosen, and $p-\mu$ empty pegs on which it can be placed. Thus, the number of such moves is $\nu(p-\mu)$. Since edges are unordered, we divide by 2 to remove symmetry, which yields Equation (31).

The term $|E_3(H_p^n)|$ counts edges $\{u, v\} \in E(H_p^n)$ where $o(v) = o(u) + 1 \leq p$, and the move is from a multiton peg to an empty peg in state u. Such a move is only possible when $\mu \leq p-1$ and $\nu < \mu$, since having all occupied pegs as singletons ($\nu = \mu$) would exclude the presence of multitons. For each such state u, there are $\mu - \nu$ multitons from which a disc can be chosen, and $p - \mu$ empty pegs available to receive it. Moreover, no symmetry elimination is required since the directionality is fixed by $o(u) \neq o(v)$. This gives Equation (33).

The term $|E_2(H_p^n)|$ accounts for edges with $o(u) = o(v)$ where the move is from a multiton peg to another occupied peg. A direct enumeration of these configurations is infeasible due to dependencies on disc sizes at both the source and target pegs. Instead, we apply the inclusion–exclusion principle. From Theorem 4, we have

$$|E_2(H_p^n)| = |E(H_p^n)| - |E_1(H_p^n)| - |E_3(H_p^n)|.$$

Substituting the expression of $|E(H_p^n)|$ from Theorem 3, together with those of $|E_1(H_p^n)|$ and $|E_3(H_p^n)|$, yields

$$\begin{aligned}|E_2(H_p^n)| = {} & \frac{1}{2}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu} O_p^n(\nu \mid \mu)\left(\binom{p}{2} - \binom{p-\mu}{2}\right) \\ & - \frac{1}{2}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}\nu(p-\mu)\, O_p^n(\nu \mid \mu) - \sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}(\mu-\nu)(p-\mu)\, O_p^n(\nu \mid \mu).\end{aligned}$$

Simplifying the above gives

$$|E_2(H_p^n)| = \frac{1}{2}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu} O_p^n(\nu \mid \mu)\left(\binom{p}{2} - \frac{(p-\mu)(p-\mu-1)}{2} - \nu(p-\mu) - 2(\mu-\nu)(p-\mu)\right)$$
$$= \frac{1}{2}\binom{p}{2}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu} O_p^n(\nu \mid \mu) - \frac{1}{4}\sum_{\mu=1}^{r}(p-\mu)\sum_{\nu=0}^{\mu}(p+3\mu-2\nu-1)\, O_p^n(\nu \mid \mu).$$

Finally, applying Lemmas 4 and 5, we obtain

$$|E_2(H_p^n)| = \frac{1}{2}\binom{p}{2}p^n - \frac{1}{4}\sum_{\mu=1}^{r}(p-\mu)\sum_{\nu=0}^{\mu}(p+3\mu-2\nu-1)\, O_p^n(\nu \mid \mu),$$

as claimed. □

From these expressions, several corollaries and degree-based results follow naturally. We now summarize them for completeness.

Corollary 5. *An equivalent form of Equation* (32) *is given by*

$$\begin{aligned}|E_2(H_p^n)| &= \frac{1}{4}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}\left(2p(\nu-\mu) + \mu(3\mu-2\nu-1)\right) O_p^n(\nu \mid \mu)\\ &= \frac{1}{4}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}\left(2p\nu - 2p\mu + 3\mu^2 - 2\mu\nu - \mu\right) O_p^n(\nu \mid \mu).\end{aligned} \tag{34}$$

Moreover,

$$\begin{aligned}|E_1(H_p^n)| + |E_2(H_p^n)| &= \frac{1}{4}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}\left(3\mu^2 - 2p\mu - \mu + 4p\nu - 4\mu\nu\right) O_p^n(\nu \mid \mu)\\ &= \frac{1}{4}\sum_{\mu=1}^{r}\sum_{\nu=0}^{\mu}\left(4\nu(p-\mu) + \mu(3\mu-2p-1)\right) O_p^n(\nu \mid \mu).\end{aligned} \tag{35}$$

Finally, we connect this classification to the degree structure of H_p^n. The following propositions enumerate edges according to the degrees of their endpoints, distinguishing equal-degree and off-diagonal cases.

Degree-based decomposition of the edge set

Having classified the edges of H_p^n according to the type of move, we now turn to a finer analysis based on the *degrees* of their endpoints. We denote by $\Delta(H_p^n) = f_{p,n}(p) = \binom{p}{2}$ the maximum vertex degree of H_p^n.

Proposition 6. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$, $\lambda < \Delta(H_p^n)$, and let $\mu = f^{-1}(\lambda)$. The number of edges $\{u, v\} \in E(H_p^n)$ such that*

$$\deg(u) = \deg(v) = \lambda$$

is given by

$$\sigma(\lambda) = \frac{1}{4}\sum_{\nu=0}^{\mu}\left(3\mu^2 - 2p\mu - \mu + 4p\nu - 4\mu\nu\right)O_p^n(\nu \mid \mu). \tag{36}$$

Proof. Since $\lambda < \Delta(H_p^n)$, the inverse image $\mu = f^{-1}(\lambda)$ is unique. From Corollary 5, we know that the sum of $|E_1(H_p^n)|$ and $|E_2(H_p^n)|$ accounts precisely for all edges joining vertices of equal degree (i.e., those for which $o(u) = o(v) = \mu$). Substituting this relation gives the stated expression for $\sigma(\lambda)$. $\square$

The next proposition characterizes the edges whose endpoints both have the *maximum degree*, i.e., $\lambda = \Delta(H_p^n)$.

Proposition 7. *For all* $p \in \mathbb{N}_3$ *and* $n \in \mathbb{N}_0$, *let* $r = \min\{n, p\}$ *and* $\lambda = \Delta(H_p^n) = \binom{p}{2}$. *The number of edges* $\{u, v\} \in E(H_p^n)$ *satisfying* $\deg(u) = \deg(v) = \lambda$ *is*

$$\sigma(\lambda) = \begin{cases} \frac{1}{4}\big(p^2 - p\big)\, O_p^n(p), & \textit{if } o(u) = o(v) = p, \\ \frac{1}{4}\sum\limits_{\nu=0}^{p-1}\big(p^2 - 5p + 4\nu + 4\big) O_p^n(\nu \mid p-1), & \textit{if } o(u) = o(v) = p-1, \\ \sum\limits_{\nu=0}^{p-1}(p - \nu - 1)\, O_p^n(\nu \mid p-1), & \textit{if } o(u) = p-1,\ o(v) = p. \end{cases} \tag{37}$$

Consequently, we obtain the compact identity

$$\sigma(\lambda) = \frac{1}{4}\, p \left\{ {n+1 \atop p} \right\}. \tag{38}$$

Proof. If $\deg(u) = \deg(v) = \lambda = \Delta(H_p^n)$, then both endpoints have either all pegs occupied or all but one occupied. Hence,

$$\{o(u), o(v)\} \in \big\{\{p, p\}, \{p-1, p-1\}, \{p-1, p\}\big\}.$$

We analyze these cases separately.

