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# HYPER-WIENER INDEX OF ZIGZAG POLYHEX NANOTUBES

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**Abstract**

The hyper-Wiener index of a connected graph $G$ is defined as $WW(G) = (1/4)\sum_{(u,v)\in V(G)\times V(G)} \left(d(u, v) + d(u, v)^2\right)$, where $V(G)$ is the set of all vertices of $G$ and $d(u, v)$ is the distance between the vertices $u, v \in V(G)$. In this paper we find an exact expression for the hyper-Wiener index of $TUHC_6[2p, q]$, the zigzag polyhex nanotube.

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## 1. Introduction

Topological indices are one of the descriptors of molecules that play an important role in structure property and structure activity studies, particularly when multivariate regression analysis, artificial neural networks, and pattern recognition are used as statistical tools. The Wiener index was the first topological index that was introduced in 1947 by Harold Wiener. He published a series of papers [27–31] showing that there are excellent correlations between the Wiener index and a variety of physicochemical properties of organic compounds. For a nice survey on this topic we encourage the reader to consult [13, 14].

Let $G$ be an undirected connected graph without loops or multiple edges. The set of vertices and edges of $G$ are denoted by $V(G)$ and $E(G)$, respectively. For vertices $x$ and $y$ in $V(G)$, we denote by $d(x, y)$ (or $d_G(x, y)$ when we deal with more than one graph) the topological distance, that is, the number of edges on a shortest path, joining

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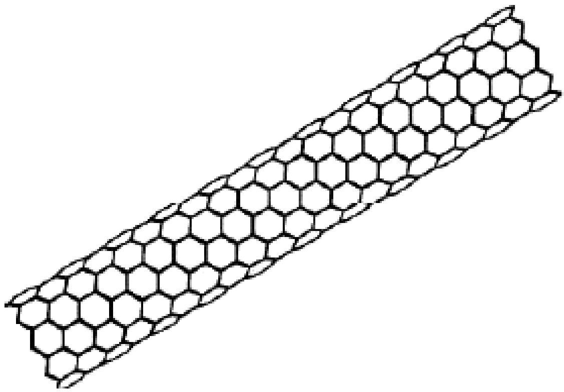

FIGURE 1. A $TUHC_6[2p, q]$ nanotube.

two vertices of $G$. The Wiener index of a graph $G$ is the half sum of all distances in the graph $G$:

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

The hyper-Wiener index is one of the recently conceived distance-based graph invariants, used as a structure-descriptor for predicting physicochemical properties of organic compounds (often significant for pharmacology, agriculture and environmental protection). Randić in [26] introduced an extension of the Wiener index for trees, and this has come to be known as the hyper-Wiener index. Klein *et al.* [25] generalized this extension to cyclic structures as

$$WW(G) = \frac{1}{2} W(G) + \frac{1}{4} \sum_{(u,v)\in V(G)\times V(G)} d(u, v)^2.$$

The hyper-Wiener index $WW(G)$ has seen widespread use in correlations; references may be found in [4] and also in [24]. In [5, 6], Diudea has treated both $W(G)$ and $WW(G)$ in a common matrix framework.

In a series of papers, Diudea and coauthors [7–12, 23] computed the Wiener index of some nanotubes as did the present authors in [15–22].

In this paper we find an exact expression for the hyper-Wiener index of the zigzag polyhex nanotubes of circumference $2p$ and length $q$, denoted by $G := TUHC_6[2p, q]$. (An example is shown in Figure 1.) For this purpose we choose coordinate labels for vertices of $G$ as shown in Figure 2. In [15] we have included a MATHEMATICA [32] program to produce the graph of $TUHC_6[2p, q]$. With this program we can compute the hyper-Wiener indices of the graphs under consideration.

