



## Research Paper

## 2-RESTRICTED OPTIMAL PEBBLING NUMBER OF SOME DENDRIMERS

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## ABSTRACT

This paper studies the 2-restricted optimal pebbling number of certain dendrimer graphs. In graph pebbling, a configuration is a distribution of pebbles on the vertices of a simple connected graph  $G$ . A pebbling move removes two pebbles from a vertex and places one on an adjacent vertex. A  $t$ -restricted pebbling configuration ( $t$ RPC) is an initial placement where no vertex holds more than  $t$  pebbles. A configuration is solvable if, for any target vertex  $v$ , a sequence of pebbling moves can place at least one pebble on  $v$ . The  $t$ -restricted optimal pebbling number, denoted  $\pi_t^*(G)$ , is the minimum number of pebbles required for a solvable  $t$ RPC on  $G$ . We focus on the case  $t = 2$  and determine  $\pi_2^*(G)$  for several classes of dendrimers.

## 1. INTRODUCTION

Graph pebbling serves as a mathematical model for resource transportation in networks, sharing similarities with network flow, transportation, and supply chain problems. While network flow aims to maximize commodity delivery under capacity constraints, and transportation models minimize costs, graph pebbling focuses on satisfying demands with minimal initial inventory. A distinctive feature, introduced by Chung [8], is the movement constraint:

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transferring a unit of commodity across an edge consumes an additional unit, analogous to fuel consumption during transport or energy dissipation in physical systems.

Let  $G = (V, E)$  be a simple connected graph. We denote by  $V(G)$  and  $E(G)$  its vertex and edge sets, respectively. The distance between vertices  $u$  and  $v$  is  $d(u, v)$ , and  $u \sim v$  indicates adjacency. The neighborhood  $N(v) = \{u \mid u \sim v\}$  consists of vertices adjacent to  $v$ , and  $d(v) = |N(v)|$  is the degree of  $v$ . For a subgraph  $H \subseteq G$ ,  $d_H(v)$  denotes the degree of  $v$  in  $H$ .

A *pebbling configuration* is a function  $f : V \rightarrow \mathbb{N} \cup \{0\}$  assigning nonnegative integers (pebbles) to vertices. The *weight*  $w(f) = \sum_{v \in V} f(v)$  is the total number of pebbles. A *pebbling move* removes two pebbles from a vertex  $v$  and places one on an adjacent vertex  $u \in N(v)$ . A vertex  $v$  is a *root* or *target* if the objective is to place a pebble on it. A configuration is *solvable* if, for every vertex  $v$ , some sequence of pebbling moves can place a pebble on  $v$ .

The *pebbling number*  $\pi(G)$  is the smallest integer  $k$  such that every configuration with  $k$  pebbles is solvable. If  $t$  pebbles can be moved to  $v$ , then  $f$  is  *$t$ -fold  $v$ -solvable*, and if this holds for all  $v$ , then  $f$  is  *$t$ -solvable*. The  *$t$ -pebbling number*  $f_t(G)$  is the minimum number  $m$  such that every configuration of size  $m$  is  $t$ -solvable. For  $t = 1$ , we write  $f(G) = f_1(G)$ .

Chung [8] introduced graph pebbling, proving that the  $n$ -cube has pebbling number  $2^n$ , which yielded an alternative proof of a number-theoretic result of Lemke and Kleitman [15]. Pebbling models find applications in transportation and physical processes such as percolation, where liquid absorption corresponds to the pebble discarded in each move.

Computing  $\pi(G)$  is computationally challenging. Determining if a configuration is  $v$ -solvable is NP-complete [16, 17], and deciding whether  $\pi(G) < k$  is  $\Pi_2^P$ -complete [17]. Recent work has explored pebbling numbers for polymers [1].

The *optimal pebbling number*  $\pi^*(G)$ , defined by Pachter et al. [20], is the minimum weight of a solvable configuration. A configuration achieving this weight is a  $\pi^*$ -configuration. This variant has been extensively studied [6, 10, 11, 12, 13, 14, 18, 19, 21, 22], and computing  $\pi^*(G)$  is NP-complete [17].