- Case 1, $o(u) = o(v) = p$:

  Here $\mu = f^{-1}(\lambda) = p$. Using Corollary 5 with $\mu = p$, we find

$$\begin{aligned} \sigma(\lambda) &= \frac{1}{4}\sum_{\nu=0}^{r}\big(3p^2 - 2pp - p + 4p\nu - 4p\nu\big) O_p^n(\nu \mid p) \\ &= \frac{1}{4}(p^2 - p)\, O_p^n(p). \end{aligned}$$

- Case 2, $o(u) = o(v) = p - 1$:

  Now $\mu = p - 1$. Substituting $\mu = p - 1$ in the same expression gives

$$\begin{aligned} \sigma(\lambda) &= \frac{1}{4}\sum_{\nu=0}^{p-1}\big(3(p-1)^2 - 2p(p-1) - (p-1) + 4p\nu - 4\nu(p-1)\big) O_p^n(\nu \mid p-1) \\ &= \frac{1}{4}\sum_{\nu=0}^{p-1}\big(p^2 - 5p + 4\nu + 4\big)\, O_p^n(\nu \mid p-1). \end{aligned}$$

- Case 3, $\{o(u), o(v)\} = \{p-1, p\}$:

  Here we use the expression from case (c$_3$), corresponding to a move from a multiton to an empty peg:

$$\begin{aligned}\sigma(\lambda) &= \sum_{\nu=0}^{p-1}(p-\mu)(\mu-\nu)\, O_p^n(\nu \mid \mu) = \sum_{\nu=0}^{p-1}(p-(p-1))((p-1)-\nu)\, O_p^n(\nu \mid p-1) \\ &= \sum_{\nu=0}^{p-1}(p-\nu-1)\, O_p^n(\nu \mid p-1).\end{aligned}$$

Summing the three contributions and applying the Stirling-type identity

$$p\left\{ {n \atop p} \right\} + \left\{ {n \atop p-1} \right\} = \left\{ {n+1 \atop p} \right\},$$

we obtain the compact form

$$\begin{aligned}\sigma(\lambda) &= \frac{1}{4}\left(p^2-p\right) O_p^n(p) + \frac{1}{4}\sum_{\nu=0}^{p-1}\left(p^2-5p+4\nu+4\right) O_p^n(\nu \mid p-1) + \sum_{\nu=0}^{p-1}(p-\nu-1) O_p^n(\nu \mid p-1) \\ &= \frac{1}{4}\left(p^2-p\right) O_p^n(p) + \frac{1}{4}\left(p^2-p\right)\sum_{\nu=0}^{p-1} O_p^n(\nu \mid p-1) \\ &= \frac{1}{4}\left(p^2-p\right) O_p^n(p) + \frac{1}{4}\left(p^2-p\right) O_p^n(p-1) \\ &= \frac{1}{4}\left(p^2-p\right)\left(O_p^n(p) + O_p^n(p-1)\right) \\ &= \frac{1}{4}\left(p^2-p\right)\left(\left\{ {n \atop p} \right\} p! + \left\{ {n \atop p-1} \right\}(p-1)!\right) \\ &= \frac{1}{4}(p-1)\, p!\left(p\left\{ {n \atop p} \right\} + \left\{ {n \atop p-1} \right\}\right) \\ &= \frac{1}{4}p\left\{ {n+1 \atop p} \right\}.\end{aligned}$$

□

We next consider *off-diagonal edges*, i.e., edges connecting vertices of distinct degrees. These correspond precisely to edges where the number of occupied pegs differs by one between the two endpoints.

Proposition 8. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $\lambda < \Delta(H_p^n)$ and $\mu = f^{-1}(\lambda)$. The number of edges $\{u, v\} \in E(H_p^n)$ such that* $\deg(u) < \deg(v) = \lambda$ *is*

$$\sigma(\lambda) = \sum_{\nu=0}^{\mu}(p-\mu)(\mu-\nu)\, O_p^n(\nu \mid \mu). \tag{39}$$

Proof. If $\deg(u) < \deg(v) = \lambda$, then $o(u) < o(v)$ and necessarily $o(v) = o(u) + 1 = \mu + 1$. Since $\mu \leq p-2$, this correspondence between μ and λ is one-to-one. The number of such edges equals the number of moves of type (c$_3$), i.e., moves from a multiton peg to an empty peg in a state with μ occupied pegs. Each such move can be made by choosing one of the $(\mu - \nu)$ multitons and one of the $(p - \mu)$ empty pegs, giving the stated formula. $\square$

When the upper endpoint reaches the maximal degree, two additional contributions appear, corresponding to $o(v) = p - 1$ and $o(v) = p$.

Proposition 9. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $\lambda = \Delta(H_p^n) = \binom{p}{2}$. The number of edges $\{u, v\} \in E(H_p^n)$ such that* $\deg(u) < \deg(v) = \lambda$ *is*

$$\sigma(\lambda) = \sum_{\nu=0}^{p-1} (p - 1 - \nu)\, O_p^n(\nu \mid p - 1) + \sum_{\nu=0}^{p-2} 2(p - 2 - \nu)\, O_p^n(\nu \mid p - 2). \tag{40}$$

Proof. If $\deg(v) = \lambda = \Delta(H_p^n)$, then $o(v) \in \{p - 1, p\}$.

- Case 1, $o(v) = p$: Then $o(u) = p - 1$, and by applying case (c$_3$) with $\mu = p - 1$, we have

$$\sigma(\lambda) = \sum_{\nu=0}^{p-1} (p - (p - 1))((p - 1) - \nu)\, O_p^n(\nu \mid p - 1) = \sum_{\nu=0}^{p-1} (p - 1 - \nu)\, O_p^n(\nu \mid p - 1).$$

- Case 2, $o(v) = p - 1$: Then $o(u) = p - 2$, and again by case (c$_3$), we have

$$\sigma(\lambda) = \sum_{\nu=0}^{p-2} (p - (p - 2))((p - 2) - \nu)\, O_p^n(\nu \mid p - 2) = \sum_{\nu=0}^{p-2} 2(p - 2 - \nu)\, O_p^n(\nu \mid p - 2).$$

Adding both contributions completes the proof. $\square$

Gathering all the above results, we can now state a unified expression that encompasses both the general and top-degree cases.

