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On Wiener Indices of Parikh Word Representable Graphs

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ABSTRACT. Graphs associated with finite sequences of symbols, called words, have been investigated in various studies. A new class of graphs introduced in the study of words, called Parikh word representable graphs, are defined using the number of symbols in the word and scattered subwords which are subsequences of the word. On the other hand, various topological indices have been computed for different classes of graphs in the area of chemical graph theory. Wiener indices of Parikh word representable graphs ($PWRG$) of binary words have also been studied. Here we obtain the Wiener indices of $PWRG$ of binary words resulting from certain word operations.

1. INTRODUCTION

Graphs of different kinds related to words have been introduced and their properties have been studied in detail [9, 8, 5, 14, 3]. In particular, a new class of graphs, called Parikh word representable graphs ($PWRG$) have been introduced in [3] based on scattered subwords of words and several graph properties have been studied. Following this study, several investigations related to $PWRG$ have been done [3, 16, 21, 22]. On the other hand various topological indices [7] associated with graphs have been introduced and investigated in the area of chemical graph theory [6]. The Wiener index [24] is the first topological index introduced by Harold Wiener. Knor et al. [11] provide a comprehensive account of results relating to Wiener index.

Studies on computing topological indices for different classes of graphs have been done (see, for example, [23, 25]). Enriching the study of structural properties of Parikh word representable graphs, expressions for computing topological indices of these graphs were derived in [21, 22]. In fact formulas for computing the Wiener index and certain other Wiener-type indices of the $PWRG$ corresponding to a binary core word [20] are derived in [21]. Motivated by these studies, here we derive formulas for computing Wiener index and Hyper Wiener index [10] of Parikh word representable graphs ($PWRG$) corresponding to binary core words formed under certain word operations. The main interest in these formulas is that the expressions in the formulas involve only certain parameters of the binary words which simplifies the computation of the indices and this is the advantage of the approach adopted here in comparison with the computation based on the graphs themselves.

2. PRELIMINARIES

Basic notions and results related to words and graphs needed in the study undertaken here are recalled in this section. For notions not recalled here, we refer to [13] for words and to [4] for graphs.

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A finite set of symbols, called an alphabet, with an ordering on the symbols, denoted by $<$, is referred to as an ordered alphabet. For example, the binary alphabet $\{a, b\}$ with an ordering $a < b$, is an ordered alphabet, written as $\{a < b\}$. In the subsequent sections, we mainly deal with the binary ordered alphabet $V = \{a < b\}$. A word over an alphabet V is a finite sequence of symbols belonging to V. The set of all words over V is denoted by V^*. The length of a word w is denoted by $|w|$. The reversal of a word $w = a_1a_2 \cdots a_n$ is the word $w^R = a_na_{n-1} \cdots a_2a_1$. The *dual* $d(w)$ of a binary word w over $\{a, b\}$ is the reversal of the word obtained from w by replacing a by b and b by a. The concatenation of two words $u = a_1a_2 \cdots a_n$ and $v = b_1b_2 \cdots b_m$, $(n, m \geq 1)$ over an alphabet is the word, written as uv, and is given by $uv = a_1 \cdots a_nb_1 \cdots b_m$. A scattered subword x of a word w, called simply as a subword x, is a subsequence of the word w. The number of subwords u in a word w is denoted by $|w|_u$. In particular, $|w|_a$ is the number of $a's$ in w. For example, $w = babaabb$ is a word over the alphabet $\{a, b\}$. If the ordering is $a < b$, the word aab is a subword of w. In fact the number of such subwords aab in w is $|w|_{aab} = 6$. Also $|w|_a = 3$ and $|w|_b = 4$. The vector $(|w|_a, |w|_b)$ is referred to as the Parikh vector [17] of the binary word w over $\{a < b\}$.

Two binary words u, v over $\{a < b\}$ are said to satisfy a weak-ratio property [19], denoted by $u \sim v$, if there exists a constant $k > 0$, such that $|v|_a = k|u|_a$ and $|v|_b = k|u|_b$. The Parikh matrix [15] $M(w)$ of a word w over $V = \{a < b\}$ is given by

$$M(w) = \begin{pmatrix} 1 & |w|_a & |w|_{ab} \\ 0 & 1 & |w|_b \\ 0 & 0 & 1 \end{pmatrix}.$$

A binary word over $\{a < b\}$ is called a core word [20] if it begins with a and ends with b. For example, the binary word $abaab$ is a core word. Two words w_1, w_2 over the binary ordered alphabet V are said to be M-equivalent, if the Parikh matrices of w_1 and w_2 are the same i.e. $M(w_1) = M(w_2)$.

