A study of First geometric-Arithmetic Index with Chemical Applications

Ammar B. Habeb, A.M. Khalaf
Department of Mathematics, Faculty of Computer Science and Mathematics, University of Kufa, Najaf, IRAQ

*Corresponding Author:
A.M. Khalaf
Email: abduljaleel.khalaf@uokufa.edu.iq

Abstract: The first geometric–arithmetic index $GA_1$ is found to be useful in compute the numerical value of certain graphs and chemical graphs, which is defined as $GA_1 = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$. We denotes $d_u$ the degree of vertex $u$ in graph $G$. In this paper, we present the general formula for the first geometric-Arithmetic Index for certain graphs and $k_r$-gluing graphs.

Keywords: First geometric-Arithmetic Index, $k_r$-gluing graph, complete graph, Web graph, wheel graph, k-bridge graph.

INTRODUCTION

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences one of these tools is topological indices [8, 10].

Topological indices are one of the main theoretical tools for studying molecular properties of chemical compounds. The definition of topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [7, 16].

we need to recall a few concepts from chemical graph theory Let $G$ be a molecular graph. Two vertices of $G$, connected by an edge, are said to be adjacent. If two vertices $u$ and $v$ are adjacent, we shall write $u \sim v$. The number of vertices of $G$, adjacent to a given vertex $v$, is the degree of this vertex, and will be denoted by $d_v(G)$. The concept of degree in graph theory is closely related (but not identical) to the concept of valence in chemistry [2,11-15].

First geometric-Arithmetic Index has been proposed in 2009 by D. VukiČeviĆ and B. Furtula. They analyzed some of its basic mathematical properties and proved that $GA_1$ to be better than well-known Randić index. $GA_1$ is defined as:

$$GA_1 = \sum_{u,v \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

We denotes $d_u$ the degree of vertex $u$ in graph $G$. The chemical applicability of the $GA_1$ index was examined and documented in detail in the paper [6], and the reviews [1,4].

Nowadays many new chemical compounds have been constructed and we need to study the chemical properties of these compounds. This process require a long time and expensive. So this paper is organized as follows. In Section 2, we specify the notation used and provide the necessary definitions. In Section 3, we will present the general formula for $GA_1$ Index to the Some Special Graphs, $k$-bridge graph, wheel graph, Web graph. In Section 4 and 5 we obtain general formula for $GA_1$ Index to vertices gluing of graphs.
2. Basic Definition and Known Result

Suppose $G_1$ and $G_2$ are graphs each containing a complete sub-graph $k_r$ ($r \geq 1$). Let $G$ be a graph obtained from the union of $G_1$ and $G_2$ by identifying the two subgraphs $k_r$ in any arbitrary way as shown in figure 1. We call $G$ a $k_r$-gluing graph of $G_1$ and $G_2$, and denoted by $e[G_1 \cup G_2]$ the family of all $k_r$-gluing graph of $G_1$ and $G_2$. In particular where $r = 1$ (resp. $r = 2$) we say $G$ is vertex-gluing graph (resp. an edge-gluing graph) of $G_1$ and $G_2$.

![Fig-1: k_r-gluing graph of G_1 and G_2.](image)

A graph is said to be complete if any two of its vertices are adjacent. The complete graph of order $n$ is denoted by $k_n$ (see Figure. 2).

![Fig-2: complete graph (k_4).](image)

A web graph $W_{(n,m)}$ is the graph obtained from the Cartesian product of the cycle $C_n$ and the path $P_m$ (see Figure. 3).

![Fig-3: web graph W_{(n,m)}](image)

A wheel $W_n$ is a graph of order $n$, $n \geq 4$ obtained from the cycle $C_{n-1}$ by adding a new vertex $v$ adjacent to each vertex of the cycle i.e. $C_{n-1} + k_1$ (see Figure. 4).
A graph consisting of $s$ paths joining two vertices is called a $k$-bridge graph, which is denoted by $\theta(a_1, ..., a_k)$, where $a_1, ..., a_k$ are the lengths of $k$ paths. Clearly a $k$-bridge graph is a generalized polygon tree (see Figure 5).

