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# THE EDGE-SZEGED INDEX OF THE TITANIA NANOTUBES TIO$_2$ (M, N)

## LI YAN [1], YING FANG LI [2], MOHAMMAD REZA FARAHANI[3] AND MUHAMMAD KAMRAN JAMIL[4*]

[1]School of Engineer, Honghe University, Mengzi 661100, China

yanli_uoh@163.com

[2]School of Engineer, Honghe University, Mengzi 661100, China

1013747460@qq.com

[3] Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran

MrFarahani88@Gmail.com, Mr_Farahani@Mathdep.iust.ac.ir

[4]Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan

m.kamran.sms@gmail.com

## ABSTRACT

Let *G* be a connected graph with vertex set *V* and edge set *E*. The edge-Szeged index of a graph *G* is defined as $Sz_e(G) = \sum_{e=uv \in E(G)} [m_u(e/G) \times m_v(e/G)]$, where $m_u(e/G)$ is the number of edges lying closer to the vertex *u* then the vertex *v*, analogously defined $m_v(e/G)$. In this paper, we computed the edge-Szeged index of Titania nanotubes, *TiO$_2$[m,n]*.

**Keywords: Titania Nanotubes TiO$_2$(m,n); Wiener index; Szeged index; orthogonal cuts.**

## INTRODUCTION

From last few years, low-dimensional nano-structural materials have gained increasing scientific and technological observation due to their physical properties and their potential applications. The finding of carbon nanotubes by *Iijima* with their diverse interesting properties has derived the quest for the synthesis of nano-structures of other

substances and chemical compounds such as $Fe_2O_3$, $MoO_3$, $TiO_2$, $SiO_2$ and $V_2O_5$. Among these compounds, *titanium dioxide* has attracted great interest since due to its photosensitivity, high chemical stability, strong photo-oxidizing potential, non-toxicity and low cost [1-7].

Let $G$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For vertices $u,v \in V(G)$, the number of edges in a shortest path connecting $u$ and $v$ in $G$ is called *distance* between $u$ and $v$, denoted as $d_G(u,v)$. Suppose $e=uv \in E(G)$ is an edge connecting the vertices $u$ and $v$, and

$$n_u(e/G)=|\{w|w \in V(G), d(u,w)<d(v,w)\}|,$$
$$n_v(e/G)=|\{w|w \in V(G), d(v,w)<d(u,w)\}|,$$
$$m_u(e/G)=|\{x|x \in E(G), d(u,x)<d(x,v)\}|,$$
$$m_v(e/G)=|\{x|x \in E(G), d(v,x)<d(x,u)\}|,$$

i.e. $m_u(e/G)$ is the number of edges of $G$ lying closer to $u$ than to $v$, analogously defined $m_v(e/G)$, and $n_u(e/G)$ is the number of vertices of $G$ lying closer to $u$ than to $v$, analogously $n_v(e/G)$.

Topological indices are numerical values related with chemical structures via their hydrogen-depleted graphs, which are used in theoretical chemistry for the design of chemical compounds with given physicochemical properties.

The *Wiener index* of a graph $G$ is defined as

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

The Wiener index is one of the oldest and the most thoroughly studied topological indices [8-14].

*I. Gutman* [15] defined a new topological index besides the Wiener index, and named it the *Szeged Index*. They abbreviated this new

topological index as $Sz(G)$, (Of course, more precisely, we abbreviate it as $Sz_v(G)$ because there exists also a edge version of the Szeged index) defined as

$$Sz_v(G)= \sum_{e \in E(G)} [n_u(e/G) \times n_v(e/G)],$$

The vertices which are equidistant from $u$ and $v$ are neglected.

The edge version of Szeged index introduced recently by *I. Gutman* and *A.R. Ashrafi* [16] and was computed for some graphs [17, 18]. Readers can find computations of this index for some graphs in [19-26]. The edge version of Szeged index is defined as

$$Sz_e(G)= \sum_{e \in E(G)} [m_u(e/G) \times m_v(e/G)].$$

The edges which are equidistant from $u$ and $v$ are neglected.

*S. Klavžar* [27] gave the general description of the *cut method* and presents its

applications in chemical graph theory. Applications include the Wiener index, the Szeged index, the hyper-Wiener index, the PI index etc. *John et.al.* [28] describes an *orthogonal cut* by using the term of *strongly co-distant.* Also, they found the PI index of some graphs with the help of orthogonal cut. In this paper, we compute the edge-Szeged index of Titania nanotubes $TiO_2[m,n]$.