We next recall the notion of a morphism [13] on words. Let V_1 and V_2 be two alphabets. A morphism on V_1^* is a mapping $\phi : V_1^* \to V_2^*$ such that $\phi(uv) = \phi(u)\phi(v)$, for words $u, v \in V_1^*$. Thue morphism [18] and Fibonacci morphism [18] are two well-known morphisms. The Thue morphism t on $\{a, b\}^*$ is given by $t(a) = ab, t(b) = ba$. The Fibonacci morphism f on $\{a, b\}^*$ is given by $f(a) = ab, t(b) = a$.

We consider simple graphs G with vertex set V and edge set E. We now recall the notion of Parikh word representable graph ($PWRG$) [3], restricting the notion to the binary ordered alphabet.

Definition [3]
For a word $w = a_1a_2 \cdots a_n$ of length n where for $1 \leq i \leq n$, $a_i \in \Sigma = \{a < b\}$, we associate a simple graph $G = G(w)$ with n vertices $\{1, 2, \cdots, n\}$. Each vertex i has the label a_i and represents the position of the letter a_i, $1 \leq i \leq n$, in w. For each occurrence of the subword ab in w, there is an edge in $G(w)$ joining the vertices corresponding to the positions of a and b in w. We say that the graph G is Parikh binary word representable by the binary word w. In other words, we say that a graph G is *Parikh binary word representable* if there exists a binary word w such that G is Parikh binary word representable by the binary word w. It is known that [16] Parikh binary word representable graph corresponding to a core word, is connected. We deal with only core words and the corresponding graphs in the rest of this paper. We will call Parikh binary word representable graph simply as Parikh

word representable graph. For example, if the core word is $w = abaab$, then in the Parikh word representable graph as shown in Fig. 1, the vertices 1,3 and 4 have label a while the vertices 2 and 5 have the label b. The graph has four edges as $|w|_{ab} = 4$. Note that in the graph there are edges joining the vertex 1 with the vertices 2 and 5 corresponding to the subword ab in w formed by the symbol a in position 1 and the symbol b in positions 2 and 5.

In a connected graph $G = (V, E)$ with vertex set V and edge set E, we denote by $d(u, v)$,

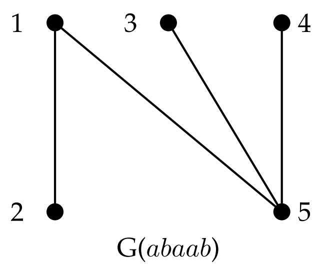

FIGURE 1. The Parikh word representable graph of the word $abaab$

the distance between the vertices u and v of G which is the length of a shortest path between u and v. The Wiener index $W(G)$ of a connected graph G, is the sum of distances $d(u, v)$ between all the vertices u and v of G. In other words

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

The Hyper-Wiener index of a connected graph G is given by

$$WW(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v) + d^2(u, v)$$

where $d(u, v)$ is the distance between the vertices u and v of G.

We now recall the formulas [21] for computing the Wiener index and the Hyper-Wiener index of Parikh word representable graph of a binary word $w = a^{n_1}ba^{n_2}b\cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$ over $\{a < b\}$. The formulas involve only the parameters related to the word.

Lemma 2.1. *(i) The Wiener index of a Parikh word representable graph $G(w)$, for $w = a^{n_1}ba^{n_2}b\cdots a^{n_l}b, n_1 \geq 1, n_k \geq 0$ for $2 \leq k \leq l$, is*

$$W(G(w)) = |w|^2 - |w| + |w|_a|w|_b - 2|w|_{ab}.$$

(ii) The Hyper-Wiener index of a Parikh word representable graph $G(w)$ for $w = a^{n_1}ba^{n_2}b...a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is

$$WW(G(w)) = 3|w|^2 - 3|w| + 6|w|_a|w|_b - 10|w|_{ab}.$$

We now illustrate computation of Wiener index of the Parikh word representable graph in Figure 1, in the two approaches, directly from the graph and from the formula given in Lemma 2.1.