We first give some examples of $GA_1$ index for certain graphs. Let $P_n, S_n, C_n$ and $K_n$ be the path, star, cycle and complete graphs respectively with $n$ vertices.

**Example 2.1.** Consider the complete graph $K_n$ of order $n$. The first geometric–arithmetic index of this graph is computed as follow:

$$GA_1(K_n) = \frac{n(n-1)}{2}.$$

**Example 2.2.** Suppose $C_n$ is a cycle of length $n$ labeled by $1, 2, ..., n$. Then the first geometric–arithmetic index of this cycle is:

$$GA_1(C_n) = n.$$

**Example 2.3.** If $S_n$ is the star on $n$ vertices, then

$$GA_1(S_n) = \frac{2\sqrt{(n-1)^3}}{n}.$$

**Example 2.4.** If $P_n$ is the Path on $n$ vertices, then

$$GA_1(P_n) = \begin{cases} 1, & \text{if } n = 2 \\ (n-3) + \frac{4\sqrt{2}}{3}, & \text{if } n \geq 3 \end{cases}.$$

3. **First Geometric-Arithmetic Index of Some Special Graphs**

In this section, we present the general formulas for some special graphs.

**Theorem 3.1.** Let $n, m$ be positive integers. Then, the first geometric–arithmetic index of web graph $W_{(n,m)}$ is:

$$GA_1(W_{(n,m)}) = \begin{cases} n(2m - 1), & \text{if } m = 1, 2 \text{ and } n = 1, 2, ... \\ n(2m - 3) + 4n\frac{\sqrt{12}}{2}, & \text{if } m \geq 3 \text{ and } n = 1, 2, ... \end{cases}.$$

Proof. We have two cases:

**Case 1.** If $m = 1$ or $m = 2$, then we have cycles containing $n(2m - 1)$ edges, and all edges in this case have the same degree two or three.

Hence by the definition of first geometric–arithmetic index, we get:

the $GA_1$ for each one of all edges equal to one ($\frac{2\sqrt{d_u d_v}}{d_u + d_v} = 1$), then
Case 2. If \( m \geq 3 \) then, we have cycles containing \( n(2m - 3) \) edges, and all edges in this case have two vertices the same degree three or four, and \( (2n) \) of the edges link the vertices of cycles [all of them are incident on two vertices of degree three and four], then

\[
GA_1(W_{(n,m)}) = n(2m - 3) + 4n\sqrt{\frac{7}{12}} \quad \text{if } m \geq 3.
\]

**Theorem 3.3.** Let \( n, m \) be positive integers. Then, the first Geometric - Arithmetic Index of complete bipartite graph \( k_{n,m} \) is

\[
GA_1(k_{n,m}) = \frac{2(nm)\sqrt{nm}}{n + m}.
\]

Proof. In complete bipartite graph \( k_{n,m} \) there are \( nm \) edges, all of them are incident on two vertices of degree \( n \) and \( m \). Hence by the definition of first geometric–arithmetic index, we get:

\[
GA_1(W_{(n,m)}) = n(2m - 1). \quad \text{if } m = 1, 2
\]

**Theorem 3.4.** Let \( K \) be a positive integer, the first Geometric - Arithmetic Index of a \( k - bridge \) graph denoted by \( \theta(a_1, a_2, ..., a_k) \) is:

\[
GA_1(\theta(a_1, a_2, ..., a_k)) = (m - 2k) + 4k\frac{\sqrt{2k}}{k^2 + 2}.
\]

Proof. We have \( (m - 2k) \) edges, and all of them have two vertices the same degree two, and \( (2k) \) of the edges are incident on two vertices of degree two and \( k \), then

\[
GA_1(\theta(a_1, a_2, ..., a_k)) = (m - 2k) + 4k\frac{\sqrt{2k}}{k^2 + 2}.
\]

4. First Geometric-Arithmetic Index of Certain Vertex Gluing Graphs

In this section, we present the general formulas for first Geometric-Arithmetic Index to the vertices Gluing graphs.