We note that $G$ is a bipartite graph which means that its vertices can be coloured with white and black so that adjacent vertices have different color, or equivalently, that

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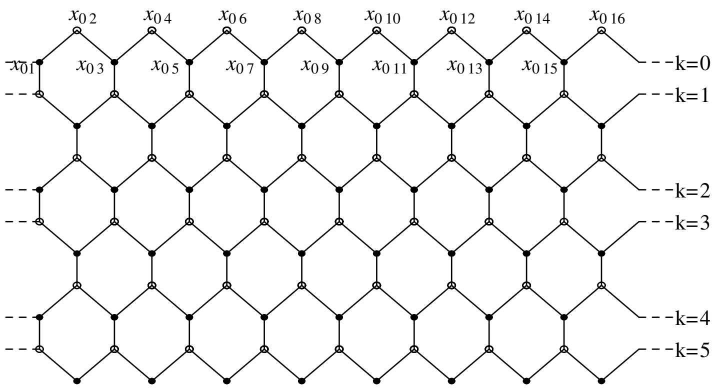


FIGURE 2. A $TUHC_6[2p, q]$ lattice with $p = 8$ and $q = 6$.

every cycle has even length (see [18, Theorem 2.4]). Obviously the number of vertices and the number of edges of $G$ is $n = |V(G)| = 2pq$ and $m = |E(G)| = 3pq - p$, respectively.

## 2. Computing the hyper-Wiener index of zigzag polyhex nanotubes

In this section we derive an exact formula for the hyper-Wiener index of $G := TUHC_6[2p, q]$. For $u \in V(G)$ we define

$$d(u) = \sum_{v \in V(G)} d(u, v), \quad d'(u) = \sum_{v \in V(G)} d(u, v)^2, \quad dd(u) = \sum_{u \in V(G)} [d(u) + d'(u)].$$

(If necessary, we show these quantities by $d_G(u)$, $d'_G(u)$ and $dd_G(u)$, respectively.) Then

$$WW(G) = \frac{1}{4} \sum_{u \in V(G)} d(u) + \frac{1}{4} \sum_{u \in V(G)} d'(u) = \frac{1}{4} \sum_{u \in V(G)} dd(u).$$

Also, for $u, v \in V(G)$, we define the hyper distance $dd(u, v)$ (or $dd_G(u, v)$) as

$$dd(u, v) = d(u, v) + d(u, v)^2.$$

In the following lemma we find a formula for the hyper distances of one white (black) vertex of level zero of the graph $TUHC_6[2p, q]$ to all vertices on the level $k < q$ (see Figure 1).

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LEMMA 2.1. *In the graph $TUHC_6[2p, q]$ we have*

$$\begin{aligned} ww_k &:= \sum_{x\in \text{ level } k} dd(x_{02}, x) \\ &= \sum_{x\in \text{ level } k} dd(x_{04}, x) \\ &\ \vdots \\ &= \begin{cases} \frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p & \text{if } 0 \le k < p \\ 2p(2k+1)^2 & \text{if } p \le k \end{cases} \end{aligned}$$

*and*

$$\begin{aligned} bb_k &:= \sum_{x\in \text{ level } k} dd(x_{01}, x) \\ &= \sum_{x\in \text{ level } k} dd(x_{03}, x) \\ &\ \vdots \\ &= \begin{cases} \frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p & \text{if } 0 \le k < p \\ 8k^2p & \text{if } p \le k. \end{cases} \end{aligned}$$

PROOF. We compute $b_k$. It is sufficient to consider $x_{01}$. For other black vertices, the argument is similar. At first note that the lattice is symmetric (with respect to the line joining $x_{01}$ to $x_{11}$). We distinguish between three cases.

*Case 1: $k \ge p$ and $k$ is even.* In this case, for all $1 \le j \le p+1$,

$$d(x_{01}, x_{kj}) = \begin{cases} 2k-1 & \text{if } j \text{ is even} \\ 2k & \text{if } j \text{ is odd.} \end{cases}$$

By considering these vertices and their symmetric vertices we obtain $p$ vertices having distance $2k-1$ from $x_{01}$, and $p$ vertices having $2k$ distance from $x_{01}$. So

$$\begin{aligned} &\sum_{u\in \text{ level } k} [d(x_{01}, u) + d(x_{01}, u)^2] \\ &\quad = \sum_{j \text{ is even}} [d(x_{01}, x_{ji}) + d(x_{01}, x_{ji})^2] + \sum_{j \text{ is odd}} [d(x_{01}, x_{ji}) + d(x_{01}, x_{ji})^2] \\ &\quad = p[(2k-1) + (2k-1)^2] + p[(2k) + (2k)^2] = 8k^2p. \end{aligned}$$

*Case 2: $k \ge p$ and $k$ is odd.* In this case, for all $1 \le j \le p+1$,

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } j \text{ is even} \\ 2k-1 & \text{if } j \text{ is odd.} \end{cases}$$