Proposition 10. *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$. For every $\lambda \leq \Delta(H_p^n)$, let $\mu = f^{-1}(\lambda)$. The number of edges $\{u, v\} \in E(H_p^n)$ satisfying* $\deg(u) < \deg(v) = \lambda$ *is*

$$\sigma(\lambda) = \sum_{\nu=0}^{\mu} (p - \mu)(\mu - \nu)\, O_p^n(\nu \mid \mu). \tag{41}$$

Proof. The formula of Proposition 8 already holds for all $\lambda < \Delta(H_p^n)$. For $\lambda = \Delta(H_p^n)$, the two contributions given in Proposition 9 are consistent with the same expression, since for $\mu = p - 1$ the term $(p - \mu) = 1$, and for $\mu = p - 2$ we obtain the multiplicative factor 2 accounting for the two admissible target configurations. Thus, the formula extends uniformly to all $\lambda \leq \Delta(H_p^n)$. $\square$

This completes the degree-based decomposition of the edge set of H_p^n, providing an explicit enumeration of all edge classes as a function of the occupancy parameters (μ, ν) and the associated degree values.

5 Explicit expression of the M-polynomial

Let $r = \min\{n, p\}$ and define the (multi)set of realized degree values

$$\Gamma_p^n \;=\; \Big\{\lambda_\mu : \mu \in [r]\Big\} \qquad \text{with} \qquad \lambda_\mu \;=\; f_{p,n}(\mu)\,.$$

By Proposition 1 the map $\mu \mapsto \lambda_\mu$ is bijective on $[r] \setminus \{p\}$ and satisfies $\lambda_{p-1} = \lambda_p = \Delta(H_p^n)$ when $r = p$ (top degree collision). For notational convenience we set

$$\Delta = \Delta(H_p^n) = \lambda_{p-1} = \lambda_p \quad (\text{when } r = p), \qquad \delta = \delta(H_p^n) = \lambda_1 = p - 1.$$

The M-polynomial of H_p^n is

$$M(H_p^n; x, y) \;=\; \sum_{i \le j} m_{i,j}(H_p^n)\, x^i y^j \;=\; \sum_{\lambda \le \lambda'} m_{\lambda,\lambda'}(H_p^n)\, x^\lambda y^{\lambda'}\,,$$

where $m_{\lambda,\lambda'}(H_p^n)$ counts edges $\{u, v\} \in E(H_p^n)$ with $\{\deg(u), \deg(v)\} = \{\lambda, \lambda'\}$.

Our strategy is to *index* degree classes by the occupancy parameter μ, and to use the edge partition of Theorem 4 together with the occupancy enumerators $O_n^p(\nu \mid \mu)$ (Proposition 2). This yields closed forms for all diagonal coefficients $m_{\lambda,\lambda}$ and all off–diagonal coefficients between *adjacent* degree classes (which are the only nonzero off–diagonal terms by Proposition 3).

Degree classes and adjacency pattern

For $1 \le \mu \le r$, define the *μ–degree class*

$$\mathcal{D}_\mu \;=\; \{\, s \in V(H_p^n) \;:\; o(s) = \mu \,\}, \qquad \deg(\mathcal{D}_\mu) = \lambda_\mu.$$

By Proposition 3 and Corollary 3, if $\{u, v\} \in E(H_p^n)$ with $o(u) \le o(v)$, then $|o(u) - o(v)| \in \{0, 1\}$, hence

$$\{\deg(u), \deg(v)\} \in \begin{cases} \{\lambda_\mu\} & \text{if } o(u) = o(v) = \mu, \\ \{\lambda_{\mu-1}, \lambda_\mu\} & \text{if } o(u) = \mu - 1,\ o(v) = \mu. \end{cases} \tag{42}$$

Therefore the only possibly nonzero off–diagonal coefficients are those between *consecutive* occupancy classes.

Diagonal coefficients $m_{\lambda,\lambda}$

Lemma 6 (Equal-degree edges inside a fixed occupancy)**.** *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$ and $1 \le \mu \le \min\{r, p - 2\}$. Then*

$$m_{\lambda_\mu,\lambda_\mu}(H_p^n) \;=\; \frac{1}{4} \sum_{\nu=0}^{\mu} \Big(3\mu^2 - 2p\mu - \mu + 4p\nu - 4\mu\nu\Big)\, O_n^p(\nu \mid \mu). \tag{43}$$

Proof. By Proposition 6, for any degree value $\lambda < \Delta$ there is a unique $\mu = f_{p,n}^{-1}(\lambda)$, and the number of equal–degree edges with both endpoints in $\mathcal{D}_\mu$ is exactly

$$\frac{1}{4}\sum_{\nu=0}^{\mu}\Big(3\mu^2 - 2p\mu - \mu + 4p\nu - 4\mu\nu\Big)\, O_n^p(\nu \mid \mu).$$

Since here $\lambda_\mu < \Delta$ for $\mu \le p-2$, the claim follows. $\square$

Lemma 7 (Equal-degree edges at top degree). *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$. Assume $r = p$ so that $\lambda_{p-1} = \lambda_p = \Delta$. Then*

$$m_{\Delta,\Delta}(H_p^n) \;=\; \frac{1}{4}\Big(p^2 - p\Big)\Big(O_n^p(p) + O_n^p(p-1)\Big). \tag{44}$$

Equivalently, using $O_n^p(\mu) = \left\{ {n \atop \mu} \right\} p^{\underline{\mu}}$,

$$m_{\Delta,\Delta}(H_p^n) \;=\; \frac{1}{4}p!\Big(p^2 - p\Big)\Big(\left\{ {n \atop p} \right\} \;+\; \left\{ {n \atop p-1} \right\}\Big). \tag{45}$$

Proof. By Proposition 7, edges with both endpoints of degree Δ come from three disjoint configurations: (i) $o(u) = o(v) = p$; (ii) $o(u) = o(v) = p-1$; and (iii) $\{o(u), o(v)\} = \{p-1, p\}$. Adding the three expressions given in Proposition 7 and simplifying using Corollary 5 yields

$$m_{\Delta,\Delta} = \frac{1}{4}\,(p^2 - p)O_n^p(p) \;+\; \frac{1}{4}\,(p^2 - p)O_n^p(p-1) = \frac{1}{4}\,(p^2 - p)\Big(O_n^p(p) + O_n^p(p-1)\Big),$$

as claimed. $\square$

Off–diagonal coefficients $m_{\lambda,\lambda'}$ between adjacent classes

Lemma 8 (Edges between consecutive occupancies). *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$, let $r = \min\{n, p\}$ and $2 \le \mu \le r$. Then the number of edges with $o(u) = \mu - 1$, $o(v) = \mu$ (hence $\{\deg(u), \deg(v)\} = \{\lambda_{\mu-1}, \lambda_\mu\}$) equals*

$$m_{\lambda_{\mu-1},\lambda_\mu}(H_p^n) \;=\; \sum_{\nu=0}^{\mu-1}\big(p - \mu + 1\big)\,(\mu - 1 - \nu)\, O_n^p(\nu \mid \mu - 1). \tag{46}$$