Let \( G \) be the graph obtained from the vertex-gluing of two cycles \( C_n \) and \( C_m \) and denoted by \( e[C_n \cup_1 C_m] \), (see Figure 6).

**Theorem 4.1.** Let \( n, m \) be positive integers. Then, the first Geometric - Arithmetic Index of the vertex-gluing of two cycles of \( e[C_n \cup_1 C_m] \) is:

\[
GA_1(e[C_n \cup_1 C_m]) = (n + m - 4) + 8\frac{\sqrt{39}}{6}.
\]

Proof. We have \( (n + m - 4) \) the numbers of edges, all of them are incident on a vertices the same degree two, and \( (4) \) of them are incident on two vertices of degree two and four, then

\[
GA_1(e[C_n \cup_1 C_m]) = (n + m - 4) + 8\frac{\sqrt{39}}{6}.
\]

Let \( G \) be the graph obtained from the edge-gluing of two cycles \( C_n \) and \( C_m \) and denoted by \( e[C_n \cup_2 C_m] \), (see Figure 7).
Theorem 4.2. Let $n, m$ be positive integers. Then, the first Geometric - Arithmetic Index of the edge-gluing of two cycles $\varepsilon [C_n \cup C_m]$ is:

$$GA_1 \left( \varepsilon \left[ C_n \cup C_m \right] \right) = (n + m - 5) + 8 \frac{\sqrt{6}}{5}.$$ 

Proof. We have $(n + m - 5)$ the numbers of edges are incident on a vertices the same degree two, and (4) of them incident on a vertex of degree three, then

Let $G$ be the graph obtained from the vertex-gluing of the two $k$ -Bridge graphs $\theta_1$ and $\theta_2$ denoted by $\varepsilon[\theta_1 \cup \theta_2]$, (see Figure. 8,9).

Theorem 4.3. Let $n, m$ be positive integers. Then, the first Geometric - Arithmetic Index of the vertex-gluing by head of $\varepsilon[\theta_1 \cup \theta_2]$ is:

$$GA_1 \left( \varepsilon \left[ \theta_1 \cup \theta_2 \right] \right) = (m - 2(k_1 + k_2)) + 2k_1 \frac{\sqrt{2k_1}}{k_1 + 2} + 2k_2 \frac{\sqrt{2k_2}}{k_2 + 2} + 2(k_1 + k_2) \frac{\sqrt{2(k_1 + k_2)}}{k_1 + k_2 + 2}.$$ 

Proof. We have $(m - 2(k_1 + k_2))$ the numbers of edges, all of them have at least one vertex of degree
two, \((k_1)\) of them incident on a vertex of degree two and a vertex of degree \(k_1\), \((k_2)\) of them incident on a vertex of degree two and a vertex of degree \(k_2\), and \((k_2 + k_2)\) of them incident on a vertex of degree two and a vertex of degree \((k_2 + k_2)\).

Hence by the definition of first geometric–arithmetic index, we get:

\[
\begin{align*}
GA_1 \left( \varepsilon \left[ \theta_1 \bigcup \theta_2 \right] \right) &= (m - 2(k_1 + k_2)) + 2k_1 \sqrt{\frac{2k_1}{k_1 + 2}} \\
&+ 2k_2 \sqrt{\frac{2k_2}{k_2 + 2}} \\
&+ 2(k_1 + k_2) \sqrt{\frac{2(k_1 + k_2)}{k_1 + k_2 + 2}}.
\end{align*}
\]

**Theorem 4.4.** Let \(n,m\) be positive integers. Then, the first Geometric - Arithmetic Index of the vertex-gluing by side of \(\varepsilon[\theta_1 \cup \theta_2]\) is:

\[
G_{\text{A}} \left( \varepsilon \left[ \theta_1 \bigcup \theta_2 \right] \right) = (m - 2(k_1 + k_2)) + 4(k_1 - 1) \frac{\sqrt{2k_1}}{k_1 + 2} \\
+ 4(k_2 - 1) \frac{\sqrt{2k_2}}{k_2 + 2} + 4 \frac{\sqrt{4k_1}}{k_1 + 4} \\
+ 4 \frac{\sqrt{4k_2}}{k_2 + 4} \text{ if } a_n, b_1 = 2
\]

\[
\text{Fig.9: vertex-gluing by side of } \varepsilon[\theta_1 \cup \theta_2].
\]

