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Notes on some Distance-Based Invariants for 2-Dimensional Square and Comb Lattices

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Abstract. We present explicit formulae for the eccentric connectivity index and Wiener index of 2-dimensional square and comb lattices with open ends. The formulae for these indices of 2-dimensional square lattices with ends closed at themselves are also derived. The index for closed ends case divided by the same index for open ends case in the limit $N \to \infty$ defines a novel quantity we call compression factor. This factor was calculated for both eccentric connectivity and Wiener index for 2-dimensional square lattice.

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1. Square lattices

1.1 The case of square graph $\mathbf{Sq}^C$ with closed ends

The translationally invariant lattice satisfying boundary cyclic conditions we describe with $\mathbf{Sq}^C$ graph. Its unit cell U contains just one site (vertex) V_1 whose valency (degree) equals $\delta_1 = 4$.

$\mathbf{Sq}^C$ graph is built by adding an increasing number L of the unit cells along both plane directions and so it possesses altogether N=L^2 vertices. The number of edges (chemical bonds) in a graph is denoted by B. The 4-regularity of $\mathbf{Sq}^C$ immediately implies that B=2N.

The Wiener index, *W,* is defined as the half of the sum of all distances in the distance matrix D of a graph, and the diameter, *M*, as the largest distance in the graph. Let further define $\underline{w}$ as the half of the minimal sum of distances in a row (column) of D and the related vertex (vertices) we call minimal vertex (vertices) $\underline{v}$ *(*$\underline{V}$*).* The eccentricity ε_i of a vertex v_i is defined as the maximal distance from v_i to any other vertex in a graph, and the sum of all local eccentricities multiplied with corresponding vertex degrees δ_i defines the *eccentric connectivity index,* ξ*(N)*, of a graph with N vertices as [5]:

$$\xi(N) = \Sigma_i \varepsilon_i \delta_i \qquad (1)$$

The eccentric connectivity index is the central subject we study in the present paper.

All the above graph-theoretical invariants, W, M, $\underline{w}$, and ξ, can be in 2-dimensional lattices expressed as polynomials in $N^{1/2}$ where the leading exponent of $N^{1/2}$ depends on the invariant under study as it is shown below:

$$W(N) = a_5 N^{5/2} + a_4 N^2 + a_3 N^{3/2} + a_2 N + a_1 N^{1/2} + a_0 \qquad (2\text{-}1)$$

$$M(N) = b_1 N^{1/2} + b_0 \qquad (2\text{-}2)$$

$$\underline{\mathrm{w}}(N) = d_3 N^{3/2} + d_2 N + d_1 N^{1/2} + d_0 \qquad (2\text{-}3)$$

$$\xi(N) = f_3 N^{3/2} + f_2 N + f_1 N^{1/2} + f_0 \qquad (2\text{-}4)$$

The coefficients in the above polynomials are rational numbers and they only depend on topological structure (connectivity) of a given graph and are easily obtained by interpolating numerical results for different values of N; see Table 1 for the case of $\mathbf{Sq}^C$ graph.

As $\mathbf{Sq}^C$ graph is highly symmetrical, all $\underline{w}(N)$ contributions to W are mutually equal and therefore we have $W(N)=N\underline{w}(N)$. Moreover, due to the cyclic boundary conditions, the eccentricity ε of any node equals graph diameter M. As all vertex degrees are also the same, for local contribution to eccentric connectivity index is:

$$e = \delta\varepsilon = 4M \qquad (3)$$

and therefore:

$$\xi(N) = Ne(N) = 4NM(N). \qquad (4)$$

In Table 1 we present numerical values of graph invariants (2) for $\mathbf{Sq}^C$ lattices for L=2 up to L=15 where the data for even L are separated from those for odd L. In the headers of this Table we give explicit formulas for invariants as functions of N. Some of these invariants for even L differ from those for odd L what is marked by an asterisk. However, diameter M for an even L equals that one for the next odd value L+1. The same holds for two consecutive values of the local contributions e to the eccentric connectivity index.

