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The Nordhaus-Goddum-type inequalities for some chemical indices

Li Zhang[1] * **and Baoyindureng Wu**[1,2]

[1]Institute of Systems Science, Academy of Mathematics and System Sciences
Chinese Academy of Sciences, Beijing 100080, P.R.China

[2] Department of Mathematics and System Sciences, Xinjiang University
Urumqi, Xinjiang 830046, P.R.China

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Abstract

Many chemical indices have been invented in theoretical chemistry, such as the Randić index, the Zagreb index and the Wiener index etc. In this paper, the Nordhaus-Goddum-type inequalities for these three kinds of chemical indices are presented. The corresponding extremal graphs for the inequalities are also given.

1 Introduction

Let $G = (V(G), E(G))$ be a graph. The degree and the neighborhood of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and $N_G(u)$ (or simply by $d(u)$ and $N(u)$), respectively. Given two adjacent vertices u and v of a graph G, the Randić weight of the edge uv is $R(uv) = (d(u)d(v))^{-\frac{1}{2}}$, and the Randić index of a graph G, $R(G)$, is the sum of the Randić weights of its edges. Randić [6] proposed the important topological index in his research on molecular structures, which is closely related with many chemical properties. Fixing $\alpha \in R - \{0\}$, the general Randić index is defined as $R_\alpha(G) = \sum_{uv \in E(G)} R_\alpha(uv) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha$. Hence, $R_{-\frac{1}{2}}(G)$ is the ordinary Randić index of G.

There are also a large number of other chemical indices of molecular graphs. Next we just give the definitions of those are particularly concerned with in this paper. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, defined in [1], are $M_1(G) = \sum_{u \in V(G)} (d(u))^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$, respectively. Note that the second Zagreb index $M_2(G)$ is just the general Randić index $R_1(G)$. By observing the common appearance of the general Randić index and the Zagreb index, Li and Zhao [4] introduced

*corresponding author. Email: zhangli@amss.ac.cn, baoyin@amss.ac.cn

the first general Zagreb index as $M_\alpha(G) = \sum_{u\in V(G)}(d(u))^\alpha$ where $\alpha \in R$ and $\alpha \neq 0$. The Wiener index of G, defined in [7], is $W(G) = \sum_{\{u,v\}} d_G(u,v)$ where $d_G(u,v)$ denotes the distance between u and v in G and the sum goes over all the unordered pairs of vertices. For the results and further references the reader may refer to the recent survey article [2].

For a graph G, the chromatic number $\chi(G)$ is the minimum number of colors needed to color the vertices of G in such a way that no two adjacent vertices are assigned the same color. Throughout the paper, the complement of a graph G, denoted by $\bar{G}$, is the graph with the same vertex set as G, where two vertices are adjacent if and only if they are not adjacent in G. In 1956, Nordhaus and Goddum [5] gave the bounds involving the chromatic number $\chi(G)$ of a graph G and its complement.

Theorem 1.1. (Nordhaus and Goddum [5]) Let G be a graph of order n, and $\bar{G}$ be its complement. Then $2\sqrt{n} \leq \chi(G) + \chi(\bar{G}) \leq n + 1$.

Motivated by this theorem, we present the corresponding Nordhaus-Goddum-type inequalities for the general Randić index, the Zagreb index and the Wiener index in the following sections.

2 General Randić Index

Lemma 2.1. Define $f(x) = x^x(a-x)^{(a-x)}$ for $x \in (0,a)$ and $f(0) = f(a) = a^a$. Then $f(x) \geq (\frac{a}{2})^a$ for $x \in [0,a]$.

Proof. By the definition of $f(x)$, both $f'(x)$ and $f''(x)$ are continuous on $[0,a]$, and it is easy to check that $\frac{a}{2}$ is the unique zero of $f'(x)$, and $f''(\frac{a}{2}) > 0$. This means that $f(x) \geq f(\frac{a}{2})$ for any $x \in [0,a]$. □

Theorem 2.2. Let G be a graph of order n. If $\alpha > 0$, then
$\binom{n}{2}(\frac{n-1}{2})^{2\alpha} \leq R_\alpha(G) + R_\alpha(\bar{G}) \leq \binom{n}{2}(n-1)^{2\alpha}$.