Let \(G\) be the graph obtained from the edge-gluing of the two \(k\)-Bridge graphs \(\theta_1\) and \(\theta_2\) denoted by \(\varepsilon[\theta_1 \cup \theta_2]\), (see Fig.10,11,12,13).

**Theorem 4.5.** Let \(n,m\) be positive integers. Then, the first Geometric - Arithmetic Index of the edge-gluing by head of \(\varepsilon[\theta_1 \cup \theta_2]\) is:

1. If \(a_n\) and \(b_m = 2\), then
GA\(_1\left(\varepsilon \left[\theta_1 \bigcup \theta_2\right]\right)\)
\[
= (m - 2(k_1 + k_2) - 1) + 2(k_1 - 1) \frac{\sqrt{2k_1}}{k_1 + 2} + 2(k_2 - 1) \frac{\sqrt{2k_2}}{k_2 + 2} + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 1} + 2\left(\frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + \frac{\sqrt{3k_1}}{3 + k_1} + \frac{\sqrt{3k_2}}{3 + k_2}\right)
\]

2. If \(a_n\) and \(b_m\) ≥ 3, then

GA\(_1\left(\varepsilon \left[\theta_1 \bigcup \theta_2\right]\right)\)
\[
= (m - 2(k_1 + k_2) + 1) + 2k_1 \frac{\sqrt{2k_1}}{k_1 + 2} + 2k_2 \frac{\sqrt{2k_2}}{k_2 + 2} + 2\left(\frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + \frac{\sqrt{3k_1}}{3 + k_1} + \frac{\sqrt{3k_2}}{3 + k_2}\right) + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 1} + 4\sqrt{6}.
\]

3. If \(a_n = 2\) and \(b_m\) ≥ 3, then

GA\(_1\left(\varepsilon \left[\theta_1 \bigcup \theta_2\right]\right)\)
\[
= (m - 2(k_1 + k_2)) + 2(k_1 - 1) \frac{\sqrt{2k_1}}{k_1 + 2} + 2\left(\frac{\sqrt{3k_1}}{k_1 + 3} + 2k_2 \frac{\sqrt{2k_2}}{k_2 + 2} + 2\frac{\sqrt{6}}{5}\right) + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 1} + 2\left(\frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + \frac{\sqrt{3k_1}}{3 + k_1} + \frac{\sqrt{3k_2}}{3 + k_2}\right).
\]

Proof. We have three cases:

Case 1. We have \(a_i, i = 1, 2, 3, \ldots, n\), \(a_n = 2\) and \(b_i, i = 1, 2, 3, \ldots, m\), \(b_m = 2\) the numbers of edges. Therefore, we have \((m - 2(k_1 + k_2) - 1)\) of them incident on a vertex of degree two, \((k_1 - 1)\) of them incident on a vertex of degree two and a vertex of degree \(k_1\), \((k_2 - 1)\) of them incident on a vertex of degree two and a vertex of degree \(k_2\), \((k_1 + k_2 - 2)\) of them incident on a vertex of degree two and a vertex of degree \((k_1 + k_2 - 1)\), one of them incident on a vertex of degree three and a vertex of degree \((k_1 + k_2 - 1)\), and finally one of them incident on a vertex of degree three and a vertex of degree \(k_1\), and finally one of them incident on a vertex of degree three and a vertex of degree \(k_2\).

