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# THE WIENER NUMBER OF KNESER GRAPHS

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**Abstract**

The Wiener number of a graph $G$ is defined as $\frac{1}{2}\sum d(u,v)$, where $u, v \in V(G)$, and $d$ is the distance function on $G$. The Wiener number has important applications in chemistry. We determine the Wiener number of an important family of graphs, namely, the Kneser graphs.

**Keywords:** Wiener number, Kneser graph, odd graph.

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## 1. Introduction

Let $G = (V, E)$ be a simple connected undirected graph with $|V(G)| = n$ and $|E(G)| = m$. Given two distinct vertices $u, v$ of $G$, let $d(u, v)$ denote the distance (= number of edges in a shortest path between $u$ and $v$ in $G$). The Wiener number (also called Wiener Index) $W(G)$ of the graph $G$ is defined by

$$W = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v).$$

Given the structure of an organic compound, the corresponding (molecular) graph is obtained by replacing the atoms by vertices and covalent bonds by edges. The Wiener number is one of the oldest molecular-graph-based structure-descriptors, first proposed by the American chemist Harold Wiener [18], as an aid to determine the boiling point of paraffins. The study of Wiener number is one of the current areas of research in mathematical chemistry (see, for example, [14] and [19]). For more details on the computation of Wiener number and its applications to chemistry, see [8]. Some recent articles in the topic are [2, 5, 6]. One of the important families of graphs is the family of Kneser graphs. There are a good number of papers in problems dealing with the coloring parameters of Kneser graphs. See for instance, [9–12, 16]. Extremal problems concerning Kneser graphs are considered in [7]. In this paper, we obtain an explicit expression, based on mathematical induction, for the Wiener number of the Kneser graphs. Our notation and terminology are as in [3].

We recall the definition of a Kneser graph.

Let $n$ and $k$ be positive integers, $m = 2n + k$, where $k \geq 1$. We denote by $[m]$ the set $\{1, 2, \ldots, m\}$ and by $\binom{[m]}{n}$ the collection of all $n$-subsets of $[m]$. The Kneser graph $KG(m, n)$ has vertex set $\binom{[m]}{n}$, in which two vertices are adjacent iff they are disjoint. It is to be noted that Kneser graphs are vertex-transitive but not distance-regular and therefore not distance-transitive.

## 2. Some Basic Results

**Lemma 2.1** (Stahl [15]). *If $A, B$ are two distinct vertices of $KG(m, n)$, with $d(A, B) = 2p$, then $|A \cap B| \geq n - kp$.*

A consequence of Lemma 2.1 is Lemma 2.2.

**Lemma 2.2.** *If $A, B$ are two distinct vertices of $KG(m, n)$, with $d(A, B) = 2p + 1$, then $|A \cap B| \leq kp$.*

***Proof.*** Let $A, B, C$ be vertices of $KG(m, n)$ such that $d(A, C) = 2p$, $d(C, B) = 1$ and $d(A, B) = 2p + 1$ so that $C$ is the vertex preceding $B$ in a $A$-$B$ distance path in $G$. By Lemma 2.1, $|A \cap C| \geq n - kp$. But since $|B \cap C| = \emptyset$, $|A \cap B| \leq n - (n - kp) = kp$. ■

Using Lemmas 2.1 and 2.2, Valencia-Pabon and Vera [13] have determined the diameter of $G$.

**Lemma 2.3** ([13]). *The diameter of the Kneser graph $KG(m, n)$ is $\lceil \frac{n-1}{k} \rceil + 1$.*

## 3. WIENER NUMBER OF $KG(m, n)$

We now compute the Wiener number of the Kneser graph $KG(m, n)$.

We first observe that for any two distinct vertices of $KG(m, n)$, $|A \cap B| \in \{0, 1, \ldots, n-1\}$. Further $d(A_0, A) = 0$ if and only if $|A_0 \cap A| = n$, and $d(A_0, A) = 1$ if and only if $|A_0 \cap A| = 0$.