Example 2.1. *Consider the Parikh word representable graph $G(w)$ in Figure 1 which corresponds to the word $w = abaab$. There are five vertices in $G(w)$ labelled 1,2,3,4,5. The distances between the vertices are listed below:*

$$d(1,2) = d(1,5) = 1, d(1,3) = d(1,4) = 2, d(2,5) = 2, d(2,3) = d(2,4) = 3,$$
$$d(3,4) = 2, d(3,5) = 1, d(4,5) = 1$$

Hence the Wiener index of the graph $G(w)$ is the sum of the distances between every two vertices of the graph which equals 18.
On the other hand, using the formula in Lemma 2.1, we obtain the same value 18 for $W(G(w))$ since $w = abaab, |w| = 5, |w|_a = 3, |w|_b = 2, |w|_{ab} = 4$. The calculations of the values of the parameters from the word are simpler as the word is linear in comparison with the corresponding calculations from the graph.

3. Word operations and Wiener index of $PWRG$

We first consider the word operations of concatenation and strict shuffle [2] on core words over the binary alphabet $V = \{a < b\}$ and derive the Wiener index of $PWRG$ corresponding to the binary core word formed by these operations.

3.1. **Concatenation and Strict shuffle.** Let V be an alphabet. For two words u, v over V, the concatenation [13] of u with v is the word $w = uv$. The strict shuffle [2] of two words u, v of the same length with $u = a_1 a_2 \cdots a_n$ and $v = b_1 b_2 \cdots b_n$ where for $1 \leq i \leq n$, $a_i, b_i \in V$ is given by $SShuf(u, v) = a_1 b_1 a_2 b_2 \cdots a_n b_n$. A result on strict shuffle of two binary words, established in [2, Theorem 3.8], is stated in the following Lemma in a slightly modified but an equivalent form.

Lemma 3.2. [2] *For any two words u, v over $\{a < b\}$ with the same Parikh vector,*
$|SShuf(u, v)|_a = 2|u|_a$, $|SShuf(u, v)|_b = 2|u|_b$ so that $|SShuf(u, v)| = 2|u|$ and
$|SShuf(u, v)|_{ab} = 2|u|_{ab} + 2|v|_{ab}$.

We obtain a formula for computing the Wiener index of the $PWRG$ of the binary core word uv.

Theorem 3.1. *Let u, v be two binary core words over $V = \{a < b\}$. The Wiener index $W(G(uv))$ of the $PWRG$ $G(uv)$ corresponding to the binary word uv is given by*

$$W(G(uv)) = W(G(u)) + W(G(v)) + 2|u||v| + |v|_a|u|_b - |u|_a|v|_b.$$

When $u \sim v$, then $W(G(uv)) = W(G(u)) + W(G(v)) + 2|u||v|$.

Proof. From Lemma 2.1, we have

$$W(G(uv)) = |uv|^2 - |uv| + |uv|_a|uv|_b - 2|uv|_{ab}$$
$$= (|u| + |v|)^2 - (|u| + |v|) + (|u|_a + |v|_a)(|u|_b + |v|_b) - 2(|u|_{ab} + |v|_{ab} + |u|_a|v|_b)$$
$$= W(G(u)) + W(G(v)) + 2|u||v| + |v|_a|u|_b - |u|_a|v|_b.$$

□

Corollary 3.1. *Let u be a binary core word over $V = \{a < b\}$. The Wiener index $W(G(ud(u)))$ of the $PWRG$ $G(ud(u))$ corresponding to the binary word $ud(u)$, where $d(u)$ is the dual of the word u, is given by*

$$W(G(ud(u))) = 2W(G(u)) + 2|u|^2 + |u|(|u|_b - |u|_a).$$

Proof. The result is a consequence of Theorem 3.1 and the following facts: (i) $d(u)$ is a binary core word, (ii) $|d(u)|_a = |u|_b$ and $|d(u)|_b = |u|_a$ so that $|d(u)| = |u|$ and (iii) $W(G(d(u))) = W(G(u))$ since the graphs $G(u)$ and $G(d(u))$ are isomorphic [16]. $\square$

We now obtain a formula for computing the Wiener index of the $PWRG$ of the strict shuffle of two binary words.

