The Harmonic index of general graphs, nanocones and triangular benzenoid graphs

LIHUI YANG, HONGBO HUA[a,*]

Department of mathematics, Hunan City University, Yiyang City, Hunan 413000, P. R. China

[a]*Faculty of Mathematics and Physics, Huaiyin Institute of Technology, Huai'an City, Jiangsu 223003, P. R. China*

The *Harmonic index* of a graph *G* is defined as $H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}$, where $d_G(v)$ is the degree of vertex *v* in *G*. In this paper, we first report some further mathematical properties of Harmonic index for general connected graphs. Then we give explicit computing formulae for Harmonic index of nanocones and triangular benzenoid graphs, respectively.

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1. Introduction

Let *G* be a graph with vertex set *V(G)* and edge set *E(G)*. The *Harmonic index* of graph *G* is defined [2] as the sum

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)},$$

where $d_G(v)$ is the degree of vertex *v* in *G*.

Harmonic index is related with other graph invariants, which is referred in [2]. The authors [3] disapproved some conjectures about the eigenvalues and Harmonic index. In [4], the author investigate the unicyclic graphs with the minimum and maximum Harmonic index among all *n*-vertex unicyclic graphs.

During the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. One pentagonal carbon nanocones originally discovered by Ge and Sattler in 1994 [9]. For mathematical properties of nanocones we encourage the reader to consult papers [10-14] and the references.

In this paper, we first report some further mathematical properties of Harmonic index. Then we give explicit computing formulae for Harmonic index of of nanocones and triangular benzenoid graphs, respectively.

2. Main results and discussion

We first report some further mathematical properties of Harmonic index, different from those have been obtained in [4].

Recall that the well-known Randic index (see [1]) is defined as $R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)d_G(v)}}$.

Theorem 1. *Let G be a connected graph with* $n\geq 2$ *vertices and m edges. Then* $H(G)\leq R(G)$, *with equality if and only if G is a* $\frac{2m}{n}-$ *regular graph of order n.*

Proof. Let *uv* be an edge in *G*. Note that $d_G(u)+d_G(v)\geq 2\sqrt{d_G(u)d_G(v)}$. Then the contribution of *uv* to *H(G)* is no more than $\frac{1}{\sqrt{d_G(u)d_G(v)}}$. Summing up the contribution of all edges, we obtain $H(G) \le \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}} = R(G)$. Obviously, the equality holds if and only if $d_G(u) = d_G(v)$ for any edge *uv* in G. Now, *G* is a regular graph. Suppose that $d_G(u) = k$ for any vertex *u*. Then we have $nk = 2m$, completing the proof.

Let $M_1(G) = \sum_{u\in V(G)} (d_G(u))^2$ denote the first Zagreb index (see [5, 6]). This topological index can be rewritten as $M_1(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))$.

Theorem 2. *Let G be a connected graph with n vertices and m edges. Then* $H(G) > \frac{2m^2}{M_1(G)}$.

Proof. By the definition of Harmonic index and the first Zagreb index, we immediately have $H(G)M_1(G) \ge 2m^2$, that is, $H(G) \ge \frac{2m^2}{M_1(G)}$. Obviously, the equality can not be attained since $\frac{1}{d_G(u)+d_G(v)} \ne d_G(u) + d_G(v)$ for any edge *uv* in a connected graph *G*. This completes the proof.

Let $\overline{M}_1(G) = \sum_{uv\notin E(G)} (d_G(u) + d_G(v))$ denote the first Zagreb coindex (see [7, 8]).

Lemma 1([7]). *Let G be a simple graph with* $n \ge 2$ *vertices and m edges. Then* $\overline{M}_1(G) = 2m(n-1) - M_1(G)$.

It then follows from Theorem 2 and Lemma 1 the following consequence.

Corollary 1. *Let G be a simple graph with* $n \ge 2$ *vertices and m edges. Then* $H(G) > \frac{2m^2}{2m(n-1) - \overline{M}_1(G)}$.