**Lemma 3.1.** *Let $G = KG(m, n)$ be a Kneser graph with diameter $D$. Fix $A_0 \in V(G)$. Then for any $A \in V(G)$, $p \geq 1$,*

(i) *$d(A_0, A) = 2p < D$, if and only if*

$$|A_0 \cap A| \in N_{2p} := \{n - kp, n - kp + 1, \ldots, n - k(p-1) - 1\},$$

(ii) *$d(A_0, A) = 2p + 1 < D$, if and only if*

$$|A_0 \cap A| \in N_{2p+1} := \{k(p-1) + 1, k(p-1) + 2, \ldots, kp\}, \text{ and}$$

(iii) *$d(A_0, A) = D$, if and only if*

$$|A_0 \cap A| \in N_D := \begin{cases} \left\{k(\frac{D}{2} - 1) + 1, \ldots, n - k(\frac{D}{2} - 1) - 1\right\} & \text{if } D \text{ is even,} \\ \left\{k(\frac{D-1}{2} - 1) + 1, \ldots, n - k(\frac{D-1}{2}) - 1\right\} & \text{if } D \text{ is odd.} \end{cases}$$

We set $N_0 = \{n\}$ and $N_1 = \{0\}$. Before we prove Lemma 3.1, we observe the following:

**Observation 3.2.** (a) *$|N_0| = 1$, $|N_1| = 1$ and $|N_i| = k$ when $2 < i < D$.*

(b) *The sets $N_{2p+1}$ are successive disjoint intervals (intervals of positive integers) that are increasing from 0 to $n$ as $p$ increases from 1, and the sets $N_{2p}$ are successive disjoint intervals that are decreasing from $n$ to 0 again as $p$ increases from 1, that is, for $i < j$ and for $x \in N_i$ and $y \in N_j$, $x < y$ if $i$ and $j$ are odd and $x > y$ if $i$ and $j$ are even.*

(c) *If $p \neq q$ and $p < D$ and $q < D$, then $N_p \cap N_q = \phi$.*

We prove (c); (a) and (b) are obvious from the definition of the sets $N_i$.

***Proof of (c).*** If $p$ and $q$ are both even or both odd, there is nothing to prove. So let one of them be odd and the other even, say, $p$ odd and $q$ even. Also let $i$ = largest even integer less than $D$, and $j$ = largest odd integer less than $D$, and $j = 2e + 1$. This implies that $i = j \pm 1$. First, let $i = j - 1$, so that $i = 2e$. Again, from the definition of $i$ and $j$, we observe that $p \leq j = 2e+1$, $q \leq i = 2e$ and therefore by (b) of Observation 3.2, it suffices to prove that $N_{2e} \cap N_{2e+1} = \emptyset$. Indeed, we verify that $ke < n-ke-1$. This is true, since $ke \geq n-ke-1$ implies that $n-1 \leq 2ke \leq k(D-2)$, a contradiction to the fact that $D = \lceil \frac{n-1}{k} \rceil + 1$. Similarly, we verify the result when $i = j+1$. ■

***Proof of Lemma* 3.1.** We prove (i) and (ii) by induction on $i$ where $d(A_0, A) = i < D$.

Let $d(A_0, A) = 2$. By Lemma 2.1, $|A_0 \cap A| \geq n-k$. If $|A_0 \cap A| = n$, then $d(A_0, A) = 0$, a contradiction. Hence $n > |A_0 \cap A| \geq n-k$ and so $|A_0 \cap A| \in N_2$.

Conversely, let $|A_0 \cap A| \in N_2 = \{n-k, n-k+1, \dots, n-1\}$, so that $|A_0 \cap A| = n-k+r$, where $0 \leq r < k$. Consequently, $|A_0 \cup A| = 2n-(n-k+r) = n+k-r$; and hence $|[m] \backslash (A_0 \cup A)| = (2n+k)-(n+k-r) = n+r$ where $0 \leq r < k$. From these $n+r$ elements, we can find a vertex $Z$ in $V(G)$ such that $|A_0 \cap Z| = 0 = |A \cap Z|$. Therefore, $d(A_0, Z) = d(A, Z) = 1$ and so $d(A_0, A) \leq 2$. Clearly, $d(A_0, A) < 2$ is not possible and therefore $d(A_0, A) = 2$.