We consider a generalization: a configuration  $f$  is a  *$t$ -restricted pebbling configuration* ( $t$ RPC) if  $f(v) \leq t$  for all  $v \in V$ . The  *$t$ -restricted optimal pebbling number*  $\pi_t^*(G)$  is the minimum weight of a solvable  $t$ RPC. This paper focuses on the 2-restricted case, investigating  $\pi_2^*(G)$  for dendrimers—highly branched, tree-like macromolecules significant in chemical applications.

## 2. 2-RESTRICTED OPTIMAL PEBBLING NUMBER OF SOME DENDRIMERS

Imagine a molecule that starts from a central point (core) and branches out radially and systematically, much like a tree or fractal structure. That's a dendrimer. Their structure consists of a core, a series of repeating units (monomers) connected in a branched manner, and surface groups.

Unlike linear or random polymers, dendrimers have a precisely defined and spherical (or pseudo-spherical) structure. These molecules are classified into different generations ( $G_0, G_1, G_2$ , etc.) based on the number of branching steps. Higher generations result in larger, more branched molecules with a higher density of surface groups. The numerous terminal groups on the dendrimer's surface allow for chemical modification and attachment

of other molecules, making dendrimers attractive for diverse applications. Dendrimers can have internal spaces (cavities) that can accommodate smaller molecules, enabling host-guest chemistry. Despite their large size, dendrimers exhibit lower viscosity compared to linear polymers of similar molecular weight, due to their spherical structure and lack of entangled chains. Dendrimers possess a uniform size, contributing to their well-defined properties. The high degree of branching distinguishes dendrimers from other polymeric materials. Some topological indices of some dendrimers have studied in [4, 5].

In this section we calculate 2-restricted optimal pebbling number of dendrimers. First we consider the dendrimer  $NS_2[n]$ . See dendrimer  $NS_2[3]$  that has grown 3 stages in Figure 1.

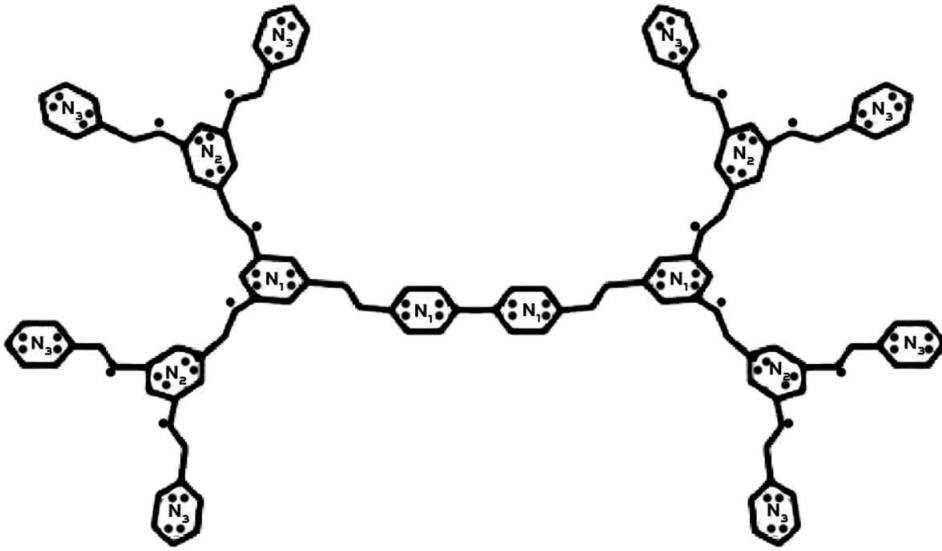


FIGURE 1. Distribution of pebbles in the dendrimer  $NS_2[n]$  that has grown 3 stages.

