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HOSOYA POLYNOMIAL OF CAYLEY GRAPHS OF D_{2n} AND Q_{2^n} WITH A FOCUS ON SPECIFIC GENERATING SETS

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Abstract. Cayley graphs are powerful tools for analyzing algebraic groups through their combinatorial and topological properties. In this paper, we investigate the Hosoya polynomial of Cayley graphs associated with the Dihedral group D_{2n} and the Generalized Quaternion group Q_{2^n}, considering specific generating subsets. General formulas for computing these polynomials are presented, and their connection with the Wiener index is examined. Our results show that both the Hosoya polynomial coefficients and the Wiener index exhibit exponential growth with group order, reflecting the increasing complexity of the graphs. This study contributes to the understanding of distance-based invariants in algebraic graph theory and provides a foundation for further exploration in network analysis.

1. Introduction

A graph $G = (V, E)$ is a mathematical structure consisting of a non-empty set of vertices and a set of edges, which are represented by $V(G)$ and $E(G)$, respectively. In any graph, vertices that are connected by an edge are called adjacent vertices. Edges can be directed or undirected, which accordingly classifies the graph as directed or undirected. A graph $G = (V, E)$ is called simple if it has no loops and each pair of vertices is connected by at most one edge. A graph G is connected if there is a path between any two vertices.

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In this study, the graphs considered are simple, undirected, and connected. The degree of a vertex u, denoted by $d(u)$, is the number of adjacent vertices to u, and the distance between two vertices is the length of the shortest path between them. The diameter of a graph, denoted by $\text{diam}(G)$, is the greatest distance between any two vertices in the graph.

Definition 1.1. Suppose G is a group with identity element 1 and S is a non-empty subset of G such that, $1 \notin S$. The Cayley graph of the group G associated with S, denoted by $\Gamma(G, S)$, is defined such that the set of vertices is the elements of the group G, and the set of edges is the set of ordered pairs (x, y) where $x^{-1}y \in S$. This means that for any vertex u in the graph, which is also an element of the group, $u \cdot s$ for each member of the set S is an adjacent vertex to u [3, 8, 14].

Remark 1.2. The Cayley graph of the group G associated with S, $\Gamma(G, S)$, has the following properties [3]:

a. $\Gamma(G, S)$ is a $|S|$-regular graph, meaning each vertex is connected to exactly $|S|$ adjacent vertices.

b. $\Gamma(G, S)$ is an undirected graph if and only if $S^{-1} = S$.

c. $\Gamma(G, S)$ is Loop-free: Given that $1 \notin S$, the Cayley graph is loop-free.

d. $\Gamma(G, S)$ is connected if and only if S is a generating set of the group G.

Let $G = (V, E)$ be a simple, connected graph, where V represents the set of vertices and E represents the set of edges. An automorphism h of G is a bijective function on V that preserves the edge structure of G; that is, if $e = uv$ is an edge of G, then $e^h = u^h v^h$ is also an edge of G. The collection of all automorphisms of G forms a group $\text{Aut}(G)$ under function composition. If, for any two arbitrary vertices u and v, there exists an automorphism $h \in \text{Aut}(G)$ such that $u^h = v$, the graph is said to be vertex-transitive. In this case, $\text{Aut}(G)$ acts transitively on V. This implies that the vertex set is acted upon transitively by the automorphism group. In particular, a Cayley graph $\Gamma = Cay(G, S)$, defined for a group G and a generating set S, possesses this property.

Lemma 1.3. *The Cayley graph of the group G associated with S, $\Gamma(G, S)$ is vertex-transitive.*

Proof. A key property of Cayley graphs is that left multiplication by elements of G induces a graph automorphism. Specifically, for any $g \in G$, the mapping

$$\phi_g : G \to G, \quad x \mapsto gx$$

preserves adjacency, as for any edge (x, y) in Γ, we have

$$(\phi_g(x))^{-1}(\phi_g(y)) = (gx)^{-1}(gy) = x^{-1}g^{-1}gy = x^{-1}y \in S.$$

For any two vertices $g_1, g_2 \in G$, there exists $g \in G$ such that $\phi_g(g_1) = g_2$. Thus, the automorphism group of Γ acts transitively on its vertex set, proving that every Cayley graph is vertex-transitive. □

A graph invariant is a numerical value that depends only on the abstract structure of the graph, not on specific representations such as labels or drawings. It remains constant under any automorphism of the graph. The topological index of a simple connected graph G is an example of such an invariant. When G represents a molecular graph, its topological indices are referred to as molecular structure descriptors, which are used to study the properties of chemical compounds. These indices remain invariant under graph isomorphisms and have a wide range of applications in fields such as social network analysis, bioinformatics, optimization of electronic systems, and various other scientific disciplines. Topological indices are categorized based on vertex degree, distance, dispersion, eccentricity, and adjacency matrix properties, [1, 2, 10, 11, 13].