Now by the definition of first geometric–arithmetic index, we get:

GA\(_1\left(\varepsilon \left[\theta_1 \bigcup \theta_2\right]\right)\)
\[
= (m - 2(k_1 + k_2) - 1) + 2(k_1 - 1) \frac{\sqrt{2k_1}}{k_1 + 2} + 2(k_2 - 1) \frac{\sqrt{2k_2}}{k_2 + 2} + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 1} + 2\left(\frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + \frac{\sqrt{3k_1}}{3 + k_1} + \frac{\sqrt{3k_2}}{3 + k_2}\right).
\]

Case 2. We have \(a_i, i = 1, 2, 3, \ldots, n\), \(a_n \geq 3\) and \(b_i, i = 1, 2, 3, \ldots, m\), \(b_m \geq 3\) the numbers of edges. Therefore, we have \((m - 2(k_1 + k_2) + 1)\) of them incident on a vertex of degree two, \(k_1\) of them incident on a vertex of degree two and a vertex of degree \(k_1\), \(k_2\) of them incident on a vertex of degree two and a vertex of degree \(k_1\), \((k_1 + k_2 - 2)\) of them incident on a vertex of degree two and a vertex of degree \((k_1 + k_2 - 1)\), one of them incident on a vertex of degree three and a vertex of degree \(k_1\), and finally two of them incident on a vertex of degree two and a vertex of degree three. Hence by the definition of first geometric–arithmetic index, we get:

GA\(_1\left(\varepsilon \left[\theta_1 \bigcup \theta_2\right]\right)\)
\[
= (m - 2(k_1 + k_2) + 1) + 2k_1 \frac{\sqrt{2k_1}}{k_1 + 2} + 2k_2 \frac{\sqrt{2k_2}}{k_2 + 2} + 2\left(\frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + \frac{\sqrt{3k_1}}{3 + k_1} + \frac{\sqrt{3k_2}}{3 + k_2}\right) + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 1} + 4\sqrt{6}.
\]

Case 3. We have \(a_i, i = 1, 2, 3, \ldots, n\), \(a_n = 2\) and \(b_i, i = 1, 2, 3, \ldots, m\), \(b_m \geq 3\) the numbers of edges. Therefore, we have \((m - 2(k_1 + k_2))\) each one of
them has two vertices that have the same degree two, 
\( (k_1 - 1) \) of them incident on a vertex of degree two and a vertex of degree \( k_1 \), one of them incident on a vertex of degree \( k_1 \), one of them incident on a vertex of degree three and a vertex of degree \( k_1, k_2 \) of them incident on a vertex of degree two and a vertex of degree \( k_2 \), one of them incident on a vertex of degree two and a vertex of degree \( k_2 \), one of them incident on a vertex of degree \( k_1 + k_2 - 2 \) of them incident on a vertex of degree two and a vertex of degree three, \( (k_1 + k_2 - 1) \), and finally one of them incident on a vertex of degree three and a vertex of degree \( (k_1 + k_2 - 1) \).

Hence by the definition of first geometric–arithmetic index, we get:

\[
GA_1 \left( \varepsilon \left[ \theta_1 \cup \theta_2 \right] \right) = m - 2(k_1 + k_2) + 4(k_1 - 1) \frac{2k_1}{k_1 + 2} + 4(k_2 - 1) \frac{2k_2}{k_2 + 2} + 4 \frac{\sqrt{3k_1}}{k_1 + 3} + 4 \frac{\sqrt{3k_2}}{k_2 + 3}.
\]

Theorem 4.6. Let \( n, m \) be positive integers. Then, the first Geometric - Arithmetic Index of the edge-gluing by side of \( \varepsilon [\theta_1 \cup \theta_2] \) is:

If \( a_n \) and \( b_m = 2 \), then

\[
GA_1 \left( \varepsilon \left[ \theta_1 \cup \theta_2 \right] \right) = m - 2(k_1 + k_2) + 4 \frac{\sqrt{3}}{5} + 2(k_1 + k_2 - 2) \frac{\sqrt{2(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} + 2 \frac{\sqrt{3(k_1 + k_2 - 1)}}{k_1 + k_2 + 2} ; \text{ if } a_n = 2 \text{ and } b_m \geq 3.
\]