Proof. For a graph $G = (V,E)$ of order n, let $\varepsilon(G) = |E(G)|$ and $N = \binom{n}{2}$. First we consider the upper bound. Since $\alpha > 0$, we have

$$\begin{aligned} R_\alpha(G) + R_\alpha(\bar{G}) &= \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha + \sum_{uv\in E(\bar{G})} (d_{\bar{G}}(u)d_{\bar{G}}(v))^\alpha \\ &\leq \varepsilon(G)[(n-1)(n-1)]^\alpha + \varepsilon(\bar{G})[(n-1)(n-1)]^\alpha \\ &= \binom{n}{2}(n-1)^{2\alpha}. \end{aligned}$$

Now we aim to the lower bound.

$$\begin{aligned} R_\alpha(G)+R_\alpha(\bar{G}) &= \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha + \sum_{uv\in E(\bar{G})} (d_{\bar{G}}(u)d_{\bar{G}}(v))^\alpha \\ &\geq N \sqrt[N]{\prod_{uv\in E(G)} (d_G(u)d_G(v))^\alpha \prod_{uv\in E(\bar{G})} (d_{\bar{G}}(u)d_{\bar{G}}(v))^\alpha} \\ &= N \sqrt[N]{\prod_{u\in V(G)} (d_G(u))^{d_G(u)\alpha} \prod_{v\in V(\bar{G})} (d_{\bar{G}}(v))^{d_{\bar{G}}(v)\alpha}} \\ &= N \ [\prod_{u\in V(G)} (d_G(u))^{d_G(u)}(n-1-d_G(u))^{(n-1-d_G(u))}]^{\frac{\alpha}{N}} \\ &\geq N \ [\prod_{u\in V(G)} (\frac{n-1}{2})^{(n-1)}]^{\frac{\alpha}{N}} \\ &= \binom{n}{2}[(\frac{n-1}{2})^{(n-1)n}]^{\frac{2\alpha}{n(n-1)}} \\ &= \binom{n}{2}(\frac{n-1}{2})^{2\alpha}. \end{aligned}$$

Similarly, we can get the bounds for $\alpha < 0$. □

Theorem 2.3. Let G be a graph of order n, and $\bar{G}$ be its complement. If $\alpha < 0$, then $\binom{n}{2}(n-1)^{2\alpha} \leq R_\alpha(G)+R_\alpha(\bar{G}) \leq \binom{n}{2}(\frac{n-1}{2})^{2\alpha}$.

Note that the bounds are best possible. The complete graph K_n is the unique graph G whose $R_\alpha(G)+R_\alpha(\bar{G})$ attains the upper bound in Theorem 2.2. For any $n = 4k+1, k \geq 1$, there exists a graph G_n with G_n and $\bar{G_n}$ are $2k$-regular. Then G_n is a graph G whose $R_\alpha(G)+R_\alpha(\bar{G})$ attains the lower bound in Theorem 2.2. For $\alpha < 0$, K_n and G_n are, in turn, the graphs whose $R_\alpha(G)+R_\alpha(\bar{G})$ attain the lower and upper bound respectively in Theorem 2.3.

3 Zagreb Indices

As we have seen before, the second Zagreb index $M_2(G)$ of a graph G is just the general Randić index $R_1(G)$. By Theorem 2.2, we have

$$\binom{n}{2}(\frac{n-1}{2})^2 \leq M_2(G)+M_2(\bar{G}) \leq \binom{n}{2}(n-1)^2.$$

Next we will determine the Nordhaus-Goddum-type inequality for the first general Zagreb index $M_\alpha(G) = \sum_{u\in V(G)}(d_G(u))^\alpha$, where $\alpha \in R, \alpha \neq 0$ and $\alpha \neq 1$.