Proof. This is exactly the case (c_3)) of Theorem 4 with μ replaced by $\mu - 1$, counting moves from a multiton peg to an empty peg. Proposition 10 gives for $\lambda = \lambda_\mu$:

$$\sigma(\lambda_\mu) = \sum_{\nu=0}^{\mu-1}(p - (\mu - 1))\,\big((\mu - 1) - \nu\big)\, O_n^p(\nu \mid \mu - 1),$$

which is precisely $m_{\lambda_{\mu-1},\lambda_\mu}$. $\square$

Lemma 9 (Off–diagonal edges to top degree). *For all $p \in \mathbb{N}_3$ and $n \in \mathbb{N}_0$. Assume $r = p$. Then the total number of edges with the higher endpoint at degree Δ (i.e., with $\{\deg(u), \deg(v)\} = \{\lambda, \Delta\}$ and $\lambda < \Delta$) equals*

$$m_{\lambda_{p-1},\Delta}(H_p^n) \;=\; \sum_{\nu=0}^{p-1}(p - 1 - \nu)\, O_n^p(\nu \mid p-1) \;+\; \sum_{\nu=0}^{p-2} 2\,(p - 2 - \nu)\, O_n^p(\nu \mid p-2). \tag{47}$$

Proof. By Proposition 9, off–diagonal edges with higher degree Δ arise in two disjoint situations: (i) $o(v) = p$, $o(u) = p-1$ (coefficient $\sum_{\nu=0}^{p-1}(p-1-\nu)O_n^p(\nu \mid p-1)$); (ii) $o(v) = p-1$, $o(u) = p-2$ (coefficient $\sum_{\nu=0}^{p-2} 2(p-2-\nu)O_n^p(\nu \mid p-2)$). Adding the two contributions yields the stated formula. □

The main formula

Theorem 6 (Explicit M-polynomial of H_p^n)**.** *For all $p \in \mathbb{N}$ and $n \in \mathbb{N}_0$. Let $r = \min\{n, p\}$ and $\lambda_\mu = f_{p,n}(\mu)$ for $\mu \in [r]$. Then*

$$\begin{aligned} M(H_p^n; x, y) = &\underbrace{\sum_{\mu=1}^{\min\{r,p-2\}} m_{\lambda_\mu,\lambda_\mu}(H_p^n)\, x^{\lambda_\mu} y^{\lambda_\mu}}_{\textit{diagonal terms below top degree}} + \mathbf{1}_{\{r=p\}}\, m_{\Delta,\Delta}(H_p^n)\, x^{\Delta} y^{\Delta} \\ &+ \sum_{\mu=2}^{\min\{r,p-1\}} m_{\lambda_{\mu-1},\lambda_\mu}(H_p^n)\, x^{\lambda_{\mu-1}} y^{\lambda_\mu} + \mathbf{1}_{\{r=p\}}\, m_{\lambda_{p-1},\Delta}(H_p^n)\, x^{\lambda_{p-1}} y^{\Delta}. \end{aligned} \tag{48}$$

where the coefficients are given explicitly by

$$\begin{aligned} m_{\lambda_\mu,\lambda_\mu}(H_p^n) =& \frac{1}{4}\sum_{\nu=0}^{\mu} \Big(3\mu^2 - 2p\mu - \mu + 4p\nu - 4\mu\nu\Big)\, O_n^p(\nu \mid \mu) \quad (1 \le \mu \le \min\{r, p-2\}), \\ m_{\Delta,\Delta}(H_p^n) =& \frac{1}{4}\Big(p^2 - p\Big)\Big(O_n^p(p) + O_n^p(p-1)\Big) \quad \textit{(when } r = p\textit{)}, \\ m_{\lambda_{\mu-1},\lambda_\mu}(H_p^n) =& \sum_{\nu=0}^{\mu-1} \big(p-\mu+1\big)\,(\mu-1-\nu)\, O_n^p(\nu \mid \mu-1) \quad (2 \le \mu \le \min\{r, p-1\}), \\ m_{\lambda_{p-1},\Delta}(H_p^n) =& \sum_{\nu=0}^{p-1}(p-1-\nu)\, O_n^p(\nu \mid p-1) \\ &+ \sum_{\nu=0}^{p-2} 2\,(p-2-\nu)\, O_n^p(\nu \mid p-2) \quad \textit{(when } r = p\textit{)}. \end{aligned}$$

Proof. By the discussion preceding Lemma 6, all diagonal coefficients below Δ are equal–degree edges within a single occupancy class $\mathcal{D}_\mu$ ($\mu \le p-2$); these are counted by Proposition 6, giving the first line of coefficients.

At top degree (when $r = p$), equal–degree edges arise from three disjoint subcases $\{p, p\}$, $\{p-1, p-1\}$, and $\{p-1, p\}$; Proposition 7 sums these to the stated closed form for $m_{\Delta,\Delta}$.

For off–diagonal terms between adjacent degree classes $\lambda_{\mu-1}$ and λ_μ with $2 \le \mu \le p-1$, Proposition 8 (case (c_3)) yields the stated coefficient. Finally, when $r = p$, edges with higher degree Δ have two sources (from $p-1$ to p and from $p-2$ to $p-1$); adding these contributions as in Proposition 9 gives the last line.

No other off–diagonal pairs occur: by Proposition 3, if $\{u, v\}$ is an edge with $o(u) \le o(v)$, then $o(v) - o(u) \in \{0, 1\}$, hence degree differences can only connect consecutive occupancy classes. Collecting all contributions produces the asserted decomposition. □

Proposition 11 (Edge count recovered)**.** *Summing all coefficients of $M(H_p^n; x, y)$ at $x = y = 1$ yields*

$$\sum_{\lambda \le \lambda'} m_{\lambda,\lambda'}(H_p^n) \;=\; |E(H_p^n)|,$$

and the right–hand side simplifies to the closed forms of Theorem 3 (equations (27) *and* (28)*).*

Proof. Directly from the definition of $m_{\lambda,\lambda'}$ and the partition of the edge set by Propositions 4 and 4; evaluating M at $(1,1)$ counts each edge exactly once. □

Remark 2 (Closed forms in Stirling numbers)**.** *Using Proposition 1 we may rewrite $O_n^p(\nu \mid \mu)$ as*

$$O_n^p(\nu \mid \mu) \;=\; \binom{n}{\nu} \left\{ {n-\nu \atop \mu-\nu} \right\}_{\ge 2} p^{\underline{\mu}}, \qquad p^{\underline{\mu}} = p(p-1)\cdots(p-\mu+1),$$

so Theorem 6 becomes a fully explicit expression in terms of (associated) Stirling numbers and falling factorials. In particular,

$$O_n^p(\mu) = \sum_{\nu=0}^{\mu} O_n^p(\nu \mid \mu) = \left\{ {n \atop \mu} \right\} p^{\underline{\mu}},$$

and the identity $\sum_{\mu=1}^{r} O_n^p(\mu) = p^n$ recovers Lemma 4.

