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Hosoya polynomials of zig-zag open-ended nanotubes*

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Abstract

For a connected graph G we denote by $d(G,k)$ the number of vertex pairs at distance k. The Hosoya polynomial of G is $H(G,x) = \sum_{k\geqslant 0} d(G,k)x^k$. In this paper, we give analytical formulae for calculating this polynomial of zig-zag open-ended nanotubes, and show it is unimodal. Furthermore, the Wiener index, derived from the first derivative of the Hosoya polynomial in $x=1$, and the hyper-Wiener index, from a half of the second derivative of the Hosoya polynomial multiplied by x in $x=1$, can be calculated.

1 Introduction

Single-walled nanotubes (briefly denoted SWNTs), one-dimensional carbon allotropes with remarkable mechanical properties, were discovered by two groups (*i.e.*, Iijima's group [14] and Bethune's group [2] from IBM) independently. They have intensive theoretical and experimental researches [4, 5, 19, 24]. For zig-zag open-ended nanotubes, a particular class of SWNTs, John and Diudea [15] have given explicit formulae of their Wiener indices.

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The *Wiener index* of a connected graph G, introduced originally for alkanes by H. Wiener [23] and denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in G [13],

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v),$$

where $d_G(u,v)$ is the distance (*i.e.* the number of edges in a shortest path) between a pair of vertices u and v of G. The *hyper-Wiener index* is proposed by Randić [20] for trees and extended by Klein et al. [17] as

$$WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G(u,v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d_G^2(u,v).$$

If we denote by $d(G,k)$ the number of vertex pairs of G at distance k, then the Wiener and hyper-Wiener indices of G can also be expressed as [28]:

$$W(G) = \sum_{k\geqslant 0} kd(G,k), \tag{1}$$

$$WW(G) = \frac{1}{2}\sum_{k\geqslant 0} k(k+1)d(G,k). \tag{2}$$

Note that $d(G,0)$ is the number of vertices of G and $d(G,1)$ is the number of edges of G.

The Wiener index is one of the oldest graph-based structure descriptors and extensively studies since the middle of 1970s. For the researches on the Wiener index we can refer to two special issues [9, 10] and references therein, whereas chemical applications and the computation of the hyper-Wiener index are referred to [1, 18, 20].

The following polynomial associated with a connected graph G

$$H(G,x) = \sum_{k\geqslant 0} d(G,k)x^k$$

was introduced by Hosoya [12] and was called the *Wiener polynomial* because (by Eq. (1)) the Wiener index $W(G)$ is equal to the first derivative of the polynomial in $x = 1$:

$$W(G) = \frac{dH(G,x)}{dx}\Big|_{x=1}. \tag{3}$$

Recently this polynomial was called *Hosoya polynomial* in the literature in honor of Hosoya. Similar to Eq. (3), from Eq. (2), the following relation holds:

$$WW(G) = \frac{1}{2}\frac{d^2(xH(G,x))}{dx^2}\Big|_{x=1}. \tag{4}$$

The Hosoya polynomial has many applications. Firstly, analogous to Eq. (3), we can consider higher derivatives of the Hosoya polynomial in $x = 1$(In Ref. [6] they are

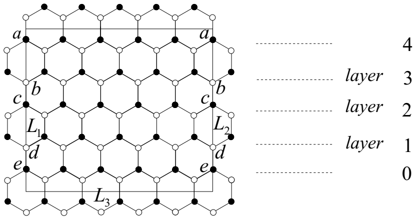


Fig. 1. A zig-zag open-ended nanotube $T(p, q)$ with $p = 5, q = 5$ and its two vertices v_0 and w_0. Note that the vertices with the same label are identified.

called *"extended Wiener indices"*), which may have some chemical applicability [6, 16]. Secondly, the Hosoya polynomial contains more information about distance in a graph than any of the hitherto proposed distance-based topological indices, not only these, but some celebrated topological indices of a graph often can be obtained directly from its Hosoya polynomial, such as the Wiener index and the hyper-Wiener index. In view of these it is imaginable that the Hosoya polynomial and the quantities derived from it will play a significant role in QSAR/QSPR studies. Therefore, abundant literature appeared on this topic for the theoretical consideration [7, 8] and computation [3, 11, 22, 25, 26].

