

Harary Index of Pericondensed Benzenoid Graphs

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Abstract

The Harary index of a connected graph is equal to the sum of reciprocal distance between all pairs of its vertices. An $\ell \times m \times n$ pericondensed benzenoid graph, denoted by $L_{\ell,m,n}$, is a graph consisting of three rows benzenoid chains with size ℓ, m, n , respectively. In this paper, we compute the Harary index of $\ell \times m \times n$ pericondensed benzenoid graphs.

1 Introduction

In theoretical chemistry and biology, molecular structure descriptors have been used for quantifying information on molecules. This relates to characterizing physico-chemical, toxicologic, pharmacologic, biological and other properties of chemical compounds by

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utilizing molecular indices. We point out that the so-called topological indices are an important class thereof. Actually, thousands of topological indices have been introduced in order to describe physical and chemical properties of molecules. Those indices can be divided into several classes, namely degree-based indices [10–13,15,16,18,21,30], distance-based indices [28,31], eigenvalue-based indices [19] and others. The Harary index is one of widely studied distance-based indices. The Harary index of a connected graph G , denoted by $H(G)$, was introduced by Plavšić et al. [22] in 1991 in honor of Professor Frank Harary on his 70th birthday, who greatly influenced the development of graph theory and chemical graph theory. The Harary index and the related indices have shown a modest success in structure property correlations, and their use in combination with other descriptors improves the QSPR models. This index is equal to the sum of reciprocal distance of all pairs of vertices of respective graph, i.e.,

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)}.$$

The study of finding explicit combinatorial expressions for topological index of several classes of connected graphs was also proposed in a few decades [1, 6, 7]. In comparison to the acyclic graphs [2, 14, 20], it has been discovered that this problem is much difficult for polycyclic graphs. Note that the majority of molecular graphs are polycyclic. This is particularly frustrating in chemical applications. Nevertheless, with the appearance of some techniques containing the method of elemental edge-cut developed by Klavžar, Gutman and Mohar [17] and combinatorial algorithm developed by Shiu et al. [23], numerous explicit formulas for Wiener index of special classes of benzenoid graphs have been deduced [23, 25, 26] to name a few. Unfortunately, these methods can not be efficiently applied to many other types of topological indices, especially Harary index. For this purpose, various topological indices for molecular graphs, including nanotubes, nanotorus, catacondensed benzenoid graphs have been investigated (see eg. [3, 4, 8, 9]).

In this paper, we consider a widely studied classes of benzenoid graphs, which is called *pericondensed benzenoid graph*. A pericondensed benzenoid graph is a benzenoid graph containing internal vertices. Actually, we consider the pericondensed benzenoid graph consisting of three rows of hexagons of various lengths. Various topological indices, including Wiener index [27], PI index [5], Omega polynomials [29] and Sadhana polynomials [29] et al., have been calculated for these molecules up to this time. The primary aim of this article is to compute the Harary index for pericondensed benzenoid graphs consisting of three rows of hexagons of various lengths.

2 Main results

The following definition of wall was first introduced in [24]. The infinite graph W is called the *wall* if its vertex set $V(W) = \{(x, y) | x \in \mathbb{Z}\}$ and edge set

$$E(W) = \{(x_1, y_1) \sim (x_2, y_2) \mid y_1 = y_2 \text{ and } |x_1 - x_2| = 1, \\ \text{or } x_1 = x_2, |y_1 - y_2| = 1 \text{ and } x_1 + y_1 + x_2 + y_2 \equiv 1 \pmod{4}\}.$$

An n -benzenoid chain, denoted by L_n , is a graph formed by a row of n hexagonal cells. We identify L_n as a subgraph of wall and describe the vertex set of L_n as $\{(x, y) \in \mathbb{Z}^2 \mid 0 \leq y \leq 1, 0 \leq x \leq 2n\}$. An $\ell \times m \times n$ pericondensed benzenoid system, denoted by $L_{\ell, m, n}$, is a graph consisting of three rows benzenoid chains with size ℓ, m, n , respectively. We identify $L_{\ell, m, n}$ as a subgraph of wall and so describe its vertex set as

$$\{(x, y) \in \mathbb{Z}^2 \mid y = 0, 0 \leq x \leq 2n, \text{ or} \\ y = 1, 0 \leq x \leq \max\{2n, 2m + 1\}, \text{ or} \\ y = 2, 0 \leq x \leq \max\{2\ell, 2m + 1\}, \text{ or} \\ y = 3, 0 \leq x \leq 2\ell\}.$$

As an example, the graphs L_4 and $L_{3,4,5}$ are depicted as follows:

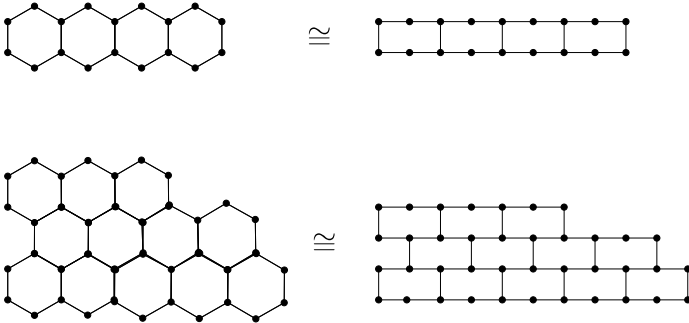


Fig. 1. The graphs L_3 and $L_{3,4,5}$.