One of the most famous topological descriptors of graphs is the Wiener index, which was first studied by a chemist named H. Wiener [6, 7, 16] as a descriptor of the molecular structure of chemical graphs and is defined as follows:

$$W(G) = \sum_{\{u,v\} \subseteq V} d(u, v)$$

Where $d(u, v)$ is the distance between vertices u and v. If the sum of distances between the vertex u with all other vertices of the graph G is denoted by $d(u)$ then we have:

$$W(G) = \frac{1}{2} \sum_{u \in V} d(u)$$

The Hosoya polynomial [12] was first introduced by Hosoya in 1988. It is defined based on the number of vertex pairs at different distances in a graph as follows:

$$H(G,x) = \sum_{k\geq 0} d(G,k)x^k \tag{1.1}$$

where $d(G,k)$ denotes the number of vertex pairs that are exactly k distance apart. The relationship between the Hosoya polynomial and the Wiener index [5, 9] is given by:

$$W(\Gamma) = \frac{\partial H}{\partial x} H(\Gamma,x)\Big|_{x=1}$$

2. **Hosoya Polynomial of the Cayley Graph of the Dihedral Group**

The dihedral group D_{2n} $(n \geq 2)$ represents the symmetries of a regular n-gon and has an order of $2n$. It is defined as follows:

$$D_{2n} = \langle a, b \mid a^2 = b^n = 1, (ab)^2 = 1\rangle.$$

We consider the subset S of the group D_{2n} as:

$$S = \{a, ab, b^{n-1}, b\}.$$

The set S generates the dihedral group D_{2n}, and since $S^{-1} = S$, the Cayley graph $\Gamma(D_{2n}, S)$ is undirected and connected. Also, $\Gamma(D_{2n}, S)$ is vertex-transitive (Lemma 1.3).

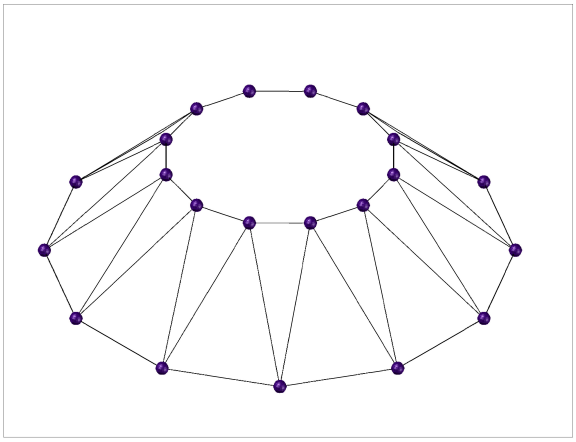


FIGURE 1. The Cayley graph $\Gamma(D_{2n}, S)$.

Proposition 2.1. *Let $\Gamma(D_{2n}, S)$ be the Cayley graph of the dihedral group D_{2n} with $n \geq 2$. Then the Hosoya polynomial of Γ is given by:*

$$H(\Gamma, x) = \begin{cases} \sum_{i=1}^{\frac{n}{2}-1} 4n \cdot x^i + 3n \cdot x^{\frac{n}{2}}, & \text{if } n = 2t,\ t \in \mathbb{N}, \\ \sum_{i=1}^{\frac{n-1}{2}} 4n \cdot x^i + n \cdot x^{\frac{n+1}{2}}, & \text{if } n = 2t+1,\ t \in \mathbb{N}. \end{cases}$$

where $\lfloor n/2 \rfloor$ denotes the greatest integer less than or equal to $n/2$.