In this paper, we focus on zig-zag open-ended nanotubes, proposing a recursive method for calculating the Hosoya polynomial H in the corresponding graph. By means of this method, explicit expressions for H are obtained (*e.*g. Theorem 3.1). Furthermore, we show that the coefficients of H are unimodal. Finally, according to relations (3) and (4) we give closed formulae for the Wiener index and the hyper-Wiener index of zig-zag open-ended nanotubes.

2 Some Lemmas about distance in tubules

A *zig-zag open-ended nanotube* (or *tubule*) is a finite section of a polyhex cylinder, described by two parameters p and q, denoted as $T(p, q)$ [15], and drawn in the plane (equipped with the regular hexagonal lattice L) using the representation of the cylinder by a rectangular R with the vertical boundary identification (see Fig. 1): The bottom side L_3 and the top side L_4 are all perpendicular to the vertical edge-direction of L such that L_3 connects the centers of two hexagons of L and passes through p edges, while L_4 connects the centers of either two hexagons or two vertical edges such that there are q vertices on a vertical side L_1 (or L_2). Then, identify points of opposite positions on vertical sides L_1 and L_2. Note that $T(p, q)$ are bipartite, its vertices can be colored such that every vertical edge connects a white top vertex with a black bottom vertex. For convenience, we denote by *layer* $0, 1, \cdots, q-1$ horizontal zig-zag lines in $T(p,q)$ from bottom to top, respectively. In fact, for every k, the layer k corresponds to a cycle of length $2p$, denoted by $C_k = v_{0,k}v_{1,k}\cdots v_{2p-1,k}v_{0,k}$. Two specific vertices, v_0 and w_0 of layer 0, one vertex being white and the other black, are shown in Fig. 1.

Let G_1 be a connected subgraph of a graph G. Then $d_{G_1}(u,v) \geqslant d_G(u,v)$ for any pair of vertices u and v of the graph. G_1 is a *convex subgraph* of G if any shortest path of G joining two vertices of G_1 is already in G_1. Hence if G_1 is convex, $d_{G_1}(u,v) = d_G(u,v)$.

Lemma 2.1 ([27]). *For any integer r with $1 \leqslant r \leqslant q-1$, $T(p,r)$ is convex in $T(p,q)$.*

For convenience, for nonnegative integers m, n and s, we define 3 sequences as follows:

$$m, \nearrow, n := (m, m+1, \cdots, n); \qquad (m \leqslant n)$$

$$m, \searrow, n := (m, m-1, \cdots, n); \qquad (m \geqslant n)$$

$$m, \leftrightsquigarrow 2s, n := \overbrace{m, n, m, n, \cdots, m, n}^{2s \text{ terms}}; \qquad (m \neq n)$$

For a vertex v of $T(p,q)$, we denote by $S_{T(p,q)}(k;v)$ the cyclic permutation of the sequence $\left(d_{T(p,q)}(v_{i,k}, v)\right)_{0 \leqslant i \leqslant 2p-1}$.

Lemma 2.2 ([27]).

$$S_{T(p,q)}(k;v_0) = \begin{cases} (2k, \nearrow, p+k, \searrow, 2k, \leftrightsquigarrow 2k, 2k+1), & 0 \leqslant k < p-1; \\ (2k, \leftrightsquigarrow 2p, 2k+1), & p-1 \leqslant k \leqslant q-1. \end{cases} \tag{5}$$

By Lemma 2.1 and the structure of $T(p,q)$,

$$\begin{array}{c} T(p,q-1) \textit{ can be considered as a convex subgraph of } T(p,q) \\ \textit{induced by layers } 1, 2, \cdots, q-1. \end{array} \tag{$*$}$$

By $(*)$ and Lemma 2.2, we have

Lemma 2.3.

$$S_{T(p,q)}(k;w_0) = \begin{cases} (0, \nearrow, p, \searrow, 1), & k = 0; \\ (2k-1, \nearrow, p+k, \searrow, 2k-1, \leftrightsquigarrow 2k-2, 2k), & 0 < k < p; \\ (2k-1, \leftrightsquigarrow 2p, 2k), & p \leqslant k \leqslant q-1. \end{cases}$$

3 Main results

In this section, we give our main results—Theorems 3.1 and 3.5. In the first theorem we present the explicit expression for the Hosoya polynomial of $T(p,q)$. The proof of the theorem will be given in the next section. The second result shows that the polynomial is unimodal.