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Now by considering these vertices and their symmetric vertices we obtain $p$ vertices having distance $2k-1$ from $x_{01}$, and $p$ vertices having $2k$ distance from $x_{01}$. So

$$\begin{aligned}\sum_{u\in \text{ level } k} &[d(x_{01},u)+d(x_{01},u)^2]\\ &= \sum_{j \text{ is even}} [d(x_{01},x_{ji})+d(x_{01},x_{ji})^2] + \sum_{j \text{ is odd}} [d(x_{01},x_{ji})+d(x_{01},x_{ji})^2]\\ &= p[(2k)+(2k)^2]+p[(2k-1)]+(2k-1)^2] = 8k^2p.\end{aligned}$$

*Case 3:* $k \le p-1$. For all $p+1 \le j$ and $j > k+1$,

$$d(x_{01},x_{kj}) = k+j-1.$$

Thus, the summation of the distances between $x_{01}$ and $x_{kj}$ (for all $j$ such that $p+1 \le j$ and $j > k+1$) and their symmetric vertices is

$$\begin{aligned}S_1 &= 2\sum_{j=k+2}^{p} [(k+j-1)+(k+j-1)^2] + [(k+p+1-1)+(k+p+1-1)^2]\\ &= \tfrac{2}{3}(p-1-k)(p^2+4pk+p+7k^2+5k)+(k+p)+(k+p)^2\\ &= 2kp+\tfrac{1}{3}p+2pk^2+2p^2k-7k^2-\tfrac{7}{3}k+p^2-\tfrac{14}{3}k^3+\tfrac{2}{3}p^3.\end{aligned}$$

Also, if $1 \le j \le k+1$, then

$$d(x_{01},x_{kj}) = \begin{cases} 2k & \text{if } k-j \text{ is odd}\\ 2k-1 & \text{if } k-j \text{ is even.}\end{cases}$$

Arguing as before we obtain $k+1$ vertices having distance $2k$ and $k$ vertices having distance $2k-1$ from $x_{01}$, respectively. Therefore, the summation of the distances between $x_{01}$ and $x_{kj}$ (for all $j$ such that $1 \le j \le k+1$) and their symmetric vertices is

$$S_2 = (k+1)[(2k)+(2k)^2]+k[(2k-1)+(2k-1)^2].$$

Hence,

$$\begin{aligned}bb_k &= S_1+S_2\\ &= 2kp+\tfrac{1}{3}p+2pk^2+2p^2k-7k^2-\tfrac{7}{3}k+p^2-\tfrac{14}{3}+\tfrac{2}{3}p^3\\ &\quad + (k+1)\big[(2k)+(2k)^2\big]+k\big[(2k-1)+(2k-1)^2\big]\\ &= \tfrac{10}{3}k^3+\tfrac{2}{3}p^3-3k^2+2k^2p+2kp+p^2+2kp^2-\tfrac{1}{3}k+\tfrac{1}{3}p.\end{aligned}$$

In a similar manner we can compute $\widehat{w}_k$. □

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COROLLARY 2.2. *We have:*
(a) $dd(x_{02}) = dd(x_{04}) = \cdots = dd(x_{0,2p}) = ww_0 + ww_1 + \cdots + ww_{q-1}$;
(b) $dd(x_{01}) = dd(x_{03}) = \cdots = dd(x_{0,2p-1}) = bb_0 + bb_1 + \cdots + bb_{q-1}$.

PROOF. By Lemma 2.1 we have

$$\begin{aligned} dd(x_{02}) &= \sum_{u\in \text{ level } 0} dd(u, x_{02}) + \sum_{u\in \text{ level } 1} dd(u, x_{02}) + \cdots + \sum_{u\in \text{ level } q-1} dd(u, x_{02}) \\ &= ww_0 + ww_1 + \cdots + ww_{q-1} \end{aligned}$$

and so $\widehat{d}(x_{01}) = \widehat{d}(x_{03}) = \cdots = \widehat{d}(x_{0,2p2}) = \widehat{b}_0 + \widehat{b}_1 + \cdots + \widehat{b}_{q-1}$. The proof of (b) is similar. □