## RESULTS AND DISCUSSIONS

Titania nanotubes are comprehensively studied in materials science. Since the growth mechanism for $TiO_2$ nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. A graphical representation of $TiO_2$ is shown in graph Figure 1. In this section we computed the edge-Szeged index of Titania nanotubes.
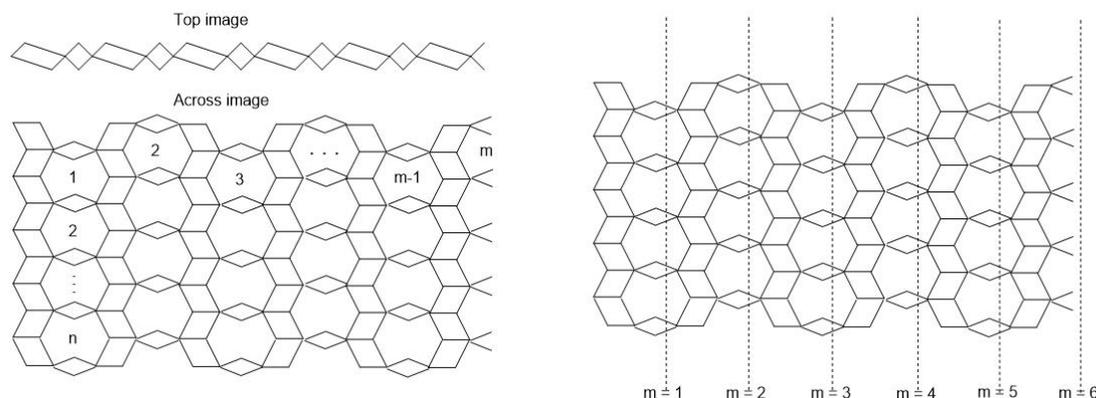


**Figure 1: A graphical representation of Titania nanotube *$TiO_2[m,n]$*.**

**Theorem 1.** The edge version of Szeged index of Titania Nanotubes *$TiO_2(m,n)$ ($\forall m,n \geq 1$)* is equal to

$$Sz_e(TiO_2(m,n)) = 4hm^2[-250hm + 250mn - 400h + 330m + 400n] + 4m^2[570mn + 778m + 534h + 871n - 1454]$$
$$-2hm[-400hm + 400mn - 480h + 460m + 480n - 216] + 2m[1080mn - 1360m + 748h + 2041n - 3755]$$
$$-2h[256h - 256n - 304] + 2[356n - 1036]$$

***Proof.*** Let *$TiO_2(m,n)$* be the Titania Nanotubes for all *$m,n \in \mathbb{N}$* with *$12(m+1)(\frac{1}{2}n)+4(m+1)=6mn+4m+6n+4=2(3n+2)(m+1)$* vertices/atoms bonds ($|V(TiO_2(m,n))|$) where $6\left(\frac{n}{2}\right)+2+4(m-1)\left(\frac{n}{2}\right)+0+7+6\left(\frac{n}{2}-1\right)+1=2mn+4n+4$ vertices have degree two, $2\left(\frac{n}{2}\right)+2\left(\frac{n}{2}\right)=2n$ vertices have degree four, $2(m)\left(\frac{n}{2}\right)=2mn$ vertices have degree five and there are $3+2\left(\frac{n}{2}-1\right)+1+5(m-1)+4(m-1)\left(\frac{n}{2}-1\right)+3(m-1)+2\left(\frac{n}{2}+1\right)=2mn+4m$ vertices with degree 3. Thus the number of edges/Chemical bonds is equal to *$|E(TiO_2(m,n))|$ $=\frac{1}{2}[2(2mn+4n+4)+3(2mn+4m)+4(2n)+5(2mn)] =10mn+6m+8n+4$* .

