

An exact expression for the wiener index of a $TUC_4C_8(R)$ nanotorus

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The Wiener index of a graph G is defined as $W(G) = 1/2 \sum_{\{x,y\} \subseteq V(G)} d(x,y)$, where $V(G)$ is the set of all vertices of G and for $x, y \in V(G)$, $d(x,y)$ denotes the length of a minimal path between x and y . AC_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8 . It can cover either a cylinder or a torus. In this paper, an algorithm for computing the distance matrix of a $C_4C_8(R)$ nanotorus $T = T[p, q]$ is given. Using this matrix, the Wiener index of T is computed.

KEY WORDS: Wiener index, chemical graph, $TUC_4C_8(R)$ nanotorus

1. Introduction

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. If the vertices $u, v \in V(G)$ are connected by an edge e then we write $e = uv$. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by edge between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be path, a tree, or in general a graph.

A real number that describes a molecular graph is called a topological index. The first use of a topological index for the correlation of the measured properties of molecules with their structural features was made in 1947 by the chemist Harold Wiener. In that year, he introduced the notion of path number of a graph as the sum of the distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Wiener originally defined his index (W) on trees and studied its use for correlations of physico-chemical properties of alkanes, alcohols, amines, and their analogous compounds (see [1] for details).

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Hosoya [2] reformulated the Wiener index in terms of distances between vertices in an arbitrary graph. He defined W as the sum of distances between all pairs of vertices of the graph under consideration, $W(G) = \sum_{u,v} d(u, v)$, where $d(u, v)$ is the number of edges in a minimum path connecting the vertices u and v . We encourage the reader to consult the special issues of MATCH Communication in Mathematics and in Computer Chemistry [3], Discrete Applied Mathematics [4], and [5–7], for information on results on the Wiener index, the chemical meaning of the index and its history.

In a series of papers, Diudea and coauthors [8–13] studied the topological indices of some chemical graphs related to nanostructures. They also computed the Wiener index of some nanotubes. In a previous paper [14], the present authors computed the Wiener index of a polyhex nanotorus. In this paper, we continue this program to find an exact expression for the Wiener index of a $TUC_4C_8(R)$ nanotorus, (figure 1).

In this paper, our notation is standard and mainly taken from [15,16]. We consider only simple molecular graphs without directed and multiple edges and without loops. $T = T[m, n]$ denotes an arbitrary $C_4C_8(R)$ nanotorus in which n is the number of rhombs on the level 1 and the length of torus is m . The main result of this paper is as follows:

Theorem. Suppose $T = T[p, q]$ is a $TUC_4C_8(R)$ nanotorus. Then we have:

$$W(T) = \begin{cases} (2m/3)(m^2 - 1) + mn(m + 3n) - k_1, & \text{if } m < n \\ (2n/3)(n^2 - 1) + mn(3m + n) - k_2, & \text{if } m > n \\ (n/3)(14n^2 - k_3), & \text{if } m = n \end{cases}$$

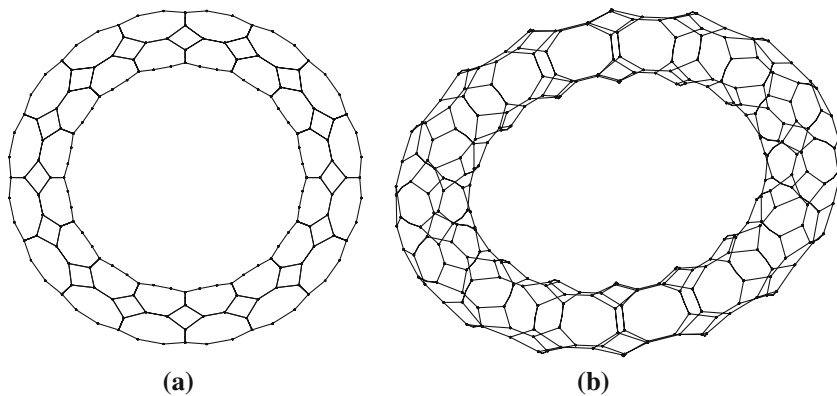


Figure 1. A $TUC_4C_8(R)$ tori (a) Top view (b) Side view.