Next, let $d(A_0, A) = 3$. By Lemma 2.2, $|A_0 \cap A| \leq k$. If $|A_0 \cap A| = 0$, then $d(A_0, A) = 1$ which is not true. Therefore $|A_0 \cap A| \in N_3 = \{1, 2, \dots, k\}$.

Conversely, let $|A_0 \cap A| \in N_3 = \{1, 2, \dots k\}$, so that $|A_0 \cap A| = k-r$ for $0 \leq r < k$. Hence if $X = A_0 \cap A$, then $A_0 = X \cup \{\alpha_1, \alpha_2, \dots, \alpha_{n-k+r}\}$, and $A = X \cup \{\beta_1, \beta_2, \dots, \beta_{n-k+r}\}$, where $\{\alpha_1, \alpha_2, \dots, \alpha_{n-k+r}\}$ is disjoint from $\{\beta_1, \beta_2, \dots, \beta_{n-k+r}\}$. Further let $C = [m] \backslash (A_0 \cup A)$. Then $|C| = (2n+k)-(2n-k+r) = 2k-r$, where $0 \leq r < k$. Choose $k$ elements $c_1, \dots c_k$ from $C$ and set $B = \big(C \backslash \{c_1, \dots c_k\}\big) \cup \{\alpha_1, \dots, \alpha_{n-k+r}\}$. Then $|B| = (2k-r)-k+(n-k+r) = n$ and so $B \in V(G)$, $|A_0 \cap B| = n-k+r$ and $|A \cap B| = 0$. Since $0 \leq r < k$, we have $|A_0 \cap B| \in N_2$ and therefore, $d(A_0, B) = 2$. Also $d(A, B) = 1$. Hence $d(A_0, A) \leq 3$, which gives $d(A_0, A) = 3$. Thus we have established the result when $d(A_0, A) = 2$ or 3.

Assume now that $d(A_0, A) = i > 3$ and that the result is true if $d(A_0, A) \in \{2, 3, \dots, i-1\}$, $i < D$.

*Case* (i). Let $i$ be odd so that $i = 2p+1 < D$.
Let $d(A_0, A) = 2p+1$. By Lemma 2.2, $|A_0 \cap A| \leq kp$. If $|A_0 \cap A| \leq k(p-1)$, by the induction hypothesis, $d(A_0, A) \leq 2(p-1)+1$ which is a contradiction. Thus $|A_0 \cap A| \in N_{2p+1} = \{k(p-1)+1, \dots, kp\}$.

Conversely, let $|A_0 \cap A| \in N_{2p+1} = \{k(p-1)+1, \dots kp\}$, so that $|A_0 \cap A| = kp-r$ where $0 \leq r < k$. Set $Y' = A_0 \cap A$, so that $A_0 =$

$Y' \cup \{a_1, \ldots, a_{n-kp+r}\}$, and $A = Y' \cup \{b_1, \ldots, b_{n-kp+r}\}$ where the sets $\{a_1, \ldots, a_{n-kp+r}\}$ and $\{b_1, \ldots, b_{n-kp+r}\}$ are disjoint. Further, let $C' = [m] \backslash \big(A_0 \cup A\big)$. Then, $|C'| = 2n + k - (2n - kp + r) = k(p+1) - r$. Now choose $k$ elements $c'_1, c'_2, \ldots c'_k$ from $C'$ and set $B' = \big(C' \backslash \{c'_1, \ldots, c'_k\}\big) \cup \{a_1, \ldots a_{n-kp+r}\}$. Hence $|B'| = n$ and so $B' \in V(G)$, $|A_0 \cap B'| = n - kp + r$ and $|A \cap B'| = 0$. Since, $0 \le r < k$, by the induction hypothesis, $d(A_0, B') = 2p$ and $d(A, B') = 1$ and so, $d(A_0, A) \le 2p + 1$. If $d(A_0, A) < 2p + 1$, by the induction hypothesis, $|A_0 \cap A| \ne kp - r$, for any $r$ in $0, 1, 2, \ldots, k-1$, which is a contradiction. Thus $d(A_0, A) = 2p + 1$.