Table 1. Graph invariants for Sq^C graphs with $N=L^2$ vertices

L=even

L	N	$M=N^{1/2}$	$W=N^{5/2}/4$	$\underline{w}= N^{3/2}/4$	e =4M	$\xi=4N^{3/2}$
2	4	2	8	2	8	32
4	16	4	256	16	16	256
6	36	6	1.944	54	24	864
8	64	8	8.192	128	32	2048
10	100	10	25.000	250	40	4000
12	144	12	62.208	432	48	6912
14	196	14	134.456	686	56	10976

L=odd

L	N	$^*M=N^{1/2}-1$	$^*W=(N^{5/2}-N^{3/2})/4$	$^*\underline{w}= (N^{3/2}-N^{1/2})/4$	e=4M	$^*\xi=4(N^{3/2}-N)$
3	9	2	54	6	8	72
5	25	4	750	30	16	400
7	49	6	4.116	84	24	1176
9	81	8	14.580	180	32	2592
11	121	10	39.930	330	40	4840
13	169	12	92.274	546	48	8112
15	225	14	189.000	840	56	12600

In summary, for even N we have

$$\underline{\mathrm{w}} = N^{3/2}/4, W(N) = N^{5/2}/4 \text{ and } \xi(N) = 4N^{3/2} \ ,$$

whereas for odd N we obtain

$$\underline{\mathrm{w}} = (N^{3/2} - N^{1/2})/4, W = (N^{5/2} - N^{3/2})/4 \text{ and } \xi = 4(N^{3/2} - N).$$

In the limit of large N, these N odd vs. N even differences vanish, leading to

$$\underline{\mathrm{w}}^C \to N^{3/2}/4, W^C \to N^{5/2}/4, \xi^C \to 4N^{3/2} \ ,$$

where by superscript C we emphasize the fact that we consider graphs closed on themselves, i.e. those satisfying cyclic boundary conditions. Later we will use the limits $W^C \to N^{5/2}/4$ and $\xi^C \to 4N^{3/2}$ to compare them with analogous limits for graphs with open ends to determine the so called *compression ratios* or factors for square graphs.

1.2 The case of square graph Sq with open ends

The square lattice graph without cyclic boundary conditions imposed on it we call the square lattice (graph) with open ends and denote by **Sq.** The number of edges is readily obtained as $B=2(N - N^{1/2})$. Again, the interpolation method quickly produces the closed forms for all previous topological lattice invariants. Opposite to $\mathbf{Sq}^C$, neither *W(N)* nor *M(N)* in lattice **Sq** do show dependence on the parity of N. However, this dependence still persists for other indices (marked by an asterisk in Table2) related to the minimal vertices $\underline{V}$ like $\underline{w}$, $\underline{e}=\underline{\delta\varepsilon}$ and the eccentric connectivity ξ.

By inspection of Table 1 and Table 2, one observes an interesting fact that numerical values of $\underline{e}=\underline{\delta\varepsilon}$ with respect to L are the same both for closed ends and open ends lattices. However, it is a simple consequence of the fact that the center of open ends lattice **Sq** can also serve as the center of closed ends lattice $\mathbf{Sq}^C$ with the same eccentricity and degree for both vertices.

It is interesting to note that for open ends graphs **Sq** the numerical values of $\underline{e}$ remain identical for consecutive lattices (e.g. for L=4,5 or L=6,7 pairs) as it was the case for closed ends lattices $\mathbf{Sq}^C$.

Asymptotic values of the Wiener index and eccentric connectivity index for **Sq** graphs are given by

$$W \to N^{5/2}/3, \xi \to 6N^{3/2},$$

and by combining this with previously obtained limits for $\mathbf{Sq}^C$, $W^C \to N^{5/2}/4$; $\xi^C \to 4N^{3/2}$, the asymptotic values of the compression ratios for W and ξ are determined as

$$W^C/W = 3/4 \qquad (5)$$

$$\xi^C/\xi = 2/3. \qquad (6)$$

It is interesting to note that the same numerical values of compression factors appear also in 1-dimensional lattices as we reported in an earlier work [3]. Also, the eccentric connectivity index of **Sq** lattices were considered in [4] as special cases of Cartesian products of two paths.

Table 2. Graph invariants for Sq graphs with $N=L^2$ vertices

L=even

L	N	$M=2(N^{1/2}-1)$	$W=(N^{5/2}- N^{3/2})/3$	$\underline{w}= N^{3/2}/4$	$\underline{e}=\underline{\delta}(M+2)/2$	$\xi=6N^{3/2}$ - $11N +6N^{1/2}$
2	4	2	8	2	4(+)	16
4	16	6	256	16	16	232
6	36	10	1.944	54	24	936
8	64	14	8.192	128	32	2.416
10	100	18	25.000	250	40	4.960
12	144	22	62.208	432	48	8.856
14	196	26	134.456	686	56	14.392