Now, by refer to definition of the edge Szeged index in the first section , we see that it is enough to compute $m_u(e/TiO_2(m,n))$ and $m_v(e/TiO_2(m,n))$ for all $e) \in E(TiO_2(m,n))$ belong to the orthogonal cut $C(e)$.
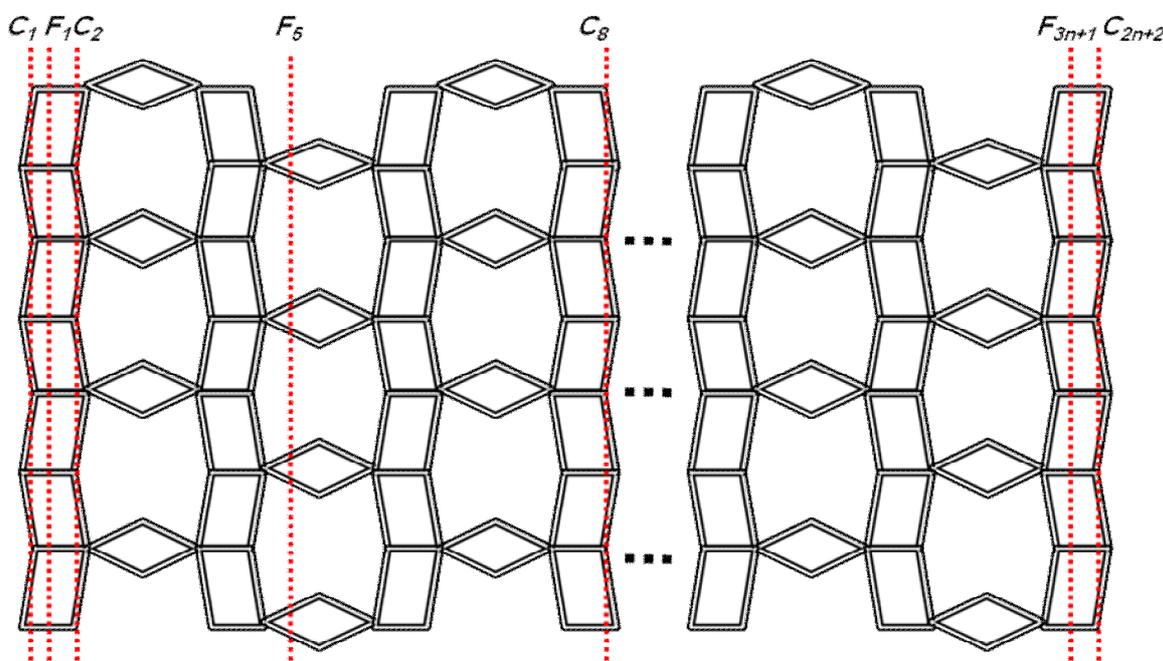


**Figure 2. Orthogonal cuts representation of the Titania nanotubes.**

Thus by using the Cut Method and finding Orthogonal Cuts of the Titania Nanotubes $TiO_2(m,n)$, we can determine all edge cuts (quasi-orthogonal) of $TiO_2(m,n)$ and compute all $m_u(e/TiO_2(m,n))$ and $m_v(e/TiO_2(m,n))$, $\forall e \in E(TiO_2(m,n))$.

We denote $m_u(e/TiO_2(m,n))$ as the number of edges in the left component of $TiO_2(m,n)$-$C(e)$ and alternatively $m_v(e/TiO_2(m,n))$ as the number of edges in the right component of $TiO_2(m,n)$-$C(e)$, $\forall e=uv \in E(TiO_2(m,n))$.

From Figure 2, we see that there are $5n+3$ vertical cuts for all edges in $TiO_2(m,n)$, $\forall$ $m,n \in \mathbb{N}$ and obviously all these orthogonal cuts are vertical. Now on based an edge e is an oblique edge or a horizontal edge, we dente its orthogonal cut by $C_i$ or $F_j$ for all $i=1,...,C=2(n+1)$ and $j=1,...,F=2n+n+1$.

Clearly from Figure 2, we can notice that the size of all orthogonal cuts $C_i$ are equivalence and is $2m+1=|C_i|$ and the size of all orthogonal cuts $F_i$ are equivalence, too and is $2(m+1)=|F_i|$ . Thus for all orthogonal cuts $C_i$ and $F_i$, we have following results.

In case the orthogonal cuts $C_i(i=1,...,2(n+1))$ , see Figure 2:

- For $C_1$: $m_u(e_1/TiO_2(m,n))=0$ and $m_v(e_1/TiO_2(m,n))=|E(TiO_2(m,n))|-|C_1|=10mn+6m+8n+4-(2m+1)=10mn+4m+8n+3$.