Theorem 3.2. *Let u, v be two binary core words over $V = \{a < b\}$ having the same Parikh vector. The Wiener index $W(G(SShuf(u,v)))$ of the $PWRG$ $G(SShuf(u,v))$ corresponding to the binary core word $SShuf(u,v)$ is given by*

$$W(G(SShuf(u,v))) = W(G(u)) + W(G(v)) + 2|u|^2 + 2|u|_a|u|_b - 2[|u|_{ab} + |v|_{ab}].$$

In particular, if the binary words are $M-$equivalent, then
$W(G(SShuf(u,v))) = W(G(u)) + W(G(v)) + 2|u|^2 + 2|u|_a|u|_b - 4|u|_{ab}$.

Proof. Since the binary words u and v have the same Parikh vector, we have $|u|_a = |v|_a$ and $|u|_b = |v|_b$ so that $|u| = |v|$. From Lemma 2.1 and Lemma 3.2, we have

$$W(G(SShuf(u,v))) = |SShuf(u,v)|^2 - |SShuf(u,v)|$$
$$+|SShuf(u,v)|_a|SShuf(u,v)|_b - 2|SShuf(u,v)|_{ab}$$
$$= 4|u|^2 - 2|u| + 4|u|_a|u|_b - 4[|u|_{ab} + |v|_{ab}]$$
$$= W(G(u)) + W(G(v)) + 2|u|^2 + 2|u|_a|u|_b - 2[|u|_{ab} + |v|_{ab}].$$

Also, if u and v are $M-$equivalent, then in addition, $|u|_{ab} = |v|_{ab}$ and so

$$W(G(SShuf(u,v))) = W(G(u)) + W(G(v)) + 2|u|^2 + 2|u|_a|u|_b - 4|u|_{ab}.$$

$\square$

Corollary 3.2. *Let u be a binary core word over $V = \{a < b\}$ with $|u|_a = |u|_b$. The Wiener index $W(G(SShuf(u,d(u))))$ of the $PWRG$ $G(SShuf(u,d(u)))$ corresponding to the binary word $SShuf(u,d(u))$ where $d(u)$ is the dual of the word u, is given by*

$$W(G(SShuf(u,d(u)))) = 2W(G(u)) + 2|u|^2 + 2|u|_a|u|_b - 4|u|_{ab}.$$

Example 3.2. *Consider the binary core words $u = aabab, v = aaabb$ so that $uv = aababaaabb$. The Wiener indices of $PWRGs$ $G(u)$, $G(v)$ and $G(uv)$ are respectively 16, 14 and 80 on using the formula in Lemma 2.1. From the formula in Theorem 3.1, $W(G(uv))$ = 16+14+50+6-6 = 80.*

The strict shuffle $SShuf(u,v) = aaaabaabbb$. The Wiener index of the $PWRG$ $G(SShuf(u,v))$ is 70 on using the formula in Lemma 2.1. From the formula in Theorem 3.1, $W(G(SShuf(u,v)))$ = 16+14+50+12-22 = 70. Thus the formulas in Theorem 3.1 and Theorem 3.2 are verified.

3.2. **Thue morphism.** We now derive formulas for computing the Wiener index of the $PWRG$ of the images under Thue morphism t and Fibonacci morphism f of binary words of the form awa over the binary ordered alphabet $\{a < b\}$. We note that the images of awa under these morphisms are core words.

We recall a result established in [1] on the count of subwords of length two in the morphic images of binary words restricting the alphabet as the binary alphabet.

Lemma 3.3. *Let ϕ be a morphism from V^* to V^* where $V = \{a, b\}$. For a non-empty word w over V, we have*

$$|\phi(w)|_{ab} = \sum_{x \in V} |w|_x |\phi(x)|_{ab} + \sum_{x,y \in V} |w|_{xy} |\phi(x)|_a |\phi(y)|_b.$$

We now obtain formulas for computing the number of $a's$, $b's$ and subword $ab's$ in the binary core word $t(awa)$ where t is the Thue morphism.

