A new sum of graphs and caterpillar trees

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Abstract. Caterpillar trees, or simply Caterpillar, are trees such that when we remove all their leaves (or end edge) we obtain a path. The number of nonisomorphic caterpillars with \( n \geq 2 \) edges is \( 2^{n-3} + 2^{\lfloor (n-3)/2 \rfloor} \). Using a new sum of graphs, introduced in this paper, we provided a new proof of this result.

Keywords: Graph, Caterpillar trees, tree graphs, sum of graphs.

MSC2010: 05C30, 05C76, 05C05, 05C60.

1. Introduction

The Caterpillar trees were initially studied by F. Harary and A. J. Schwenk \cite{1} in a series of articles. The name was introduced by Arthur Hobbs, an American mathematician. In 1973, F. Harary and A.J. Schwenk \cite{1} showed that the number of nonisomorphic caterpillars with \( n \geq 2 \) edges is \( 2^{n-3} + 2^{\lfloor (n-3)/2 \rfloor} \). They found this formula in two ways: first, derived as a special case of an application of Pólya’s enumeration Theorem which counts graphs with integer-weighted points; secondly, by an appropriate labelling of the
lines of the caterpillar. In this paper, we gave a new proof of this result using a new sum of graphs, introduced in [3, 2] and studied with great attention in [4].

The paper is organized as follows. In Section 2, we study a combinatorial problem which will be used in the proof of the main Theorem (see Theorem 3.7). In Section 3, we introduce the sum of graphs and use it to build the caterpillar trees, and, thus, give a new proof of the formula enumerating caterpillar trees on \( n \geq 2 \) edges.

2. Combinatorial lemma

Let \( \mathbb{B} = \{0, 1\} \) and \( \mathbb{B}^m = \mathbb{B} \times \cdots \times \mathbb{B} \), the \( m \)-times Cartesian product of \( \mathbb{B} \). We define the following functions:

\[
\begin{align*}
  i & : \mathbb{B}^m \rightarrow \mathbb{B}^m, & \quad r & : \mathbb{B}^m \rightarrow \mathbb{B}^m, \\
  (x_1, x_2, \ldots, x_m) & \mapsto (x_1, x_2, \ldots, x_m), & \quad (x_1, x_2, \ldots, x_m) & \mapsto (x_m, x_{m-1}, \ldots, x_1), \\
  c & : \mathbb{B}^m \rightarrow \mathbb{B}^m, & \quad (x_1, x_2, \ldots, x_m) & \mapsto (x_1, x_2, \ldots, x_m),
\end{align*}
\]

where, for \( k = 1, \ldots, m \),

\[
\pi_k = \begin{cases} 0 & \text{if } x_k = 1, \\ 1 & \text{if } x_k = 0. \end{cases}
\]

Here, we consider for all \( f, g : \mathbb{B}^m \rightarrow \mathbb{B}^m \) the composition \( f \circ g : \mathbb{B}^m \rightarrow \mathbb{B}^m \).

**Proposition 2.1.** Let \( i, r, c : \mathbb{B}^m \rightarrow \mathbb{B}^m \) the functions defined above and take \( x \in \mathbb{B}^m \).

Then, the following properties hold:

1. \( i(x) = x \),
2. \( r^2 = i \),
3. \( c^2 = i \),
4. \( c \circ r = r \circ c \),
5. \( (c \circ r)^2 = i \),

where \( c^2 = c \circ c \).

**Proof.** By definition of \( i, r \) and \( c \), it is clear that (1), (2), (3) and (4) follows. And (5) follows from (4), (2) and (3).

**Definition 2.2.** Let \( x, y \in \mathbb{B}^m \). We will say that \( x \) is related to \( y \) when \( i(x) = y \) or \( r(x) = y \) or \( c(x) = y \) or \( (c \circ r)(x) = y \), and it will be denoted by \( x \sim y \).

**Remark 2.3.** The relation \( \sim \) defined in Definition 2.2 is an equivalence relation.

In this section we prove the following combinatorial lemma for the equivalence classes associated with points in \( \mathbb{B}^m \).