**Theorem 2.1.** For  $n \geq 1$ ,  $\pi_2^*(NS_2[n]) = 5 \times 2^{n+1} - 4$ .

*Proof.* As can be seen in Figure 1, initially there are 2 hexagons in the core connected by a path  $P_2$ , and the 2-restricted optimal pebbling number of each of these hexagons is 4. In the first stage of dendrimer growth, there are two hexagons whose sum of the 2-restricted optimal pebbling number is also equal to 16. From this stage onwards, each hexagon is divided into 2 hexagons by a path  $P_4$ , and this process can continue. The pebbles can be distributed in such a way that in each hexagon all vertices are accessible by 4 pebbles, and each path  $P_4$  between two hexagons can also be made accessible by placing one pebble on the second vertex. So if we assume  $\pi_2^*(NS_2[1]) = 16$  to be the stage before dividing the hexagons into two hexagons, when the 2-restricted optimal pebbling number is equal to 16, we can obtain the following sequence:

$$\pi_2^*(NS_2[n]) = \pi_2^*(NS_2[n-1]) + 5 \times 2^n, \quad n \geq 2.$$

By solving this recurrence relation, we have the result. □

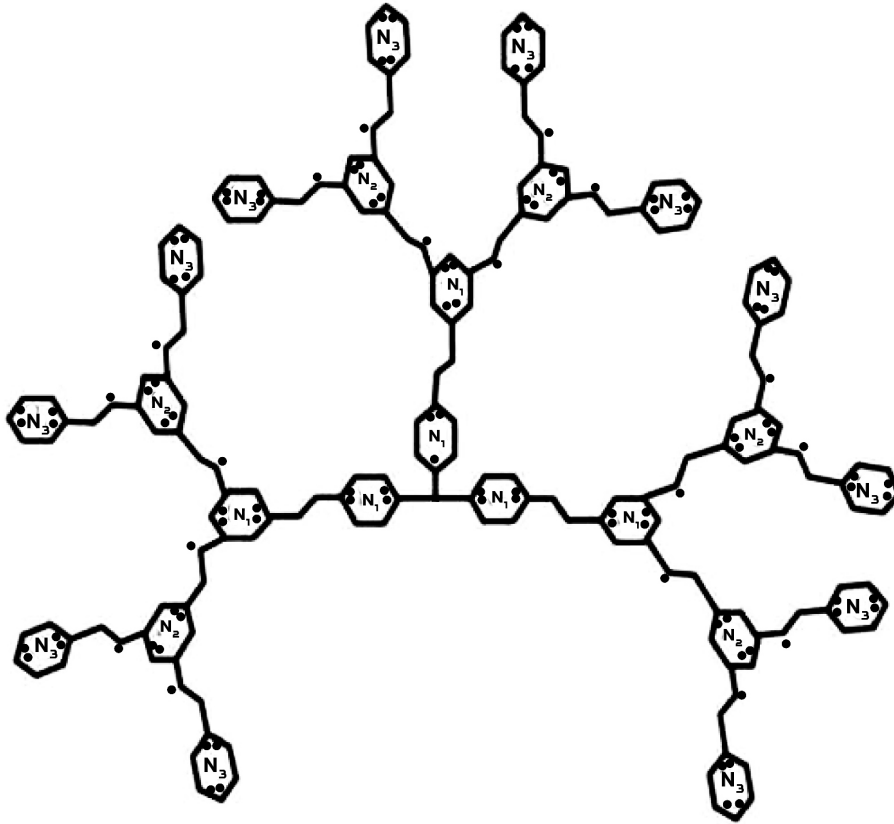


FIGURE 2. Distribution of pebbles in the dendrimer  $NS_1[n]$  that has grown 3 stages.

Now we consider the dendrimer  $NS_1[n]$ . See dendrimer  $NS_1[3]$  that has grown 3 stages in Figure 2.

**Theorem 2.2.** For  $n \geq 1$ ,  $\pi_2^*(NS_1[n]) = 15 \times 2^n - 7$ .

*Proof.* As we can see in Figure 2, there are 3 hexagons in the core, and in the first stage, each hexagon is connected to another hexagon by a path  $P_4$ , which is the 2-restricted optimal pebbling number of the core 11. By calculating the optimal pebble number of three hexagons connected to the core, we can say that in the first stage, the the 2-restricted optimal pebbling number is 23, and as is clear from the graph, in the next stage, each hexagon is divided into two hexagons by a path  $P_4$ , and this process can continue. So we have the following recurrence relation:

$$\pi_2^*(NS_1[n]) = \pi_2^*(NS_1[n - 1]) + 15 \times 2^{n-1}, \quad n \geq 2.$$

Therefore we have the result. □

Here, we consider the dendrimer of generation 1-3 denoted by  $D_{1,3}[n]$  (see dendrimer  $D_{1,3}[3]$  that has grown 3 stages in Figure 3), then