Theorem 3.1. Let G be a graph of order n, then

(i) $2n(\frac{n-1}{2})^\alpha \leq M_\alpha(G)+M_\alpha(\bar{G}) \leq n(n-1)^\alpha$, if $\alpha > 1$.

(ii) $n(n-1)^\alpha \leq M_\alpha(G)+M_\alpha(\bar{G}) \leq 2n(\frac{n-1}{2})^\alpha$, if $0 < \alpha < 1$.

(iii) $2n(\frac{n-1}{2})^\alpha \leq M_\alpha(G)+M_\alpha(\bar{G}) \leq n(1+(n-2)^\alpha)$, if $\alpha < 0$.

Proof. By the definition,

$$M_\alpha(G)+M_\alpha(\bar{G})=\sum_{u\in V(G)}(d_G(u))^\alpha+\sum_{u\in V(\bar{G})}(d_{\bar{G}}(u))^\alpha=\sum_{u\in V(G)}((d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha).$$

Let $f(x)=x^\alpha$, where $x\geq 0$, $\alpha\in R$, $\alpha\neq 0$ and $\alpha\neq 1$. The second derivative $f''(x)=\alpha(\alpha-1)x^{\alpha-2}$ satisfies that $f''(x)>0$ if $\alpha>1$ or $\alpha<0$ and $f''(x)<0$ if $0<\alpha<1$. This implies that $f(x)$ is a convex function if $\alpha\in(-\infty,0)\cup(1,+\infty)$ and is a concave function if $\alpha\in(0,1)$.

By the definition of convex function, $(d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha\geq 2(\frac{d_G(u)+d_{\bar{G}}(u)}{2})^\alpha=2(\frac{n-1}{2})^\alpha$ if $\alpha\in(-\infty,0)\cup(1,+\infty)$. Thus,

$$M_\alpha(G)+M_\alpha(\bar{G})\geq 2n(\frac{n-1}{2})^\alpha,\quad \alpha\in(-\infty,0)\cup(1,+\infty). \tag{1}$$

On the other hand, $f(x)=x^\alpha$ is a concave function if $\alpha\in(0,1)$. Hence,

$$M_\alpha(G)+M_\alpha(\bar{G})\leq 2n(\frac{n-1}{2})^\alpha,\quad \alpha\in(0,1). \tag{2}$$

If $\alpha>1$, then $(d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha\leq(d_G(u)+d_{\bar{G}}(u))^\alpha$ since $(\frac{d_G(u)}{d_G(u)+d_{\bar{G}}(u)})^\alpha+(\frac{d_{\bar{G}}(u)}{d_G(u)+d_{\bar{G}}(u)})^\alpha\leq\frac{d_G(u)}{d_G(u)+d_{\bar{G}}(u)}+\frac{d_{\bar{G}}(u)}{d_G(u)+d_{\bar{G}}(u)}=1$. We have

$$M_\alpha(G)+M_\alpha(\bar{G})\leq\sum_{u\in V(G)}(d_G(u)+d_{\bar{G}}(u))^\alpha=n(n-1)^\alpha,\ \alpha\in(1,+\infty). \tag{3}$$

Similarly, if $0<\alpha<1$, then $(d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha\geq(d_G(u)+d_{\bar{G}}(u))^\alpha$. We have

$$M_\alpha(G)+M_\alpha(\bar{G})\geq n(n-1)^\alpha,\quad \alpha\in(0,1). \tag{4}$$