For a benzenoid graph $L_{\ell, m, n}$, we will also use the following notation. Let $S_0 = \{(x, 0) | 0 \leq x \leq 2n\}$, $S_1 = \{(x, 1) | 0 \leq x \leq \max\{2n, 2m + 1\}\}$, $S_2 = \{(x, 2) | 0 \leq x \leq \max\{2\ell, 2m + 1\}\}$, and $S_3 = \{(x, 3) | 0 \leq x \leq 2\ell\}$. It is easy to see that $V(L_{\ell, m, n}) = S_0 \cup S_1 \cup S_2 \cup S_3$. For convenient, we define the following three functions for integers ℓ, m and n :

$$\begin{aligned}
 h_1(\ell, m, n) &= (10n + 8)f(2n + 1) + (6n + 10)f(2n + 3) + (4\ell + 3)f(2\ell + 1) + (6\ell + 9)f(2\ell + 2) \\
 &\quad + (2\ell + 2)f(2\ell + 3) + (6m + 8)f(2m + 2) + (2m + 4)f(2m + 3) - (4n - 4m + 1)f(2n \\
 &\quad - 2m) + (4n - 4\ell + 3)f(2n - 2\ell + 1) - (4n - 4\ell + 5)f(2n - 2\ell + 2) - (4n - 4\ell + 7)f(\\
 &\quad 2n - 2\ell + 3) + f(2n - 2\ell + 4) + 2f(2n - 2\ell + 5) + f(2n - 2\ell + 6) - (2m - 2\ell + 2)f(2m \\
 &\quad - 2\ell + 1) - (10n + 18m + 30\ell + 42) - \left(\frac{140n + 91m - 27\ell}{210} - \frac{15}{28} \right),
 \end{aligned}$$

$$\begin{aligned}
 h_2(\ell, m, n) &= (4n + 3)f(2n + 1) + (4n + 7)f(2n + 3) + (8m + 10)f(2m + 2) + (8m + 14)f(2m + 3) \\
 &\quad + (8\ell + 7)f(2\ell + 1) + 2f(2\ell + 2) + f(2\ell + 3) - (2n - 2\ell + 4)f(2n - 2\ell + 5) + f(2n - 2\ell \\
 &\quad + 6) - (4m - 4\ell + 5)f(2m - 2\ell + 2) - (4m - 4n + 5)f(2m - 2n + 2) - (18n + 10m \\
 &\quad + 30\ell + 38) - \left(\frac{140m + 91n + 113\ell}{210} + \frac{9}{140} \right),
 \end{aligned}$$

$$\begin{aligned}
 h_3(\ell, m, n) &= (10n + 8)f(2n + 1) + (6n + 10)f(2n + 3) + (10\ell + 8)f(2\ell + 1) + (6\ell + 10)f(2\ell + 3) \\
 &\quad + (8m + 20)f(2m + 4) - (4m + 12)f(2m + 5) + (4n + 4\ell - 8m + 1)f(2n + 2\ell - 4m) \\
 &\quad + (4n + 4\ell - 8m + 3)f(2n + 2\ell - 4m + 1) - (4n - 4m + 1)f(2n - 2m) - (8n - 8m \\
 &\quad + 7)f(2n - 2m + 1) - (4n - 4m + 5)f(2n - 2m + 3) + f(2n - 2m + 4) - (8\ell - 8m \\
 &\quad - 10)(f(2\ell - 2m - 3) - f(2\ell - 2m - 1)) - (6\ell - 6m + 2)f(2\ell - 2m) - (10\ell - 10m \\
 &\quad + 12)f(2\ell - 2m + 2) + f(2\ell - 2m + 3) + f(2\ell - 2m + 4) - \frac{32(n + \ell)}{3} - (38m + 15) \\
 &\quad + \left(\frac{38m}{105} + \frac{37}{210} \right).
 \end{aligned}$$

To deduce our main result, we need several lemmas as follows.

Lemma 2.1 Let $f(n) = \sum_{i=1}^n \frac{1}{i}$. Then

$$\sum_{i=1}^n f(i) = (n + 1)f(n + 1) - (n + 1) = (n + 1)f(n) - n.$$

Lemma 2.2 For $n \geq 2$, $H(P_n) = nf(n) - n$.

Lemma 2.3 For $n \geq 1$, $H(L_n) = (8n + 6)f(2n + 1) - \frac{32n}{3} - 5$.

Proof: Let $V(L_n) = S_0 \cup S_1$, where $S_i = \{(x, i) \mid 0 \leq x \leq 2n\}$ for $0 \leq i \leq 1$. Then

$$H(L_n) = \sum_{\{u,v\} \subseteq S_0} \frac{1}{d(u,v)} + \sum_{\{u,v\} \subseteq S_1} \frac{1}{d(u,v)} + \sum_{u \in S_0, v \in S_1} \frac{1}{d(u,v)}.$$

Given two vertices $u = (a, 0)$ and $v = (b, 1)$, $d(u, v) = |a - b| + 1$ if $a \neq b$, or $a = b$ and a, b are even, and $d(u, v) = 3$ if $a = b$ and a, b are odd. Thus, we have

$$\begin{aligned}
 \sum_{u \in S_0, v \in S_1} \frac{1}{d(u,v)} &= \sum_{i=0}^{2n} \sum_{j=0}^{2n} \frac{1}{|i - j| + 1} + n \left(\frac{1}{3} - 1 \right) \\
 &= \sum_{i=0}^{2n} \sum_{j=0}^i \frac{1}{i - j + 1} + \sum_{i=0}^{2n-1} \sum_{j=i+1}^{2n} \frac{1}{j - i + 1} - \frac{2n}{3}
 \end{aligned}$$

$$\begin{aligned}
 &= \sum_{i=1}^{2n+1} f(i) + \sum_{i=1}^{2n+1} (f(i) - 1) - \frac{2n}{3} \\
 &= (4n + 4)f(2n + 1) - \left(\frac{20n}{3} + 3 \right).
 \end{aligned}$$

Notice that $\sum_{\{u,v\} \subseteq S_0} \frac{1}{d(u,v)} = \sum_{\{u,v\} \subseteq S_1} \frac{1}{d(u,v)} = H(P_{2n+1})$. Hence, by Lemma 2.2 and some elementary calculations, we have $H(L_n) = (8n + 6)f(2n + 1) - \left(\frac{32n}{3} + 5 \right)$. \blacksquare

Lemma 2.4 For $n \geq 1$, $H(L_{n+1,n,n+1}) = (20n + 36)f(2n + 3) + (8n + 20)f(2n + 4) + (4n + 12)f(2n + 5) - (58n + 104) - \left(\frac{102n}{105} + \frac{103}{210} \right)$.