Remark 3 (Adjacency constraint)**.** *By Proposition 3 and Corollary 3, edges only connect equal occupancies ($\mu \to \mu$) or* adjacent *occupancies ($\mu \to \mu+1$). Therefore, in $M(H_p^n; x, y)$ only diagonal terms $x^{\lambda_\mu} y^{\lambda_\mu}$ and consecutive off–diagonal terms $x^{\lambda_\mu} y^{\lambda_{\mu+1}}$ appear (with $i \le j$), exactly as enforced in Theorem 6.*

Worked examples and index extraction

We illustrate Theorem 6 with two concrete instances: the classical three–peg, three–disc graph H_3^3, and the four–peg, two–disc graph H_4^2. In each case we (i) compute the occupancy enumerators $O_n^p(\nu \mid \mu)$, (ii) assemble the edge counts by the (c_1)–(c_3) decomposition of Theorem 4, and (iii) synthesize $M(H_p^n; x, y)$. Finally we verify by extracting M_1 and M_2 via the operator table.

Example 1: H_3^3. Here $p = 3$, $n = 3$, $r = \min\{n, p\} = 3$; the realized degrees are

$$\lambda_1 = f_{3,3}(1) = 2, \qquad \lambda_2 = f_{3,3}(2) = 3, \qquad \lambda_3 = f_{3,3}(3) = 3 = \Delta,$$

so $\Gamma_3^3 = \{2, 3\}$ and the top degree is $\Delta = 3$ (with a collision at $\mu = 2, 3$).

Occupancy counts. Using Proposition 2,

$$O_3^3(\nu \mid \mu) = \binom{3}{\nu} \left\{ {3-\nu \atop \mu-\nu} \right\}_{\ge 2} (3)_\mu, \qquad (3)_1 = 3,\ (3)_2 = 6,\ (3)_3 = 6.$$

A direct check gives

$\mu \backslash \nu$	0	1	2, 3
1	3	0	0
2	0	18	0
3	0	0	6

$$\Longrightarrow \qquad O_3^3(1) = 3,\ O_3^3(2) = 18,\ O_3^3(3) = 6,$$

and $O_3^3(1) + O_3^3(2) + O_3^3(3) = 27 = 3^3$.

Edges between occupancy classes. By (c_3), edges from μ to $\mu+1$ are counted (with orientation) by $(\mu-\nu)(p-\mu)$ from a state of type $(\nu \mid \mu)$; for undirected edges and fixed μ this is a *single* count (no symmetry division because $\mu \neq \mu+1$).

• Between $\mu = 1$ (all three discs on one peg: $\nu = 0$) and $\mu = 2$: each such state contributes $(\mu-\nu)(p-\mu) = 1 \cdot 2 = 2$ edges; there are $O_3^3(0 \mid 1) = 3$ such states, hence

$$|E(\mu = 1 \leftrightarrow \mu = 2)| \;=\; 3 \cdot 2 \;=\; 6.$$

These are edges of *degree pair* $(2, 3)$, thus they contribute to $m_{2,3}$.

• Between $\mu = 2$ (necessarily $\nu = 1$) and $\mu = 3$ (necessarily $\nu = 3$): each $\mu = 2$ state contributes $(\mu-\nu)(p-\mu) = 1 \cdot 1 = 1$; there are $O_3^3(1 \mid 2) = 18$ such states, hence

$$|E(\mu = 2 \leftrightarrow \mu = 3)| \;=\; 18.$$

Here *both* endpoints have degree 3 (since $\lambda_2 = \lambda_3 = 3$), so these edges contribute to $m_{3,3}$.

Edges within occupancy classes. For $\mu = 1$ there are no within-class edges (only one occupied peg, so any legal move increases μ). For $\mu = 3$ there are again no within-class edges: from a state with three singletons, any legal move decreases the number of occupied pegs. Thus the only within-class contribution is for $\mu = 2$.

At $\mu = 2$ we necessarily have $\nu = 1$ (one singleton, one multiton). Edges that keep $\mu = 2$ are of types (c_1) SP→EP and (c_2) MP→OP. The (c_1) contribution depends only on $(\nu \mid \mu)$, but (c_2) depends on the top-disc size ordering at both pegs and is not directly multiplicative in (ν, μ). Instead of a delicate direct count, we now *balance* using the total edge count. Indeed,

$$|E(H_3^3)| \;=\; \frac{1}{2}\sum_{s \in V} \deg(s) = \frac{1}{2}\big(O_3^3(1) \cdot 2 + (O_3^3(2) + O_3^3(3)) \cdot 3\big) = \frac{1}{2}(3 \cdot 2 + 24 \cdot 3) = 39.$$

Subtracting the already-counted cross–class edges (6 between $\mu = 1, 2$ and 18 between $\mu = 2, 3$) leaves

$$|E(\text{within } \mu = 2)| \;=\; 39 - (6 + 18) = 15,$$

and these are all of degree pair $(3, 3)$.

M-polynomial. Collecting all contributions,

$$m_{2,2} = 0, \qquad m_{2,3} = 6, \qquad m_{3,3} = 18 + 15 = 33,$$

and therefore

$$M(H_3^3; x, y) \;=\; 6\,x^2y^3 \;+\; 33\,x^3y^3.$$

Checks via indices. Applying the operators at $(x, y) = (1, 1)$:

$$M_1(H_3^3) = (D_x + D_y)M\big|_{1,1} = 6(2+3) + 33(3+3) = 30 + 198 = 228.$$

This equals $\sum_{v \in V} \deg(v)^2 = 3 \cdot 2^2 + 24 \cdot 3^2 = 12 + 216 = 228$. Also

$$M_2(H_3^3) = (D_xD_y)M\big|_{1,1} = 6(2 \cdot 3) + 33(3 \cdot 3) = 36 + 297 = 333.$$

Finally, $M(1, 1) = 6 + 33 = 39 = |E(H_3^3)|$.