Let $\alpha<0$ and u be any vertex of G. Next we will prove that $(d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha\leq(n-2)^\alpha+1$. We may assume $d_G(u)\geq d_{\bar{G}}(u)$, and let $a=d_G(u)$ and $b=d_{\bar{G}}(u)$. If $b\leq 1$, clearly the inequality holds. If $b\geq 2$, then $(a+1)^\alpha+(b-1)^\alpha-(a^\alpha+b^\alpha)=((a+1)^\alpha-a^\alpha)-(b^\alpha-(b-1)^\alpha)$. Using Lagrange's mean-value theorem, we conclude that there exist $\xi_1\in(a,a+1)$ and $\xi_2\in(b-1,b)$ such that $((a+1)^\alpha-a^\alpha)-(b^\alpha-(b-1)^\alpha)=\alpha\xi_1^{(\alpha-1)}-\alpha\xi_2^{(\alpha-1)}=\alpha(\xi_1^{(\alpha-1)}-\xi_2^{(\alpha-1)})>0$. Consequently, by $d_G(u)+d_{\bar{G}}(u)=n-1$, we have $(d_G(u))^\alpha+(d_{\bar{G}}(u))^\alpha\leq(d_G(u)+1)^\alpha+(d_{\bar{G}}(u)-1)^\alpha\leq\cdots\leq(n-2)^\alpha+1^\alpha$. Therefore, we obtain $M_\alpha(G)+M_\alpha(\bar{G})\leq n((n-2)^\alpha+1),\quad \alpha\in(-\infty,0).$ (5)

So (1) and (3) imply (i), (2) and (4) imply (ii), and (1) and (5) imply (iii). □

Note that the bounds are best possible. The upper bound of (i) and the lower bound of (ii) are same and are attained uniquely on K_n. On the other hand, The lower bound of (i) and (iii), and the upper bound of (ii) are same and are attained on the $(\frac{n-1}{2})$-regular graphs (so $n=4k+1$ for some positive integer k). Also, the upper bound of (iii) is attained on the graph H_n obtained from K_n by deleting a perfect matching (so, this occurs only if n is even).

4 Wiener Index

The Wiener index has no much meaning for disconnected graphs, and so we only consider it for connected graphs. The path of order n is denoted by P_n, and the star of order n is denoted by S_n. A tree is called a double star $S_{p,q}$ if it is obtained from S_p and S_q by connecting the center of S_p with that of S_q. The diameter of a graph G, denoted by $diam(G)$, is the largest distance between two vertices in G. Since the Wiener index is concerned with the distance of vertices, the diameter is important for us to study the index. The following facts might be found in some graph theory textbook.

Lemma 4.1. Let G be a connected graph with the connected complement. Then

(1) if $diam(G) > 3$, then $diam(\bar{G}) = 2$,

(2) if $diam(G) = 3$, then $\bar{G}$ has a spanning subgraph which is a double star.

Proof. (1) is an easy exercise. To prove (2), we take two vertices u, v in G such that $d_G(u, v) = 3$. Then, $w \notin N_G(u) \cap N_G(v)$ for any vertex $w \in V(G) \setminus \{u, v\}$, which means $w \in N_{\bar{G}}(u) \cup N_{\bar{G}}(v)$ in $\bar{G}$. Therefore, $\bar{G}$ contains a spanning double star whose two centers are u and v. □

Theorem 4.2. (Entringer et al. [3]) Among all trees with n vertices, P_n is the unique extremal structure with the largest Wiener index.

Note that P_4 is the unique graph of oder 4 whose complement is connected, and $\bar{P_4} \cong P_4$. So, $W(P_4) + W(\bar{P_4}) = 2W(P_4) = 20$. Next, we calculate the value of $W(P_n) + W(\bar{P_n})$ for $n \geq 5$. Let $P_n = v_1 v_2 \cdots v_n$, then, in P_n, it is easy to see that $d(v_i, v_{i+k}) = k$ for $i = 1, 2, \cdots, n-k$ and those pairs of vertices are all the pairs with distance k in P_n. Therefore,

$$W(P_n) = \sum_{i=1}^{n-1} i(n-i) = n \sum_{i=1}^{n-1} i - \sum_{i=1}^{n-1} i^2 = \frac{n^3 - n}{6}.$$

On the other hand, since $diam(\bar{P_n}) = 2$, we have $W(\bar{P_n}) = \varepsilon(\bar{P_n}) + 2\varepsilon(P_n) = [\binom{n}{2} - (n-1)] + 2(n-1) = \frac{n^2}{2} + \frac{n}{2} - 1$. Hence, $W(P_n) + W(\bar{P_n}) = \frac{n^3-n}{6} + \frac{n^2}{2} + \frac{n}{2} - 1 = \frac{n^3+3n^2+2n-6}{6}$.