(+) for L=2: $\underline{\delta}=2$, $\underline{e}=M+2$

L=odd

L	N	$M=2(N^{1/2}-1)$	$W=(N^{5/2}-N^{3/2})/3$	$*\underline{w}= (N^{3/2})/4- (N^{1/2})/4$	$*\underline{e}=\underline{\delta}M/2$	$*\xi=6N^{3/2}$ - $11N +4N^{1/2} +1$
3	9	4	72	6	8	76
5	25	8	1.000	30	16	496
7	49	12	5.488	84	24	1548
9	81	16	19.440	180	32	3.520
11	121	20	53.240	330	40	6.700
13	169	24	123.032	546	48	11.376
15	225	28	252.000	840	56	17.836

2. Comb latices

2.1 The case of square comb lattice Cq with pen ends

A few first square comb lattice graphs **Cq** are depicted in Figure 1.

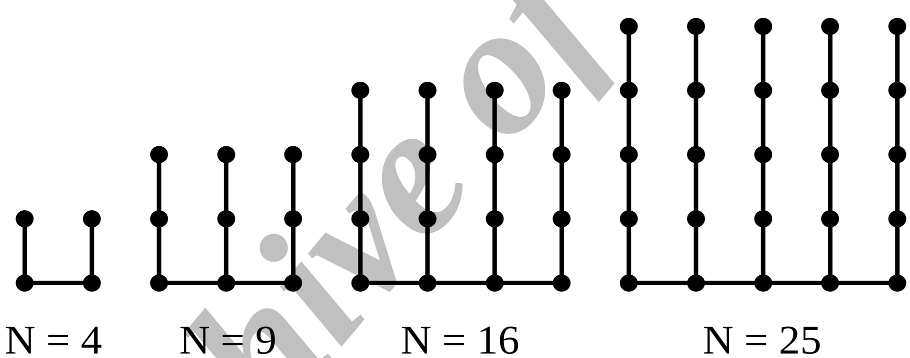

Figure 1. Graphs of **Cq** comb lattices for N=4,9,16,25.

Numerical interpolation for increasing number of nodes $N=L^2$ allows a fast determination of closed forms of lattice invariants for graphs **Cq**. The results are given in Table 3. Similarly to the case of square lattices with open ends, the Wiener index of **Cq** graphs, $W(N)= (4N^{5/2} - 5N^2 + 2N^{3/2} -N)/6$, does not show dependence on parity of N. However, parity plays role in $\underline{w}$ and eccentric connectivity index $\xi(N)$ as for even N we have $\xi=(9N^{3/2} -10N -6N^{1/2}+8)/2$ whereas for odd N we obtain $\xi=(9N^{3/2} -10N -7N^{1/2}+8)/2$. Generally, a tree has one or two centers and this is, of course, also seen in **Cq**. One center configuration is one for odd N where $\underline{\varepsilon}=M/2$ and for even N two centers are present with $\underline{\varepsilon}=1+M/2$ but for both configurations minim

al vertices have the same degree: $\underline{\delta}=3$ (except for $N=4$). It is clear that for an increase of L by 2, the corresponding values of $\underline{e}$ grow by 9 as seen in Table 3.

Table 3. Graph invariants for Cq graphs with $N=L^2$ vertices

L=even

L	N	$M=3(N^{1/2}-1)$	$W(N)=(4N^{5/2}-5N^2+2N^{3/2}-N)/6$	$\underline{w}=(3N^{3/2}-2N)/8$	$\underline{e}=\underline{\delta}(M+1)/2=3(M+1)/2$	$\xi=(9N^{3/2}-10N-6N^{1/2}+8)/2$
2	4	3	10	2	4(+)	14
4	16	9	488	20	15	200
6	36	15	4170	72	24	778
8	64	21	18592	176	33	1964
10	100	27	58650	350	42	3974
12	144	33	149160	612	51	7024
14	196	39	327418	980	60	11330

(+) for L=2 $\underline{e}=\underline{\delta\varepsilon}=2^2=4$

L=odd

L	N	$M=3(N^{1/2}-1)$	$W(N)=(4N^{5/2}-5N^2)/6+(2N^{3/2}-N)/6$	$^*\underline{w}=(3N^{3/2}-2N)/8-(N^{1/2})/8$	$^*\underline{e}=3M/2$	$^*\xi=(9N^{3/2}-10N)/2-(7N^{1/2}-8)/2$
3	9	6	102	7,50	9	70
5	25	12	1600	40	18	424
7	49	18	9310	115,5	27	1278
9	81	24	34128	252	36	2848
11	121	30	95590	467,5	45	5350
13	169	36	224432	780	54	9000
15	225	42	465150	1207,5	63	14014

2.2 The case of Van Hove comb lattice CvH with open ends

Some of smallest van Hove comb lattice graphs **CvH** are depicted in Figure 2.