**Theorem 2.3.** For  $n \geq 1$ ,  $\pi_2^*(D_{1,3}[n]) = 21 \times 2^n - 10$ .

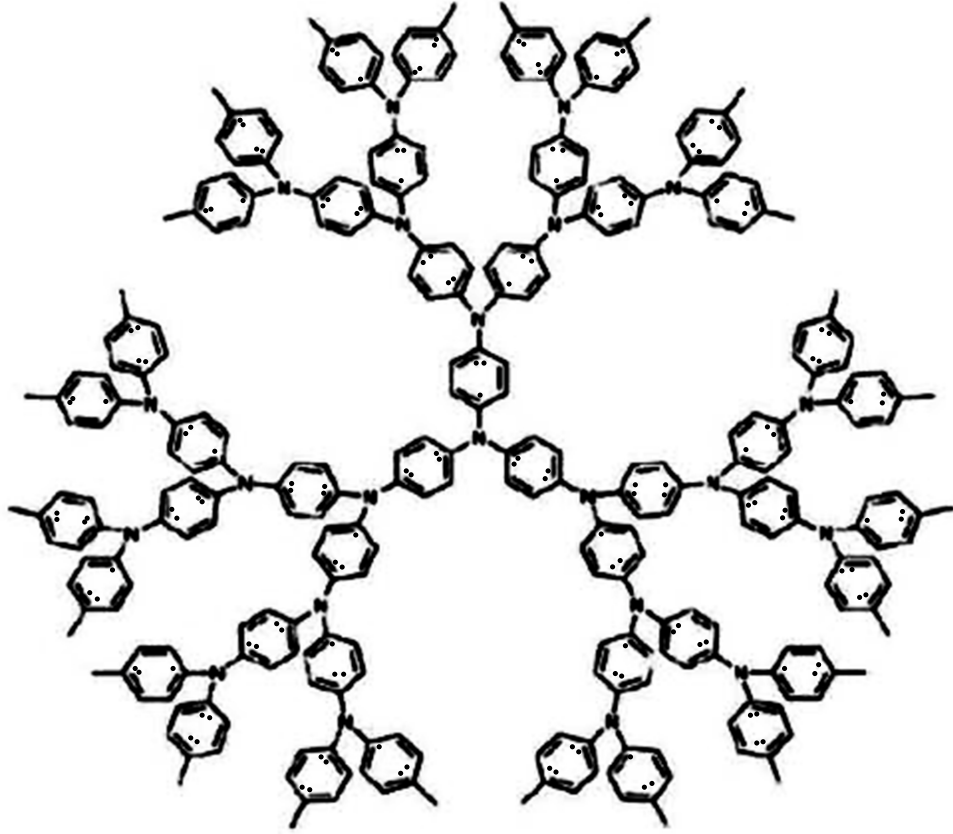


FIGURE 3. Distribution of pebbles in the first kind of dendrimer of generation 1 – 3,  $D_{1,3}[3]$  that has grown 3 stages.

*Proof.* As see in Figure 3 in the first step, the three hexagons can be optimized with 11 pebbles. This process, where each hexagon is transformed into two other hexagons, continues, and the 2-restricted optimization process can be continued. We have the following recurrence relation:

$$\pi_2^*(D_{1,3}[n]) = \pi_2^*(D_{1,3}[n-1]) + 21 \times 2^{n-1}, \quad n \geq 1.$$

Therefore we have the result.  $\square$

Here, we consider the dendrimer of generation 1-3 denoted by  $D_{1,2}[n]$  (see dendrimer  $D_{1,2}[4]$  that has grown 4 stages in Figure 4), then

**Theorem 2.4.** For  $n \geq 2$ ,

$$\pi_2^*(D_{1,2}[n]) = \begin{cases} 2\pi_2^*(D_{1,2}[n-1]) + 4, & \text{if } n \text{ is odd} \\ 2\pi_2^*(D_{1,2}[n-1]) - 4, & \text{if } n \text{ is even} \end{cases}$$

with the initial conditions  $\pi_2^*(D_{1,2}[0]) = 4$  and  $\pi_2^*(D_{1,2}[1]) = 16$ .