Proof: Note that $S_i = \{(x, i) | 0 \leq x \leq 2n + 2\}$ for $0 \leq i \leq 3$. Since $\sum_{\{u,v\} \subseteq S_0 \cup S_1} \frac{1}{d(u,v)} = \sum_{\{u,v\} \subseteq S_2 \cup S_3} \frac{1}{d(u,v)} = H(L_{n+1})$ and $\sum_{u \in S_1, v \in S_3} \frac{1}{d(u,v)} = \sum_{u \in S_0, v \in S_2} \frac{1}{d(u,v)}$, we have

$$\begin{aligned}
 H(L_{n+1,n,n+1}) &= \sum_{\{u,v\} \subseteq S_0 \cup S_1} \frac{1}{d(u,v)} + \sum_{\{u,v\} \subseteq S_2 \cup S_3} \frac{1}{d(u,v)} + \sum_{u \in S_0, v \in S_2} \frac{1}{d(u,v)} + \sum_{u \in S_0, v \in S_3} \frac{1}{d(u,v)} \\
 &\quad + \sum_{u \in S_1, v \in S_2} \frac{1}{d(u,v)} + \sum_{u \in S_1, v \in S_3} \frac{1}{d(u,v)} \\
 &= 2H(L_{n+1}) + \sum_{u \in S_1, v \in S_2} \frac{1}{d(u,v)} + 2 \sum_{u \in S_1, v \in S_3} \frac{1}{d(u,v)} + \sum_{u \in S_0, v \in S_3} \frac{1}{d(u,v)}.
 \end{aligned}$$

Firstly, we consider $\sum \frac{1}{d(u,v)}$ for $u \in S_1$ and $v \in S_2$. For two vertices $u = (a, 1)$ and $v = (b, 2)$, $d(u, v) = |a - b| + 1$ if $|a - b| \neq 0$ or $a = b$ and a is odd, and $d(u, v) = 3$ if $a = b$ and a is even. Thus, we have

$$\begin{aligned}
 \sum_{u \in S_1, v \in S_2} \frac{1}{d(u,v)} &= \sum_{i=0}^{2n+2} \sum_{j=0}^{2n+2} \frac{1}{|i - j| + 1} + (n + 2) \left(\frac{1}{3} - 1 \right) \\
 &= \sum_{i=0}^{2n+2} \sum_{j=0}^i \frac{1}{i - j + 1} + \sum_{i=0}^{2n+1} \sum_{j=i+1}^{2n+2} \frac{1}{j - i + 1} - \frac{2n + 4}{3} \\
 &= \sum_{i=1}^{2n+3} f(i) + \sum_{i=1}^{2n+3} (f(i) - f(1)) - \frac{2n + 4}{3} \\
 &= (4n + 8)f(2n + 3) - (6n + 10) - \left(\frac{2n + 1}{3} \right).
 \end{aligned}$$

Secondly, we compute $\sum \frac{1}{d(u,v)}$ for $u \in S_1$ and $v \in S_3$. For two vertices $u = (a, 1)$ and $v = (b, 3)$, $d(u, v) = |a - b| + 2$ if $|a - b| \geq 2$ or $|a - b| = 1$ and a is odd, and $d(u, v) = |a - b| + 4$ if $a = b$ or $|a - b| = 1$ and a is even. Thus, we have

$$\sum_{u \in S_1, v \in S_3} \frac{1}{d(u,v)} = \sum_{i=0}^{2n+2} \sum_{j=0}^{2n+2} \frac{1}{|i - j| + 2} + 2(n + 1) \left(\frac{1}{5} - \frac{1}{3} \right) + (2n + 3) \left(\frac{1}{4} - \frac{1}{2} \right)$$

$$\begin{aligned}
 &= \sum_{i=0}^{2n+2} \sum_{j=0}^i \frac{1}{i-j+2} + \sum_{i=0}^{2n+1} \sum_{j=i+1}^{2n+2} \frac{1}{j-i+2} - \frac{46n+61}{60} \\
 &= \sum_{i=1}^{2n+4} (f(i) - f(1)) + \sum_{i=1}^{2n+4} (f(i) - f(2)) + \frac{1}{2} - \left(\frac{23n}{30} + \frac{61}{60} \right) \\
 &= (4n+10)f(2n+4) - (9n+18) - \left(\frac{23n}{30} + \frac{31}{60} \right).
 \end{aligned}$$

Lastly, we determine $\sum \frac{1}{d(u,v)}$ for $u \in S_0$ and $v \in S_3$. For two vertices $u = (a, 0)$ and $v = (b, 3)$, $d(u, v) = |a-b|+3$ if $|a-b| \geq 3$ or $|a-b| = 2$ and a is even, $d(u, v) = |a-b|+5$ if $|a-b| = 2$ and a is odd, or $|a-b| = 1$, or $a = b$ and a is even, and $d(u, v) = 7$ if $a = b$ and a is odd. Thus, we have

$$\begin{aligned}
 \sum_{u \in S_0, v \in S_3} \frac{1}{d(u, v)} &= \sum_{i=0}^{2n+2} \sum_{j=0}^{2n+2} \frac{1}{|i-j|+3} + 2n \left(\frac{1}{7} - \frac{1}{5} \right) + 2(2n+2) \left(\frac{1}{6} - \frac{1}{4} \right) \\
 &\quad + (n+2) \left(\frac{1}{5} - \frac{1}{3} \right) + (n+1) \left(\frac{1}{7} - \frac{1}{3} \right) \\
 &= \sum_{i=0}^{2n+2} \sum_{j=0}^i \frac{1}{i-j+3} + \sum_{i=0}^{2n+1} \sum_{j=i+1}^{2n+2} \frac{1}{j-i+3} - \frac{81n+83}{105} \\
 &= \sum_{i=1}^{2n+5} (f(i) - f(2)) + \frac{1}{2} + \sum_{i=1}^{2n+5} (f(i) - f(3)) + \frac{7}{6} - \left(\frac{27n}{35} + \frac{83}{105} \right) \\
 &= (4n+12)f(2n+5) - (11n+25) - \frac{46n+83}{105}.
 \end{aligned}$$