Proof. Based on Equation 1.1, the Hosoya polynomial of the Cayley graph $\Gamma(D_{2n}, S)$ is expressed as:

$$H(\Gamma, x) = \sum_{k \geq 0} d(\Gamma, k) x^k.$$

Here, the coefficients $d(\Gamma, k)$ represent the number of vertex pairs in Γ that are exactly k distance apart. The diameter of Γ, denoted as $\mathrm{diam}(\Gamma)$, is the largest shortest path between any pair of vertices in the graph. Hence, the polynomial degree equals $\mathrm{diam}(\Gamma)$, and it can be rewritten as:

$$H(\Gamma, x) = \sum_{k=0}^{\mathrm{diam}(\Gamma)} d(\Gamma, k) x^k. \tag{2.1}$$

Let $V(\Gamma)$ denote the vertex set of the Cayley graph $\Gamma(D_{2n}, S)$. The graphs C_1 and C_2 are both n-cycles, whose vertex sets are denoted by $V(C_1)$ and $V(C_2)$, respectively (Figure 1).

Accordingly, the vertex set of Γ can be expressed as:

$$V(\Gamma) = V(C_1) \cup V(C_2).$$

In general, the set of all two-element subsets of $V(\Gamma)$ can be partitioned into the following categories:

$$V_1 = \{\{x, y\} \mid \{x, y\} \subset C_1\}, V_2 = \{\{x, y\} \mid \{x, y\} \subset C_2\}, V_3 = \{\{x, y\} \mid x \in C_1,\ y \in C_2\}.$$

Case 1: n is even.

In this case, considering the diameter of cycles with even length, we obtain:

$$\max\{d(x, y) \mid \{x, y\} \in V_1\} = \max\{d(x, y) \mid \{x, y\} \in V_2\} = \max\{d(x, y) \mid \{x, y\} \in V_3\} = \frac{n}{2}.$$

Thus, the diameter of the graph is given by:

$$\mathrm{diam}(\Gamma) = \max\{d(x, y) \mid \{x, y\} \in V_1 \cup V_2 \cup V_3\} = \frac{n}{2}.$$

The coefficient of the highest-degree term in the polynomial is calculated as follows:

$$d(\Gamma, diam(\Gamma)) = |\{\{x,y\} \in V_1 | d(x,y) = \frac{n}{2}\}| + |\{\{x,y\} \in V_2 | d(x,y) = \frac{n}{2}\}| + |\{\{x,y\} \in V_3 | d(x,y) = \frac{n}{2}\}|$$

$$= \frac{n}{2} + \frac{n}{2} + 2n = 3n.$$

Case 2: n is odd.

In this case, considering the diameter of cycles with odd length, we obtain:

$$\max\{d(x,y) \mid \{x,y\} \in V_1\} = \max\{d(x,y) \mid \{x,y\} \in V_2\} = \lfloor n/2 \rfloor = \frac{n-1}{2},$$

$$\max\{d(x,y) \mid \{x,y\} \in V_3\} = \lfloor n/2 \rfloor + 1 = \frac{n+1}{2}.$$

Thus, the diameter of the graph is given by:

$$\text{diam}(\Gamma) = \max\{d(x,y) \mid \{x,y\} \in V_1 \cup V_2 \cup V_3\} = \lfloor n/2 \rfloor + 1 = \frac{n+1}{2}.$$

The coefficient of the highest-degree term in the polynomial is computed as follows:

$$d(\Gamma, diam(\Gamma)) = |\{\{x,y\} \in V_1 | d(x,y) = \frac{n+1}{2}\}| +$$

$$|\{\{x,y\} \in V_2 | d(x,y) = \frac{n+1}{2}\}| + |\{\{x,y\} \in V_3 | d(x,y) = \frac{n+1}{2}\}|$$

$$= 0 + 0 + n = n.$$

Therefore, the degree of the polynomial in the cases where n is even or odd is given by $\frac{n}{2}$ and $\frac{n+1}{2}$, respectively. Additionally, the coefficient of the highest-degree term in the polynomial for even and odd n is $3n$ and n, respectively. On the other hand, since $1 \notin S$, the Cayley graph Γ is a simple graph, meaning it has no loops, implying that $d(\Gamma, 0) = 0$. Hence, the constant term in the polynomial is zero. Furthermore, since $d(\Gamma, 1)$ represents the number of vertex pairs at a distance of one, it is exactly equal to the number of edges in the graph:

$$d(\Gamma, 1) = |E(C_1)| + |E(C_2)| + 2|E(C_1)| = n + n + 2n = 4n.$$

Thus, the coefficient of x in the polynomial is $4n$. For each value of k, $1 \leq k < \text{diam}(\Gamma)$, we have:

$$|\{\{x,y\} \in V_1 \mid d(x,y) = k\}| = |\{\{x,y\} \in V_2 \mid d(x,y) = k\}| = n,$$

$$|\{\{x,y\} \in V_3 \mid d(x,y) = k\}| = 2n.$$

Thus, for values of k where $1 \leq k < \text{diam}(\Gamma)$, it follows that:

$$d(\Gamma, k) = n + n + 2n = 4n.$$

Therefore, by Equation (2.1), the proof is complete. □

2.1. **Verification of the relationship between the Hosoya polynomial and the Wiener index for the Cayley graph $\Gamma(D_{2n}, S)$.**