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Lemma 2.4 (Combinatorial Lemma). Let $x \in \mathbb{B}^m$ and set $[x] = \{y \in \mathbb{B}^m \mid x \sim y\}$. Then,
\[
\# \left( \frac{\mathbb{B}^m}{\sim} \right) = 2^{m-2} + 2^{\left\lfloor \frac{m-2}{2} \right\rfloor},
\]
where $\frac{\mathbb{B}^m}{\sim} = \{[x] \mid x \in \mathbb{B}^m\}$ and $\lfloor z \rfloor$ is the largest integer smaller than or equal to $z$.

Proof. First, let’s show the following: The class $[x] \in \frac{\mathbb{B}^m}{\sim}$ has 2 or 4 representatives. Indeed, if $x, r(x), c(x)$ and $(c \circ r)(x) = (r \circ c)(x)$ are different from each other, we will get that the class $[x]$ has 4 representatives, namely
\[
[x] = \{x, r(x), c(x), (c \circ r)(x)\}.
\]

On the other hand:

i) If $x = r(x)$, then $c(x) = (c \circ r)(x)$ and, thus, $[x] = \{x, c(x)\}$.

ii) If $x = (r \circ c)(x)$, then $r(x) = c(x)$ and, thus, $[x] = \{x, r(x) = c(x)\}$.

The cases i) and ii) have only 2 representatives for the class $[x]$ and the affirmation follows.

Remark: $x \neq c(x)$ by definition.

Now, let $[x] \in \frac{\mathbb{B}^m}{\sim}$ be a class that only has 2 representatives. Set $x = (x_1, x_2, \ldots, x_m)$. We have the following cases:

I) If $x = r(x)$ then
\[
x_1 = x_m, x_2 = x_{m-1}, \ldots, x_i = x_{m-i+1}, \ldots, x_{\lceil \frac{m}{2} \rceil} = x_{m-\lceil \frac{m}{2} \rceil+1}.
\]

II) If $x = (r \circ c)(x)$ then
\[
x_1 = x_m, x_2 = x_{m-1}, \ldots, x_i = x_{m-i+1}, \ldots, x_{\lfloor \frac{m}{2} \rfloor} = x_{m-\lfloor \frac{m}{2} \rfloor+1}.
\]

In case (I), if $m$ is even, we have to know the $\left\lfloor \frac{m}{2} \right\rfloor$ first entries of $x = (x_1, x_2, \ldots, x_m)$, that is, we can form $2^{\left\lfloor \frac{m}{2} \right\rfloor}$ elements. Now, as pairwise elements belong to the same class, we have that $2^{\left\lfloor \frac{m}{2} \right\rfloor-1}$ belong to the same class, and, therefore, we will have two representatives. On the other hand, if $m$ is odd, we first delete the central coordinate $x_{\lfloor \frac{m}{2} \rfloor} + 1$ of $x$, to obtain the $m - 1$ even case, which leads us to have $2^{\left\lfloor \frac{m-1}{2} \right\rfloor-1}$ classes with two representatives. Now, considering the central coordinate $x_{\lfloor \frac{m}{2} \rfloor} + 1$ of $x$, we see that it can take the values 0 or 1, and thus, when $m$ is odd there are $2\left(2^{\left\lfloor \frac{m-1}{2} \right\rfloor-1}\right) = 2^{\left\lfloor \frac{m-1}{2} \right\rfloor} = 2^{\left\lfloor \frac{m}{2} \right\rfloor}$ classes with two representatives.

Analogously, we have a similar result in case (II) when $m$ is even. Note that when $m$ is odd there are no representatives, since no $x$ with $m$ odd entries satisfies this case.