Thus by Lemma 2.3, we get $H(L_{n+1, n, n+1}) = (20n+36)f(2n+3) + (8n+20)f(2n+4) + (4n+12)f(2n+5) - (58n+104) - \left(\frac{102n}{105} + \frac{103}{210} \right)$. ■

Lemma 2.5 *Let $m, n \in N$ with $m \geq n$. Then $H(L_{n, m, n}) = (8m+10)f(2m+2) + (8m+14)f(2m+3) + (12n+10)f(2n+1) + 2f(2n+2) + (4n+8)f(2n+3) - (8m-8n+10)f(2m-2n+2) - \frac{32m}{3} - (48n+44) - \left(\frac{32n}{105} + \frac{109}{210} \right)$.*

Proof: Note that $S_i = \{(x, i) | 0 \leq x \leq 2n\}$ for $i = 0, 3$ and $S_i = \{(x, i) | 0 \leq x \leq 2m+1\}$ for $i = 1, 2$. Let $S'_i = \{(x, i) | 2n+1 \leq x \leq 2m+1\}$ for $i = 1, 2$. Then $L_{n, m, n} - S'_1 - S'_2 \cong L_{n, n-1, n}$. Let $V' = V(L_{n, m, n}) - S'_1 - S'_2$. Hence, by symmetry,

$$\begin{aligned}
 H(L_{n, m, n}) &= \sum_{\{u, v\} \subseteq V'} \frac{1}{d(u, v)} + \sum_{\{u, v\} \subseteq S'_1 \cup S'_2} \frac{1}{d(u, v)} + \sum_{u \in S'_1, v \in V'} \frac{1}{d(u, v)} + \sum_{u \in S'_2, v \in V'} \frac{1}{d(u, v)} \\
 &= H(L_{n, n-1, n}) + H(L_{m-n}) + 2 \sum_{u \in S'_1, v \in V'} \frac{1}{d(u, v)},
 \end{aligned}$$

where $L_{m-n} = K_2$ if $m = n$. For $u = (a, b) \in S'_1$ and $v = (c, d) \in V'$, we have $d(u, v) = a - c + |b - d|$. Thus, we obtain

$$\begin{aligned}
 & \sum_{u \in S'_1, v \in V'} \frac{1}{d(u, v)} \\
 &= \sum_{i=0}^{2n} \sum_{j=0}^{2m-2n} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} + \frac{1}{i+j+2} + \frac{1}{i+j+3} \right) \\
 &= \left[\sum_{i=1}^{2m+1} f(i) - \sum_{i=1}^{2n} f(i) - \sum_{i=1}^{2m-2n} f(i) \right] + 2 \left[\sum_{i=1}^{2m+2} f(i) - \sum_{i=1}^{2n+1} f(i) - \sum_{i=1}^{2m-2n+1} f(i) \right] \\
 & \quad + \left[\sum_{i=1}^{2m+3} f(i) - \left(\sum_{i=1}^{2n+2} f(i) - f(1) \right) - \sum_{i=1}^{2m-2n+2} f(i) \right] \\
 &= (4m+5)f(2m+2) + (4m+7)f(2m+3) - (4n+3)f(2n+1) - (4n+5)f(2n \\
 & \quad + 2) - (4m-4n+3)f(2m-2n+1) - (4m-4n+5)f(2m-2n+2) + 3.
 \end{aligned}$$

By Lemmas 2.3 and 2.4, we get the desired result. \blacksquare

Lemma 2.6 *Let $m, n \in \mathbb{N}$ with $n \geq m$. Then $H(L_{m,m-1,n}) = (10n+8)f(2n+1) + (6n+10)f(2n+3) + (10m+8)f(2m+1) + (8m+12)f(2m+2) - (2m+2)f(2m+3) - (4n-4m+5)f(2n-2m+2) - (4n-4m+7)f(2n-2m+3) + f(2n-2m+4) + 2f(2n-2m+5) + f(2n-2m+6) - \frac{32n}{3} - (48m+34) - \left(\frac{32m}{105} + \frac{2}{7} \right)$.*

Proof: Notice that $S_i = \{(x, i) | 0 \leq x \leq 2n\}$ for $0 \leq i \leq 1$ and $S_i = \{(x, i) | 0 \leq x \leq 2m\}$ for $2 \leq i \leq 3$. Let $S'_i = \{(x, i) | 2m+1 \leq x \leq 2n\}$ for $i = 0, 1$. Then $L_{m,m-1,n} - S'_0 - S'_1 \cong L_{m,m-1,m}$. Let $V' = V(L_{m,m-1,n}) - S'_0 - S'_1$. Hence,

$$\begin{aligned}
 H(L_{m,m-1,n}) &= \sum_{\{u,v\} \subseteq V'} \frac{1}{d(u,v)} + \sum_{\{u,v\} \subseteq S'_0 \cup S'_1} \frac{1}{d(u,v)} + \sum_{u \in S'_0, v \in V'} \frac{1}{d(u,v)} + \sum_{u \in S'_1, v \in V'} \frac{1}{d(u,v)} \\
 &= H(L_{m,m-1,m}) + \left[H(L_{n-m-1}) + 2f(2n-2m-1) + 2f(2n-2m) - 2 + \frac{1}{3} \right] \\
 & \quad + \sum_{u \in S'_0, v \in V'} \frac{1}{d(u,v)} + \sum_{u \in S'_1, v \in V'} \frac{1}{d(u,v)}.
 \end{aligned}$$