- For $C_2$: $m_u(e_2/TiO_2(m,n))=|C_1|+|F_1|=2m+1+2m+2=4m+3$ and $m_v(e_2/TiO_2(m,n))=|E(TiO_2(m,n))|-(|C_1|+|F_1|+|C_2|)=10mn+6m+8n+4-(6m+4)=10mn+2m+8n.$

- For $C_3$: $m_u(e_3/TiO_2(m,n))=2|C_1|+3|F_1|=10m+8$ and $m_v(e_3/TiO_2(m,n))=|E(TiO_2(m,n))|-(3|C_1|+3|F_1|)=10mn+6m+8n+4-(12m+9)=10mn+8n-6m-5.$

- For $C_4$: $m_u(e_4/TiO_2(m,n))=3|C_1|+4|F_1|=14m+11$ and $m_v(e_4/TiO_2(m,n))=|E(TiO_2(m,n))|-(3|C_1|+4|F_1|)=10mn+6m+8n+4-(16m+12)=10mn+8n-10m-8.$

- For $C_{(2h-1)}$:

$m_u(e_{(2h-1)}/TiO_2(m,n))=(2h-2)|C_1|+(3h-3)|F_1|=(2h-2)(2m+1)+(3h-3)(2m+2)=(10m+8)(h-1)$

and

$m_v(e_{(2h-1)}/TiO_2(m,n))=|E(TiO_2(m,n))|-((2h-1)|C_1|+(3h-3)|F_1|)$

$=10mn+6m+8n+4-(10m+8)(h-1)-(2m+1)$

- For $C_{(2h)}$:

$m_u(e_{(2h)}/TiO_2(m,n))=(2h-1)|C_1|+(3h-2)|F_1|=(2h-1)(2m+1)+(3h-2)(2m+2)=10hm+8h-6m-5$

*and*

$m_v(e_{(2h)}/TiO_2(m,n))=|E(TiO_2(m,n))|-(2h|C_1|+(3h-1)|F_1|)=10m(n-h)+10m+8(n-h)+8.$

- For $C_{2n+2}$:

$m_u(e_{2n+2}/TiO_2(m,n))=(2n+1)|C_1|+(3n+1)|F_1|=(2h-1)(2m+1)+(3h-2)(2m+2)=10nm+8n+4m+3$

and                                    $m_v(e_{2n+2}/TiO_2(m,n))=0.$

In case the orthogonal cuts $F_j$ (j=1,…,3n+1) , see Figure 2:

*For* $F_1$: $m_u(e_1/TiO_2(m,n))=2m+1=|C_i|$ *and* $m_v(e_1/TiO_2(m,n))=|E(TiO_2(m,n))|-(|C_1|+|F_1|)=10mn+6m+8n+4-(4m+3)=10mn+8n+2m+1.$

*For* $F_2$: $m_u(e_2/TiO_2(m,n))=2|C_1|+|F_1|=6m+4$ *and* $m_v(e_2/TiO_2(m,n))=|E(TiO_2(m,n))|-(2|C_1|+2|F_1|)=10mn+6m+8n+4-(8m+6)=10mn+8n-2m-2.$

*For* $F_3$: $m_u(e_3/TiO_2(m,n))=2|C_1|+2|F_1|=8m+6$ *and* $m_v(e_3/TiO_2(m,n))=|E(TiO_2(m,n))|-(2|C_1|+3|F_1|)=10mn+6m+8n+4-(10m+8)=10mn+8n-4m-4.$

*For* $F_4$: $m_u(e_4/TiO_2(m,n))=3|C_1|+3|F_1|=12m+9$ *and* $m_v(e_4/TiO_2(m,n))=|E(TiO_2(m,n))|-(3|C_1|+4|F_1|)=10mn+6m+8n+4-(14m+11)=10mn+8n-8m-7.$

*For   $F_5$:   $m_u(e_5|TiO_2(m,n))=4|C_1|+4|F_1|=16m+12$   and   $m_v(e_5|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+5|F_1|)=10mn+6m+8n+4-(18m+14)=10mn+8n-12m-10$.*

*For   $F_6$:   $m_u(e_6|TiO_2(m,n))=4|C_1|+5|F_1|=18m+13$   and   $m_v(e_6|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(20m+15)=10mn+8n-14m-11$.*