$$\text{in which } k_1 = \begin{cases} 0, & \text{if } 2|n \ \& \ 2|m \\ n - m & \text{if } 2|n \ \& \ 2 \nmid m \\ m, & \text{if } 2 \nmid n \ \& \ 2|m \\ n, & \text{if } 2 \nmid n \ \& \ 2 \nmid m \end{cases} \quad k_2 = \begin{cases} 0, & \text{if } 2|m \\ m, & \text{if } 2 \nmid m \end{cases} \quad k_3 = \begin{cases} 2, & \text{if } 2|n \\ 5, & \text{if } 2 \nmid n \end{cases}$$

and, “|” denotes the divisibility relation.

2. Main result

In this section, the Wiener index of the molecular graph of an arbitrary $TUC_4C_8(R)$ nanotorus $T = T[m, n]$ were computed. To compute the Wiener index of this graph, we first consider a base vertex b for the 2-dimensional lattice of T (figure 2), and compute $S_b = \sum_{x \in V(G)} d(x, b)$. It is clear that the value of S_b is independent from the base vertex b . Therefore, $W(T) = 2mnS_b$ and so it is enough to compute S_b . To do this, we define a matrix $X_{m,n} = [x_{ij}]$ in which x_{ij} is the sum of distances between vertices of (i, j) th rhomb of the 2-dimensional lattice of T from the base vertex b . Since $S_b = \sum_{i,j} x_{ij}$, we must find an algorithm for computing $X_{m,n}$. From figure 2, it is obvious that T has exactly $4mn$ vertices, $6mn$ edges, and $x_{11} = \begin{cases} 3, & m = 1, \\ 4, & m > 1. \end{cases}$

Lemma 1. For $2 \leq j \leq n, x_{ij} = x_{i(n-j+2)}$.

Proof. The proof is straightforward.

In the following theorem, we compute the Wiener index of $T[n, n]$. Suppose $X_{1,1} = [3]$ and $X_{2,2} = \begin{bmatrix} 4 & 10 \\ 8 & 14 \end{bmatrix}$.

Lemma 2. $W(T[n, n]) = (2n^3)/3 (14n^2 - k_3)$.

Proof. To prove the theorem, it is enough to compute $X_{n,n}$. Obviously, the 2-dimensional lattice of $T[n - 2, n - 2]$ is a part of the 2-dimensional lattice of $T[n, n]$. So, we can proceed with induction on n . Suppose $X_{n,n} = [x_{ij}]$ and $X_{n-2,n-2} = [a_{i,j}]$. Our main proof will consider two cases that n is odd or even.

Case 1 n is odd. In this case, it can easily seen that $x_{i,j} = x_{i,n-j+2}, (n + 1)/2 < j \leq n$. From 2-dimensional lattice of $T[n, n]$ (figure 2), we have $x_{(n+1)/2,1} = a_{(n-1)/2,1} + 11$ and $x_{(n+1)/2,j} = x_{(n+1)/2,j-1} + 4, 2 \leq j \leq (n + 1)/2$. This relation determines the $((n + 1)/2)$ th row of the matrix $X_{n,n}$. On the other hand,

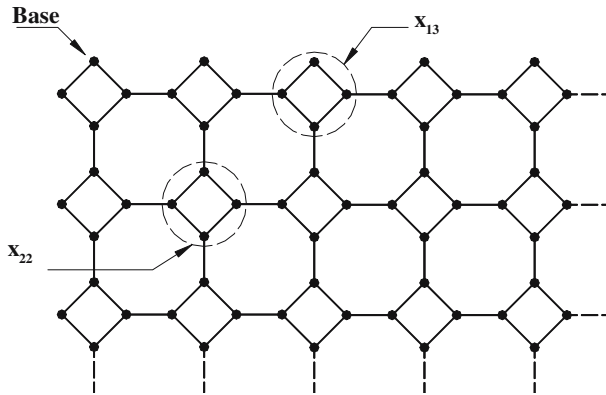


Figure 2. The 2-Dimensional lattice of $TUC_4C_8(R)$ nanotorus with $m = 3$ and $n = 5$.