So, from (I) and (II), if $m$ is even, we get $2^{\left\lceil \frac{m}{2} \right\rceil-1} + 2^{\left\lfloor \frac{m}{2} \right\rfloor-1} = 2^{\left\lceil \frac{m}{2} \right\rceil}$ classes with two representatives each. If $m$ is odd, we get $2^{\left\lfloor \frac{m}{2} \right\rfloor}$. Therefore, in both cases we have the same number of representatives.
The next step consists of computing \(\#(\overline{B^m})\). It follows from the Affirmation that \(\overline{B^m}\) is made up of classes that have 2 or 4 elements. Thus, we can divide \(\overline{B^m}\) into a collection of disjoint classes of 2 or 4 elements each. Thus, one gets

\[2^m = \#(\overline{B^m}) = 2\mu + 4\eta,\]  

where \(\mu\) is the number of classes of \(\overline{B^m}\) with two representatives, namely \(\mu = 2^m - 1 + 2^{m-1} = 2^m - 1\); and \(\eta\) is the number of classes of \(\overline{B^m}\) with four representatives. Then, substituting these values in (1), one gets

\[\Rightarrow \eta = \frac{2^m - 2 - 2^{m-1}}{2}.\]  

Therefore,

\[\#(\overline{B^m}) = \mu + \eta = 2^m - 2 - 2^{m-1} = 2^{m-2} + 2^{m-1} = 2^{m-2} + 2^{m-2}.\]

3. **Sum of graph and Caterpillar tree**

Let us denote by \(\mathcal{A}\) the set of all tree graphs.

The *sum of graphs* in \(\mathcal{A}\) is an operation that is performed between two graphs of \(\mathcal{A}\). This sum is defined as follows:

\[\mathcal{G} \oplus \mathcal{H} = (V \cup V' - \{a', b'\}, E \cup E' - \{e'\})\]

is a new graph such that \(e\) and \(e'\) and their respective vertices, connecting \(\mathcal{G}\) and \(\mathcal{H}\), are identified. The graph \(\mathcal{G} \oplus_{\{e, e'\}} \mathcal{H}\) is the sum between \(\mathcal{G}\) and \(\mathcal{H}\). This sum will be denoted by \(\mathcal{G} \oplus \mathcal{H}\) if there is no confusion in the identification of the edges. See Figure 1 for a graphical representation of this sum.

**Definition 3.1.** Let \(\mathcal{G} = (V, E)\) and \(\mathcal{H} = (V', E')\) be distinct graphs in \(\mathcal{A}\) and let \(e = (a, b) \in E\) and \(e' = (a', b') \in E'\) be edges. Then,

\[\mathcal{G} \oplus_{\{e, e'\}} \mathcal{H} = (V \cup V' - \{a', b'\}, E \cup E' - \{e'\})\]

is a new graph such that \(e\) and \(e'\) and their respective vertices, connecting \(\mathcal{G}\) and \(\mathcal{H}\), are identified. The graph \(\mathcal{G} \oplus_{\{e, e'\}} \mathcal{H}\) is the sum between \(\mathcal{G}\) and \(\mathcal{H}\). This sum will be denoted by \(\mathcal{G} \oplus \mathcal{H}\) if there is no confusion in the identification of the edges. See Figure 1 for a graphical representation of this sum.

**Definition 3.2.** Consider the path \(P_3\) and \(\mathcal{J} = P_3\). We denote by \(\mathcal{J}^+\) the graph derived of \(\mathcal{J}\) with two positive signs in the extreme vertices and a negative sign in the middle vertex, and by \(\mathcal{J}^-\) to the graph derived of \(\mathcal{J}\) with two negative signs in the extreme vertices and a positive sign in the middle vertex. See Figure 2.
Definition 3.3. Let \( \{J_i\}_{i=1}^k \) be a family of graphs, where \( J_i \in \{\mathcal{J}_+, \mathcal{J}_-\} \). We define \( J_1 \oplus J_2 \oplus \cdots \oplus J_k \), as follows:

- For \( k = 1 \), we have \( J_1 \).
- For \( k = 2 \), we choose an edge in \( J_1 \) and add with \( J_2 \) in the chosen edge. Thus, we obtain \( J_1 \oplus J_2 \). Finally, we mark in \( J_1 \oplus J_2 \) the edge of \( J_2 \) where the addition was not performed. (See part (i) of Figure 3).
- For \( k = j \), we add \( J_1 \oplus \cdots \oplus J_{j-1} \) with \( J_j \) on the marked edge of \( J_1 \oplus \cdots \oplus J_{j-1} \), and, thus, obtaining \( J_1 \oplus \cdots \oplus J_j \). Finally, we mark in \( J_1 \oplus \cdots \oplus J_j \) the edge of \( J_j \), where the addition was not performed.