*Case* (ii). Let $i$ be even so that $i = 2p < D$, $p \ge 2$.
Let $d(A_0, A) = 2p$. By Lemma 2.1, $|A_0 \cap A| \ge n - kp$. If $|A_0 \cap A| \ge n - k(p-1)$, by the induction hypothesis, $d(A_0, A) \le 2(p-1)$, which is a contradiction. Thus $|A_0 \cap A| \in N_{2p} = \{n - kp, n - kp + 1, \ldots, n - k(p-1) - 1\}$.

Conversely, let $|A_0 \cap A| \in N_{2p}$, so that $|A_0 \cap A| = n - kp + r$, where $0 \le r < k$. Set $Y'' = A_0 \cap A$, $A_0 = Y'' \cup \{x_1, x_2, \ldots x_{kp-r}\}$, and $A = Y'' \cup \{y_1, y_2, \ldots y_{kp-r}\}$ where the set $\{x_1, x_2, \ldots x_{kp-r}\}$ is disjoint from $\{y_1, y_2, \ldots y_{kp-r}\}$. Further, if $B'' = Y'' \cup \{x_1, \ldots x_k, y_{k+1}, \ldots, y_{kp-r}\}$, then $|B''| = n$ and so $B'' \in V(G)$. Also $|A_0 \cap B''| = n - k(p-1) + r$, and $|A \cap B''| = n - k$. Since $0 \le r < k$, by the induction hypothesis, $d(A_0, B'') = 2(p-1)$ and $d(A, B'') = 2$ and so $d(A_0, A) \le 2p$. If $d(A_0, A) < 2p$, by the induction hypothesis, $|A_0 \cap A| \ne n - kp + r$ for any $r$ in $0, 1, \ldots, k-1$, which is a contradiction. Thus $d(A_0, A) = 2p$.

We have settled all the cases for which $d(A_0, A) \le D - 1$. We now dispose of the case when $d(A_0, A) = D$. There are two possibilities according to whether $D$ is even or odd.

*Case* (a). $D$ is even. Let $d(A_0, A) = D$, so that $d(A_0, A) \not\le D - 1$. Consequently,

$$|A_0 \cap A| \notin \bigcup_{i=2}^{D-1} N_i \cup \{0, n\} = \bigcup_{\substack{i \text{ even} \\ 2 \le i \le D-1}} N_i \bigcup_{\substack{j \text{ odd} \\ 2 \le j \le D-1}} N_j \cup \{0, n\}.$$

In 2 to $D-1$, there are $\frac{D}{2} - 1$ odd numbers and $\frac{D}{2} - 1$ even numbers. Hence

$$\bigcup_{\substack{i \text{ even} \\ 2 \le i \le D-1}} N_i = \bigcup_{i=1}^{\frac{D}{2}-1} N_{2i} = \Big\{n - k\Big(\frac{D}{2} - 1\Big), \ldots, n - 1\Big\},$$

and

$$\bigcup_{\substack{j \text{ odd} \\ 2\le j\le D-1}} N_j = \bigcup_{j=1}^{\frac{D}{2}-1} N_{2j+1} = \Big\{1, 2, \ldots, k\Big(\frac{D}{2}-1\Big)\Big\},$$

and hence

$$|A_0 \cap A| \in \Big\{k\Big(\frac{D}{2}-1\Big)+1, \ldots, n-k\Big(\frac{D}{2}-1\Big)-1\Big\}.$$

Conversely, let

$$|A_0 \cap A| \in \Big\{k\Big(\frac{D}{2}-1\Big)+1, \ldots, n-k\Big(\frac{D}{2}-1\Big)-1\Big\}.$$

Then $|A_0 \cap A| \notin \bigcup_{i=2}^{D-1} N_i \cup \{0, n\}$, and so $d(A_0, A) = D$.

