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GENERATING FUNCTIONS FOR THE HARARY-READ NUMBERS CLASSIFIED ACCORDING TO SYMMETRY

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Abstract

The studies of the "Harary-Read numbers" for catafusenes are continued. The generating functions were derived separately for the different symmetries of interest. Numerical values are supplemented.

1. Introduction

In 1970 Harary and Read [1] published a generating function for the numbers of catafusenes. This work is considered as a major achievement in the enumeration of polyhexes. More than twenty years later, the present authors [2] produced formulas for the numbers of catafusenes belonging to the different symmetry groups. The problem was solved by elementary combinatorics without invoking generating functions. This method resulted in summation formulas. In the conclusion of the same work [2], it was suggested that the problem of symmetry-classified Harary-Read numbers might also be solved in terms of generating functions, and perhaps easier. The combinatorial methods were supposed to provide a useful alternative.

In the present paper, we report the generating functions for the numbers of catafusenes (Harary-Read numbers) separately for the different symmetries. It seems to be a matter of taste which one of the methods is easier than the other. We would say that the application of generating functions is not much easier, if easier at all, than the previously applied method leading to the summation formulas.

It should be repeated here that the catafusenes [3] are defined as the catacondensed (without internal vertices) simply connected polyhexes. In particular, it should be noted that the helicenic systems (catahelicenes) are included.

2. Edge-rooted catafusenes

Harary and Read [1] start their analysis by deducing the generating function, viz. $U(x)$, for the numbers of catafusenes rooted at an edge. Here, we define

$$N(x) = 1 + U(x). \tag{1}$$

Hence,

$$N(x) = \tfrac{1}{2} x^{-1}[1 - x - (1-x)^{1/2}(1-5x)^{1/2}]$$
$$= \sum_{i=0}^{\infty} N_i x^i = 1 + x + 3x^2 + 10x^3 + 36x^4 + \dots \; . \tag{2}$$

3. Example: dihedral symmetry

As a example, we show the derivation of the generating function, say $D(x)$, for the numbers of (unrooted) catafusenes with dihedral (D_{2h}) symmetry. These numbers occur in groups of four [2]:

$$D(x) = x^2 + x^3 + x^4 + x^5 + 2x^6 + 2x^7 + 2x^8 + 2x^9 + 5x^{10} + 5x^{11} + 5x^{12} + 5x^{13}$$
$$+ 15x^{14} + 15x^{15} + 15x^{16} + 15x^{17} + 51x^{18} + \dots \; . \tag{3}$$

Let us first derive the auxiliary function

$$\mathcal{D}(w) = \sum_{j=1}^{\infty} \mathcal{D}_j w^j = w + 2w^2 + 5w^3 + 15w^4 + 51w^5 + \dots \; , \tag{4}$$

which generates all the *different* coefficients in (3). One has, consistently with the previous analysis [2],

$$\mathcal{D}_j = \sum_{k=0}^{j-1} N_k \; ; \quad \mathcal{D}_{j+1} - \mathcal{D}_j = N_j \; . \tag{5}$$

Consequently,

$$\mathcal{D}(w) - w\,\mathcal{D}(w) = w + w^2 + 3w^3 + 10w^4 + 36w^5 + \dots = w\,N(w). \tag{6}$$

Herefrom, it is readily obtained, with the aid of eq. (2), that

$$\mathcal{D}(w) = w(1-w)^{-1}N(w) = \tfrac{1}{2}[1 - (1-w)^{-1/2}(1-5w)^{1/2}]. \tag{7}$$

The next step is to insert $w = x^4$. Then,

$$\mathcal{D}(x^4) = x^4 + 2x^8 + 5x^{12} + 15x^{16} + 51x^{20} + \dots$$
$$= \tfrac{1}{2}[1 - (1-x^4)^{-1/2}(1-5x^4)^{1/2}]. \tag{8}$$

This equation should be compared with eq. (3). It is seen that the expansion of $\mathcal{D}(x^4)$ possesses the same coefficients as $D(x)$ for x^i when $i = 4, 8, 12, 16, \dots$, but all the other terms in $\mathcal{D}(x^4)$ vanish. In order to obtain the coefficients repeated for two units before and one unit after the i values specified above, one should take

$$D(x) = x^{-2}\,\mathcal{D}(x^4) + x^{-1}\,\mathcal{D}(x^4) + \mathcal{D}(x^4) + x\,\mathcal{D}(x^4), \tag{9}$$

which, together with eq. (8), readily gives the $D(x)$ function in closed form (see below).

4. Unrooted catafusenes of the different symmetries

For the sake of brevity, no further details of the derivation of the different generating functions are reported here. Only the final results are listed in the following. The functions are identified as

$$F(x) = \sum_{i=1}^{\infty} F_i x^i, \tag{10}$$

where F stands for I, T, D, C, R, $M^{(a)}$, $M^{(b)}$ or A, referring to the symmetries D_{6h}, D_{3h}, D_{2h}, C_{2h}, C_{3h}, C_{2v}(a), C_{2v}(b) and C_s, respectively. Within the symmetry group C_{2v}, one distinguishes between two types, viz. (a) and (b), depending on whether the twofold symmetry axis cuts edges or goes through vertices, respectively.