Next we consider the last two items in the above equation. Firstly, we have

$$\begin{aligned}
 & \sum_{u \in S'_0, v \in V'} \frac{1}{d(u, v)} \\
 &= \sum_{i=0}^{2m} \sum_{j=0}^{2n-2m-1} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} \right) + \sum_{i=0}^{2m-1} \sum_{j=0}^{2n-2m-1} \frac{1}{i+j+4} + \sum_{j=0}^{2n-2m-1} \frac{1}{j+5}
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{i=0}^{2m-2} \sum_{j=0}^{2n-2m-1} \frac{1}{i+j+6} + \sum_{j=0}^{2n-2m-1} \left(\frac{1}{j+6} + \frac{1}{j+7} \right) \\
= & \left[\sum_{i=1}^{2n} f(i) - \sum_{i=1}^{2m} f(i) - \sum_{i=1}^{2n-2m-1} f(i) \right] + \left[\sum_{i=1}^{2n+1} f(i) - \sum_{i=1}^{2m+1} f(i) - \sum_{i=1}^{2n-2m} f(i) \right] \\
& + \left[\sum_{i=1}^{2n+2} f(i) - \left(\sum_{i=1}^{2m+2} f(i) - f(1) - f(2) \right) - \sum_{i=1}^{2n-2m+2} f(i) \right] + f(2n-2m+4) \\
& - f(4) + \left[\sum_{i=1}^{2n+3} f(i) - \left(\sum_{i=1}^{2m+3} f(i) - \sum_{i=1}^4 f(i) \right) - \sum_{i=1}^{2n-2m+4} f(i) \right] \\
& + f(2n-2m+5) - f(5) + f(2n-2m+6) - f(6) \\
= & (4n+3)f(2n+1) + (4n+7)f(2n+3) - (4m+3)f(2m+1) - (4m+7)f(2m \\
& + 3) - (4n-4m+1)f(2n-2m) - (4n-4m+7)f(2n-2m+3) + f(2n-2m \\
& + 5) + f(2n-2m+6) + \frac{81}{10}.
\end{aligned}$$

Then we compute the last one and obtain

$$\begin{aligned}
& \sum_{u \in S'_1, v \in V'} \frac{1}{d(u, v)} \\
= & \sum_{i=0}^{2m} \sum_{j=0}^{2n-2m-1} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} \right) + \sum_{i=0}^{2m-1} \sum_{j=0}^{2n-2m-1} \frac{1}{i+j+3} + \sum_{j=0}^{2n-2m-1} \frac{1}{j+4} \\
& + \sum_{i=0}^{2m-2} \sum_{j=0}^{2n-2m-1} \frac{1}{i+j+5} + \sum_{j=0}^{2n-2m-1} \left(\frac{1}{j+5} + \frac{1}{j+6} \right) \\
= & \left[\sum_{i=1}^{2n} f(i) - \sum_{i=1}^{2m} f(i) - \sum_{i=1}^{2n-2m-1} f(i) \right] + \left[\sum_{i=1}^{2n+1} f(i) - \sum_{i=1}^{2m+1} f(i) - \sum_{i=1}^{2n-2m} f(i) \right] \\
& + \left[\sum_{i=1}^{2n+1} f(i) - \left(\sum_{i=1}^{2m+1} f(i) - f(1) \right) - \sum_{i=1}^{2n-2m+1} f(i) \right] + f(2n-2m+3) - f(3) \\
& + \left[\sum_{i=1}^{2n+2} f(i) - \left(\sum_{i=1}^{2m+2} f(i) - \sum_{i=1}^3 f(i) \right) - \sum_{i=1}^{2n-2m+3} f(i) \right] + f(2n-2m+4) - f(4) \\
& + f(2n-2m+5) - f(5) \\
= & (6n+5)f(2n+1) + (2n+3)f(2n+3) - (6m+5)f(2m+1) - (2m+3)f(2m \\
& + 3) - (4n-4m+1)f(2n-2m) - (4n-4m+5)f(2n-2m+2) + f(2n-2m \\
& + 4) + f(2n-2m+5) + \frac{47}{15}.
\end{aligned}$$

Then by Lemmas 2.3 and 2.4, we get the desired result. ■

Lemma 2.7 *Let $\ell, m, n \in \mathbb{N}$ with $m < \ell \leq n$. Then $H(L_{\ell, m, n}) = h_3(\ell, m, n)$.*

Proof: Notice that $S_i = \{(x, i) | 0 \leq x \leq 2n\}$ for $0 \leq i \leq 1$ and $S_i = \{(x, i) | 0 \leq x \leq 2\ell\}$ for $2 \leq i \leq 3$. Let $S'_i = \{(x, i) | 2m+3 \leq x \leq 2\ell\}$ for $i = 2, 3$. Then $L_{\ell, m, n} - S'_2 - S'_3 \cong L_{m+1, m, n}$. Let $V' = V(L_{\ell, m, n}) - S'_2 - S'_3$. Hence,

$$\begin{aligned} H(L_{\ell, m, n}) &= \sum_{\{u, v\} \subseteq V'} \frac{1}{d(u, v)} + \sum_{\{u, v\} \subseteq S'_2 \cup S'_3} \frac{1}{d(u, v)} + \sum_{u \in S'_2, v \in V'} \frac{1}{d(u, v)} + \sum_{u \in S'_3, v \in V'} \frac{1}{d(u, v)} \\ &= H(L_{m+1, m, n}) + \left[H(L_{\ell-m-2}) + 2f(2\ell-2m-3) + 2f(2\ell-2m-2) - 2 \right. \\ &\quad \left. + \frac{1}{3} \right] + \sum_{u \in S'_2, v \in V'} \frac{1}{d(u, v)} + \sum_{u \in S'_3, v \in V'} \frac{1}{d(u, v)}. \end{aligned}$$