*Case* (b). $D$ is odd. In this case,

$$|A_0 \cap A| \notin \bigcup_{i=2}^{D-1} N_i \cup \{0, n\} = \bigcup_{\substack{i \text{ even} \\ 2\le i\le D-1}} N_i \bigcup_{\substack{j \text{ odd} \\ 2\le j\le D-1}} N_j \cup \{0, n\}.$$

In 2 to $D-1$, there are $\frac{D-1}{2}-1$ odd numbers and $\frac{D-1}{2}$ even numbers. Hence,

$$\bigcup_{\substack{i \text{ even} \\ 2\le i\le D-1}} N_i = \bigcup_{i=1}^{\frac{D-1}{2}} N_{2i} = \Big\{n-k\Big(\frac{D-1}{2}\Big), \ldots, n-1\Big\},$$

and

$$\bigcup_{\substack{j \text{ odd} \\ 2\le j\le D-1}} N_j = \bigcup_{j=1}^{\frac{D-1}{2}-1} N_{2j+1} = \Big\{1, 2, \ldots, k\Big(\frac{D-1}{2}-1\Big)\Big\}.$$

Therefore, $|A_0 \cap A| \in \big\{k(\frac{D-1}{2}-1)+1, \ldots, n-k(\frac{D-1}{2})-1\big\}$. Conversely, if $|A_0 \cap A| \in \big\{k(\frac{D-1}{2}-1)+1, \ldots, n-k(\frac{D-1}{2})-1\big\}$, then $|A_0 \cap A| \notin \bigcup_{i=2}^{D-1} N_i \cup \{0, n\}$, and hence $d(A_0, A) = D$. ■

**Remark 3.3.** Let $A_0 \in V\big(KG(m, n)\big)$. Let $0 \le j \le n$. Then the number of vertices $A$ of $KG(m, n)$ such that $|A_0 \cap A| = j$ is equal to $\binom{n}{j}\binom{n+k}{n-j}$.

**Theorem 3.4.** *The Wiener number $W$ of the Kneser graph $KG(m,n)$is given by*

$$W = \frac{1}{2}\binom{2n+k}{n}\left[\sum_{i=0}^{\lceil\lfloor\frac{D-1}{2}\rfloor}(2i)\sum_{j=n-ki}^{\min\{n-k(i-1)-1,n\}}\binom{n}{j}\binom{n+k}{n-j} + \sum_{i=0}^{\lceil\frac{D-1}{2}\rceil-1}(2i+1)\sum_{j=\max\{k(i-1)+1,0\}}^{ki}\binom{n}{j}\binom{n+k}{n-j}+S\right],$$

*where*

$$S = \begin{cases} D\displaystyle\sum_{j=k(\frac{D}{2}-1)+1}^{n-k(\frac{D}{2}-1)-1}\binom{n}{j}\binom{n+k}{n-j} & \text{if } D \text{ is even,}\\ D\displaystyle\sum_{j=k(\frac{D-1}{2}-1)+1}^{n-k(\frac{D-1}{2})-1}\binom{n}{j}\binom{n+k}{n-j} & \text{if } D \text{ is odd.}\end{cases}$$

(Note: the min and max symbols are used in the summation to take care of the case $i = 0$.)

***Proof.*** Let $A_0$ be a fixed vertex of $KG(m,n)$. By Lemma 3.1 and Remark 3.3, we see that the number of vertices at distance $l < D$ is given by

$$\sum_{j=n-ki}^{\min\{n-k(i-1)-1,n\}}\binom{n}{j}\binom{n+k}{n-j}, \quad \text{if } l = 2i, \quad \text{and}$$

$$\sum_{j=\max\{k(i-1)+1,0\}}^{ki}\binom{n}{j}\binom{n+k}{n-j}, \quad \text{if } l = 2i+1.$$

and the number of vertices at distance $D$ is given by

$$\sum_{j=k(\frac{D}{2}-1)+1}^{n-k(\frac{D}{2}-1)-1}\binom{n}{j}\binom{n+k}{n-j}, \quad \text{if } D \text{ is even, and}$$

$$\sum_{j=k(\frac{D-1}{2}-1)+1}^{n-k(\frac{D-1}{2})-1}\binom{n}{j}\binom{n+k}{n-j}, \quad \text{if } D \text{ is is odd.}$$

Since $KG(m,n)$ is vertex-transitive, we get the expression given in Theorem 3.4 for $W$. ■

