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Maximal trees with log-concave independence polynomials

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Abstract: If s_k denotes the number of independent sets of cardinality k in graph G, and $\alpha(G)$ is the size of a maximum independent set, then $I(G;x) = \sum_{k=0}^{\alpha(G)} s_k x^k$ is the *independence polynomial* of G (I. Gutman and F. Harary, 1983, [8]). The *Merrifield–Simmons index* $\sigma(G)$ (known also as the *Fibonacci number*) of a graph G is defined as the number of all independent sets of G. Y. Alavi, P. J. Malde, A. J. Schwenk and P. Erdös (1987, [2]) conjectured that $I(T;x)$ is unimodal whenever T is a tree, while, in general, they proved that for each permutation π of $\{1, 2, ..., \alpha\}$ there is a graph G with $\alpha(G) = \alpha$ such that $s_{\pi(1)} < s_{\pi(2)} < ... < s_{\pi(\alpha)}$. By *maximal tree* on n vertices we mean a tree having a maximum number of maximal independent sets among all the trees of order n. B. Sagan proved that there are three types of maximal trees, which he called batons [24].

In this paper we derive closed formulas for the independence polynomials and Merrifield–Simmons indices of all the batons. In addition, we prove that $I(T;x)$ is log-concave for every maximal tree T having an odd number of vertices. Our findings give support to the above mentioned conjecture.

Keywords: Independent set, Independence polynomial, Log-concave sequence, Tree.
AMS Classification: 05C05, 05C69, 05C31.

1 Introduction

Throughout this paper $G = (V, E)$ is a finite, undirected, loopless and without multiple edges graph, with vertex set $V = V(G)$ and edge set $E = E(G)$. As usual, a *tree* is an acyclic connected graph. $G[A]$ is the subgraph of G induced by $A \subset V$, and $G - W$ means the subgraph $G[V - W]$. We write shortly $G - w$, whenever $W = \{w\}$. The *neighborhood* of a vertex $v \in V$ is the set $N(v) = \{w : w \in V \textit{ and } vw \in E\}$, while $N[v] = N(v) \cup \{v\}$. A *spider* is a tree having at most one vertex of degree ≥ 3. $K_n, P_n, K_{m,n}$ denote respectively, the complete graph on $n \geq 1$ vertices, the chordless path on $n \geq 1$ vertices, and the complete bipartite graph on $m + n$ vertices, $m, n \geq 1$. The *disjoint union* of the graphs G_1, G_2 is the graph $G = G_1 \cup G_2$ having $V(G) = V(G_1) \cup V(G_2)$ and $E(G) = E(G_1) \cup E(G_2)$. In particular, nG denotes the disjoint union of $n > 1$ copies of the graph G. If G_1, G_2 are disjoint graphs, then their *Zykov sum* [27] is the graph $G_1 + G_2$ with $V(G_1 + G_2) = V(G_1) \cup V(G_2)$, and

$$E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{v_1v_2 : v_1 \in V(G_1), v_2 \in V(G_2)\}.$$

An *independent* set in G is a set of pairwise non-adjacent vertices, and the *independence number* $\alpha(G)$ is the maximum size of an independent set in G. Let $m(G)$ denotes the cardinality of the family of all independent sets that are *maximal under inclusion* in G. In [21] it is proved that $m(G) \leq \sqrt{3^n}$ holds for any graph G on n vertices. For trees, Wilf [26] proved that the base $\sqrt{3}$ can be reduced to $\sqrt{2}$. In [24], Sagan characterized all the trees on n vertices having the largest possible number of maximal independent sets.

Theorem 1. *[24] Among all labelled trees T with n vertices, the maximum value of $m(T)$ is $m(T) = 1 + 2^{k-1}$ for $n = 2k$, and $m(T) = 2^k$ for $n = 2k + 1$. Furthermore, this maximum is attained by the batons of length 0 (when n is odd) or by the batons of lengths 1 and 3 (when n is even).*

A number of batons of each kind are depicted in Figures 2, 3 and 4.