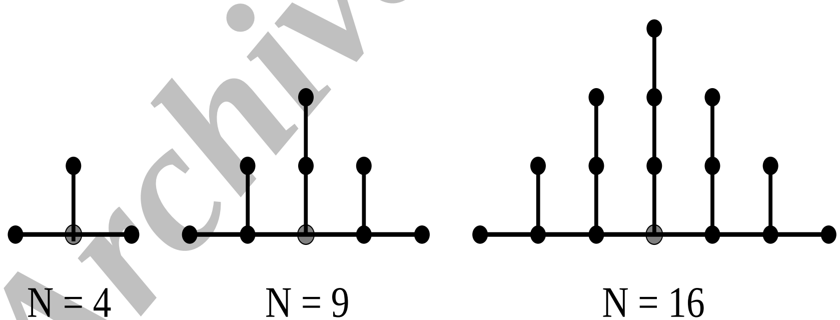

FIGURE 2. Graphs of **CvH** comb lattices for N=4,9,16; graph minimal vertices are in gray.

Numerical interpolation for increasing number of nodes N allows us again to determine closed forms of lattice invariants for graphs **CvH**. The results are

given in Table 4. Note that for these graphs, invariants are insensitive on parity of N, and they are all expressed as polynomials in $N^{1/2}$ like in Eq. (2) which is valid for all 2-dimensional lattices studied so far. So, Eq. (2) is of a general interest and applicability as it holds for lattices of rather different topologies like those studied here but also for other structures as translationally invariant graphs (crystals), pentagonal nanocones [2] and heptagonal nanocones [1].
The results are summarized in Table 4, where polynomials for all invariants studied are given: $W(N) = (17N^{5/2} - 20N^2 + 10N^{3/2} - 10N + 3N^{1/2})/30$, $\underline{w} = (4N^{3/2} - 3N - N^{1/2})/12$, etc. Note that for **CvH** graphs there is only a single center we mark by grey node at the bottom of figures. Let also note that $\underline{e}$ values of Table 4 increase by 3 (except for the first two lattices) as one moves from any **CvH** graph up to its next graph.

Table 4. Graph invariants for CvH graphs with N vertices.

N	$M=2(N^{1/2}-1)$	$W(N)=(17N^{5/2}-20N^2)/30 + (10N^{3/2}-10N+3N^{1/2})/30$	$\underline{w}= (4N^{3/2}-3N)/12-(N^{1/2})/12$	$\underline{e}=3\ M/2$	$\xi=(10N^{3/2}-12N)/3-(7N^{1/2}-9)/3$
4	2	9	1,5	3	9
16	6	426	17	9	143
25	8	1.388	35	12	308
36	10	3.603	62,5	15	565
49	12	8.022	101,5	18	934
64	14	15.988	154	21	1435
81	16	29.304	222	24	2088
100	18	50.301	307,5	27	2913
121	20	81.906	412,5	30	3930
144	22	127.710	539	33	5159
169	24	192.036	689	36	6620
196	26	280.007	864,5	39	8333
225	28	397.614	1067,5	42	10318

3. Conclusions

In the present paper it has been demonstrated that the Wiener index, the eccentric connectivity index and a couple of other invariants (see Eq. (2)), can be all represented as polynomials in $N^{1/2}$, where N stands for the number of vertices of the lattice under study.
The asymptotic values of the Wiener index and the eccentric connectivity index for N being large are given below for all lattices studied in the present note. The leading coefficient of W is a measure of compactness of a given lattice and, as it should be expected, the lattices have to be ordered as shown below. Note that the comb lattices are by no means topologically different from square lattices in filling the plane, i.e. the comb lattices do not exhibit any fractal nature.

Table 5. Asymptotic behaviors of the Wiener and the eccentric connectivity index.

Graph kind	*W (N)*	*W (N)/* $N^{5/2}$	ξ *(N)*
SqC	1/4 $N^{5/2}$	0,25	4 $N^{3/2}$
Sq	1/4 $N^{5/2}$	0,33	6 $N^{3/2}$
CvH	17/30 $N^{5/2}$	0,57	10/3 $N^{3/2}$
Cq	2/3 $N^{5/2}$	0,67	9/2 $N^{3/2}$

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