4.1. REGULAR HEXAGONAL SYMMETRY, D_{6h}

$$I(x) = x. \tag{11}$$

4.2. REGULAR TRIGONAL SYMMETRY, D_{3h}

$$T(x) = \tfrac{1}{2}x^{-2}(1+x^3)[1-(1-x^6)^{-1/2}(1-5x^6)^{1/2}]. \tag{12}$$

4.3. DIHEDRAL SYMMETRY, D_{2h}

$$D(x) = \tfrac{1}{2}x^{-2}(1+x)(1+x^2)[1-(1-x^4)^{-1/2}(1-5x^4)^{1/2}]. \tag{13}$$

4.4. CENTROSYMMETRY, C_{2h}

$$C(x) = \tfrac{1}{4}x^{-2}(1-x)[1-(1-x^2)^{1/2}(1-5x^2)^{1/2}] - \tfrac{3}{4}(1+x) - \tfrac{1}{2}D(x), \tag{14}$$

where $D(x)$ is given by eq. (13).

4.5. NON-REGULAR TRIGONAL SYMMETRY, C_{3h}

$$R(x) = \tfrac{1}{4}x^{-2}[1-(1-x^3)^{1/2}(1-5x^3)^{1/2}] - \tfrac{3}{4}x - \tfrac{1}{2}T(x), \tag{15}$$

where $T(x)$ is given by eq. (12).

4.6. MIRROR SYMMETRY OF THE TYPE C_{2v}(a)

$$M^{(a)}(x) = \tfrac{1}{4}x^{-2}(1+3x)[1-(1-x^2)^{1/2}(1-5x^2)^{1/2}] - \tfrac{3}{4}(1+3x) - \tfrac{1}{2}D(x) - T(x), \tag{16}$$

where $D(x)$ and $T(x)$ are given by eqs. (13) and (12), respectively.

4.7. MIRROR SYMMETRY OF THE TYPE C_{2v}(b)

$$M^{(b)}(x) = C(x) \tag{17}$$

as in eq. (14).

4.8. ASYMMETRICAL SYSTEMS C_s

$$A(x) = \tfrac{1}{24}x^{-2}[(1-x)^{3/2}(1-5x)^{3/2} + 3(1+3x)(1-x^2)^{1/2}(1-5x^2)^{1/2} - 4(1-x^3)^{1/2}(1-5x^3)^{1/2}] - \tfrac{1}{2} + x - C(x) - R(x), \tag{18}$$

where $C(x)$ and $R(x)$ are given by eqs. (14) and (15), respectively.

4.9. TOTAL

The generating function for the numbers of catafusenes in total is

$$H(x) = I(x) + T(x) + R(x) + D(x) + C(x) + M^{(a)}(x) + M^{(b)}(x) + A(x). \tag{19}$$

This function was derived by Harary and Read [1] and it is not necessary to repeat it here.

5. Numerical values

The derived generating functions were expanded by means of a simple computer program to give the numbers of non-isomorphic (unrooted) catafusenes of the different symmetries. The computations reproduced (as they should, of course) the numbers obtained from the summation formulas [2]. Those numbers were given up to $h = 15$, where h is the number of hexagons. For the sake of brevity, we do not repeat these previously published numbers here, but give a continuation of the listing. These supplementary numbers are divided into two tables.

Table 1 pertains to the systems with a nontrivial plane of (mirror) symmetry other than the plane of the hexagonal lattice. Here, the symmetry groups of interest

Table 1

Numbers of large catafusenes ($h > 15$) of the symmetries $D_{3h}(T)$, $D_{2h}(D)$ and $C_{2v}(M)$

h	T	D	M	Total (W)
16	5	15	9265	9285
17	0	15	18555	18570
18	0	51	39536	39587
19	5	51	79118	79174
20	0	51	171318	171369
21	0	51	342687	342738
22	15	188	751033	751236
23	0	188	1502284	1502472
24	0	188	3328030	3328218
25	15	188	6656233	6656436

are D_{3h}, D_{2h} and C_{2v}, both C_{2v}(a) and C_{2v}(b). The generating function for these symmetries together, viz.

$$W(x) = I(x) + T(x) + D(x) + M(x), \tag{20}$$

is particularly simple, as has been deduced by Harary and Read [1]. It has also been quoted in our previous work [2]. In the above equation,

$$M(x) = M^{(a)}(x) + M^{(b)}(x). \tag{21}$$

Table 2 pertains to the systems without a nontrivial plane of symmetry, viz. C_{3h}, C_{2h} and C_s. Define the generating function

$$V(x) = R(x) + C(x) + A(x) \tag{22}$$

for the appropriate subtotals. Then of course,

$$H(x) = W(x) + V(x). \tag{23}$$

Table 2

Numbers of large catafusenes ($h > 15$) of the symmetries $C_{3h}(R)$, $C_{2h}(C)$ and $C_s(A)$

h	R	C	A	Total (V)
16	66	4635	36681383	36686084
17	0	4635	159894915	159899550
18	0	19768	701898184	701917952
19	269	19768	3100972840	3100992877
20	0	85659	13779678410	13779764069
21	0	85659	61557361263	61557446922
22	1102	375524	276326335318	276326711944
23	0	375524	1245934013926	1245934389450
24	0	1664015	5640863040825	5640864704840
25	4635	1664015	25635343582986	25635345251636

The numbers for the symmetry types C_{2v}(a) and C_{2v}(b) separately are easily accessible from tables 1 and 2 by virtue of the relations:

$$M^{(a)}(x) = M(x) - C(x), \quad M^{(b)}(x) = C(x). \tag{24}$$

6. Conclusion

This paper completes our studies of the Harary–Read numbers for catafusenes classified according to the symmetries of the systems. The two methods, which lead to summation formulas or generating functions, are supposed to be useful complementary alternatives.

References

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