Let s_k be the number of independent sets in G of cardinality $k \in \{0, 1, ..., \alpha(G)\}$. The polynomial

$$I(G; x) = s_0 + s_1x + s_2x^2 + ... + s_\alpha x^\alpha, \alpha = \alpha(G),$$

is called the *independence polynomial* of G (Gutman and Harary, [8]). It is easy to deduce that

$$I(G_1 \cup G_2; x) = I(G_1; x) \cdot I(G_2; x), I(G_1 + G_2; x) = I(G_1; x) + I(G_2; x) - 1$$

(see also [12, 13, 14, 17]). For a survey on independence polynomials see [16]. In [8, 10] is proved the following result.

Proposition 2. *If $v \in V(G)$, then $I(G; x) = I(G - v; x) + xI(G - N[v]; x)$.*

A polynomial $P = a_0 + a_1x + a_2x^2 + ... + a_nx^n$ is called *unimodal (log-concave)* if the sequence of its coefficients is unimodal (log-concave, respectively), where the sequence of real numbers $(a_0, a_1, a_2, ..., a_n)$ is said to be:

- *unimodal* if there is some $k \in \{0, 1, ..., n\}$, called the *mode* of the sequence, such that $a_0 \leq ... \leq a_{k-1} \leq a_k \geq a_{k+1} \geq ... \geq a_n$,
- *log-concave* if $a_i^2 \geq a_{i-1} \cdot a_{i+1}$ for $i \in \{1, 2, ..., n-1\}$.

It is known that every log-concave sequence of positive numbers is also unimodal.

It is worth noticing that the independence polynomial of a graph is not necessarily log-concave or unimodal. For instance, the independence polynomial:

(a) $I(K_{40} + 3K_7; x) = 1 + 61x + 147x^2 + 343x^3$ is log-concave;

(b) $I(K_{50} + 3K_7; x) = 1 + 71x + 147x^2 + 343x^3$ is unimodal, but non-log-concave;

(c) $I(K_{150} + 3K_7; x) = 1 + 171x + 147x^2 + 343x^3$ is not unimodal.

However, there exist families of graphs whose independence polynomials are log-concave; e.g., recall the following result, due to Hamidoune.

Theorem 3. *[9] The independence polynomial of a $K_{1,3}$-free graph is log-concave.*

On the other side, Alavi *et al.* [2] showed that for any permutation σ of $\{1, 2, ..., \alpha\}$ there is a graph G with $\alpha(G) = \alpha$ such that$s_{\sigma(1)} < s_{\sigma(2)} < ... < s_{\sigma(\alpha)}$. Nevertheless, for trees, they stated the following conjecture.

Conjecture 4. *[2] The independence polynomial of every tree is unimodal.*

For instance, the independence polynomials of chordless paths and chordless cycles are log-concave, by Theorem 1. Moreover, one may assert that for every $\alpha \geq 1$, there exists a tree T with $\alpha(T) = \alpha$, whose $I(T; x)$ is log-concave (e.g., $P_{2\alpha}$).

The product of two unimodal polynomials is not always unimodal, even if they are independence polynomials; e.g., $I(K_{110} + (K_7 \cup K_7 \cup K_7); x) = 1 + 131x + 147x^2 + 343x^3$ and $I(K_{125} + (K_7 \cup K_7 \cup K_7); x) = 1 + 146x + 147x^2 + 343x^3$, while their product is not unimodal:

$$1 + 277x + 19\,420x^2 + 41\,405x^3 + 116\,620x^4 + \mathbf{100\,842}x^5 + 117\,649x^6.$$

Theorem 5. *[11] If P, Q are polynomials, such that P is log-concave and Q is unimodal, then $P \cdot Q$ is unimodal, while the product of two log-concave polynomials is log-concave.*

Recall that a graph G is called *well-covered* if all its maximal independent sets are of the same cardinality, (Plummer, [22]). The well-covered spider $S_n, n \geq 2$, has n vertices of degree 2, one vertex of degree $n+1$, and $n+1$ vertices of degree 1 (see Figure 1).

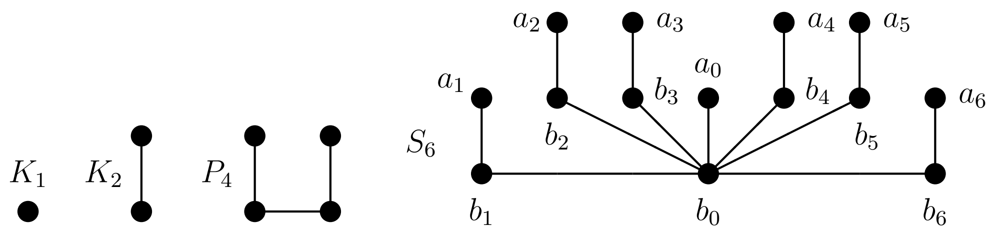

Figure 1. Well-covered spiders.