Next we consider the last two items in the above equation. Firstly, we have

$$\begin{aligned} &\sum_{u \in S'_2, v \in V'} \frac{1}{d(u, v)} \\ &= \sum_{i=0}^{2m+2} \sum_{j=0}^{2\ell-2m-3} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} \right) + \sum_{i=0}^{2m+1} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+3} + \sum_{i=0}^{2n-2m-2} \\ &\quad \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+4} + \sum_{i=0}^{2m} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+5} + \sum_{i=0}^{2n-2m-2} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+5} \\ &\quad + \sum_{j=0}^{2\ell-2m-3} \frac{1}{j+6} \\ &= \left[\sum_{i=1}^{2\ell} f(i) - \sum_{i=1}^{2m+2} f(i) - \sum_{i=1}^{2\ell-2m-3} f(i) \right] + \left[\sum_{i=1}^{2\ell+1} f(i) - \sum_{i=1}^{2m+3} f(i) - \sum_{i=1}^{2\ell-2m-2} f(i) \right] \\ &\quad + \left[\sum_{i=1}^{2\ell+1} f(i) - \left(\sum_{i=1}^{2m+3} f(i) - f(1) \right) - \sum_{i=1}^{2\ell-2m-1} f(i) \right] + \left[\sum_{i=1}^{2n+2\ell-4m-1} f(i) - \right. \\ &\quad \left(\sum_{i=1}^{2n-2m+1} f(i) - \sum_{i=1}^2 f(i) \right) - \sum_{i=1}^{2\ell-2m} f(i) \right] + \left[\sum_{i=1}^{2\ell+2} f(i) - \left(\sum_{i=1}^{2m+4} f(i) - \sum_{i=1}^3 f(i) \right) \right. \\ &\quad \left. - \sum_{i=1}^{2\ell-2m+1} f(i) \right] + \left[\sum_{i=1}^{2n+2\ell-4m} f(i) - \left(\sum_{i=1}^{2n-2m+2} f(i) - \sum_{i=1}^3 f(i) \right) - \sum_{i=1}^{2\ell-2m+1} f(i) \right] \\ &\quad + f(2\ell-2m+3) - f(5) \\ &= (6\ell+5)f(2\ell+1) + (2\ell+3)f(2\ell+3) + (4n+4\ell-8m+1)f(2n+2\ell-4m) \\ &\quad - (6m+11)f(2m+3) - (2m+5)f(2m+5) - (4n-4m+5)f(2n-2m+2) \\ &\quad - (4\ell-4m-3)f(2\ell-2m-2) - (4\ell-4m+1)f(2\ell-2m) - (4\ell-4m+4)f(2\ell \\ &\quad - 2m+2) + f(2\ell-2m+3) + 21 + \frac{53}{60}. \end{aligned}$$

Then we compute the last one and obtain

$$\begin{aligned}
 & \sum_{u \in S'_3, v \in V'} \frac{1}{d(u, v)} \\
 = & \sum_{i=0}^{2m+2} \sum_{j=0}^{2\ell-2m-3} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} \right) + \sum_{i=0}^{2m+1} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+4} + \sum_{i=0}^{2n-2m-2} \\
 & \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+5} + \sum_{i=0}^{2m} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+6} + \sum_{i=0}^{2n-2m-2} \sum_{j=0}^{2\ell-2m-3} \frac{1}{i+j+6} \\
 & + \sum_{j=0}^{2\ell-2m-3} \frac{1}{j+7} \\
 = & \left[\sum_{i=1}^{2\ell} f(i) - \sum_{i=1}^{2m+2} f(i) - \sum_{i=1}^{2\ell-2m-3} f(i) \right] + \left[\sum_{i=1}^{2\ell+1} f(i) - \sum_{i=1}^{2m+3} f(i) - \sum_{i=1}^{2\ell-2m-2} f(i) \right] \\
 & + \left[\sum_{i=1}^{2\ell+2} f(i) - \left(\sum_{i=1}^{2m+4} f(i) - f(1) - f(2) \right) - \sum_{i=1}^{2\ell-2m} f(i) \right] + \left[\sum_{i=1}^{2n+2\ell-4m} f(i) - \right. \\
 & \left. \left(\sum_{i=1}^{2n-2m+2} f(i) - \sum_{i=1}^3 f(i) \right) - \sum_{i=1}^{2\ell-2m+1} f(i) \right] + \left[\sum_{i=1}^{2\ell+3} f(i) - \left(\sum_{i=1}^{2m+5} f(i) - \sum_{i=1}^4 f(i) \right) \right. \\
 & \left. - \sum_{i=1}^{2\ell-2m+2} f(i) \right] + \left[\sum_{i=1}^{2n+2\ell-4m+1} f(i) - \left(\sum_{i=1}^{2n-2m+3} f(i) - \sum_{i=1}^4 f(i) \right) - \sum_{i=1}^{2\ell-2m+2} f(i) \right] \\
 & + f(2\ell - 2m + 4) - f(6) \\
 = & (4\ell + 3)f(2\ell + 1) + (4\ell + 7)f(2\ell + 3) + (4n + 4\ell - 8m + 3)f(2n + 2\ell - 4m \\
 & + 1) - (4m + 7)f(2m + 3) - (4m + 11)f(2m + 5) - (4n - 4m + 7)f(2n - 2m \\
 & + 3) - (4\ell - 4m - 3)f(2\ell - 2m - 2) - (2\ell - 2m + 1)f(2\ell - 2m) - (6\ell - 6m \\
 & + 8)f(2\ell - 2m + 2) + f(2\ell - 2m + 4) + 31 + \frac{13}{60}.
 \end{aligned}$$