$$x_{i,(n+1)/2} = \begin{cases} a_{i,(n+1)/2} + 2, & 1 \leq i \leq (n-1)/2, \\ a_{i-1,(n+1)/2} + 2, & (n+1)/2 < i \leq n, \end{cases}$$

which defines the $((n+1)/2)$ th column of the matrix $X_{n,n}$. For other entries of $X_{n,n}$, we have:

$$x_{i,j} = \begin{cases} a_{i,j}, & 1 \leq i \leq (n-1)/2, & 1 \leq j \leq (n-1)/2 \\ a_{i-1,j}, & (n+1)/2 \leq i \leq n, & 1 \leq j \leq (n-1)/2. \end{cases}$$

Case 2 n is even. In this case, we can see that $x_{i,j} = x_{i,n-j+2, n/2 + 1} < j \leq n$. Again since from 2-dimensional lattice of $T[n-2, n-2]$ is a part of 2-dimensional

lattice of $T[n-2, n-2]$, $x_{i,j} = \begin{cases} a_{i,j}, & 1 \leq i \leq n/2 - 1, & 1 \leq j \leq n/2, \\ a_{i-1,j}, & n/2 + 1 < i \leq n, & 1 \leq j \leq n/2. \end{cases}$

To complete this case, we must determine the entries of $((n/2 + 1))$ th row and column and $(n/2)$ th row of the matrix $X_{n,n}$. From figure 1, it can be seen that

$$x_{1,n/2+1} = a_{1,n/2} + 10, \quad x_{i,n/2+1} = \begin{cases} x_{i-1,n/2+1} + 4, & 2 \leq i \leq n/2 + 1, \\ x_{i-1,n/2+1} - 4, & n/2 + 1 < i \leq n, \end{cases}$$

which determines the entries of $(n/2 + 1)$ th column of $X_{n,n}$. Finally, for the entries of the $(n/2)$ th and $(n/2 + 1)$ th rows of $X_{n,n}$ we have:

$$x_{n/2,j} = a_{n/2,j} + 1 \quad x_{n/2+1,j} = a_{n/2,j} + 5 \quad 1 \leq j \leq n/2.$$

Suppose S_n denotes the sum of entries of $X_{n,n}$. To compute the Wiener index of $T[n, n]$, we first assume that n is odd. Then by our calculation in case

1, we have $S_n = S_{n-1} + (14n^2 - 15n + 4)$. But this recurrence relation is linear and so $S_n = A + B$ in which A is the general solution of its associated homogeneous equation and B is one particular solution for the main equation. By a well-known method for solving such equations, we have $S_n = (n/3)(14n^2 - 5)$. If n is even, then the case 2 implies that $S_n = (n/3)(14n^2 - 2)$. Therefore,

$$S_n = (n/3)(14n^2 - k_3), \quad k_3 = \begin{cases} 2, & \text{if } 2|n \\ 5, & \text{if } 2 \nmid n \end{cases},$$

which completes the proof.

To explain our algorithm for computing the matrix $X_{n,n}$, we calculate $X_{8,8}$, $X_{9,9}$, and $X_{10,10}$.

$$X_{8,8} = \begin{bmatrix} 4 & 12 & 24 & 36 & 46 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 50 & 40 & 28 & 20 \\ 28 & 32 & 36 & 44 & 54 & 44 & 36 & 32 \\ 40 & 44 & 48 & 52 & 58 & 52 & 48 & 44 \\ 44 & 48 & 52 & 56 & 62 & 56 & 52 & 48 \\ 32 & 36 & 40 & 48 & 58 & 48 & 40 & 36 \\ 20 & 24 & 32 & 44 & 54 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 50 & 40 & 28 & 16 \end{bmatrix}, \quad X_{9,9} = \begin{bmatrix} 4 & 12 & 24 & 36 & 48 & 48 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 52 & 52 & 40 & 28 & 20 \\ 28 & 32 & 36 & 44 & 56 & 56 & 44 & 36 & 32 \\ 40 & 44 & 48 & 52 & 60 & 60 & 52 & 48 & 44 \\ 51 & 55 & 59 & 63 & 67 & 67 & 63 & 59 & 55 \\ 44 & 48 & 52 & 56 & 64 & 64 & 56 & 52 & 48 \\ 32 & 36 & 40 & 48 & 60 & 60 & 48 & 40 & 36 \\ 20 & 24 & 32 & 44 & 56 & 56 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 52 & 52 & 40 & 28 & 16 \end{bmatrix},$$