Lemma 4.3. Let G be a graph of order $n \geq 5$. If $diam(\bar{G}) = 2$, then $W(G) + W(\bar{G}) \leq W(P_n) + W(\bar{P_n})$.

Proof. Let T be a spanning tree of G. Then $\bar{G}$ is a spanning subgraph of $\bar{T}$, and so $\bar{T}$ has diameter 2. Therefore, $W(G) + W(\bar{G}) - W(\bar{T}) = W(G) + (\varepsilon(\bar{T}) - \varepsilon(\bar{G})) = W(G) + (\varepsilon(G) - \varepsilon(T)) \leq W(T) \leq W(P_n)$ by Theorem 4.2. The result follows by noting that $W(\bar{T}) = W(\bar{P_n})$. □

It is ready for giving the Nordhaus-Goddum-type inequality for the Wiener index.

Theorem 4.4. Let G be a graph of order $n \geq 5$, and $\bar{G}$ be its complement. Then $3\binom{n}{2} \leq W(G) + W(\bar{G}) \leq \frac{n^3+3n^2+2n-6}{6}$.

Proof. The lower bound is immediate from $W(G) + W(\bar{G}) \geq (\varepsilon(G) + 2\varepsilon(\bar{G})) + (\varepsilon(\bar{G}) + 2\varepsilon(G)) = 3\binom{n}{2}$.

For the upper bound, it remains to consider the case $diam(G) = diam(\bar{G}) = 3$ in view of Lemma 4.1(1) and 4.3. Let s_i be the number of pair of vertices with distance i in G, for $i = 1, 2, 3$, and $\bar{s_i}$ be that in $\bar{G}$. Then $W(G) + W(\bar{G}) = \sum_{i=1}^{3} i(s_i + \bar{s_i}) = s_1 + \bar{s_1} + 2(s_2 + \bar{s_2} + s_3 + \bar{s_3}) + s_3 + \bar{s_3} = 3\binom{n}{2} + s_3 + \bar{s_3}$. By Lemma 4.1(2), let S_{p_1,q_1} be a spanning subgraph of G and S_{p_2,q_2} be that of $\bar{G}$, where $p_j + q_j = n$ for $j = 1, 2$. Hence, $s_3 \leq (p_1 - 1)(q_1 - 1) = p_1q_1 - n + 1$ and $\bar{s_3} \leq p_2q_2 - n + 1$. Since $p_iq_i \leq g(n)$ for $i = 1$ and 2, where $g(n) = \frac{n^2}{4}$ if n is even, and otherwise $\frac{n^2-1}{4}$, we have $s_3 \leq g(n) - n + 1$ and $\bar{s_3} \leq g(n) - n + 1$, and thus $W(G) + W(\bar{G}) \leq 3\binom{n}{2} + 2(g(n) - n + 1)$. One can easy to check that $3\binom{n}{2} + 2(g(n) - n + 1) \leq \frac{n^3+3n^2+2n-6}{6}$ if $n \geq 5$. This completes the proof. □

Note that the bounds are sharp. Obviously, the upper bound can be obtained on the graph P_n. To see the lower bound is best possible, we construct a sequence of graphs. Let G_n be graph of order n, which is obtained from C_5 by replacing a vertex of C_5 by complete graph of order $n - 4$. It is easy to see that $diam(G_n) = diam(\bar{G_n}) = 2$ and so $W(G_n) + W(\bar{G_n}) = 3\binom{n}{2}$.

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