Theorem 3.1. *(1) If $q \leqslant \frac{p}{2}$,*

$$H(T(p,q),x) = 2pq + p\sum_{i=1}^{2q-1}(-i^2+3qi)x^i + 2pq^2\sum_{i=2q}^{p-1}x^i + pq(2q-1)x^p + 2p\sum_{i=p+1}^{p+q-1}(p+q-i)^2x^i. \tag{6}$$

(2) If $\frac{p}{2} < q \leqslant p$,

$$\begin{aligned} H(T(p,q),x) = {} & 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq-p^2-q)x^p \\ & + p\sum_{i=p+1}^{2q-1}(2p^2+4pq+i^2-4pi-qi)x^i + 2p\sum_{i=2q}^{p+q-1}(p+q-i)^2x^i. \end{aligned} \tag{7}$$

(3). If $q \geqslant p+1$,

$$\begin{aligned} H(T(p,q),x) = {} & 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq-p^2-q)x^p \\ & + p\sum_{i=p+1}^{2p-1}(2p^2+4pq+i^2-4pi-qi)x^i + p^2\sum_{i=2p}^{2q-1}(2q-i)x^i. \end{aligned} \tag{8}$$

Corollary 3.2.

(i) $H(T(1,q),x) = H(P_{2q},x) = \sum_{i=0}^{2q-1}(2q-i)x^i.$

(ii) $H(T(p,1),x) = H(C_{2p},x) = 2p\sum_{i=0}^{p-1}x^i + px^p.$

Taking the derivatives of the Eqs. (6)-(8) and setting $x=1$ it results in the Wiener index of $T(p,q)$ according to Eq. (3), which are consistent with Eqs. (9) and (10) of [15].

Corollary 3.3 ([15])**.** *In the case of short tubes, i.e. $0 < q \leqslant p$,*

$$W(T(p,q)) = \frac{pq}{6}[6p^2q + (4p+q)(q^2-1)].$$

While in the case of long tubes, i.e. $p \leqslant q$,

$$W(T(p,q)) = \frac{p^2}{6}[p^2(4q-p) + q(8q^2-6) + p].$$

Analogously, according to Eq. (4) we obtain the hyper-Wiener index of $T(p,q)$.

Corollary 3.4. *In the case of short tubes, i.e.* $0 < q \leqslant p$,

$$WW(T(p,q)) = \frac{pq}{12}[2pq(2p+1)(p+1)+2pq(q+1)^2-(2p+1)^2+(2pq-1)^2+q(q^2-1)(2q+1)];$$

While in the case of long tubes, i.e. $p \leqslant q$,

$$WW(T(p,q)) = \frac{p^2}{12}[-p(p^2-1)(2p+1) + 2q(p^2-1)(3p+2) + 2q(q+1)(4q^2-1)].$$

We say a sequence $(a_i)_{i\geqslant 0}$ is *unimodal* if, for some index k,

$$a_0 \leqslant a_1 \leqslant \cdots \leqslant a_k \geqslant a_{k+1} \geqslant a_{k+2} \geqslant \cdots .$$

Unimodal sequences appear in many areas of mathematics. For a survey, see Stanley's article [21].

Theorem 3.5. *The coefficients of* $H(T(p,q),x)$ *are unimodal.*

Proof. Let $a_0 = 2pq$, $a_i = p(-i^2+3qi)$ for $i \geqslant 1$. Then the sequence $(a_i)_{i\geqslant 0}$ is unimodal. It is obvious that the sequences $\big(p(2p^2+4pq+i^2-4pi-qi)\big)_{p+1\leqslant i\leqslant 2p}$, $\big(2p(p+q-i)^2\big)_{1\leqslant i\leqslant p+q-1}$ and $\big(p^2(2q-i)\big)_{2p\leqslant i\leqslant 2q-1}$ are all monotone decreasing. In the following we distinguish two cases.