Theorem 3. *Let G be a connected triangle-free graph with* $n \ge 2$ *vertices and m edges. Then* $H(G) \ge \frac{2m}{n}$ *with equality if and only if G is an n-vertex star* S_n.

Proof. Let *uv* be an edge in *G*. Since *G* is triangle-free, we have $d_G(u) \le n - d_G(v)$. Summing up the contribution of all edges gives $H(G) \ge \frac{2m}{n}$. If *G* is the *n*-vertex star S_n , then $H(G) = \frac{2(n-1)}{n} = \frac{2m}{n}$, as claimed. Conversely, we assume that $H(G) = \frac{2m}{n}$ but *G* is not isomorphic to S_n. Then there must exist an edge *uv* such that $d_G(u) < n - d_G(v)$, implying that $H(G) > \frac{2m}{n}$, a contradiction. This completes the proof.

Theorem 4. *Let G be a 2-edge-connected graph with n vertices and m edges. Then* $H(G) \le \frac{m}{2}$ *with equality if and only if G is an n-vertex cycle* C_n.

Proof. Let *uv* be an edge in *G*. Since *G* is *2-edge-connected*, we have $d_G(u) \ge 2$ and . $d_G(v) \ge 2$. So we have $H(G) \le \frac{m}{2}$ *with equality if and only if* $d_G(v) = 2$ for any vertex *v* in *G*, that is, $G \cong C_n$, as desired.

Note that a 2-connected graph is necessarily a 2-edge-connected graph. By Theorem 4, we thus have

Theorem 5. Let G be a 2-connected graph with *n* vertices and m edges. Then $H(G) \le \frac{m}{2}$ with equality if and only if G is an n-vertex cycle C_n.

The nanocones are constructed from a graphene sheet by removing a wedge and joining the edges produces a cone with a single triangle, square or pentagonal defects at the apex. In some recent papers [10-14] the authors investigated the mathematical properties of this interesting class of nano-materials.

Suppose $NC_n(k)$ denotes an arbitrary nanocone, where n denotes the number of edges in the single triangle, square, pentagon, etc. See Fig.s 1-3 for examples of this type of nanocones.

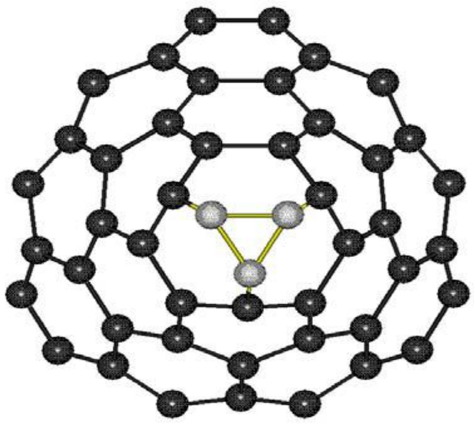

Fig. 1. A NC3(3) Nanocone.

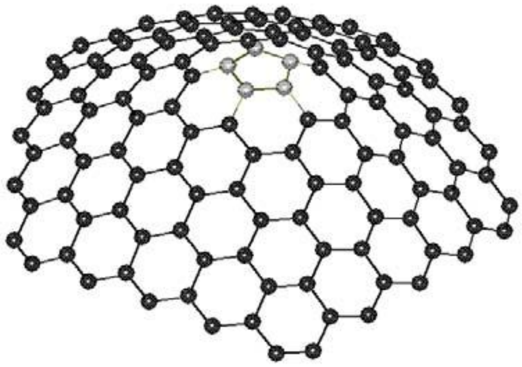

Fig. 2. A NC5(4) Nanocone..