It is easy to check that the independence polynomial of every well-covered tree T with $\alpha(T) \leq 2$ (i.e., of K_1, K_2, P_4) is log-concave.

In [13] it is proved that the independence polynomial of every well-covered spider is unimodal, and its mode is unique and equals $1 + (n-1) \bmod 3 + 2(\lceil n/3 \rceil - 1)$. Later, using the facts that

$$I(S_n; x) = (1+x) \cdot \sum_{k=0}^{n} \left[\binom{n}{k} \cdot 2^k + \binom{n-1}{k-1} \right] \cdot x^k, n \geq 2,$$

and that the product of two log-concave polynomials is again log-concave, (Theorem 5), this result was strengthened to the following.

Theorem 6. *[15] The independence polynomial of each well-covered spider is log-concave.*

In [4] it is shown that $I(G; x)$ of every graph G with $\alpha(G) = 2$ has real roots. The assertion fails for graphs having stability number greater than 2. For instance, the independence polynomial of the "claw", i.e., $I(K_{1,3}; x) = 1 + 4x + 3x^2 + x^3$, is log-concave, but has non-real roots. Hence, Newton's theorem (stating that if a polynomial with positive coefficients has only real roots, then its coefficients form a log-concave sequence) is not useful in solving Conjecture 4.

If $I(G; x) = s_0 + s_1 x + s_2 x^2 + ... + s_a x^a$ is the the independence polynomial of G, then:

(i) $I(G; 1) = s_0 + s_1 + s_2 + ... + s_a$ equals the total number $\sigma(G)$ of the independent sets of G, known as *Merrifield–Simmons index* [20] or the *Fibonacci number* [23], of G;

(ii) $I(G; -1) = s_0 - s_1 + s_2 - ... + (-1)^a s_a$ is the so-called *alternating number of independent sets* of G [3], denoted $alt(G)$.

The Merrifield–Simmons index is one of the most studied topological indices related to a structural graph of a molecule (see, for instance, [6, 7, 20, 25]). In [19] is determined the largest value that $\sigma(T)$ can attained in the family of all the trees on a given number of vertices and diameter. An algorithm for computing the Merrifield–Simmons index useful for small graphs is given in [1]. For some bounds concerning the alternating number of independent sets of a graph see [5, 18].

In this paper provide closed formulas for all the batons mentioned in Theorem 1. As a by-product, we obtain the Merrifield–Simmons indices and the alternating numbers of independent sets for these trees. We also show that the independence polynomials of all the batons on an odd number of vertices are log-concave, which give a support to Conjecture 4.

2 Results

Batons of length 0 on $2n+1$ vertices are denoted by T_{2n+1} (see Figure 4 for some examples).

Theorem 7. *The independence polynomial of* T_{2n+1} *is* $I(T_{2n+1}; x) = (1+2x)^n + x \cdot (1+x)^n$ *and it is log-concave.*

Proof. Let us notice that $I(T_3; x) = 1 + 3x + x^2$, $I(T_5; x) = 1 + 5x + 6x^2 + x^3$ and they both are log-concave. For $n \geq 3$, using Proposition 2, we deduce (see Figure 2) that:

$$I(T_{2n+1}; x) = I(T_{2n+1} - v; x) + xI(T_{2n+1} - N[v]; x) =$$

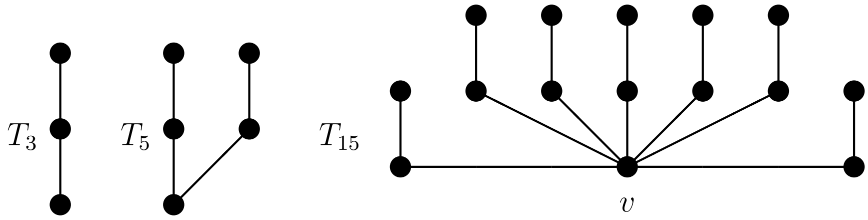

Figure 2. Batons of length 0.