Case 1. $q \leqslant \frac{p}{2}$. Since we have the following relation:

$$p(-(2q)^2 + 3q\cdot 2q) = 2pq^2 > pq(2q-1) > 2p(p+q-(p+1))^2,$$

the assertion holds.

Case 2. $q > \frac{p}{2}$. Since

$$p(-p^2+3qp) > p(3pq-p^2-q) > p\big(2p^2+4pq+(p+1)^2-4p(p+1)-q(p+1)\big),$$

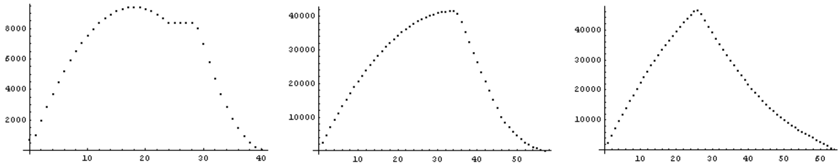
$$p\big(2p^2+4pq+(2q)^2-4p(2q)-q(2q)\big) = 2p(p+q-2q)^2$$

and

$$p\big(2p^2+4pq+(2p)^2-4p(2p)-q(2p)\big) = p^2(2q-2p),$$

the assertion holds according to Eqs. (7) and (8). $\square$

Fig. 2 illustrates the transformation of the coefficients of $H(T(p,q),x)$.



(a) (b)

Fig. 2. The coefficients of $H(T(p,q),x)$ for three cases: (a) $p=29, q=12$; (b) $p=35, q=23$ and (c) $p=26, q=32$.

4 Proof of Theorem 3.1

In this section, we prove Theorem 3.1, *i.e.* calculate $H(T(p,q),x)$. For convenience, we denote by $H(p,q,x)$ the Hosoya polynomial of $T(p,q)$. We first consider the corresponding *difference polynomial*:

$$\Delta H(p,q,x) := H(p,q,x) - H(p,q-1,x).$$

For convenience we set $\Delta H(p,1,x) = H(p,1,x)$.

Lemma 4.1.

$$H(p,q,x) = \sum_{j=1}^{q} \Delta H(p,j,x).$$

From the above lemma, our aim is changed into calculating $\Delta H(p,q,x)$. By $(*)$, if $\Delta H(p,q,x) = \sum_{k\geqslant 0} a_k x^k$, then a_k is the number of vertex pairs $\{w,v\}$ of $T(p,q)$ lying at distance k such that either w or v belongs to layer 0. By the structure of $T(p,q)$, the status of all p white vertices in layer 0 are equivalent, as well all p black vertices in layer 0. So, if we define

$$d_i(v) = |\{u \in T(p,q) | d_{T(p,q)}(v,u) = i\}|$$

for nonnegative integer i and a vertex v, then we get (Note that v_0 and u_0 are a white vertex and a black one in layer 0 respectively.)

Lemma 4.2.

$$\Delta H(p,q,x) = p\sum_{i\geqslant 0} \big(d_i(v_0) + d_i(w_0)\big)x^i - H(C_{2p},x) + 2p.$$

In the following we discuss the value of $d_i(v_0)$. Note first that if layer k has a contribution to $d_i(v_0)$, by Lemma 2.2, then k must satisfy:

(i) if $k < p-1$, then $2k \leqslant i \leqslant p+k$, *i.e.*

$$k < p-1 \text{ and } i-p \leqslant k \leqslant \frac{i}{2}, \tag{9}$$

and layer k has the contribution $1, \frac{i-1}{2}+2$ and $\frac{i}{2}+1$ to $d_i(v_0)$ when $k = i-p, \frac{i-1}{2}$ and $\frac{i}{2}$ respectively, otherwise 2 to $d_i(v_0)$, or

(ii) if $k \geqslant p-1$, then $2k \leqslant i \leqslant 2k+1$, *i.e.*

$$k \geqslant p-1 \text{ and } \frac{i-1}{2} \leqslant k \leqslant \frac{i}{2}, \tag{10}$$

and layer k has contribution p to $d_i(v_0)$.

We distinguish the following cases in discussing the value of $d_i(v_0)$ (Note that $k \leqslant q-1$).

Case 1. $0 \leqslant i < p$.