*For   $F_7$:   $m_u(e_7|TiO_2(m,n))=5|C_1|+6|F_1|=22m+17$   and   $m_v(e_7|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(24m+19)$.*

*For   $F_8$:   $m_u(e_8|TiO_2(m,n))=6|C_1|+7|F_1|=22m+17$   and   $m_v(e_8|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(24m+19)$.*

- *For $F_{3h+1}$ ($h=0,...,n$):*

*$m_u(F_{3h+1}|TiO_2(m,n))=(2h+1)|C_1|+(3h)|F_1|=(2h+1)(2m+1)+(3h)(2m+2)=10hm+2m+8h+1$.*

*$m_v(F_{3h+1}|TiO_2(m,n))= |E(TiO_2(m,n))|-(10hm+2m+8h+1)=(10m+8)(n-h)+4m+3$.*

- *For $F_{3h-1}$ ($h=1,...,n$):*

*$m_u(F_{3h-1}|TiO_2(m,n))=(2h)|C_1|+(3h-2)|F_1|$*

*$=(2h)(2m+1)+(3h-2)(2m+2)= (10m+8)h-2|F_1|=10hm-4m+8h-4$.*

*$m_v(F_{3h-1}|TiO_2(m,n))= (10mn+6m+8n+4)-(10hm-4m+8h-4)=(10m+8)(n-h)+10m+8$.*

- *For $F_{3h}$ ($h=1,...,n$):*

*$m_u(F_{3h}|TiO_2(m,n))= m_u(F_{3h-1}|TiO_2(m,n))+ |F_1|$*

*$=2h|C_1|+(3h-1)|F_1|=(10m+8)h-|F_1|= (10m+8)h-2m-2$.*

*$m_v(F_{3h}|TiO_2(m,n))= m_v(F_{3h-1}|TiO_2(m,n))-|F_1|=(10m+8)(n-h)+8m+6$.*

Now, we can compute the edge Szeged index of the Titania Nanotubes $TiO_2(m,n)$ ($\forall m,n>1$) as:

$$SZ_e(TiO_2(m,n))= \sum_{e_i=uv\in E(TiO_2(m,n))} (m_u(e_i|TiO_2(m,n))\times m_v(e_i|TiO_2(m,n)))$$

$$= \sum_{\substack{e_i=vu\in C_i \\ i=1,...,2n+2}} |C_i|\left[m_u\left(e_i|TiO_2(m,n)\right)\times m_v\left(e_i|TiO_2(m,n)\right)\right]+ \sum_{\substack{f_i=vu\in F_i \\ i=1,...,3n+1}} |F_i|\left[m_u\left(f_i|TiO_2(m,n)\right)\times m_v\left(f_i|TiO_2(m,n)\right)\right]$$

$$= |C_1| \sum_{\substack{e_{2h-1}=vu\in C_{2h-1} \\ h=1,\dots,n+1}} \left[ m_u\left(e_{2h-1}\,|TiO_2(m,n)\right) \times m_v\left(e_{2h-1}\,|TiO_2(m,n)\right) \right]$$

$$+ |C_1| \sum_{\substack{e_{2h}=vu\in C_{2h} \\ h=1,\dots,n+1}} \left[ m_u\left(e_i\,|TiO_{2h}(m,n)\right) \times m_v\left(e_{2h}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k+1}=vu\in F_{3k+1} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k+1}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k+1}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k}=vu\in F_{3k} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k-1}=vu\in F_{3k-1} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k-1}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k-1}\,|TiO_2(m,n)\right) \right]$$

$$= |C_1| \sum_{\substack{e_{2h-1}=vu\in C_{2h-1} \\ h=1,\dots,n+1}} \left[ m_u\left(e_{2h-1}\,|TiO_2(m,n)\right) \times m_v\left(e_{2h-1}\,|TiO_2(m,n)\right) \right]$$

$$+ |C_1| \sum_{\substack{e_{2h}=vu\in C_{2h} \\ h=1,\dots,n+1}} \left[ m_u\left(e_i\,|TiO_{2h}(m,n)\right) \times m_v\left(e_{2h}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k+1}=vu\in F_{3k+1} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k+1}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k+1}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k}=vu\in F_{3k} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k}\,|TiO_2(m,n)\right) \right]$$

$$+ |F_1| \sum_{\substack{f_{3k-1}=vu\in F_{3k-1} \\ k=1,\dots,n}} \left[ m_u\left(f_{3k-1}\,|TiO_2(m,n)\right) \times m_v\left(f_{3k-1}\,|TiO_2(m,n)\right) \right]$$