Example 2: H_4^2**.** Here $p=4$, $n=2$, $r=2$; realized degrees are

$$\lambda_1 = f_{4,2}(1) = 3, \qquad \lambda_2 = f_{4,2}(2) = 5,$$

so $\Gamma_4^2 = \{3,5\}$.

Occupancy counts. Using $O_2^4(\nu \mid \mu) = \binom{2}{\nu} \left\{ \begin{matrix} 2-\nu \\ \mu-\nu \end{matrix} \right\}_{\geq 2} (4)_\mu$ with $(4)_1 = 4$, $(4)_2 = 12$, we obtain

$$O_2^4(0 \mid 1) = 4, \quad O_2^4(1 \mid 1) = 0, \qquad O_2^4(2 \mid 2) = 12, \quad O_2^4(0 \mid 2) = O_2^4(1 \mid 2) = 0,$$

hence $O_2^4(1) = 4$, $O_2^4(2) = 12$, and $4 + 12 = 16 = 4^2$.

Edges between classes. By (c_3), from $\mu = 1$ ($\nu = 0$) to $\mu = 2$: each state contributes $(\mu-\nu)(p-\mu) = 1 \cdot 3 = 3$ moves; there are 4 such states, hence

$$|E(\mu = 1 \leftrightarrow \mu = 2)| \;=\; 4 \cdot 3 \;=\; 12.$$

These have degree pair $(3,5)$ and contribute to $m_{3,5}$.

Edges within classes. Within $\mu = 1$ there are none (any move increases occupancy). Within $\mu = 2$ we are in the case $\nu = 2$ (two singletons). The only moves that keep $\mu = 2$ are of type (c_1) SP$\to$EP (since (c_2) needs a multiton, which is absent). Each $\nu = 2$ state has $\nu(p-\mu) = 2 \cdot 2 = 4$ such moves; dividing by 2 to remove symmetry yields 2 undirected edges per state, hence

$$|E(\mu = 2 \text{ within})| \;=\; 12 \cdot 2 \;=\; 24,$$

all with degree pair $(5,5)$.

Total and M-polynomial. The total number of edges is

$$|E(H_4^2)| = \frac{1}{2}\big(O_2^4(1) \cdot 3 + O_2^4(2) \cdot 5\big) = \frac{1}{2}(4 \cdot 3 + 12 \cdot 5) = 36,$$

in agreement with $12 + 24 = 36$ counted above. Therefore

$$M(H_4^2; x, y) \;=\; 12\, x^3 y^5 \;+\; 24\, x^5 y^5.$$

Checks via indices.

$$M_1(H_4^2) = 12(3+5) + 24(5+5) = 96 + 240 = 336 = \sum_v \deg(v)^2 = 4 \cdot 3^2 + 12 \cdot 5^2 = 36 + 300 = 336,$$

$$M_2(H_4^2) = 12(3 \cdot 5) + 24(5 \cdot 5) = 180 + 600 = 780, \qquad M(1,1) = 12 + 24 = 36 = |E(H_4^2)|.$$

Remark 4 (How to automate larger instances)**.** *For general (p,n), Theorem 6 reduces the computation of $M(H_p^n; x, y)$ to:*

1. *tabulate $O_n^p(\nu \mid \mu)$ for $1 \leq \mu \leq r = \min\{n,p\}$ and $0 \leq \nu \leq \mu$ using $O_n^p(\nu \mid \mu) = \binom{n}{\nu} \left\{ \begin{matrix} n-\nu \\ \mu-\nu \end{matrix} \right\}_{\geq 2} p^{\underline{\mu}}$,*
2. *evaluate the coefficient sums in Theorem 6 for $m_{\lambda_\mu,\lambda_\mu}$ and $m_{\lambda_{\mu-1},\lambda_\mu}$,*

3. *assemble M and, if desired, apply the differential/integral operators of Table 1 to extract the indices in closed form.*

This workflow is quasi–linear in n for fixed p assuming precomputed associated Stirling numbers.

This scheme is illustrated through the three sequential Tables 3, 4, and 5. Table 5 presents the coefficients of $M(H_4^n; x, y)$ for $n = 1, \ldots, 8$, which are computed from the values of $O_4^n(\nu \mid \mu)$ shown in Table 4. These values, in turn, are obtained using the associated Stirling numbers provided in Table 3.

$j \backslash i$	0	1	2	3	4	5	6	7	8
0	1	0	0	0	0	0	0	0	0
1	0	0	1	1	1	1	1	1	1
2	0	0	0	0	3	10	25	52	105
3	0	0	0	0	0	0	15	70	280
4	0	0	0	0	0	0	0	0	105

Table 3: Associated Stirling numbers of the second kind $\left\{ {i \atop j} \right\}_{\geq 2}$ used in the computation of $O_4^n(\nu \mid \mu)$ for $n \leq 8$, with $i = n - \nu$ and $j = \mu - \nu$.

(μ, ν)	$n = 1$	2	3	4	5	6	7	8
(1,0)	0	4	4	4	4	4	4	4
(1,1)	4	0	0	0	0	0	0	0
(2,0)	0	0	0	36	120	300	672	1428
(2,1)	0	0	36	48	60	72	84	96
(2,2)	0	12	0	0	0	0	0	0
(3,0)	0	0	0	0	0	360	2520	11760
(3,1)	0	0	0	0	360	1440	4200	10752
(3,2)	0	0	0	144	240	360	504	672
(3,3)	0	0	24	0	0	0	0	0
(4,0)	0	0	0	0	0	0	0	2520
(4,1)	0	0	0	0	0	0	2520	20160
(4,2)	0	0	0	0	0	1080	5040	16800
(4,3)	0	0	0	0	240	480	840	1344
(4,4)	0	0	0	24	0	0	0	0

Table 4: Values of $O_4^n(\nu \mid \mu)$ for $1 \leq n \leq 8$.

n	$m_{3,3}$	$m_{3,5}$	$m_{5,5}$	$m_{5,6}$	$m_{6,6}$	$\lvert E(H_4^n)\rvert$
1	6	0	0	0	0	6
2	0	12	24	0	0	36
3	0	12	48	72	36	168
4	0	12	84	240	384	720
5	0	12	144	600	2220	2976
6	0	12	252	1344	10488	12096
7	0	12	456	2856	45444	48768
8	0	12	852	5904	189072	195840

Table 5: $M(H_4^n; x, y)$ coefficients for $n = 1, \ldots, 8$ (only $i \leq j$ pairs).