LEMMA 2.3. *If* $0 \le j \le q-1$ *is an odd number, then*

(a) $$\begin{aligned} dd_G(x_{j1}) &= dd_G(x_{j3}) = \cdots = dd_G(x_{j,2p-1}) \\ &= ww_0 + ww_1 + \cdots + ww_{q-(j+1)} + bb_1 + \cdots + bb_j; \end{aligned}$$

(b) $$\begin{aligned} dd_G(x_{j2}) &= dd_G(x_{j4}) = \cdots = dd_G(x_{j,2p}) \\ &= bb_0 + bb_1 + \cdots + bb_{q-(j+1)} + ww_1 + \cdots + ww_j. \end{aligned}$$

PROOF. First suppose that $j = 1$. We consider the tube that can be built up from two halves collapsing at level one. The bottom part is the graph $G_1 = TUHC_6[2p, q-1]$ and we can consider $x_{11}$ as one of the white edges in the first row of the graph $G_1$. According to Corollary 2.2,

$$dd_{G_1}(x_{11}) = dd_{G_1}(x_{13}) = \cdots = dd_{G_1}(x_{1,2p-1}) = ww_0 + ww_1 + \cdots + ww_{q-2}.$$

The top part is the graph $TUHC_6[2p, 2] = \widehat{G_1}$, level one of graph $G$ is the first its row and $x_{11}$ is, as such, a black vertex of $\widehat{G}_1$. Therefore, by Corollary 2.2, $dd_{\widehat{G}_1}(x_{11}) = bb_0 + bb_1$ and

$$dd_{\widehat{G}_1}(x_{11}) = dd_{\widehat{G}_1}(x_{13}) = \cdots = dd_{\widehat{G}_1}(x_{1(2p-1)}) = bb_0 + bb_1.$$

Since $ww_0 = bb_0$ and $dd_G(x_{11}) = dd_{G_1}(x_{11}) + dd_{\widehat{G}_1}(x_{11}) - bb_0$, we have $dd_G(x_{11}) = ww_0 + \cdots + ww_{q-2} + bb_1$ and, similarly,

$$dd_G(x_{11}) = dd_G(x_{13}) = \cdots = dd_G(x_{1,2p-1}) = ww_0 + \cdots + ww_{q-2} + bb_1.$$

Similarly, for $x_{12}$ we can see that

$$dd_G(x_{12}) = dd_G(x_{14}) = \cdots = dd_G(x_{1,2p}) = bb_0 + \cdots + bb_{q-2} + ww_1.$$

By repetition of this argument, we obtain the result. □

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LEMMA 2.4. *If $0 \leq j \leq q-1$ is an even number, then*

$$\begin{aligned}\text{(a)}\quad dd_G(x_{j1}) &= dd_G(x_{j3}) = \cdots = dd_G(x_{j,2p-1})\\ &= bb_0 + bb_1 + \cdots + bb_{q-(j+1)} + ww_1 + \cdots + ww_j;\end{aligned}$$

$$\begin{aligned}\text{(b)}\quad dd_G(x_{j2}) &= dd_G(x_{j4}) = \cdots = dd_G(x_{j,2p})\\ &= ww_0 + ww_1 + \cdots + ww_{q-(j+1)} + bb_1 + \cdots + bb_j.\end{aligned}$$

PROOF. First suppose that $j = 2$. We consider the tube can be built up from two halves collapsing at level two. The bottom part is the graph $G_2 = TUHC_6[2p, q-2]$, level two of $G$ is the first level of $G_2$ and we can consider $x_{21}$ as one of the black edges in the first row of graph $G_2$. According to Corollary 2.2,

$$dd_{G_2}(x_{21}) = dd_{G_2}(x_{23}) = \cdots = dd_{G_2}(x_{2,2p-1}) = bb_0 + bb_1 + \cdots + bb_{q-3}.$$

The top part is the graph $TUHC_6[2p, 3] = \widehat{G_2}$, level two of graph $G$ is the first level of $\widehat{G_2}$ and $x_{21}$ is, as such, a white vertex of $\widehat{G_2}$. Therefore, by Corollary 2.2,

$$dd_{\widehat{G_2}}(x_{21}) = ww_0 + ww_1 + ww_2$$

and

$$dd_{\widehat{G_2}}(x_{21}) = dd_{\widehat{G_2}}(x_{23}) = \cdots = dd_{\widehat{G_2}}(x_{2,2p-1}) = ww_0 + ww_1 + ww_2.$$