$$X_{10,10} = \begin{bmatrix} 4 & 12 & 24 & 36 & 48 & 58 & 48 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 52 & 62 & 52 & 40 & 28 & 20 \\ 28 & 32 & 36 & 44 & 56 & 66 & 56 & 44 & 36 & 32 \\ 40 & 44 & 48 & 52 & 60 & 70 & 60 & 52 & 48 & 44 \\ 52 & 56 & 60 & 64 & 68 & 74 & 68 & 64 & 60 & 56 \\ 56 & 60 & 64 & 68 & 72 & 78 & 72 & 68 & 64 & 60 \\ 44 & 48 & 52 & 56 & 64 & 74 & 64 & 56 & 52 & 48 \\ 32 & 36 & 40 & 48 & 60 & 70 & 60 & 48 & 40 & 36 \\ 20 & 24 & 32 & 44 & 56 & 66 & 56 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 52 & 62 & 52 & 40 & 28 & 16 \end{bmatrix}.$$

We now present another algorithm to compute the matrix $X_{n,n} = [x_{ij}]$. To do this, two cases that n is odd or even are considered. We first assume that n is odd. Define two $n \times (n + 1)/2$ matrices $A = [a_{ij}]$ and $B = [b_{ij}]$ as follows:

$$a_{1,j} = 12(j - 1) \quad 1 \leq j \leq (n + 1)/2, \quad a_{i,j} = \begin{cases} a_{i-1,j} + 4, & 2 \leq i \leq (n + 1)/2, \\ a_{n-i+2,j}, & (n + 1)/2 < i \leq n. \end{cases}$$

$$b_{i,1} = \begin{cases} 12(i - 1) + 4, & 1 \leq i \leq (n - 1)/2, \\ b_{i-1,1} - 12, & (n + 3)/2 < i \leq n, \end{cases}$$

$$b_{(n+1)/2,1} = 6n - 3, \quad b_{(n+3)/2,1} = 6n - 10, \quad b_{i,j} = b_{i,j-1} + 4; \quad 2 \leq j \leq (n + 1)/2.$$

If n is even then the matrices A and B are defined as follows:

$$\begin{aligned}
 a_{1,j} &= 12(j - 1), & 1 \leq j \leq n/2, & & a_{1, \frac{n}{2}+1} &= 6n - 2, \\
 a_{i,j} &= \begin{cases} a_{i-1,j} + 4, & 2 \leq i \leq n/2 + 1, \\ a_{n-i+2,j}, & n/2 + 1 < i \leq n, \end{cases} \\
 b_{i,1} &= \begin{cases} 12(i - 1) + 4, & 1 \leq i \leq n/2, \\ b_{i-1,1} - 12, & n/2 + 1 < i \leq n, \end{cases} & & & b_{n/2+1,1} &= 6n - 4.
 \end{aligned}$$

For other entries of the matrix B , we define $b_{i,j} = b_{i,j-1} + 4, 2 \leq j \leq n/2 + 1$. Then, we can see that $x_{i,j} = \text{Max}\{a_{i,j}, b_{i,j}\}$, where Max denotes the maximum function. In what follows, we compute the matrix $X_{8,8}$ from $A_{8,5}$ and $B_{8,5}$.