Remark 2.2. If G is a connected simple graph, then:

$$W(G) = \frac{\partial H}{\partial x} H(G, x)\Big|_{x=1}.$$

Proof. The Hosoya polynomial of Cayley graph $\Gamma(D_{2n}, S)$ is defined as:

$$H(\Gamma, x) = \sum_{k \geq 0} d(\Gamma, k) \cdot x^k.$$

where $d(\Gamma, k)$ represents the count of vertex pairs in Γ that have an exact distance of k between them. It is clear that:

$$\frac{\partial H}{\partial x} H(\Gamma, x) = \sum_{k \geq 1} k \cdot d(\Gamma, k) \cdot x^{k-1}$$

and ,

$$W(\Gamma) = \frac{\partial H}{\partial x} H(\Gamma, x)\Big|_{x=1} = \sum_{k \geq 1} k \cdot d(\Gamma, k)$$

It is easily observed that this is another form of representing the Wiener index. □

Next, we examine the validity of the above relation numerically and pointwise. The general formula for the Wiener index of the Cayley graph $\Gamma(D_{2n}, S)$ has previously been determined in [14] using its vertex-transitivity property, [4] as follows:

$$W(\Gamma) = \frac{n^2(n+1)}{2}.$$

For both even and odd values of n. In Table 1, a comparison of the Hosoya polynomial and the Wiener index of the Cayley graph of the dihedral group is presented for values of n ranging from 2 to 10.

TABLE 1. Comparison of the Wiener index and the Hosoya polynomial for $\Gamma(D_{2n}, S)$

n	D_{2n}	$W(\Gamma)$	$H(\Gamma, x)$	$\frac{\partial H}{\partial x} H(\Gamma, x)$	$\frac{\partial H}{\partial x} H(\Gamma, x)\Big\|_{x=1}$
3	D_6	18	$12x + 3x^2$	12 + 6x	18
4	D_8	40	$16x + 12x^2$	16 + 24x	40
5	D_{10}	75	$20x + 20x^2 + 5x^3$	$20 + 40x + 15x^2$	75
6	D_{12}	126	$24x + 24x^2 + 18x^3$	$24x + 48x + 54x^2$	126
7	D_{14}	196	$28x + 28x^2 + 28x^3 + 7x^4$	$28 + 56x + 84x^2 + 28x^3$	196
8	D_{16}	288	$32x + 32x^2 + 32x^3 + 24x^4$	$32 + 64x + 96x^2 + 96x^3$	288
9	D_{18}	405	$36x + 36x^2 + 36x^3 + 36x^4 + 9x^5$	$36 + 72x + 108x^2 + 144x^3 + 45x^4$	405
10	D_{20}	550	$40x + 40x^2 + 40x^3 + 40x^4 + 30x^5$	$40 + 80x + 120x^2 + 160x^3 + 150x^4$	550

3. The Hosoya Polynomial of the Cayley Graph of the generalized Quaternion Q_{2^n}

The generalized quaternion group Q_{2^n} is a non-abelian group of order 2^n with the following presentation:

$$Q_{2^n} = \langle a, b \mid a^{2^{n-1}} = 1,\ a^{2^{n-2}} = b^2,\ b^{-1}ab = a^{-1} \rangle$$

for some integer $n \geq 3$. Now, we consider the subset T of the group Q_{2^n} as:

$$T = \{a, a^{2^{n-1}-1}, b, a^{2^{n-2}}\}.$$

The set T generates the generalized Quaternion group Q_{2^n}, and since $T^{-1} = T$, the Cayley graph is undirected and connected. Also, $\Omega = Cay(Q_{2^n}, T)$ is vertex-transitive Lemma 1.3.