Numerical validation

In this section we validate the explicit formulation of the M-polynomial in Theorem 6 and the operator–based extraction of degree–based indices summarized in Table 1. For each family H_p^n with $p \in \{3, 4, 5\}$ and $n = 1, \ldots, 8$, we proceed as follows:

1. We *enumerate all regular states* (assignments of n discs to p pegs), compute the *top disc* on each peg, and generate *all legal moves* (top disc to an empty peg or onto a larger top disc).
2. From the generated adjacency, we compute vertex degrees and the set of unordered edges. We then tabulate the *edge multiplicities by degree pairs* $m_{i,j}(H_p^n)$ for $i \leq j$.
3. We compute the M-polynomial and evaluate the corresponding invariants $M(1,1)$, M_1, M_2, MM_2, SSD, H, ISI, A, and F as reported in Table 1. The value $M(1,1)$ is compared with the exact number of edges $E(H_p^n)$ to ensure consistency. We then compare all evaluated invariants with the exact results obtained using an algorithm that performs a complete enumeration of the graph and extracts the desired quantities.

For each family we list $|E|$, M_1, M_2, MM_2, SSD, H, ISI, A, and F, computed directly from the edge degree–pair counts $m_{i,j}$:

- H_3^n has degree spectrum $\{2, 3\}$; all indices reduce to combinations of $m_{2,2}, m_{2,3}, m_{3,3}$.
- H_4^n has degree spectrum $\{3, 5, 6\}$; the nonzero $m_{i,j}$ appear only for

$$(i, j) \in \{(3, 3), (3, 5), (5, 5), (5, 6), (6, 6)\}.$$

- H_5^n (with degree spectrum $\{4, 7, 9, 10\}$) is included to illustrate the generality of the pipeline and to stress the scalability of the operator extraction once $m_{i,j}$ are known.

Tables 6, 7, and 8 present the computational results.

We also implement computations for fixed values of n while varying p. Thus, to complement our vertical exploration (fixed p and increasing n), we fix $n \in \{1, 2, 3\}$ and vary $p = 1, \ldots, 8$. Tables 9, 10, and 11 report the nine degree-based indices for H_p^n in this regime and confirm consistency with Theorem 6 and Table 1.

n	$\lvert E\rvert$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	3	12	12	0.75	6.00	1.50	3.00	24.00	24
2	12	66	90	1.67	25.00	4.40	16.20	116.34	186
3	39	228	333	4.67	79.00	13.40	56.70	423.89	672
4	120	714	1062	13.67	241.00	40.40	178.20	1346.53	2130
5	363	2172	3249	40.67	727.00	121.40	542.70	4114.45	6504
6	1092	6546	9810	121.67	2185.00	364.40	1636.20	12418.22	19626
7	3279	19668	29493	364.67	6559.00	1093.40	4916.70	37329.52	58992
8	9840	59034	88542	1093.67	19681.00	3280.40	14758.20	112063.41	177090

Table 6: Degree-based indices for H_3^n, $n = 1, \ldots, 8$.

n	$\lvert E\rvert$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	6	36	54	0.67	12.00	2.00	9.00	68.34	108
2	36	336	780	1.76	75.20	7.80	82.50	919.92	1608
3	168	1800	4836	6.12	341.60	31.69	446.86	5998.63	9792
4	720	8184	23304	22.83	1451.20	127.44	2039.05	29555.77	46896
5	2976	34776	101700	88.23	5975.20	510.89	8678.86	130380.57	204048
6	12096	143256	424368	347.01	24240.00	2045.76	35781.95	546983.84	850128
7	48768	581400	1733244	1376.57	97634.40	8187.47	145283.59	2240116.56	3469392
8	195840	2342424	7005192	5483.68	391880.00	32758.85	585470.32	9066198.38	14016336

Table 7: Degree-based indices for H_4^n, $n = 1, \ldots, 8$.

n	$\lvert E\rvert$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	10	80	160	0.63	20.00	2.50	20.00	189.63	320
2	80	1060	3500	1.94	166.43	12.21	260.91	4687.28	7180
3	490	7880	31870	8.04	997.86	61.85	1954.66	47848.32	64640
4	2720	48100	213740	36.16	5492.52	310.81	11973.94	340076.03	430780
5	14410	268280	1252870	170.22	28975.00	1557.83	66909.00	2056518.36	2516720
6	74480	1427860	6857180	821.77	149419.76	7799.23	356466.70	11456712.90	13749580
7	379690	7404680	36143590	4025.16	760754.43	39023.97	1849636.50	61017378.45	72398240
8	1920320	37831300	186448940	19882.77	3844775.57	195198.92	9453118.41	316716078.91	373244380

Table 8: Degree-based indices for H_5^n, $n = 1, \ldots, 8$.

Remark 5 (Analytic notes on thresholds and degree spectra (fixed n, varying p).). *Let $r = \min\{n,p\}$ and recall that the vertex degree depends only on occupancy μ via*

$$\deg(s) = f_{p,n}(\mu) = \binom{p}{2} - \binom{p-\mu}{2}, \qquad \mu \in [r].$$

Hence the set of realized degrees is

$$\Gamma_p^n = \{\, f_{p,n}(1), f_{p,n}(2), \ldots, f_{p,n}(r) \,\},$$

with the top-degree collision *when $r = p$: $f_{p,n}(p-1) = f_{p,n}(p) = \Delta(H_p^n)$.*

- *Threshold $p = 1$: No legal move is ever possible (only one peg), hence $E(H_1^n) = 0$ for all n and all degrees are* 0*.*
- *Threshold $p = 2$: There are always moves (top disc can shuttle between the two pegs), and*

  $$\Gamma_2^n = \{\,1\,\} \quad (\textit{since } r = \min\{n,2\} \geq 1,\ f_{2,n}(1) = 1,\ f_{2,n}(2) = 1).$$

  Thus H_2^n is 1–regular (a union of cycles/paths depending on n), and every edge contributes the same degree pair $(1,1)$. Consequently, all degree–based indices reduce to simple multiples of $|E|$.
- *First nontrivial heterogeneity $p = 3$: Degrees split into $\Gamma_3^n = \{2,3\}$ for all $n \geq 2$ (and $\{2\}$ if $n = 1$). Only the pairs $(2,2)$, $(2,3)$, $(3,3)$ may occur. This is precisely what our H_3^n tables show.*
- *Rich spectra for $p \geq 4$: The realized degrees are*

  $$\Gamma_p^n = \{\,p{-}1,\ 2p{-}3,\ 3p{-}6,\ \ldots,\ \Delta(H_p^n)\,\}, \qquad \Delta(H_p^n) = \binom{p}{2} - 1 \ \ (r = p),\ \ \textit{or}\ \ \binom{p}{2} - \binom{p-r}{2}.$$

  For example:

  $$\begin{aligned} p = 4:&\quad \Gamma_4^n = \{\,3,5,6\,\}, \\ p = 5:&\quad \Gamma_5^n = \{\,4,7,9,10\,\}, \\ p = 6:&\quad \Gamma_6^n = \{\,5,9,12,14,15\,\}, \end{aligned}$$

  with the last two values equal when $r = p$ (collision at $\mu = p-1, p$). This matches the growth and diversity visible in the H_4^n and H_5^n tables.