$$= (2m+1)\left[ \begin{array}{l} 0\times(10mn+4m+8n+3)+(10m+8)\times(10mn+8n-6m-5)+\cdots+ \\ (10m+8)(h-1)\times(10mn+6m+8n+4-(10m+8)(h-1)-(2m+1)) \end{array} \right] +$$

$$(2m+1)\left[ \begin{array}{l} (4m+3)\times(10mn+2m+8n)+(14m+11)\times(10mn+8n-10m-8)+\cdots+ \\ (10hm+8h-6m-5)\times(10m(n-h)+10m+8(n-h)+8) \end{array} \right] +$$

$$2(m+1)\left[ \begin{array}{l} (2m+1)\times(10mn+8n+2m+1)+(12m+9)\times(10mn+8n-8m-7)+ \\ (22m+17)\times(10mn+6m+8n+4-24m-19)+\cdots+ \\ (10hm+2m+8h+1)\times((10m+8)(n-h)+4m+3) \end{array} \right] +$$

$$2(m+1)\left[ \begin{array}{l} (8m+6)\times(10mn+8n-4m-4)+(18m+13)\times(10mn+8n-14m-11)+\cdots+ \\ ((10m+8)h-2m-2)\times((10m+8)(n-h)+8m+6) \end{array} \right] +$$

$$2(m+1)\left[ \begin{array}{l} (6m+4)\times(10mn+8n-2m-2)+(16m+12)\times(10mn+8n-12m-10)+ \\ (22m+17)\times(10mn+6m+8n+4-(24m+19))+\cdots+ \\ (10hm-4m+8h-4)\times((10m+8)(n-h)+10m+8) \end{array} \right]$$

$$= (2m+1)\left[ \begin{array}{l} -100h^2m^2-160h^2m-64h^2+100hm^2n+240hm^2+160hmn+382hm+ \\ 64hn+152h-200m^2-320m-128 \end{array} \right]$$

$$+(2m+1)\begin{bmatrix} -100h^2m^2 -160h^2m -64h^2 +100hm^2n +160hm^2 +160hmn + \\ 258hm +64hn +104h -192m^2 -314m +120m^2n +186mn +72n -128 \end{bmatrix}$$

$$+2(m+1)\begin{bmatrix} -100h^2m^2 -160h^2m -64h^2 +100hm^2n +20hm^2 +160hmn +36hm + \\ 64hn +16h -480m^2 -778m +380m^2n +584mn +224n -314 \end{bmatrix}$$

$$+2(m+1)\begin{bmatrix} -100h^2m^2 -160h^2m -64h^2 +100hm^2n +100hm^2 +160hmn +160hm + \\ 64hn +64h +240m^2n -44m^2 +362mn -464m -136n -179 \end{bmatrix}$$

$$+2(m+1)\begin{bmatrix} -100h^2m^2 -160h^2m -64h^2 +100hm^2n +140hm^2 +160hmn +232hm + \\ 64hn +96h +400m^2n -640m^2 +610mn -1032m +232n -415 \end{bmatrix}$$

$$=2m\begin{bmatrix} -500h^2m^2 +500hm^2n -800h^2m +660hm^2 +800hmn +1140m^2n -320h^2 - \\ 1556m^2 +1068hm +320hn +1742mn +432h -2908m +392n -1164 \end{bmatrix}$$

$$+\begin{bmatrix} -800h^2m^2 +800hm^2n -1280h^2m +920hm^2 +1280hmn +2160m^2n -512h^2 - \\ 2720m^2 +1496hm +512hn +3298mn +608h -5182m +712n -2072 \end{bmatrix}$$

$$=4hm^2\begin{bmatrix} -250hm +250mn -400h +330m +400n \end{bmatrix}$$
$$+4m^2[570mn +778m +534h +871n -1454]$$
$$-2hm\begin{bmatrix} -400hm +400mn -480h +460m +480n -216 \end{bmatrix}$$
$$+2m\begin{bmatrix} 1080mn -1360m +748h +2041n -3755 \end{bmatrix}$$
$$-2h\begin{bmatrix} 256h -256n -304 \end{bmatrix}+2[356n -1036]$$

And these complete the proof of Theorem.∎

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