We note that the identification of edges should be done while preserving the signs.

Notation. Given \( \{J_i\}_{i=1}^k \), where \( J_i \in \{\mathcal{J}_+, \mathcal{J}_-\} \), we will denote by \( \bigoplus_{i=1}^k J_i \) the sum \( J_1 \oplus J_2 \oplus \cdots \oplus J_k \) in Definition 3.3. Thus:

\[
\bigoplus_{i=1}^k J_i = J_1 \oplus J_2 \oplus \cdots \oplus J_k.
\]

By convention, \( \bigoplus_0^0 J_i = I \), where \( I \) is the graph of one edge.

Example 3.4. In Figure 3 (i), we have the construction of \( \mathcal{J}_+ + \mathcal{J}_+ \) and \( \mathcal{J}_- + \mathcal{J}_- \), according to the Definition 3.3, where we can see that \( \mathcal{J}_+ + \mathcal{J}_+ \cong \mathcal{J}_- + \mathcal{J}_- \), as graphs. Similarly, in Figure 3 (ii) we have the construction of \( \mathcal{J}_+ + \mathcal{J}_- \) and \( \mathcal{J}_- + \mathcal{J}_+ \), where we can see that \( \mathcal{J}_+ + \mathcal{J}_- \cong \mathcal{J}_- + \mathcal{J}_+ \).

Proposition 3.5. Let \( \{J_i\}_{i=1}^k \) be a family of graphs such that \( J_i \in \{\mathcal{J}_+, \mathcal{J}_-\} \). Then, the following statements holds:

1. \( \bigoplus_{i=1}^k J_i \cong \bigoplus_{i=1}^k \mathcal{J}_i \), where \( \mathcal{J}_i = \begin{cases} \mathcal{J}_+, & \text{if } J_i = \mathcal{J}_-, \\ \mathcal{J}_-, & \text{if } J_i = \mathcal{J}_+ \end{cases} \)

2. \( \bigoplus_{i=1}^k J_i \cong \bigoplus_{i=1}^k J_{k+1-i} \).

Proof. For (1), since \( \mathcal{J}_+ \cong \mathcal{J}_- \) we have \( J_i \cong \mathcal{J}_i \) for all \( i = 1, \cdots, k \). Then, if we replace \( J_i \) by \( \mathcal{J}_i \) in \( \bigoplus_{i=1}^k J_i \), we get \( \bigoplus_{i=1}^k \mathcal{J}_i \) and since the sums of the graphs continue to be performed on the same edges, we have \( \bigoplus_{i=1}^k J_i \cong \bigoplus_{i=1}^k \mathcal{J}_i \), see Figure 4.

For (2), we note that the sum \( \bigoplus_{i=1}^k J_i = J_1 \oplus J_2 \oplus \cdots \oplus J_{k-1} \oplus J_k \) is built starting from \( J_1 \) which is added to \( J_2 \) to obtain \( J_1 \oplus J_2 \), latter we added \( J_3 \) to obtain \( J_1 \oplus J_2 \oplus J_3 \), and, thus,
Figure 3. Sum between $J_+$ and $J_-$, where "$\cong$" is the isomorphism of graphs.

until we get the sum of $J_1 \oplus J_2 \oplus \cdots \oplus J_{k-1}$ and $J_k$ to finally get $J_1 \oplus J_2 \oplus \cdots \oplus J_{k-1} \oplus J_k = \bigoplus_{i=1}^{k} J_i$, but we also noted that this same sum is built as the sum of $J_k$ and $J_{k-1}$, and, thus, until we get to add $J_k \oplus \cdots \oplus J_2$ with $J_1$ to get $J_k \oplus J_{k-1} \oplus \cdots \oplus J_2 \oplus J_1 = \bigoplus_{i=1}^{k} J_{k+1-i}$. Thus, $\bigoplus_{i=1}^{k} J_i \cong \bigoplus_{i=1}^{k} J_{k+1-i}$.