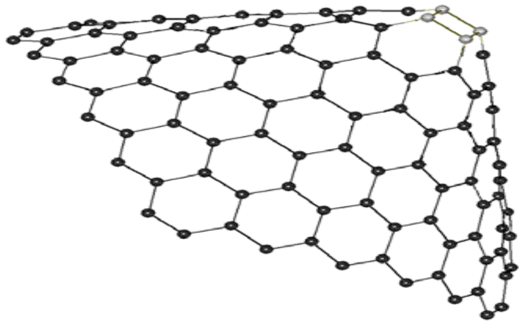

Fig. 3. A NC4(5) Nanocone.

In the following, we give an explicit computing formula for Harmonic index of an infinite class of nanocones $NC_n(k)$, as shown in above graphs.

Theorem 6. *Let* $NC_n(k)$ *be the nanocone as introduced above. Then* $H(NC_n(k)) = \frac{n}{2} + \frac{17kn}{30} + \frac{nk^2}{2}$.

Proof. For the sake of brevity, if an edge whose two ends are of degree i and j, respectively, then this edge is simply said to be an $(i, j)-$edge in the subsequent part of this paper. According to the definition of Harmonic index, it is sufficient to compute $\frac{2}{d(u)+d(v)}$ for each edge $e=uv$ in $NC_n(k)$.

We consider the contribution of three types of edges, namely, (2,2)-edge, (2,3)-edge and (3,3)-edge to Harmonic index. One can see that both (2,2)-edge and (2,3)-edge lie only within the last layer.

If we denote the number of edges in $NC_n(k)$ by t_k, then we obtain the following recursive relations: $t_k - t_{k-1} = n(3k+1)$. So we obtain $E(NC_n(k)) = \frac{n(k+1)(3k+2)}{2}$. By these calculations one can see that the number of vertices in the last layer is $n(2k+1)$. It is then obvious that the number of (2, 2)-edges in $NC_n(k)$ is *n*. So the number of (2, 3)-edges in $NC_n(k)$ equals to *2kn* and the number of (3, 3)-edges in $NC_n(k)$ equals to $\frac{n(k+1)(3k+2)}{2} - n(2k+1) = \frac{kn(3k+1)}{2}$. An elementary computation gives $H(NC_n(k)) = \frac{n}{2} + \frac{2nk}{5} + \frac{k(3k+1)n}{6} = \frac{n}{2} + \frac{17kn}{30} + \frac{k^2 n}{2}$, as desired. ■

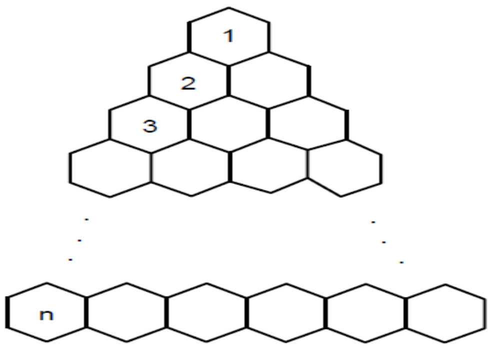

Fig. 4. The triangular benzenoid graph T(n).

Let *T(n)* denote a triangular benzenoid graph possessing *n* layer, see Fig. 4. It can be seen that there are $\frac{3(n^2+3n)}{2}$ edges in *T(n)*. Also, the number of (2, 2)-edges in *T(n)* is 6, the number of (3, 3)-edges in *T(n)* is $\frac{3n(n-1)}{2}$ and the number of (2, 3)-edges in *T(n)* is $6(n-1)$. Adding up the contribution of all edges in *T(n)* to Harmonic index gives

Theorem 7. *Let* $T(n)$ *be the triangular benzenoid graphs as introduced above. Then* $H(T(n)) = \frac{n^2}{2} + \frac{19n}{10} + \frac{3}{5}$.

3. Concluding remarks

In this paper, we reported some new mathematical properties of a new vertex- degree based topological index, namely, Harmonic index. Also, exact computing formulae for Harmonic index of nanocones and triangular benzenoid graphs were obtained. It may be interesting to investigate the relations between Harmonic index and other graph invariants and compute this new index for other nano structures.

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*Corresponding author: hongbo.hua@gmail.com
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