$$\begin{aligned}
 A_{8,5} &= \begin{bmatrix} 0 & 12 & 24 & 36 & 46 \\ 4 & 16 & 28 & 40 & 50 \\ 8 & 20 & 32 & 44 & 54 \\ 12 & 24 & 36 & 48 & 58 \\ 16 & 28 & 40 & 52 & 62 \\ 12 & 24 & 36 & 48 & 58 \\ 8 & 20 & 32 & 44 & 54 \\ 4 & 16 & 28 & 40 & 50 \end{bmatrix}, & & B_{8,5} &= \begin{bmatrix} 4 & 8 & 12 & 16 & 20 \\ 16 & 20 & 24 & 28 & 32 \\ 28 & 32 & 36 & 40 & 44 \\ 40 & 44 & 48 & 52 & 56 \\ 44 & 48 & 52 & 56 & 60 \\ 32 & 36 & 40 & 44 & 48 \\ 20 & 24 & 28 & 32 & 36 \\ 8 & 12 & 16 & 20 & 24 \end{bmatrix}, \\
 X_{8,8} &= \begin{bmatrix} 4 & 12 & 24 & 36 & 46 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 50 & 40 & 28 & 20 \\ 28 & 32 & 36 & 44 & 54 & 44 & 36 & 32 \\ 40 & 44 & 48 & 52 & 58 & 52 & 48 & 44 \\ 44 & 48 & 52 & 56 & 62 & 56 & 52 & 48 \\ 32 & 36 & 40 & 48 & 58 & 48 & 40 & 36 \\ 20 & 24 & 32 & 44 & 54 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 50 & 40 & 28 & 16 \end{bmatrix}.
 \end{aligned}$$

We now are ready to prove the main result of the paper.

Theorem. Suppose $T = T[p, q]$ is a $TUC_4C_8(R)$ nanotorus. Then we have:

$$W(T) = \begin{cases} (2m/3)(m^2 - 1) + mn(m + 3n) - k_1, & \text{if } m < n \\ (2n/3)(n^2 - 1) + mn(3m + n) - k_2, & \text{if } m > n, \\ (n/3)(14n^2 - k_3), & \text{if } m = n, \end{cases}$$

in which $k_1 = \begin{cases} 0, & \text{if } 2|n \ \& \ 2|m, \\ n - m, & \text{if } 2|n \ \& \ 2 \nmid m, \\ m, & \text{if } 2 \nmid n \ \& \ 2|m, \\ n, & \text{if } 2 \nmid n \ \& \ 2 \nmid m, \end{cases}$ $k_2 = \begin{cases} 0, & \text{if } 2|m, \\ m, & \text{if } 2 \nmid m, \end{cases}$

$k_3 = \begin{cases} 2, & \text{if } 2|n, \\ 5, & \text{if } 2 \nmid n \end{cases}$ and, “ $|$ ” denotes the divisibility relation.

Proof. The case of $m = n$ is proved before in lemma 2. According to the first paragraph of this section, we have to compute $X_{m,n}$. To compute $X_{m,n}$, we consider two cases that $m < n$ and $m > n$.

Case 1 $m < n$. In this case, we can compute $X_{m,n}$ by omitting $n - m$ rows of $X_{n,n}$. Suppose m is even. Then the first $m/2$ rows of the matrix $X_{m,n}$ and $X_{n,n}$ are the same. Similarly, the last $m/2$ rows of the matrix $X_{m,n}$ and $X_{n,n}$ are also the same. In other words if $X_{m,n} = [x_{ij}]$ and $X_{n,n} = [a_{ij}]$ then we have:

$$x_{i,j} = \begin{cases} a_{i,j}, & \text{if } 1 \leq i \leq m/2, 1 \leq j \leq n, \\ a_{n-m+i,j} & \text{if } m/2 < i \leq m, 1 \leq j \leq n. \end{cases}$$

If m is odd, then the first $(m-1)/2$ rows of the matrices $X_{m,n}$ and $X_{n,n}$ and the last $(m-1)/2$ rows of these matrices are the same. Also, the $(m+1)/2$ th row of $X_{m,n}$ is as follows:

$$x_{i,j} = \begin{cases} a_{i,j}, & 1 \leq i \leq (m-1)/2, 1 \leq j \leq n \\ a_{n-m+i,j} & (m+1)/2 < i \leq m, 1 \leq j \leq n \end{cases} ,$$

$$x_{(m+1)/2,j} = \begin{cases} a_{(m+1)/2,j}, & -1 \leq j \leq (m+1)/2, n - (m-1)/2 < j \leq n \\ a_{(m+1)/2,j}, & (m+1)/2 < j \leq n - (m-1)/2 \end{cases} .$$

Using a simple calculation, we can see that $W(T) = (2m/3)(m^2 - 1) + mn(m + 3n) - k_1$, where k_1 is defined as in theorem.