$$= (1+2x)^n + x\cdot(1+x)^n = 1 + \sum_{k=1}^{n}\left[\binom{n}{k}\cdot 2^k + \binom{n}{k-1}\right]\cdot x^k + x^{n+1} =$$
$$= \sum_{k=0}^{n+1}\left[\binom{n}{k}\cdot 2^k + \binom{n}{k-1}\right]\cdot x^k = \sum_{k=0}^{n+1} s_k x^k.$$

It is easy to check that

$$s_1^2 = (1+2n)^2 \geq s_0\cdot s_2 = 2n^2 - n,$$
$$s_n^2 - s_{n-1}\cdot s_{n+1} = 1 + 2^{n+1} + 2^{2n} - \frac{1}{2}(n^2 + n\cdot(2^n - 1)) \geq 0.$$

Further, for $2 \leq k \leq n-1$, we have:

$$s_k^2 - s_{k-1}\cdot s_{k+1} =$$
$$= \left[\binom{n}{k-1} + 2^k\binom{n}{k}\right]^2 - \left[\binom{n}{k-2} + 2^{k-1}\binom{n}{k-1}\right]\left[\binom{n}{k} + 2^{k+1}\binom{n}{k+1}\right]$$
$$= \binom{n}{k-1}^2 + 2^{k+1}\binom{n}{k-1}\binom{n}{k} + 2^{2k}\binom{n}{k}^2 -$$
$$- \binom{n}{k-2}\binom{n}{k} - 2^{k+1}\binom{n}{k+1}\binom{n}{k-2} - 2^{k-1}\binom{n}{k-1}\binom{n}{k} - 2^{2k}\binom{n}{k-1}\binom{n}{k+1}$$
$$= \left[\binom{n}{k-1}^2 - \binom{n}{k-2}\binom{n}{k}\right] + 2^{k-1}\binom{n}{k}^2 A,$$

where

$$A = 4\binom{n}{k-1}/\binom{n}{k} + 2^{k+1} - 4\binom{n}{k+1}\binom{n}{k-2}/\binom{n}{k}^2 -$$
$$- \binom{n}{k-1}/\binom{n}{k} - 2^{k+1}\binom{n}{k-1}\binom{n}{k+1}/\binom{n}{k}^2.$$

Since

$$A = \frac{1}{(k+1)(n-k+1)}\left[2^{k+1}(n+1) + \frac{k\left(3(k+1)(n-k+2) - 4(k-1)(n-k)\right)}{n-k+2}\right]$$
$$= \frac{1}{(k+1)(n-k+1)}\left[2^{k+1}(n+1) + \frac{k}{n-k+2}\left(7n - k - kn + k^2 + 6\right)\right]$$
$$= \frac{1}{(k+1)(n-k+1)}\left[2^{k+1}(n+1) + \frac{k(7n+k+6)}{n-k+2} - k^2\right] \geq 0,$$

we infer that $s_k^2 - s_{k-1}s_{k+1} \geq 0$, for $2 \leq k \leq n-1$.

In conclusion, $I(T_{2n+1};x)$ is log-concave, and this completes the proof. □

Batons of length 1 on $2m+2n+2, m \geq 0, n \geq 0$, vertices are denoted by $T_{m,n}$.

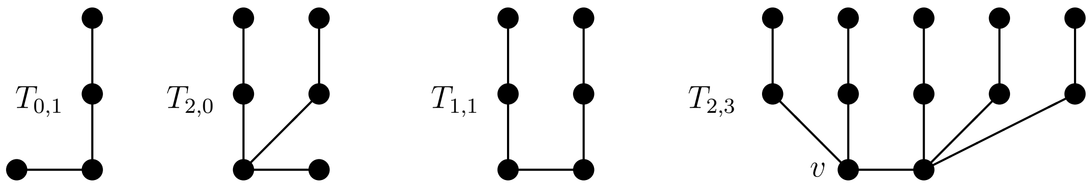

Figure 3. Batons of length 1.