Example 3.6. The graphs $J_+ \oplus J_- \oplus J_+ \oplus J_-$ and $J_- \oplus J_+ \oplus J_- \oplus J_-$ are built in (i) and (ii) of Figure 4, respectively. Furthermore, $J_- \oplus J_+ \oplus J_- \oplus J_- \cong J_- \oplus J_+ \oplus J_- \oplus J_- = J_- \oplus J_+ \oplus J_- \oplus J_-$, and, thus:

$$J_- \oplus J_+ \oplus J_- \oplus J_- \cong J_- \oplus J_+ \oplus J_- \oplus J_-.$$

Figure 4. $J_+ \oplus J_- \oplus J_+ \oplus J_+ \oplus J_- \cong J_- \oplus J_+ \oplus J_- \oplus J_-$, for which we gave an alternative proof.
Theorem 3.7. Let $\mathcal{J} = \{J_1 \oplus \cdots \oplus J_i \oplus \cdots \oplus J_m \in \mathcal{A} \mid J_i = J_+ \text{ or } J_i = J_-, \forall i = 1, \ldots, m, \text{ and } m \in \mathbb{N}\}$. Then, the number of different nonisomorphic graphs with $n \geq 2$ edges in $\mathcal{J}$, is given by

$$2^{n-3} + 2^{\lfloor\frac{n-2}{2}\rfloor}.$$ 

Proof. Given $m \in \mathbb{N}$, we define the functions $\iota, \varphi, \psi : \mathcal{J} \longrightarrow \mathcal{J}$ by

$$\iota(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} J_i,$$

$$\varphi(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} J_i,$$

$$\psi(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} J_{m+1-i}.$$ 

We say that $\bigoplus_{i=1}^{m} J_i$ and $\bigoplus_{i=1}^{m} L_i$ are $\sim_m$ related in $\mathcal{J}$, denoted by

$$\bigoplus_{i=1}^{m} J_i \sim_m \bigoplus_{i=1}^{m} L_i,$$

if

$$\iota(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} L_i \text{ or } \varphi(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} L_i \text{ or } \psi(\bigoplus_{i=1}^{m} J_i) = \bigoplus_{i=1}^{m} L_i.$$

Now, we affirm that the relation $\sim_m$ is an equivalence relation. Indeed, it follows immediately by the combinatorial Lemma (Lemma 2.4), where we take $J_i = x_i$, $J_+ = 1$, $J_- = 0$, $\bigoplus_{i=1}^{m} J_i = (x_1, \ldots, x_m)$ and $\iota = i$, $\varphi = f$, $\psi = g$, $\sim_m = \sim$. Furthermore,

$$\#(\mathcal{J} \sim_m) = \# (B^m) = 2^{m-2} + 2^{\lfloor\frac{m-2}{2}\rfloor}. \quad (3)$$

Thus, we have $2^{m-2} + 2^{\lfloor\frac{m-2}{2}\rfloor}$ different graphs of the form $\bigoplus_{i=1}^{m} J_i$, where $J_i \in \{J_+, J_-\}$. Since the graphs $\bigoplus_{i=1}^{m} J_i$ have $m + 1$ edges, making $n = m + 1$ and substituting in (3) we have that the number of nonisomorphic different graphs, with $n \geq 2$ edges in $\mathcal{J}$, is given by

$$2^{n-3} + 2^{\lfloor\frac{n-3}{2}\rfloor}.$$ 

\[\Box\]

Given a Caterpillar tree fixed, the following result allows us to obtain a family $\{J_i\}_{i=1}^{k}$, where $J_i \in \{J_+, J_-\}$, such that $K \cong \bigoplus_{i=1}^{k} J_i$. 