Lemma 3.4. *For a binary word w over the binary ordered alphabet $V = \{a < b\}$,*
(i) $|t(awa)|_x = |w| + 2$ for $x \in \{a < b\}$ so that $|t(awa)| = 2|w| + 4$
(ii) $|t(awa)|_{ab} = \frac{1}{2}|w|^2 + \frac{1}{2}(|w|_a - |w|_b) + 2|w| + 3$
where t is the Thue morphism.

Proof. Since $t(a) = ab, t(b) = ba$, we have $|t(awa)|_a = 2|t(a)|_a + |t(w)|_a = 2 + |w|$. Similarly, $|t(awa)|_b = 2 + |w|$.
Also

$$\begin{aligned}|t(awa)|_{ab} &= 2|t(a)|_{ab} + |t(w)|_{ab} + |t(a)|_a(|t(w)|_b + |t(a)|_b) + |t(w)|_a |t(a)|_b \\ &= |t(w)|_{ab} + 2|w| + 3.\end{aligned}$$

Now using Lemma 3.3,

$$\begin{aligned}|t(w)|_{ab} &= \sum_{x \in V} |w|_x |t(x)|_{ab} + \sum_{x,y \in V} |w|_{xy} |t(x)|_a |t(y)|_b \\ &= |w|_a + |w|_{aa} + |w|_{bb} + |w|_{ab} + |w|_{ba} \\ &= \frac{1}{2}|w|^2 + \frac{1}{2}(|w|_a - |w|_b)\end{aligned}$$

since $|w|_{aa} = \frac{1}{2}(|w|_a - 1)|w|_a, |w|_{bb} = \frac{1}{2}(|w|_b - 1)|w|_b$ and $|w|_{ab} + |w|_{ba} = |w|_a |w|_b$. This proves the formula in statement (ii). □

We derive a formula for computing the Wiener index of the $PWRG$ $G(t(awa))$ of the binary core word $t(awa)$, where w is a binary word over $\{a < b\}$ and t is the Thue morphism.

Theorem 3.3. *Let $V = \{a < b\}$ and w be a non-empty binary word in V^*. The Wiener index $W(G(t(awa)))$ of the $PWRG$ $G(t(awa))$ where t is the Thue morphism, is given by the formula*

$$W(G(t(awa))) = 4|w|^2 + 14|w| - |w|_a + |w|_b + 10.$$

Proof. From Lemma 2.1 and Lemma 3.4, we have

$$\begin{aligned}W(G(t(awa))) &= |t(awa)|^2 - |t(awa)| + |t(awa)|_a |t(awa)|_b - 2|t(awa)|_{ab} \\ &= (2|w| + 4)^2 - (2|w| + 4) + (|w| + 2)^2 \\ &\quad -2[\frac{1}{2}|w|^2 + \frac{1}{2}(|w|_a - |w|_b) + 2|w| + 3] \\ &= 4|w|^2 + 14|w| - |w|_a + |w|_b + 10.\end{aligned}$$

□

3.3. **Fibonacci morphism.** We now obtain formulas for computing the number of $a's, b's$ and subword $ab's$ in the binary core word $f(awa)$ where f is the Fibonacci morphism.

Lemma 3.5. *For a binary word w over the binary ordered alphabet $V = \{a < b\}$,*
(i) $|f(awa)|_a = |w| + 2$, $|f(awa)|_b = |w|_a + 2$, so that $|f(awa)| = |w| + |w|_a + 4$
(ii) $|f(awa)|_{ab} = \frac{1}{2}(|w|_a^2 + |w|_a) + |w|_{ba} + |w| + |w|_a + 3$
where f is the Fibonacci morphism.

Proof. Since $f(a) = ab, f(b) = b$, we have $|f(awa)|_a = 2 + |w|$ and $|f(awa)|_b = 2 + |w|_a$. Also

$$|f(awa)|_{ab} = 2 + |f(w)|_{ab} + (|f(w)|_b + 1) + |f(w)|_a$$

$$= |f(w)|_{ab} + |w| + |w|_a + 3.$$

Now using Lemma 3.3,

$$|f(w)|_{ab} = |w|_a + |w|_{aa} + |w|_{ba}$$

$$= \frac{1}{2}(|w|_a^2 + |w|_a) + |w|_{ba}.$$

This proves the formula in statement (ii). □

We derive a formula for computing the Wiener index of the $PWRG$ $G(f(awa))$ of the binary core word $f(awa)$, where w is a binary word over $\{a < b\}$ and f is the Fibonacci morphism.