Case 2 $m > n$. In this case, we can compute $X_{m,n}$ by omitting $m-n$ columns of $X_{m,m}$. Suppose n is odd. Then the first $(n+1)/2$ columns of the matrices $X_{m,n}$ and $X_{m,m}$ and the last $(n-1)/2$ rows of these matrices are the same. In other words if $X_{m,n} = [x_{ij}]$ and $X_{m,m} = [a_{ij}]$ then we have:

$$x_{i,j} = \begin{cases} a_{i,j}, & 1 \leq j \leq (n+1)/2, 1 \leq i \leq m \\ a_{i,m-n+j} & (n+1)/2 < j \leq n, 1 \leq i \leq m \end{cases} .$$

If n is even then the first $n/2$ columns and the last $n/2-1$ columns of matrices $X_{m,m}$ and $X_{m,n}$ are equal. Moreover, the $(n/2 + 1)$ th column of $X_{m,n}$ is as follows:

$$x_{i,j} = \begin{cases} a_{i,j} & 1 \leq j \leq n/2, 1 \leq i \leq m, \\ a_{i,m-n+j}, & n/2 + 1 < j \leq n, 1 \leq i \leq m, \end{cases}$$

$$x_{i,n/2+1} = \begin{cases} a_{i,n/2+1} - 2, & 1 \leq i \leq n/2, m - n/2 < i \leq m. \\ a_{i,n/2+1}, & n/2 < i \leq m - n/2. \end{cases}$$

Now a simple calculation shows that $W(T) = (2n/3)(n^2 - 1) + mn(3m + n) - k_2$. This completes the proof.

To explain our algorithm, we end this paper with the calculation of the matrices $X_{8,5}$, $X_{8,6}$, $X_{5,8}$, and $X_{6,8}$.

$$X_{6 \times 8} = \begin{bmatrix} 4 & 12 & 24 & 36 & 46 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 50 & 40 & 28 & 20 \\ 28 & 32 & 36 & 44 & 54 & 44 & 36 & 32 \\ 32 & 36 & 40 & 48 & 58 & 48 & 40 & 36 \\ 20 & 24 & 32 & 44 & 54 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 50 & 40 & 28 & 16 \end{bmatrix}, \quad X_{5 \times 8} = \begin{bmatrix} 4 & 12 & 24 & 36 & 46 & 36 & 24 & 12 \\ 16 & 20 & 28 & 40 & 50 & 40 & 28 & 20 \\ 27 & 31 & 35 & 44 & 54 & 44 & 35 & 31 \\ 20 & 24 & 32 & 44 & 54 & 44 & 32 & 24 \\ 8 & 16 & 28 & 40 & 50 & 40 & 28 & 16 \end{bmatrix}$$

$$X_{8 \times 5} = \begin{bmatrix} 4 & 12 & 24 & 24 & 12 \\ 16 & 20 & 28 & 28 & 20 \\ 28 & 32 & 36 & 36 & 32 \\ 40 & 44 & 48 & 48 & 44 \\ 44 & 48 & 52 & 52 & 48 \\ 32 & 36 & 40 & 40 & 36 \\ 20 & 24 & 32 & 32 & 24 \\ 8 & 16 & 28 & 28 & 16 \end{bmatrix}, \quad X_{8 \times 6} = \begin{bmatrix} 4 & 12 & 24 & 34 & 24 & 12 \\ 16 & 20 & 28 & 38 & 28 & 20 \\ 28 & 32 & 36 & 42 & 36 & 32 \\ 40 & 44 & 48 & 52 & 48 & 44 \\ 44 & 48 & 52 & 56 & 52 & 48 \\ 32 & 36 & 40 & 46 & 40 & 36 \\ 20 & 24 & 32 & 42 & 32 & 24 \\ 8 & 16 & 28 & 38 & 28 & 16 \end{bmatrix}.$$

Acknowledgments

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