p	$\lvert E\rvert$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	0	0	0	0.00	0.00	0.00	0.00	0.00	0
2	1	2	1	1.00	2.00	1.00	0.50	0.00	2
3	3	12	12	0.75	6.00	1.50	3.00	24.00	24
4	6	36	54	0.67	12.00	2.00	9.00	68.34	108
5	10	80	160	0.63	20.00	2.50	20.00	189.63	320
6	15	150	375	0.60	30.00	3.00	37.50	457.76	750
7	21	252	756	0.58	42.00	3.50	63.00	979.78	1512
8	28	392	1372	0.57	56.00	4.00	98.00	1906.35	2744

Table 9: Degree-based indices for H_p^1, $p = 1, \ldots, 8$.

p	$\|E\|$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	0	0	0	0.00	0.00	0.00	0.00	0.00	0
2	2	4	2	2.00	4.00	2.00	1.00	0.00	4
3	12	66	90	1.67	25.00	4.40	16.20	116.34	186
4	36	336	780	1.76	75.20	7.80	82.50	919.92	1608
5	80	1060	3500	1.94	166.43	12.21	260.91	4687.28	7180
6	150	2580	11070	2.15	310.67	17.62	636.43	17151.59	22620
7	252	5334	28182	2.37	519.91	24.03	1318.06	50081.20	57414
8	392	9856	61880	2.60	806.15	31.45	2438.80	124554.21	125776

Table 10: Degree-based indices for H_p^2, $p = 1, \ldots, 8$.

p	$\|E\|$	M_1	M_2	MM_2	SSD	H	ISI	A	F
1	0	0	0	0.00	0.00	0.00	0.00	0.00	0
2	4	8	4	4.00	8.00	4.00	2.00	0.00	8
3	39	228	333	4.67	79.00	13.40	56.70	423.89	672
4	168	1800	4836	6.12	341.60	31.69	446.86	5998.63	9792
5	490	7880	31870	8.04	997.86	61.85	1954.66	47848.32	64640
6	1140	24720	135000	10.34	2320.67	106.90	6132.86	246376.18	273720
7	2289	62748	433419	13.00	4655.00	169.86	15574.64	941151.50	877968
8	4144	137648	1152088	16.01	8417.85	253.71	34183.57	2913039.64	2331392

Table 11: Degree-based indices for H_p^3, $p = 1, \ldots, 8$.

Connections to Known Integer Sequences (OEIS)

Table 12 summarizes several striking correspondences between degree-based topological indices of the Hanoi graphs studied in this work and well–known sequences from the On-Line Encyclopedia of Integer Sequences (OEIS) [21]. For each index and each family of graphs, we list the first eight values computed via the M-polynomial formulas established in this paper, together with the OEIS entry that seems to match the sequence. The column *Ment.* ("mentioned") indicates whether the corresponding OEIS page explicitly refers to the same graph invariant.

All correspondences were checked for the first 30 terms and appear to hold consistently. Of course, a rigorous mathematical identification requires proving that the closed-form expressions of the corresponding indices are *exactly* equal to the OEIS formulas. Establishing such identities may constitute an interesting direction for future research.

Remark 6. *The first value listed in OEIS entry* `A277105` *is incorrect: the page reports* `A277105`$(1) = 9$, *whereas the correct value is* $MM_2(H_3^1) = 12$, *as confirmed in Tables 6 and 12. This discrepancy can be easily verified by direct computation.*

k	1	2	3	4	5	6	7	8	OEIS	Condition	Ment.
$M_1(H_3^k)$	12	66	228	714	2172	6546	19668	59034	A277104(k)		yes
$M_2(H_3^k)$	12	90	333	1062	3249	9810	29493	88542	A277105(k)	$k \geq 2$	yes
$\lfloor MM_2(H_3^k) \rfloor$	0	1	4	13	40	121	364	1093	A003462($k-1$)		no
$SSD(H_3^k)$	6	25	79	241	727	2185	6559	19681	A058481($k+1$)	$k \geq 2$	no
$\lfloor H(H_3^k) \rfloor$	1	4	13	40	121	364	1093	3280	A003462(k)		no
$M_1(H_k^1)$	0	2	12	36	80	150	252	392	A011379($k-1$)		yes
$M_2(H_k^1)$	0	1	12	54	160	375	756	1372	A019582(k)		yes
$SSD(H_k^1)$	0	2	6	12	20	30	42	56	A002378($k-1$)		no
$F(H_k^1)$	0	2	24	108	320	750	1512	2744	A179824(k)	$k \geq 2$	no
$\lfloor MM_2(H_k^3) \rfloor$	0	4	4	6	8	10	13	16	A008748($k+1$)	$k \geq 3$	no
$\lceil MM_2(H_k^3) \rceil$	0	4	5	7	9	11	14	17	A008750($k+2$)	$k \geq 2$	no

Table 12: Correspondences between degree-based topological indices of H_p^n and known integer sequences in OEIS. For each index, we list its first eight values, the associated OEIS entry (if any), the range of validity (when applicable), and whether the index is explicitly mentioned on the OEIS page.

6 Conclusion

In this work, we derived the first complete and explicit formulation of the M-polynomial of the generalized Hanoi graphs H_p^n, a natural yet previously unexplored family of graphs arising from the Tower of Hanoi problem with an arbitrary number of pegs p and discs n. Our contribution intersects combinatorial enumeration, algebraic graph theory, and the theory of degree-based topological indices, significantly expanding the applicability of the M-polynomial framework introduced by Deutsch and Klavžar [8].

The central achievement of this paper is a detailed combinatorial decomposition of the edge set of H_p^n based on occupancy transitions, distinguishing moves between singleton, multiton, empty, and occupied pegs. This structural analysis yields fully explicit formulas for all coefficients of the M-polynomial. Remarkably, the entire polynomial can be expressed using only falling factorials and (associated) Stirling numbers of the second kind, ensuring computational tractability for arbitrary p and n.

Our approach simultaneously characterizes the degree structure of the generalized Hanoi graphs, the adjacency relations between degree classes, and the combinatorial constraints imposed by the Tower of Hanoi rules. These insights culminate in Theorem 6, which provides the first exact M-polynomial for H_p^n in full generality. Furthermore, substituting this expression into the differential identities of Table 1 yields closed formulas for all classical degree-based indices (Zagreb, Randić, harmonic, symmetric division, forgotten index, etc.). The correctness of these results has been validated through explicit enumeration for representative instances, confirming the structural predictions and functional extraction properties of our formulas.

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