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Proposition 3.8. Let \( n \) be a positive integer and \( K \) be a Caterpillar tree with \( n+1 \) edges, then there exists a family \( \{ J_i \}_{i=1}^{n} \), where \( J_i \in \{ J_+ , J_- \} \), such that
\[
K \cong \bigoplus_{i=1}^{n} J_i.
\]

Proof. By induction on the number \( E \) of edges of \( K \).

- For a graph with 1 edge, then by convention we have \( K \cong \bigoplus_{i=1}^{0} J_i \).
- For a graph with 2 edges, we take \( K \cong \bigoplus_{i=1}^{1} J_i \), where \( J_i = J_+ \) or \( J_i = J_- \).
- Suppose that it is true for a graph with \( n \) edges, then \( K \cong \bigoplus_{i=1}^{n-1} J_i \).

Now, we show that it is true for a graph with \( n+1 \) edges. Indeed, \( K' \) is the graph that is obtained when deleting an edge from \( K \). Thus, \( K' \) has \( E' = n \) edges. Then, by induction, we have that \( K' \cong \bigoplus_{i=1}^{n-1} J_i \). Now, in \( \bigoplus_{i=1}^{n-1} J_i \), we insert an end edge by adding conveniently \( J_+ \) or \( J_- \), so that \( \bigoplus_{i=1}^{n} J_i \cong K \) as follows: first, we identify the sign of the vertex where the edge will be inserted (it is clear that said vertex is positive or negative). Then there will be a \( j \) such that \( \bigoplus_{i=1}^{n-1} J_i = (\bigoplus_{i=1}^{n-1} J_i) \oplus (\bigoplus_{i=n-j}^{n-1} J_i) \) so that the last vertex to the right of \( \bigoplus_{i=1}^{n-1} J_i \) become the vertex where the missing edge will be inserted. If the vertex is positive (resp. negative) we immediately add \( \bigoplus_{i=n-j}^{n-1} J_i \) with \( J_- \) (resp. \( J_+ \)), and adding \( \bigoplus_{i=n-j}^{n-1} J_i \), we get \( \bigoplus_{i=1}^{n-1} J_i \oplus J_- \oplus (\bigoplus_{i=n-j}^{n-1} J_i) \) (resp. \( \bigoplus_{i=1}^{n-1} J_i \oplus J_+ \oplus (\bigoplus_{i=n-j}^{n-1} J_i) \)). As was inserted the missing edge to \( \bigoplus_{i=1}^{n-1} J_i \) to be isomorphic to \( K \), we have that
\[
(\bigoplus_{i=1}^{n-1-j} J_i) \oplus J \oplus (\bigoplus_{i=n-j}^{n-1} J_i) \cong \bigoplus_{k=1}^{n} J_k \cong K,
\]

where \( J = J_- \), if the last vertex created in \( \bigoplus_{i=1}^{n-1-j} J_i \) has a positive sign and \( J = J_+ \), if the last vertex created in \( \bigoplus_{i=1}^{n-1-j} J_i \) has a negative sign.

An example for Proposition 3.8 is given in Figure 5.

Theorem 3.9. Let \( J_0 \) be the set of all different nonisomorphic graphs in \( J \) and let \( K \) be the set of nonisomorphic Caterpillar trees, then
\[
\#(J_0) = #(K) = 2^{n-3} + 2^{\frac{n-3}{2}}.
\]

Proof. By Definition 3.3 we have that the graphs in \( J_0 \) are Caterpillar trees (thus \( J_0 \subseteq K \)) then, by Proposition 3.8, we get that every Caterpillar tree is isomorphic to an element of \( J_0 \), thus \( K \subseteq J_0 \) and therefore \( J_0 = K \). Furthermore,
\[
\#(J_0) = #(K) = 2^{n-3} + 2^{\frac{n-3}{2}}.
\]
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Figure 5. Way to insert an edge in positive vertex (i) or in negative vertex (ii).

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