Since $ww_0 = bb_0$ and $dd_G(x_{21}) = dd_{G_2}(x_{21}) + dd_{\widehat{G_2}}(x_{21}) - ww_0$, then

$$dd_G(x_{21}) = bb_0 + \cdots + bb_{q-3} + ww_1 + ww_2$$

and, similarly,

$$dd_G(x_{21}) = dd_G(x_{23}) = \cdots = dd_G(x_{2,2p-1}) = bb_0 + \cdots + bb_{q-3} + ww_1 + ww_2.$$

We can repeat the process in a similar way for $x_{22}$ and see that

$$dd_G(x_{22}) = dd_G(x_{24}) = \cdots = dd_G(x_{2,2p}) = ww_0 + \cdots + ww_{q-3} + bb_1 + bb_2.$$

By repetition of this argument we obtain the result. □

For all $0 \leq j \leq q-1$, put

$$f(j) = ww_0 + ww_1 + \cdots + ww_{q-(j+1)} + bb_1 + \cdots + b_j \quad \text{and}$$
$$g(j) = bb_0 + bb_1 + \cdots + bb_{q-(j+1)} + ww_1 + \cdots + ww_j.$$

We are now in a position to prove the main result of the paper.

THEOREM 2.5. *The hyper-Wiener index, $WW(G)$, of $G := TUHC_6[2p, q]$ nanotubes is given by*

$$\frac{pq}{12}(4p^2q^2 + 4p^3q - 4p^2 + 2q^4 - 2q^2 + 4pq^2 - 4p - q + 6p^2q + q^3 + 2pq^3),$$
$$\frac{p^2}{12}(-2q^2 - 6pq - p^3 + p + 8q^4 - 2p^4 + 6p^3q + 2p^2 + 8q^3 - 6q + 4p^2q),$$

*respectively, according to whether $p \geq q$ or $p < q$.*

PROOF. Let

$$A_1 = \{i \mid 1 \le i \le 2p,\ i \text{ even}\}, \quad A_2 = \{i \mid 1 \le i \le 2p,\ i \text{ odd}\},$$
$$B_1 = \{j \mid 0 \le j \le q-1,\ j \text{ even}\}, \quad B_2 = \{j \mid 0 \le j \le q-1,\ j \text{ odd}\}.$$

Then $WW(G)$ is equal to

$$\begin{aligned}
&\frac{1}{4} \sum_{x_{ji} \in V(G)} dd(x_{ji}) \\
&= \frac{1}{4}\Big[\sum_{j\in B_1}\sum_{i\in A_1} dd(x_{ji}) + \sum_{j\in B_1}\sum_{i\in A_2} dd(x_{ji}) + \sum_{j\in B_2}\sum_{i\in A_1} dd(x_{ji}) \\
&\quad + \sum_{j\in B_2}\sum_{i\in A_2} dd(x_{ji})\Big] \\
&= \frac{1}{4}\Big[\sum_{j\in B_1}\sum_{i\in A_1} f(j) + \sum_{j\in B_1}\sum_{i\in A_2} g(j) + \sum_{j\in B_2}\sum_{i\in A_1} g(j) + \sum_{j\in B_2}\sum_{i\in A_2} f(j)\Big] \\
&= \frac{1}{4}\Big[\sum_{j\in B_1}\sum_{i\in A_1} f(j) + \sum_{j\in B_1}\sum_{i\in A_2} g(j) + \sum_{j\in B_2}\sum_{i\in A_1} g(j) + \sum_{j\in B_2}\sum_{i\in A_2} f(j)\Big] \\
&= \frac{1}{4}\Big[\sum_{j\in B_1} f(j)\sum_{i\in A_1} 1 + \sum_{j\in B_1} g(j)\sum_{i\in A_2} 1 + \sum_{j\in B_2} g(j)\sum_{i\in A_1} 1 \\
&\quad + \sum_{j\in B_2} f(j)\sum_{i\in A_2} 1\Big] \\
&= \frac{1}{4}\Big[\sum_{j\in B_1} pf(j) + \sum_{j\in B_1} pg(j) + \sum_{j\in B_2} pg(j) + \sum_{j\in B_2} pf(j)\Big] \\
&= \frac{p}{4}\Big[\sum_{j\in B_1}(f(j)+g(j)) + \sum_{j\in B_2}(f(j)+g(j))\Big] = \frac{p}{4}\sum_{j=0}^{q-1}(f(j)+g(j)).
\end{aligned}$$