We now deduce the Wiener number of the odd graphs $O_k$. The graph $O_k$ is the Kneser graph $KG(2k-1,k-1)$ so that it is obtained by setting $k=1$ and $n=k-1$ in $KG(m,n)$. By Lemma 2.3, the diameter of $O_k = D = \lceil \frac{k-2}{1} \rceil + 1 = k-1$. Substituting $k=1$ and $n=k-1$ in Theorem 3.4, the Wiener number of odd graphs is given by

$$W(O_k) = \frac{1}{2}\binom{2k-1}{k-1}\left[\sum_{i=0}^{\lfloor \frac{D-1}{2} \rfloor}(2i)\sum_{j=k-1-i}^{k-1-i}\binom{k-1}{j}\binom{k}{k-1-j}\right.$$
$$\left. + \sum_{i=0}^{\lceil \frac{D-1}{2}\rceil -1}(2i+1)\sum_{j=i}^{i}\binom{k-1}{j}\binom{k}{k-1-j} + S\right]$$

where

$$S = \begin{cases} D\displaystyle\sum_{j=\frac{D}{2}}^{k-1-\frac{D}{2}}\binom{k-1}{j}\binom{k}{k-1-j} & \text{if } D \text{ is even,} \\ D\displaystyle\sum_{j=\frac{D-1}{2}}^{k-2-\frac{D-1}{2}}\binom{k-1}{j}\binom{k}{k-1-j} & \text{if } D \text{ is odd,} \end{cases}$$

$$= \frac{1}{2}\binom{2k-1}{k-1}\left[\sum_{i=0}^{\lfloor \frac{k-2}{2} \rfloor}(2i)\binom{k-1}{k-1-i}\binom{k}{i}\right.$$

$$\text{(A)} \qquad \left. + \sum_{i=0}^{\lceil \frac{k-2}{2}\rceil -1}(2i+1)\binom{k-1}{i}\binom{k}{k-1-i} + S\right],$$

where

$$S = \begin{cases} D\dbinom{k-1}{k-1-\frac{D}{2}}\dbinom{k}{\frac{D}{2}} & \text{if } D \text{ is even,} \\ D\dbinom{k-1}{(\frac{D-1}{2})}\dbinom{k}{k-1-(\frac{D-1}{2})} & \text{if } D \text{ is odd.} \end{cases}$$

Now,

$$\binom{k-1}{k-1-i}\binom{k}{i} = \frac{(k-1)!}{i!(k-1-i)!}\frac{k!}{i!(k-i)!}$$
$$= \frac{k}{k-i}\frac{(k-1)!^2}{(i!)^2(k-i-1)!^2} = \frac{k(k-1)^2\cdots(k-i+1)^2(k-i)}{1^2\cdots i^2}$$

and

$$\binom{k-1}{i}\binom{k}{k-1-i} = \frac{(k-1)!}{i!(k-i-1)!}\frac{k!}{(1+i)!(k-1-i)!}$$
$$= \frac{k}{i+1}\frac{(k-1)!^2}{(i!)^2(k-i-1)!^2} = \frac{k(k-1)^2\cdots(k-i)^2}{1^2\cdots i^2(1+i)}.$$

When $D$ is even, we can add $S$ to the first summation by taking $i = \lceil \frac{k-2}{2} \rceil$ in (A) and when $D$ is odd, to the second summation by taking $i = \lfloor \frac{k-2}{2} \rfloor$ in (A). This gives

$$(B) \quad W(O_k) = \frac{1}{2}\binom{2k-1}{k-1}\left[\sum_{i=0}^{\lceil \frac{k-2}{2} \rceil}(2i)\frac{k(k-1)^2\cdots(k-i+1)^2(k-i)}{1^2\cdot 2^2\cdots i^2} + \sum_{i=0}^{\lfloor \frac{k-2}{2} \rfloor}(2i+1)\frac{k(k-1)^2\cdots(k-i)^2}{1^2\cdot 2^2\cdots i^2\cdot(1+i)}\right].$$

Expression (B) has also been established by Tilakam [17] using intersection arrays [4]. Another equivalent expression for $W(O_k)$ is given in [1].

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