*Proof.* As see in Figure 4 the first hexagon can be optimally pebbled with four pebbles. Subsequently, this hexagon transforms into two other hexagons through two  $P_4$  paths. These two paths and the two hexagons can collectively be optimally pebbled with a total of 12

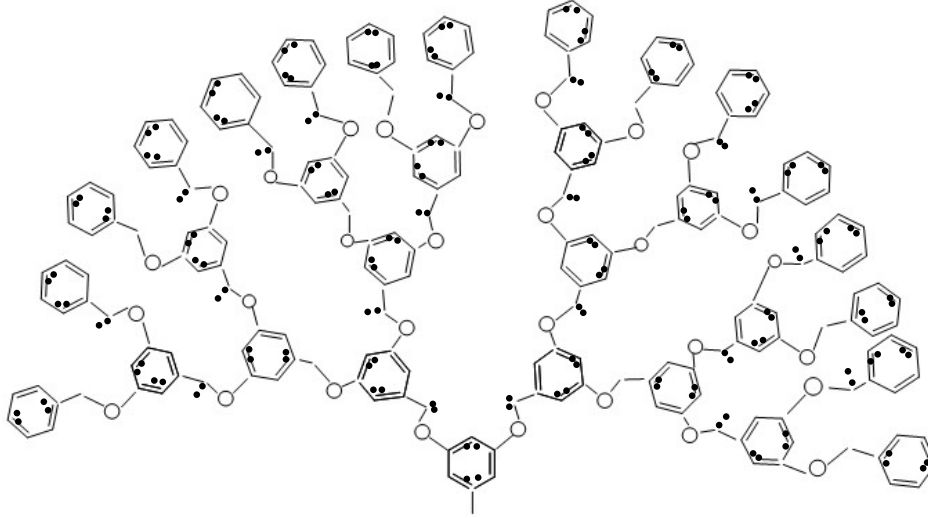


FIGURE 4. Distribution of pebbles in the first kind of dendrimer of generation 1-3,  $D_{1,2}[4]$  that has grown 4 stages.

pebbles. This process, where each hexagon transforms into two other hexagons via two paths, continues, and the optimization process can be extended. If  $t_0$  represents the 2-restricted optimal pebbling number of the first hexagon, which equals 4, and we consider the distribution of pebble increments at each stage, the number of pebbles at each even and odd stage can be obtained from the following relations:

$$\pi_2^*(D_{1,2}[n]) = \begin{cases} 2\pi_2^*(D_{1,2}[n-1]) + 4, & \text{if } n \text{ is odd} \\ 2\pi_2^*(D_{1,2}[n-1]) - 4, & \text{if } n \text{ is even} \end{cases}$$

with the initial condition:  $\pi_2^*(D_{1,2}[0]) = 4$  and  $\pi_2^*(D_{1,2}[1]) = 16$ . Therefore we have the result.  $\square$

Finally, we consider Polyphenylene dendrimer ( $PPD$ ) with  $n$  growth stages, where  $n \geq 0$ . The molecular structure of ( $PPD$ ) with 2 growth stages is shown in Figure 5.

**Theorem 2.5.** For  $n \geq 0$ ,  $\pi_2^*(PPD[n]) = 17 \times 2^{n+2} - 54$ .

*Proof.* In the first stage, which is the core and denoted by  $\pi_2^*(PPD[0])$ , there are four hexagons that are optimally pebbled with 14 pebbles. In the second stage, denoted as  $\pi_2^*(PPD[1])$ , each core hexagon connects to a graph with 5 hexagons. This graph, consisting of 5 hexagons, can be optimally pebbled with 17 pebbles. Therefore, in the second stage, the optimal pebble number is  $2^2 \times 17$ . In the third stage, two hexagons from each graph of the previous stage transform into two graphs, and in this stage, the 2-restricted optimal pebble number is  $2^3 \times 17$ . Similarly, this process continues. Thus, we have the following recursive relation:

$$\pi_2^*(PPD[n]) = \pi_2^*(PPD[n-1]) + 17 \times 2^{n+1}.$$

Therefore:

$$\pi_2^*(PPD[n]) = 17 \times 2^{n+2} - 54.$$

$\square$

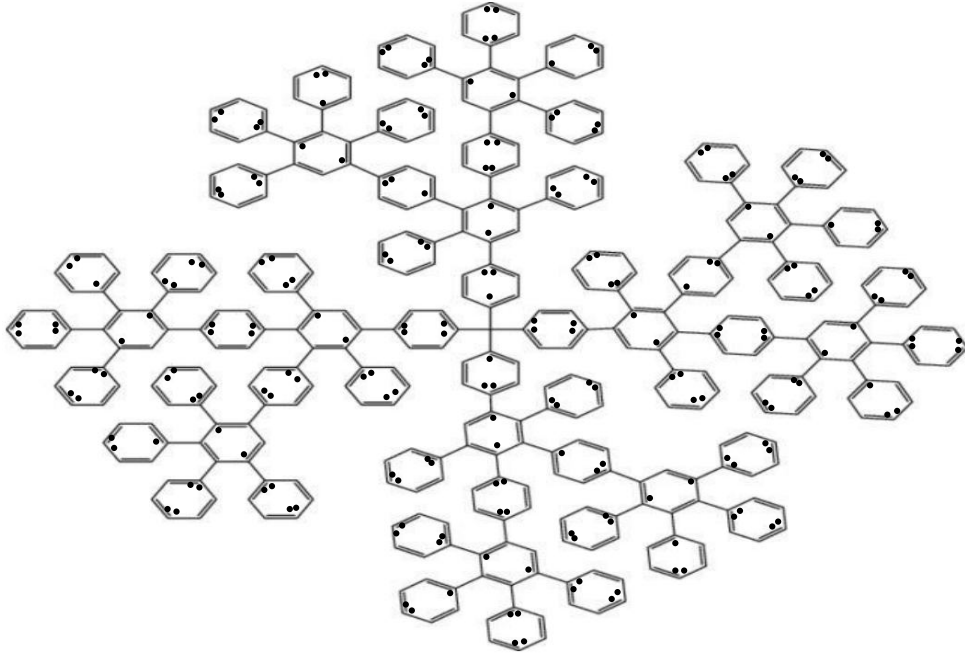


FIGURE 5. Distribution of pebbles in the Polyphenylene dendrimer of generations  $G_n$  with 2 growth stages.

### CONCLUSION

In this paper, we investigated the 2-restricted optimal pebbling number for several families of dendrimer graphs, including  $NS_2[n]$ ,  $NS_1[n]$ ,  $D_{1,3}[n]$ ,  $D_{1,2}[n]$ , and polyphenylene dendrimers  $PPD[n]$ . By analyzing the recursive structural growth patterns of these dendrimers, we established explicit formulas for  $\pi_2^*(G)$  in each case. Specifically, we proved that:

- $\pi_2^*(NS_2[n]) = 5 \times 2^{n+1} - 4$  for  $n \geq 1$ ;
- $\pi_2^*(NS_1[n]) = 15 \times 2^n - 7$  for  $n \geq 1$ ;
- $\pi_2^*(D_{1,3}[n]) = 21 \times 2^n - 10$  for  $n \geq 1$ ;
- $\pi_2^*(D_{1,2}[n])$  satisfies a recurrence relation with initial conditions  $\pi_2^*(D_{1,2}[0]) = 4$  and  $\pi_2^*(D_{1,2}[1]) = 16$ ;
- $\pi_2^*(PPD[n]) = 17 \times 2^{n+2} - 54$  for  $n \geq 0$ .

Our results demonstrate that the 2-restricted optimal pebbling number of these dendrimers grows exponentially with the number of generations, reflecting the self-similar, branching nature of dendrimeric structures. The recursive approach used here provides a systematic framework for analyzing pebbling problems on tree-like macromolecules and may be extended to other families of dendrimers or related hierarchical networks. Future work could explore the  $t$ -restricted optimal pebbling number for  $t \geq 3$  on these structures, or investigate the computational complexity of determining  $\pi_t^*(G)$  for dendrimer graphs.

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