Theorem 3.4. *Let $V = \{a < b\}$ and w be a non-empty binary word in V^*. The Wiener index $W(G(f(awa)))$ of the $PWRG$ $G(f(awa))$ where f is the Fibonacci morphism, is given by the formula*

$$W(G(f(awa))) = |w|^2 + 7|w| + 6|w|_a + 3|w||w|_a - 2|w|_{ba} + 10.$$

Proof. From Lemma 2.1 and Lemma 3.5, we have

$$W(G(f(awa))) = |f(awa)|^2 - |f(awa)| + |f(awa)|_a|f(awa)|_b - 2|f(awa)|_{ab}$$

$$= (|w| + |w|_a + 4)^2 - (|w| + |w|_a + 4) + (|w| + 2)(|w|_a + 2)$$

$$-2[\frac{1}{2}|w|_a^2 + |w|_a) + |w|_{ba} + |w| + |w|_a + 3]$$

$$= |w|^2 + 7|w| + 6|w|_a + 3|w||w|_a - 2|w|_{ba} + 10.$$

□

Example 3.3. *Consider the binary core word $w = aabab$ so that $t(awa) = abababaabaab$. The Wiener index of $PWRG$ of $t(awa)$ is 179 on using the formula in Lemma 2.1. From the formula in Theorem 3.3, $W(G(t(awa)))$ = 100+70-3+2+10 = 179. This verifies the formula in Theorem 3.3.*
The Wiener index of $PWRG$ of $f(awa)$ is 131 on using the formula in Lemma 2.1. From the formula in Theorem 3.4, $W(G(f(awa)))$ = 25+35+18+45-2+10 = 131. This verifies the formula in Theorem 3.4.

4. Word operations and Hyper-Wiener index of $PWRG$

Formulas for computing the Hyper-Wiener index of $PWRG$ of concatenation, strict shuffle of two binary core words and images under Thue morphism and Fibonacci morphism of a binary core word are now stated in the following Theorems. We omit the proofs as the proofs are analogous to the proofs of the corresponding results in the case of Wiener index dealt with in Section 3.

Theorem 4.5. *Let u, v be two binary core words over $V = \{a < b\}$. The Hyper-Wiener index $WW(G(uv))$ of the $PWRG$ $G(uv)$ corresponding to the binary word uv is given by*

$$WW(G(uv)) = WW(G(u)) + WW(G(v)) + 6|u||v| + 6|v|_a|u|_b - 4|u|_a|v|_b.$$

Theorem 4.6. *Let u, v be two binary core words over $V = \{a < b\}$ having the same Parikh vector. The Hyper-Wiener index $WW(G(SShuf(u, v)))$ of the $PWRG$ $G(SShuf(u, v))$ corresponding to the binary core word $SShuf(u, v)$ is given by*

$$WW(G(SShuf(u, v))) = WW(G(u)) + WW(G(v)) + 6|u|^2 + 12|u|_a|u|_b - 10[|u|_{ab} + |v|_{ab}].$$

Theorem 4.7. *Let $V = \{a < b\}$ and w be a non-empty binary word in V^*. The Hyper-Wiener index $WW(G(t(awa)))$ of the $PWRG$ $G(t(awa))$ where t is the Thue morphism, is given by the formula*

$$WW(G(t(awa))) = 13|w|^2 + 46|w| - 5|w|_a + 5|w|_b + 30.$$

Theorem 4.8. *Let $V = \{a < b\}$ and w be a non-empty binary word in V^*. The Hyper-Wiener index $WW(G(f(awa)))$ of the $PWRG$ $G(f(awa))$ where f is the Fibonacci morphism, is given by the formula*

$$WW(G(f(awa))) = 3|w|^2 - 2|w|_a^2 + 23|w| + 18|w|_a + 12|w||w|_a - 10|w|_{ba} + 30.$$

5. Conclusion

We have obtained formulas for computing Wiener and Hyper-Wiener indices of Parikh word representable graphs of binary core words under certain word operations. The formulas involve only certain parameters of the words considered. It will be of interest to study other word operations not considered here. Also other types of topological indices of $PWRG$ that can be expressed as formulas in terms of the word parameters can be considered.

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