Subcase 1.1. i is odd. By relations (9) and (10), $0 \leqslant k \leqslant \frac{i-1}{2} (< p-1)$.

Subsubcase 1.1.1. $i \leqslant 2q-1$. Then $\frac{i-1}{2} \leqslant q-1$. By (i),

$$d_i(v_0) = \sum_{k=0}^{\frac{i-1}{2}-1} 2 + \big(\frac{i-1}{2}+2\big) = \frac{3i+1}{2}.$$

Subsubcase 1.1.2. $i \geqslant 2q+1$. Then $\frac{i-1}{2} > q-1$. By (i),

$$d_i(v_0) = \sum_{k=0}^{q-1} 2 = 2q.$$

Subcase 1.2. i is even. By analogy to Subcase 1.1, we have

$$d_i(v_0) = \begin{cases} \frac{3i}{2}+1, & i \leqslant 2q-2; \\ 2q, & i \geqslant 2q. \end{cases}$$

Similar to Case 1, we have

Case 2. $p \leqslant i \leqslant 2(p-1)$.

$$d_i(v_0) = \begin{cases} 2p - \lceil \frac{i}{2} \rceil, & i \leqslant 2q-1; \\ 2(p+q-i)-1, & 2q \leqslant i \leqslant p+q-1; \\ 0, & p+q \leqslant i. \end{cases}$$

Case 3. $2p-1 \leqslant i$.

$$d_i(v_0) = \begin{cases} p, & i \leqslant 2q-1; \\ 0, & i \geqslant 2q. \end{cases}$$

Tidy up the above discussions, we obtain

Lemma 4.3. *(1) If $q \leqslant \frac{p}{2}$,*

$$d_i(v_0) = \begin{cases} \lfloor \frac{3}{2}i \rfloor + 1, & 0 \leqslant i \leqslant 2q-1; \\ 2q, & 2q \leqslant i \leqslant p-1; \\ 2(p+q-i)-1, & p \leqslant i \leqslant p+q-1; \\ 0, & p+q \leqslant i. \end{cases}$$

(2) If $\frac{p}{2} < q \leqslant p$,

$$d_i(v_0) = \begin{cases} \lfloor \frac{3}{2}i \rfloor + 1, & 0 \leqslant i \leqslant p-1; \\ 2p - \lceil \frac{i}{2} \rceil, & p \leqslant i \leqslant 2q-1; \\ 2(p+q-i)-1, & 2q \leqslant i \leqslant p+q-1; \\ 0, & p+q \leqslant i. \end{cases}$$

(3) If $p+1 \leqslant q$,

$$d_i(v_0) = \begin{cases} \lfloor \frac{3}{2}i \rfloor + 1, & 0 \leqslant i \leqslant p-1; \\ 2p - \lceil \frac{i}{2} \rceil, & p \leqslant i \leqslant 2p-1; \\ p, & 2p \leqslant i \leqslant 2q-1; \\ 0, & 2q \leqslant i. \end{cases}$$

By Lemma 2.3, similar to the discussion of $d_i(v_0)$, we obtain

Lemma 4.4. *(1) If $q \leqslant \frac{p}{2}$,*

$$d_i(w_0) = \begin{cases} \lceil \frac{3}{2}i \rceil + 1, & 0 \leqslant i \leqslant 2q-2; \\ 2q, & 2q-1 \leqslant i \leqslant p-1; \\ 2(p+q-i)-1, & p \leqslant i \leqslant p+q-1; \\ 0, & p+q \leqslant i. \end{cases}$$

(2) If $\frac{p}{2} < q \leqslant p$,

$$d_i(w_0) = \begin{cases} \lceil \frac{3}{2}i \rceil + 1, & 0 \leqslant i \leqslant p-1; \\ 2p - \lfloor \frac{i}{2} \rfloor, & p \leqslant i \leqslant 2q-2; \\ 2(p+q-i)-1, & 2q-1 \leqslant i \leqslant p+q-1; \\ 0, & p+q \leqslant i. \end{cases}$$