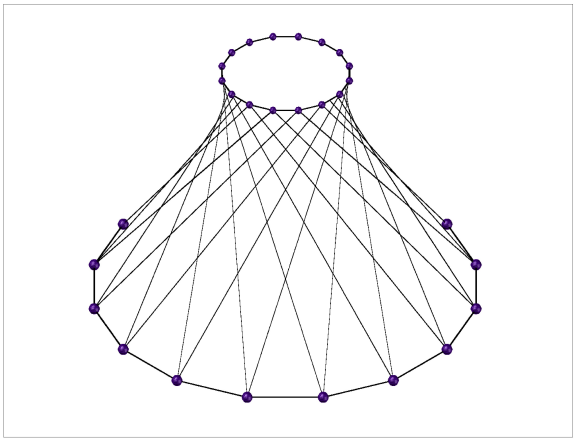


FIGURE 2. The Cayley graph $\Omega(Q_{2^n}, T)$.

Proposition 3.1. *The Hosoya polynomial of the Cayley graph $\Omega(Q_{2^n}, T)$ $(n > 3)$ is given as follows:*

$$H(\Omega, x) = 2^{n+1} \cdot x + 7 \cdot 2^{n-1} \cdot x^2 + 2^{n+2} \cdot x^3 + 2^{n+2} \cdot x^4 + \cdots + 2^{n+1} \cdot x^{2^{n-3}+1}.$$

Proof. For this proof, we employ an approach distinct from the one utilized in the proof of the preceding theorem. Based on Equation 1.1, the Hosoya polynomial of the Cayley graph $\Omega(Q_{2^n}, T)$ is expressed as:

$$H(\Omega, x) = \sum_{k \geq 0} d(\Omega, k) \cdot x^k.$$

The coefficients $d(\Omega, k)$ are the number of vertex pairs in Ω that are exactly k distance apart. Hence, the polynomial degree equals the diameter of Γ so,

$$H(\Omega, x) = \sum_{k=0}^{\text{diam}(\Omega)} d(\Omega, k) \cdot x^k. \tag{3.1}$$

Let $V(\Omega)$ denote the vertex set of the Cayley graph $\Omega(Q_{2^n}, T)$, which includes the vertices of cycles C_1 and C_2 and denoted by $V(C_1)$ and $V(C_2)$, respectively (Figure 2).

$$V(\Omega) = V(C_1) \cup V(C_2).$$

The set of all two-element subsets of $V(\Omega$ can be partitioned as follows:

$$V_1 = \{\{x, y\} \mid \{x, y\} \subset C_1\}, V_2 = \{\{x, y\} \mid \{x, y\} \subset C_2\}, V_3 = \{\{x, y\} \mid x \in C_1,\, y \in C_2\}$$

The polynomial degree, which corresponds to the graph's diameter diam(Ω) and is calculated as follows:

$$\text{diam}(\Omega) = \max\{d(x, y) \mid \{x, y\} \in V_1 \cup V_2 \cup V_3\} = 2^{n-3} + 1.$$

Let $x \in V(C_1)$, Then:

$$|\{y \in V(C_1) \mid d(x, y) = diam(\Omega)\}| = |\{y \in V(C_2) \mid d(x, y) = diam(\Omega)\}| = 2$$

In the case where $x \in V(C_2)$, similar results are obtained. Therefore, the coefficient of the highest-degree term is:

$$d(\Omega, diam\Omega) = \frac{1}{2}|V(\Omega)|(4) = \frac{1}{2}|Q_{2^n}|(4) = 2^{n+1}.$$

Since, $1 \notin T$, the Cayley graph Ω is a simple graph, meaning it has no loops, implying that $d(\Omega, 0) = 0$. Hence, the constant term in the polynomial is zero. Also, $d(\Omega, 1)$ is the number of vertex pairs at a distance of one. So, it is the number of edges in the graph, and Since the order of T is 4, $\Omega(Q_{2^n}, T)$ is 4-regular:

$$d(\Omega, 1) = |E(\Omega(Q_{2^n}, T))| = \frac{1}{2}\sum_{u \in V(\Omega)} deg(u) = \frac{1}{2}(4)|Q_{2^n}| = 2^{n+1}.$$

Where deg(u) is the degree of vertex u. To determine the coefficient x^2, we proceed as follows: For each vertex in a cycle, there are three other vertices in the same cycle and four vertices in another cycle, all of which are at a distance of 2 from the given vertex. In other words, Let $x \in V(C_1)$, Then:

$$|\{y \in V(C_1) \mid d(x, y) = 2\}| = 3, \quad |\{y \in V(C_2) \mid d(x, y) = 2\}| = 4$$