Proof. In \( n, m \)-Bridge graph the edge-gluing by side of \( \varepsilon [\theta_1 \cup \theta_2] \) there are \( a_i, i = 1, 2, 3, ..., n \), \( a_n = 2 \) and \( b_m, i = 1, 2, 3, ..., m \), \( b_m = 2 \) edges. \( m - 2(k_1 + k_2) \) the edges are also incident on a vertex of degree two, \( 2(k_1 - 1) \) of them incident on a vertex of degree two and a vertex of degree \( k_1 \), \( 2(k_2 - 1) \) of them incident on a vertex of degree two and a vertex of degree \( k_2 \), two of them incident on a vertex of degree three and a vertex of degree \( k_1 \), and finally two of them incident on a vertex of degree three and a vertex of degree \( k_2 \).

Now by the definition of first geometric–arithmetic index, we get:

\[
GA_1 \left( \varepsilon \left[ \theta_1 \cup \theta_2 \right] \right) = m - 2(k_1 + k_2) + 4(k_1 - 1) \frac{2k_1}{k_1 + 2} + 4(k_2 - 1) \frac{2k_2}{k_2 + 2} + 4 \frac{\sqrt{3k_1}}{k_1 + 3} + 4 \frac{\sqrt{3k_2}}{k_2 + 3}.
\]
Fig-10: Edge-gluing by head of $\varepsilon[\theta_1 \cup \varepsilon \theta_2]$.

Fig-11: Edge-gluing by head of $\varepsilon[\theta_1 \cup \varepsilon \theta_2]$.

Fig-12: Edge-gluing by head of $\varepsilon[\theta_1 \cup \varepsilon \theta_2]$. 
5. First Geometric-Arithmetic Index of Some Special $k_3$-Gluing Graphs

In this section, we present the general formulas for first Geometric-Arithmetic Index for some special $k_3$-Gluing graphs.

Let $G$ be the graph obtained from the $k_3$-gluing of two graphs $k_5$ and $W_n$ and denoted by $\varepsilon[k_5 \cup W_n]$, (see Figure. 14).

**Theorem 5.1**

Let $n, m$ be positive integers. Then, the first Geometric-Arithmetic Index of $k_3$-gluing of $\varepsilon[k_5 \cup W_n]$ is:

\[
GA_1\left(\varepsilon[k_5 \cup W_n]\right) = (n - 2) + 4\sqrt{\frac{15}{8}} + 8\sqrt{\frac{20}{9}} + 4\left(\sqrt{\frac{4(n + 1)}{n + 5}} + \sqrt{\frac{5(n + 1)}{n + 6}}\right) + 2(n - 3)\sqrt{\frac{3(n + 1)}{n + 4}}.
\]

**Proof.** We have the edges of complete graph $k_5$ and wheel graph $W_n$, $(n - 2)$ of them has two vertices that have the same degree, two of them incident on a vertex of degree three and a vertex of degree five, four of them incident on a vertex of degree four and a vertex of degree five, two of them incident on a vertex of degree four and a vertex of degree five, two of them incident on a vertex of degree five and a vertex of degree five, and finally two of them incident on a vertex of degree three and a vertex of degree five.

Hence by the definition of first geometric-arithmetic index, we get:
Example 5.2
Let $G$ be a graph of $k_3$-gluing of complete graph $k_5$ and wheel graph $w_n$, $n = 6$, then the first geometric–arithmetic index of the $k_3$-gluing of $k_5$ and $w_n$ is

$$GA_1\left(\varepsilon \left\{ k_5 \bigcup_3 w_n \right\} \right)$$

$$= (n - 2) + 4 \frac{\sqrt{15}}{8} + 8 \frac{\sqrt{20}}{9}$$

$$+ 4 \left( \frac{\sqrt{4(n + 1)}}{n + 5} + \frac{\sqrt{5(n + 1)}}{n + 6} \right)$$

$$+ 2(n - 3) \frac{\sqrt{3(n + 1)}}{n + 4}$$

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