Theorem 8. *(i) The independence polynomial of* $T_{m,n}$ *is*

$$I(T_{m,n};x) = (1+2x)^m \cdot \sum_{k=0}^{n+1} \left\{ \left[\binom{n}{k} \cdot 2^k + \binom{n}{k-1} \right] \cdot x^k \right\} + x \cdot (1+x)^m \cdot (1+2x)^n .$$

(ii) The independence polynomial of every $T_{m,m}$ *is log-concave.*

Proof. (i) Firstly, let us remark that:

(a) $I(T_{0,1};x) = I(T_{1,0};x) = I(P_4;x) = 1 + 4x + 3x^2$ and is log-concave;

(b) $I(T_{1,1};x) = I(P_6;x)$ and is log-concave, since P_6 is $K_{1,3}$-free;

(c) $I(T_{0,m};x) = I(T_{m,0};x) = I(S_m;x)$ and is log-concave, by Theorem 6.

For $m \geq n \geq 1$, using Proposition 2, we deduce that:

$$\begin{aligned} I(T_{m,n};x) &= I(T_{m,n} - v;x) + xI(T_{m,n} - N[v];x) = \\ &= (1+2x)^m \cdot I(T_{2n+1};x) + x \cdot (1+x)^m \cdot (1+2x)^n . \end{aligned}$$

Since, by Theorem 7, we have

$$I(T_{2n+1};x) = \sum_{k=0}^{n+1} \left\{ \left[\binom{n}{k} \cdot 2^k + \binom{n}{k-1} \right] \cdot x^k \right\}$$

we infer that

$$I(T_{m,n};x) = (1+2x)^m \cdot \sum_{k=0}^{n+1} \left\{ \left[\binom{n}{k} \cdot 2^k + \binom{n}{k-1} \right] \cdot x^k \right\} + x\,(1+x)^m\,(1+2x)^n .$$

(ii) If $m = n$, then

$$\begin{aligned} I(T_{m,m};x) &= (1+2x)^m \cdot \sum_{k=0}^{m+1} \left\{ \left[\binom{m}{k} \cdot 2^k + \binom{m}{k-1} \right] \cdot x^k \right\} + x \cdot (1+x)^m \cdot (1+2x)^m = \\ &= (1+2x)^m \cdot \left[\sum_{k=0}^{m+1} \left\{ \left[\binom{m}{k} \cdot 2^k + \binom{m}{k-1} \right] \cdot x^k \right\} + x \cdot (1+x)^m \right] = \\ &= (1+2x)^m \cdot \left[1 + \sum_{k=1}^{m+1} \left[\binom{m}{k} 2^k + 2\binom{m}{k-1} \right] x^k \right] = (1+2x)^m \cdot \sum_{k=0}^{m+1} a_k x^k . \end{aligned}$$

According to Theorem 5, in order to show that $I(T_{m,m};x)$ is log-concave, it is enough to verify that $\sum\limits_{k=0}^{m+1} a_k x^k$ is log-concave, i.e., $a_k^2 - a_{k-1}a_{k+1} \geq 0$ for all $1 \leq k \leq m$.

First, we have

$$a_k = \binom{m}{k}2^k + 2\binom{m}{k-1}, \quad a_{k+1} = \binom{m}{k+1}2^{k+1} + 2\binom{m}{k}, \quad a_{k-1} = \binom{m}{k-1}2^{k-1} + 2\binom{m}{k-2}.$$

It is not difficult to see that $a_1^2 = (2+2m)^2 \geq a_0 a_2 = 2m^2$, and

$$a_2^2 - a_1 a_3 = 4m^4 - \frac{8m^4 - 10m^3 - 8m^2 + 10m}{3} \geq 0.$$

In addition, we have $a_m^2 = 2^{2m} + m \cdot 2^{m+2} + 4m^2 \geq a_{m-1}a_{m+1} = m2^m + 4m^2 - 4$.

Now, for $2 < k < m$ we get

$$\begin{aligned} a_k^2 - a_{k-1}a_{k+1} &= \binom{m}{k}^2 2^{2k} + 2^{k+2}\binom{m}{k}\binom{m}{k-1} + 4\binom{m}{k-1}^2 - \\ &- \binom{m}{k+1}\binom{m}{k-1}2^{2k} - 2^{k+2}\binom{m}{k+1}\binom{m}{k-2} - \\ &- 2^k\binom{m}{k}\binom{m}{k-1} - 4\binom{m}{k}\binom{m}{k-2} = \\ &= \frac{(m!)^2}{(k-2)!(k-1)!(m-k-1)!(m-k)!}(A+B+C) \geq 0, \end{aligned}$$

because

$$\begin{aligned} A &= \frac{4 \cdot (m+1)}{k(k-1)(m-k)(m-k+1)^2(m-k+2)} \geq 0, \\ B &= \frac{2^{2k} \cdot (m+1)}{(k-1)k^2(m-k)(k+1)(m-k+1)} \geq 0, \\ C &= \frac{2^k \cdot (k+7m+6)}{(k-1)k(k+1)(m-k)(m-k+1)(m-k+2)} \geq 0. \end{aligned}$$