Likewise, for each vertex in the second cycle, analogous relations hold. So, The number of vertex pairs that are at a distance of 2 from each other is 7. And,

$$d(\Omega, 2) = \frac{1}{2}|Q_{2^n}|(7) = 7 \cdot 2^{n-1}.$$

For each value of k, where $2 < k < \text{diam}\Omega$ (Figure 2). Let $x \in V(C_1)$, Then:

$$|\{y \in V(C_1) \mid d(x, y) = k)\}| = |\{y \in V(C_2) \mid d(x, y) = k\}| = 4,$$

$$d(\Omega, k) = \frac{1}{2}|Q_{2^n}|(4) = 2^{n+1}.$$

Finally, based on Equation (3.1), the proof is now complete. □

Next, we examine the validity of the above relation numerically and pointwise.

3.1. **Verification of the relationship between the Hosoya polynomial and the Wiener index for the Cayley graph of the $\Omega(Q_{2^n}, T)$.**

The general formula for the Wiener index of the cayley graph $\Omega = Cay(Q_{2^n}, T)$ has previously been determined in [14] using its vertex-transitivity property, [4] as follows:

$$W(\Omega) = 2^{n-1}(2^n(2^{n-4} + 1) - 2).$$

For both even and odd values of n.

Considering Remark (2.2), in Table 2, a comparison of the Hosoya polynomial and the Wiener index of the Cayley graph of the generalized quaternion group Q_{2^n} is presented for values of n ranging from 2 to 10.

Conclusion This study compares the Hosoya polynomial and Wiener index for the Cayley graphs of the Dihedral groups D_{2n} and Generalized Quaternion groups Q_{2^n}. Both metrics exhibit exponential growth as n increases, reflecting the increasing complexity of the graphs. The Hosoya polynomial provides detailed information on vertex distances, while the Wiener index offers a global measure of graph complexity. These complementary metrics enhance our understanding of the graph's structure. Our findings highlight the relevance of these descriptors in network theory, cryptography, and optimization, paving the way for further exploration of algebraic group-based Cayley graphs.

TABLE 2. Comparison of the Wiener index and the Hosoya polynomial for $\Omega = Cay(Q_{2^n}, T)$

n	Q_{2^n}	$W(\Omega)$	$H(\Omega, x)$	$\frac{\partial H}{\partial x} H(\Omega, x)$	$\frac{\partial H}{\partial x} H(\Omega, x)\|_{x=1}$
4	Q_{2^4}	240	$2^5x + 7.2^3x^2 + 2^5x^3$	$32 + 112x + 96x^2$	240
5	Q_{2^5}	1504	$2^6x + 7.2^4x^2 + 2^7x^3 + 2^7x^4 + 2^6x^5$	$2^6 + 7.2^5x + 3.2^7x^2 + 2^9x^3 + 5.2^6x^4$	1504
6	Q_{2^6}	10176	$2^7x + 7.2^5x^2 + 2^8x^3 + ... + 2^7x^9$	$2^7 + 7.2^6x + 3.2^8x^2 + ... + 9.2^7x^8$	10176
7	Q_{2^7}	73600	$2^8x + 7.2^6x^2 + 2^9x^3 + ... + 2^9x^{16} + 2^8x^{17}$	$2^8 + 7.2^7x + 3.2^9x^2 + ... + 2^{13}x^{15} + 17.2^8x^{16}$	73600
8	Q_{2^8}	556800	$2^9x + 7.2^7x^2 + 2^{10}x^3 + ... + 2^{10}x^{32} + 2^9x^{33}$	$2^9 + 7.2^8x + 3.2^{10}x^2 + ... + 2^{15}x^{31} + 33.2^9x^{32}$	556800
9	Q_{2^9}	4324864	$2^{10}x + 7.2^8x^2 + 2^{11}x^3 + ... + 2^{11}x^{64} + 2^{10}x^{65}$	$2^{10} + 7.2^9x^2 + 3.2^{11}x^2 + ... + 2^{17}x^{63} + 65.2^{10}x^{64}$	4324864
10	$Q_{2^{10}}$	34077696	$2^{11}x + 7.2^9x^2 + 2^{12}x^3 + ... + 2^{12}x^{128} + 2^{10}x^{129}$	$2^{11} + 7.2^{10}x + 3.2^{12}x^2 + ... + 2^{19}x^{127} + 129.2^{10}x^{128}$	34077696

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