(3) If $p+1 \leqslant q$,

$$d_i(w_0) = \begin{cases} \lceil \frac{3}{2}i \rceil + 1, & 0 \leqslant i \leqslant p-1; \\ 2p - \lfloor \frac{i}{2} \rfloor, & p \leqslant i \leqslant 2p-1; \\ p, & 2p \leqslant i \leqslant 2q-2; \\ 0, & 2q-1 \leqslant i. \end{cases}$$

By the previous three lemmas, we obtain (Note that $H(C_{2p}, x) = 2p\sum\limits_{i=0}^{p-1} x^i + px^p$)

Lemma 4.5. *(1) If $q \leqslant \frac{p}{2}$,*

$$\begin{aligned} \Delta H(p,q,x) = {} & 2p + 3p\sum_{i=1}^{2q-2} ix^i + p(5q-3)x^{2q-1} + 2p\sum_{i=2q}^{p-1}(2q-1)x^i + p(4q-3)x^p \\ & + 2p\sum_{i=p+1}^{p+q-1}(2p+2q-2i-1)x^i. \end{aligned}$$

(2) If $\frac{p}{2} < q \leqslant p$,

$$\Delta H(p,q,x) = 2p + 3p\sum_{i=1}^{p-1} ix^i + p(3p-1)x^p + p\sum_{i=p+1}^{2q-2}(4p-i)x^i + p(4p-3q+1)x^{2q-1} + 2p\sum_{i=2q}^{p+q-1}(2p+2q-2i-1)x^i;$$

(3) If $p+1 \leqslant q$,

$$\Delta H(p,q,x) = 2p + 3p\sum_{i=1}^{p-1} ix^i + p(3p-1)x^p + p\sum_{i=p+1}^{2p-1}(4p-i)x^i + 2p^2\sum_{i=2p}^{2q-2}x^i + p^2x^{2q-1}.$$

Proof of Theorem 3.1. According to Lemma 4.5 we distinguish here three cases.

Case 1. $q \leqslant \frac{p}{2}$,

$$\begin{aligned}
H(p,q,x) &= \sum_{j=1}^{q}\Delta H(p,j,x)\\
&= 2pq + 3p\sum_{j=1}^{q}\sum_{i=1}^{2j-2} ix^i + p\sum_{j=1}^{q}(5j-3)x^{2j-1} + 2p\sum_{j=1}^{q}\sum_{i=2j}^{p-1}(2j-1)x^i\\
&\quad + p\sum_{j=1}^{q}(4j-3)x^p + 2p\sum_{j=1}^{q}\sum_{i=p+1}^{p+j-1}(2p+2j-2i-1)x^i\\
&= 2pq + 3p\sum_{i=1}^{2q-2}(q-\lceil\frac{i}{2}\rceil)ix^i + p\sum_{\substack{i=1\\ i\text{ odd}}}^{2q-1}(\frac{5}{2}i-\frac{1}{2})x^i + 2p\Big(\sum_{i=1}^{2q-1}(\lfloor\frac{i}{2}\rfloor)^2x^i + \sum_{i=2q}^{p-1}q^2x^i\Big)\\
&\quad + pq(2q-1)x^p + 2p\sum_{i=p+1}^{p+q-1}(p+q-i)^2x^i\\
&= 2pq + p\sum_{i=1}^{2q-1}(-i^2+3qi)x^i + 2pq^2\sum_{i=2q}^{p-1}x^i + pq(2q-1)x^p + 2p\sum_{i=p+1}^{p+q-1}(p+q-i)^2x^i.
\end{aligned}$$

Case 2. $\frac{p}{2} < q \leqslant p$. We distinguish two subcases to discuss according to the parity of p. Firstly, if p is even,

$$\begin{aligned}
H(p,q,x) &= \sum_{j=1}^{q}\Delta H(p,j,x)\\
&= \sum_{j=1}^{\frac{p}{2}}\Delta H(p,j,x) + \sum_{j=\frac{p}{2}+1}^{q}\Delta H(p,j,x)
\end{aligned}$$

$$= H(p,\frac{p}{2},x) + 2p(q-\frac{p}{2}) + 3p\sum_{j=\frac{p}{2}+1}^{q}\sum_{i=1}^{p-1} ix^i + p(3p-1)(q-\frac{p}{2})x^p + p\sum_{j=\frac{p}{2}+1}^{q}\sum_{i=p+1}^{2j-2}(4p-i)x^i$$