First we prove the formula for the case $p \ge q$. Then, for each $0 \le k \le q-1$,

$$ww_k = \tfrac{10}{3}k^3 + \tfrac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \tfrac{5}{3}k + \tfrac{1}{3}p,$$
$$bb_k = \tfrac{10}{3}k^3 + \tfrac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \tfrac{1}{3}k + \tfrac{1}{3}p.$$

So

$$\begin{aligned}
WW(G) &= \frac{p}{4}\sum_{j=0}^{q-1}(f(j)+g(j)) \\
&= \frac{pq}{12}(4p^2q^2 + 4p^3q - 4p^2 + 2q^4 - 2q^2 + 4pq^2 - 4p - q \\
&\quad + 6p^2q + q^3 + 2pq^3).
\end{aligned}$$

Now we consider the case $p < q$. We break down this case into three subcases: $2p > q$, $2p < q$ and $2p = q$. Let

$$\begin{aligned}
C_1 &:= \{0 \le j \le p-1 \mid 0 \le q-j-1 \le p-1\}\\
C_2 &:= \{0 \le j \le p-1 \mid p \le q-j-1 \le q-1\}\\
C_3 &:= \{p \le j \le q-1 \mid 0 \le q-j-1 \le p-1\}\\
C_4 &:= \{p \le j \le q-1 \mid p \le q-j-1 \le q-1\}.
\end{aligned}$$

We note that if $C_1 \neq \emptyset$, then $2p > q$. Also if $C_4 \neq \emptyset$, then $2p < q$. Therefore, first suppose that $C_1 \neq \emptyset$. Then $C_4 = \emptyset$ and $2p > q$. Therefore, if $j \in C_1$, then

$$\begin{aligned}
f(j) = {}& \sum_{k=0}^{q-j-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=1}^{j}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right),
\end{aligned}$$

if $j \in C_2$, then

$$\begin{aligned}
f(j) = {}& \sum_{k=0}^{p-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=1}^{j}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=p}^{q-j-1} 2p(2k+1)^2,
\end{aligned}$$

and if $j \in C_3$, then

$$\begin{aligned}
f(j) = {}& \sum_{k=0}^{q-j-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=1}^{p-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=p}^{j} 8k^2p.
\end{aligned}$$

Also if $j \in C_1$, then

$$\begin{aligned}
g(j) = {}& \sum_{k=0}^{j-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right)\\
&+ \sum_{k=1}^{q-j-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right),
\end{aligned}$$

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if $j \in C_2$, then

$$
\begin{aligned}
g(j) = &\sum_{k=0}^{j}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right) \\
&+ \sum_{k=1}^{p-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right) \\
&+ \sum_{k=p}^{q-j-1} 8k^2p,
\end{aligned}
$$

and if $j \in C_3$, then

$$
\begin{aligned}
g(j) = &\sum_{k=0}^{p}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 + 5k^2 + 2k^2p + 2kp + p^2 + 2kp^2 + \frac{5}{3}k + \frac{1}{3}p\right) \\
&+ \sum_{k=1}^{q-j-1}\left(\frac{10}{3}k^3 + \frac{2}{3}p^3 - 3k^2 + 2k^2p + 2kp + p^2 + 2kp^2 - \frac{1}{3}k + \frac{1}{3}p\right) \\
&+ \sum_{k=p}^{j} 2p(2k+1)^2.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
WW(G) &= \frac{p}{4}\sum_{j=0}^{q-1}[f(j) + g(j)] \\
&= \frac{p}{4}\left(\sum_{j\in C_1}[f(j) + g(j)] + \sum_{j\in C_2}[f(j) + g(j)] + \sum_{j\in C_3}[f(j) + g(j)]\right) \\
&= \frac{p^2}{12}(-2q^2 - 6pq - p^3 + p + 8q^4 - 2p^4 + 6p^3q + 2p^2 + 8q^3 - 6q \\
&\quad + 4p^2q),
\end{aligned}
$$

and so the formula is true for the case $p < q$ and $2p > q$. Using this method we can handle other conditions. □

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