By Lemmas 2.3 and 2.6, we get $H(L_{\ell, m, n}) = h_3(\ell, m, n)$. ■

Lemma 2.8 *Let $\ell, m, n \in N$ with $\ell \leq m < n$. Then $H(L_{\ell, m, n}) = h_1(\ell, m, n)$.*

Proof: Notice that $S_i = \{(x, i) | 0 \leq x \leq 2n\}$ for $0 \leq i \leq 1$, $S_2 = \{(x, 2) | 0 \leq x \leq 2m + 1\}$ and $S_3 = \{(x, 3) | 0 \leq x \leq 2\ell\}$. Let $S'_2 = \{(x, 2) | 2\ell + 1 \leq x \leq 2m + 1\}$. Then $L_{\ell, m, n} - S'_2 \cong L_{\ell, \ell-1, n}$. Let $V' = V(L_{\ell, m, n}) - S'_2$. Hence, $H(L_{\ell, m, n}) = \sum_{\{u, v\} \subseteq V'} \frac{1}{d(u, v)} + \sum_{\{u, v\} \subseteq S'_2} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_2 \\ v \in V'}} \frac{1}{d(u, v)}$. Next we consider the last one item in the above equation. For $u = (a, 2) \in S'_2$ and $v = (b, 1) \in S_1$, $d(u, v) = |a - b| + 1$ if $a - b \neq 0$, or $a = b$ and a is odd, and $d(u, v) = 3$ if $a = b$ and a is even. For $u = (a, 2) \in S'_2$

and $v = (b, 0) \in S_0$, $d(u, v) = |a - b| + 2$ if $|a - b| \geq 2$, or $|a - b| = 1$ and a is odd, and $d(u, v) = |a - b| + 4$ if $|a - b| = 1$ and a is even, or $a = b$. Thus, we have

$$\begin{aligned}
 & \sum_{\substack{u \in S'_2 \\ v \in V'}} \frac{1}{d(u, v)} \\
 = & \sum_{\substack{u \in S'_2 \\ v \in S_3 \cup (S_2 - S'_2)}} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_2 \\ v \in S_1}} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_2 \\ v \in S_0}} \frac{1}{d(u, v)} \\
 = & \left[\sum_{i=0}^{2\ell} \sum_{j=0}^{2m-2\ell} \left(\frac{1}{i+j+1} + \frac{1}{i+j+2} \right) \right] + \left[\sum_{i=0}^{2n} \sum_{j=2\ell+1}^{2m+1} \frac{1}{|i-j|+1} + (m-\ell) \left(\frac{1}{3} - 1 \right) \right] \\
 & + \left[\sum_{i=0}^{2n} \sum_{j=2\ell+1}^{2m+1} \frac{1}{|i-j|+2} + 2(m-\ell) \left(\frac{1}{5} - \frac{1}{3} \right) + (2m-2\ell+1) \left(\frac{1}{4} - \frac{1}{2} \right) \right] \\
 = & \left[\sum_{i=1}^{2m+1} f(i) - \sum_{i=1}^{2\ell} f(i) - \sum_{i=1}^{2m-2\ell} f(i) + \sum_{i=1}^{2m+2} f(i) - \sum_{i=1}^{2\ell+1} f(i) - \sum_{i=1}^{2m-2\ell+1} f(i) \right] + \left[\sum_{i=1}^{2m+2} f(i) \right. \\
 & - \sum_{i=1}^{2\ell+1} f(i) - \sum_{i=1}^{2m-2\ell+1} f(i) + \sum_{i=1}^{2n-2\ell} f(i) - \sum_{i=1}^{2n-2m-1} f(i) - \sum_{i=1}^{2m-2\ell+1} f(i) + \sum_{i=1}^{2m-2\ell+1} f(i) + \\
 & \left. \sum_{i=1}^{2m-2\ell+1} (f(i) - f(1)) - \frac{2m-2\ell}{3} \right] + \left[\sum_{i=1}^{2m+3} f(i) - \left(\sum_{i=1}^{2\ell+2} f(i) - f(1) \right) - \sum_{i=1}^{2m-2\ell+2} f(i) \right. \\
 & + \sum_{i=1}^{2n-2\ell+1} f(i) - \left(\sum_{i=1}^{2n-2m} f(i) - f(1) \right) - \sum_{i=1}^{2m-2\ell+2} f(i) + \sum_{i=1}^{2m-2\ell+2} (f(i) - f(1)) \\
 & \left. + \sum_{i=1}^{2m-2\ell+2} (f(i) - f(2)) - \frac{23m-23\ell}{30} - \frac{1}{4} \right] \\
 = & (6m+8)f(2m+2) + (2m+4)f(2m+3) - (6\ell+5)f(2\ell+1) - (2\ell+3)f(2\ell+2) \\
 & - (4m-4\ell+3)f(2m-2\ell+1) + (4n-4\ell+3)f(2n-2\ell+1) - (4n-4m+1)f(2n \\
 & - 2m) - (16m-16\ell+7) - \frac{13m-13\ell}{30} - \frac{1}{4}.
 \end{aligned}$$

By Lemmas 2.2 and 2.6, we get $H(L_{\ell, m, n}) = h_1(\ell, m, n)$. ■

Lemma 2.9 *Let $\ell, m, n \in \mathbb{N}$ such that $\ell \leq n \leq m$. Then $H(L_{\ell, m, n}) = h_2(\ell, m, n)$.*

Proof: We have $S_0 = \{(x, 0) | 0 \leq x \leq 2n\}$, $S_i = \{(x, i) | 0 \leq x \leq 2m+1\}$ for $1 \leq i \leq 2$ and $S_3 = \{(x, 3) | 0 \leq x \leq 2\ell\}$. Let $S'_0 = \{(x, 0) | 2\ell+1 \leq x \leq 2n\}$. Then $L_{\ell, m, n} - S'_0 \cong L_{\ell, m, \ell}$.