$$+ p\sum_{j=\frac{p}{2}+1}^{q}(4p-3j+1)x^{2j-1} + 2p\sum_{j=\frac{p}{2}+1}^{q}\sum_{i=2j}^{p+j-1}(2p+2j-2i-1)x^i$$

$$= \big(p^2 + p\sum_{i=1}^{p-1}(-i^2+\frac{3pi}{2})x^i + (\frac{p^3}{2}-\frac{p^2}{2})x^p + 2p\sum_{p+1}^{\frac{3}{2}p-1}(\frac{3}{2}p-i)^2x^i\big) + 2p(q-\frac{p}{2})$$

$$+ 3p(q-\frac{p}{2})\sum_{i=1}^{p-1} ix^i + p(3p-1)(q-\frac{p}{2})x^p + p\sum_{i=p+1}^{2q-2}(q-\lceil\frac{i}{2}\rceil)(4p-i)x^i$$

$$+ p\sum_{\substack{i=p+1\\ i\text{ odd}}}^{2q-1}(4p-\frac{3}{2}i-\frac{1}{2})x^i + 2p\Big(\sum_{i=p+1}^{\frac{3}{2}p-1}(q-\frac{p}{2})(\frac{5}{2}p+q-2i)x^i + \sum_{i=\frac{3}{2}p}^{p+q-1}(q+p-i)^2x^i$$

$$- \sum_{i=p+1}^{2q}(q-\lfloor\frac{i}{2}\rfloor)(2p+q+\lfloor\frac{i}{2}\rfloor-2i)x^i\Big)$$

$$= 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq-p^2-q)x^p + 2p\sum_{i=p+1}^{\frac{3}{2}p-1}(q+p-i)^2x^i$$

$$+ 2p\sum_{i=\frac{3}{2}p}^{p+q-1}(q+p-i)^2x^i + p\sum_{i=p+1}^{2q}(i-q)(2q-i)x^i$$

$$= 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq-p^2-q)x^p$$

$$+ p\sum_{i=p+1}^{2q-1}(2p^2+4pq+i^2-4pi-qi)x^i + 2p\sum_{i=2q}^{p+q-1}(q+p-i)^2x^i.$$

Second, if p is odd, we can obtain the same result as above.

Case 3. $p+1\leqslant q$,

$$\begin{aligned} H(p,q,x) &= \sum_{j=1}^{q}\Delta H(p,j,x) \\ &= \sum_{j=1}^{p}\Delta H(p,j,x) + \sum_{j=p+1}^{q}\Delta H(p,j,x) \\ &= H(p,p,x) + 2p(q-p) + 3p\sum_{j=p+1}^{q}\sum_{i=1}^{p-1} ix^i + p(3p-1)(q-p)x^p \\ &\quad + p\sum_{j=p+1}^{q}\sum_{i=p+1}^{2p-1}(4p-i)x^i + 2p^2\sum_{j=p+1}^{q}\sum_{i=2p}^{2j-2}x^i + p^2\sum_{j=p+1}^{q}x^{2j-1} \end{aligned}$$

$$= \big(2p^2 + p\sum_{i=1}^{p-1}(-i^2+3pi)x^i + p^2(2p-1)x^p + p\sum_{i=p+1}^{2p-1}(6p^2+i^2-5pi)x^i\big)$$

$$+ 2p(q-p) + 3p(q-p)\sum_{i=1}^{p-1} ix^i + p(3p-1)(q-p)x^p + p(q-p)\sum_{i=p+1}^{2p-1}(4p-i)x^i$$

$$+ 2p^2\sum_{i=2p}^{2q-2}(q-\lceil\frac{i}{2}\rceil)x^i + p^2\sum_{\substack{i=2p+1\\ i \text{ odd}}}^{2q-1} x^i$$

$$= 2pq + p\sum_{i=1}^{p-1}(-i^2+3qi)x^i + p(3pq-p^2-q)x^p + p\sum_{i=p+1}^{2p-1}(2p^2+4pq+i^2-4pi-qi)x^i$$

$$+ p^2\sum_{i=2p}^{2q-1}(2q-i)x^i.$$

□

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