In conclusion, $I(T_{m,m};x)$ is log-concave. □

Batons of length 3 on $2m+2n+4, m \geq 0, n \geq 0$, vertices are denoted by $B_{m,n}$.

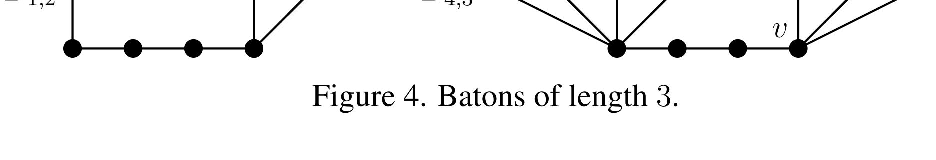

Figure 4. Batons of length 3.

Clearly, $I(B_{0,0};x) = I(P_4;x) = 1 + 4x + 3x^2$ and it is log-concave.

Applying Proposition 2, we deduce that:

$I(B_{0,n};x) = I(B_{0,n} - v;x) + xI(B_{0,n} - N[v];x) = (1+3x+x^2)(1+2x)^n + (1+2x)(1+x)^n$.

For $m \geq n \geq 1$ we obtain:

$$I(B_{m,n};x) = I(B_{m,n}-v;x) + xI(B_{m,n}-N[v];x) = \\ = I(T_{2m+1};x)\cdot I(S_n;x) + x\cdot(1+2x)^m \cdot I(T_{2n+1};x).$$

Substituting the corresponding expressions for $I(T_{2n+1};x)$ and $I(S_n;x)$ we obtain the following.

Proposition 9. *The independence polynomial of $B_{m,n}$ is*

$$I(B_{m,n};x) = \sum_{k=0}^{n+1}\left\{\left[\binom{n}{k}\cdot 2^k + \binom{n}{k-1}\right]\cdot x^k\right\}\cdot\left\{(1+x)\cdot\sum_{k=0}^{m}\left[\binom{m}{k}\cdot 2^k+\binom{m-1}{k-1}\right]\cdot x^k\right\}+ \\ +x\cdot(1+2x)^n\cdot\sum_{k=0}^{m+1}\left\{\left[\binom{m}{k}\cdot 2^k+\binom{m}{k-1}\right]\cdot x^k\right\} = \\ =\sum_{k=0}^{m+1}\left\{\left[\binom{m}{k}\cdot 2^k+\binom{m}{k-1}\right]\cdot x^k\right\}\cdot\left\{(1+x)\cdot\sum_{k=0}^{m}\left[\binom{m}{k}\cdot 2^k+\binom{m-1}{k-1}\right]\cdot x^k\right\}+ \\ +x\cdot(1+2x)^m\cdot\sum_{k=0}^{n+1}\left\{\left[\binom{n}{k}\cdot 2^k+\binom{n}{k-1}\right]\cdot x^k\right\}.$$

Using the above derived closed formulas for the independence polynomials of all the batons, we are able now to compute their Merrifield–Simmons indices and alternating number of independent sets.

Corollary 10. *The following equalities hold :*
(i) $\sigma(T_{2n+1}) = 3^n + 2^n$ *and* $alt(T_{2n+1}) = (-1)^n$*;*
(ii) $\sigma(T_{m,n}) = 3^{m+n} + 3^m\cdot 2^n + 2^m\cdot 3^n$ *and* $alt(T_{m,n}) = (-1)^{m+n}$*;*
(iii) $\sigma(B_{m,n}) = 3^n(2\cdot 3^m + 2^m) + 2^n(3^{m+1} + 2^{m+1})$ *and* $alt(B_{m,n}) = (-1)^{n+m+1}$.

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