Let $V' = V(L_{\ell, m, n}) - S'_0$. Hence, $H(L_{\ell, m, n}) = \sum_{\{u, v\} \subseteq V'} \frac{1}{d(u, v)} + \sum_{\{u, v\} \subseteq S'_0} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_0 \\ v \in V'}} \frac{1}{d(u, v)} =$

$H(L_{\ell, m, \ell}) + H(P_{2n-2\ell}) + \sum_{\substack{u \in S'_0 \\ v \in V'}} \frac{1}{d(u, v)}$. Next we consider the last one item in the above equation.

For $u = (a, 0) \in S'_0$ and $v = (b, 1) \in S_1$, $d(u, v) = |a - b| + 1$ if $a - b \neq 0$, or $a = b$ and a

is even, and $d(u, v) = 3$ if $a = b$ and a is odd. For $u = (a, 0) \in S'_0$ and $v = (b, 2) \in S_2$, $d(u, v) = |a - b| + 2$ if $|a - b| \geq 2$, or $|a - b| = 1$ and a is even, and $d(u, v) = |a - b| + 4$ if $|a - b| = 1$ and a is odd, or $a = b$. Thus, we have

$$\begin{aligned}
 & \sum_{\substack{u \in S'_0 \\ v \in V'}} \frac{1}{d(u, v)} \\
 = & \sum_{\substack{u \in S'_0 \\ v \in S_3}} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_0 \\ v \in S_1}} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_0 \\ v \in S_2}} \frac{1}{d(u, v)} + \sum_{\substack{u \in S'_0 \\ v \in S_0 - S'_0}} \frac{1}{d(u, v)} \\
 = & \left[\sum_{i=0}^{2\ell-2} \sum_{j=0}^{2n-2\ell-1} \frac{1}{i+j+6} + \sum_{j=0}^{2n-2\ell-1} \left(\frac{1}{j+6} + \frac{1}{j+7} \right) \right] + \left[\sum_{i=0}^{2m+1} \sum_{j=2\ell+1}^{2n} \frac{1}{|i-j|+1} + (n \right. \\
 & \left. - \ell) \left(\frac{1}{3} - 1 \right) \right] + \left[\sum_{i=0}^{2m+1} \sum_{j=2\ell+1}^{2n} \frac{1}{|i-j|+2} + 2(n-\ell) \left(\frac{1}{5} - \frac{1}{3} \right) + (2n-2\ell) \left(\frac{1}{4} - \frac{1}{2} \right) \right] \\
 & + \left[\sum_{i=0}^{2\ell} \sum_{j=0}^{2n-2\ell-1} \frac{1}{i+j+1} \right] \\
 = & \left[\sum_{i=1}^{2n+3} f(i) - \left(\sum_{i=1}^{2\ell+3} f(i) - \sum_{i=1}^4 f(i) \right) - \sum_{i=1}^{2n-2\ell+4} f(i) + f(2n-2\ell+5) + f(2n-2\ell+6) \right] \\
 & + \left[\sum_{i=1}^{2n+1} f(i) - \sum_{i=1}^{2\ell+1} f(i) - \sum_{i=1}^{2n-2\ell} f(i) + \sum_{i=1}^{2m-2\ell+1} f(i) - \sum_{i=1}^{2m-2n+1} f(i) - \sum_{i=1}^{2n-2\ell} f(i) + \sum_{i=1}^{2n-2\ell} \right. \\
 & \left. f(i) + \sum_{i=1}^{2n-2\ell} (f(i) - f(1)) - \frac{2n-2\ell}{3} \right] + \left[\sum_{i=1}^{2n+2} f(i) - \left(\sum_{i=1}^{2\ell+2} f(i) - f(1) \right) - \sum_{i=1}^{2n-2\ell+1} f(i) \right. \\
 & \left. + \sum_{i=1}^{2m-2\ell+2} f(i) - \left(\sum_{i=1}^{2m-2n+2} f(i) - f(1) \right) - \sum_{i=1}^{2n-2\ell+1} f(i) + \sum_{i=1}^{2n-2\ell+1} (f(i) - f(1)) + \sum_{i=1}^{2n-2\ell+1} \right. \\
 & \left. (f(i) - f(2)) - \frac{23n-23\ell}{30} \right] + \left[\sum_{i=1}^{2n} f(i) - \sum_{i=1}^{2\ell} f(i) - \sum_{i=1}^{2n-2\ell-1} f(i) \right] \\
 = & (4n+3)f(2n+1) + (4n+7)f(2n+3) - (4\ell+3)f(2\ell+1) - (4\ell+7)f(2\ell+3) - (2n \\
 & - 2\ell)f(2n-2\ell) - (2n-2\ell+4)f(2n-2\ell+5) + f(2n-2\ell+6) + (4m-4\ell+5)f(2m \\
 & - 2\ell+2) - (4m-4n+5)f(2m-2n+2) - (16n-16\ell-6) - \frac{13n-13\ell}{30} + \frac{7}{12}.
 \end{aligned}$$

By Lemmas 2.2 and 2.5, we get $H(L_{\ell, m, n}) = h_2(\ell, m, n)$. ■

From Lemmas 2.7, 2.8 and 2.9, we obtain our main result as follows.

Theorem 2.10 *Let $\ell, m, n \in N$. Then*

$$H(L_{\ell, m, n}) = \begin{cases} h_1(\ell, m, n), & \ell \leq m < n \\ h_2(\ell, m, n), & \ell \leq n \leq m \\ h_3(\ell, m, n), & m < \ell \leq n. \end{cases}$$

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