Polycubes with Small Perimeter Defect*

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Abstract
A polycube is a face-connected set of cubical cells on $\mathbb{Z}^3$. To-date, no formulae enumerating polycubes by volume (number of cubes) or perimeter (number of empty cubes neighboring the polycube) are known. We present a few formulae enumerating polycubes with a fixed deviation from the maximum possible perimeter.

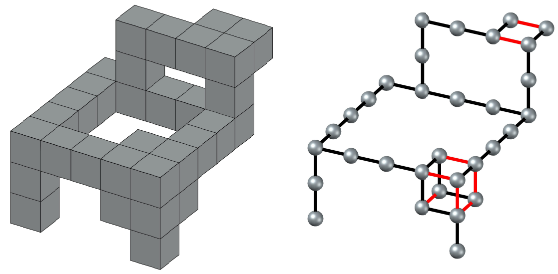
Keywords: Polycubes, linear recurrence, generating functions.

1 Introduction

A *polyomino* of area n is an edge-connected set of n squares on $\mathbb{Z}^2$. Likewise, a d-dimensional *polycube* of volume n is a connected set of n cubes on $\mathbb{Z}^d$, where connectivity is through $(d-1)$-dimensional faces. Two *fixed* polycubes are considered identical if one can be translated into the other; in this paper we consider only fixed polycubes. The study of polycubes (in two and higher dimensions) began in the 1950s in statistical physics [5] and in the 1960s in enumerative combinatorics [6].

Let $A_3(n)$ denote the number of polycubes of volume n (sequence A001931 in the On-line Encyclopedia of Integer Sequences [1]). Lunnon computed $A_3(n)$ manually up to $n = 6$ [7] and later up to $n = 12$ [8]. Aleksandrowicz and Barequet [3] provided counts up to $n = 18$. Luther and Mertens [9] set the current record by computing $A_3(19)$, improving and extending the original algorithm of Redelmeier [10] for counting polyominoes in the plane. To-date, no formula is known for $A_3(n)$ (or for the number of polycubes in any dimension).

In statistical physics, the *perimeter* of a polycube P is defined as the number of *perimeter cells*—empty cells neighboring P. (A similar definition is used for other combinatorial structures, e.g., by Blecher et al. [4].) We denote by $A_3(n, p)$ the number of polycubes having volume n and perimeter p. It is easy to observe that we always have $p \le 4n+2$. Let, then, $k = (4n+2)-p$ denote the "perimeter defect" of P. Our main result is that for each fixed non-negative value of k, the generating function of the sequence $(A_3(n, 4n+2-k))$ is rational. This work generalizes a previous work [2], in which we investigated polyominoes (polycubes in two dimensions) with fixed defect.



(a) (b)

Figure 1: A polycube and its dual graph

2 Formulae for Small Defect

2.1 Notation and Basic Facts Along with a polycube P, we will consider its dual graph P^*: The vertices of P^* correspond to the cells of P, and two vertices of P^* are adjacent if the corresponding cells of P share a face. Figure 1 shows a polycube and its dual graph. Occasionally, we shall use the graph-theoretic terminology of P^* for P: For example, we shall refer to the degree of a cell of P, the number of edges in P, etc.

The volume of a given polycube P will be denoted by n, and its perimeter by p. In Proposition 2.1(1), we show that we always have $p \le 4n + 2$. Hence, we introduce a new parameter $k = (4n + 2) - p$, to be referred to as the *(perimeter) defect* of P.

The *excess* of a perimeter cell X of P is the number of neighbors of X that belong to P, minus 1. An *excess cell* is a perimeter cell with non-zero excess (*i.e.*, an empty cell with at least two occupied neighboring cells). Let e be the total excess of P, that is, the sum of excesses over all perimeter cells of P. Finally, let r be the *circuit rank* of the dual graph of P (also known as

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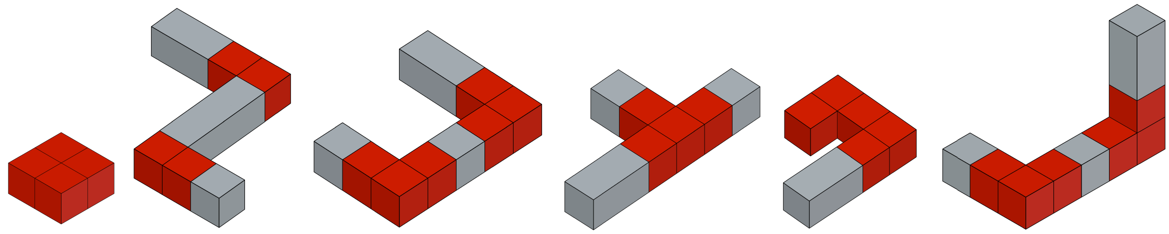


Figure 2: Cases for $k = 2$ (Proposition 2.3)

the *cyclomatic number* of P), *i.e.*, the minimal number of edges that must be removed from P in order to obtain a tree. (It is well known that in a connected graph $G = (V, E)$, we have $r = |E| - |V| + 1$.) For example, the circuit rank of the polycube in Figure 1(a) is 8, and it is manifested by eight red edges in the graph shown in Figure 1(b). We then have the following basic facts:

PROPOSITION 2.1. *For every polycube of size n and perimeter p, we have (1) $p \leq 4n+2$; and (2) $k = e+2r$.*

Proof. Consider a polycube P of size n and its dual graph $P^* = (V, E)$. If no cube of P had touched any other cube, then the total perimeter of P would have been $6n$. However, there are two factors that can contribute to the loss in the perimeter of P: excess cells, and pairs of adjacent occupied cells. The contribution of excess cells is obviously e, the total loss caused by free cells that have more than one occupied neighboring cell. The contribution of pairs of adjacent occupied cells is $2|E|$. Therefore, we have $p = 6n - e - 2|E|$. Since $e \geq 0$ and $|E| \geq n - 1$, we have

$$p \leq 6n - 2(n-1) = 4n + 2,$$

and, thus, claim (1) is proven. For claim (2), we have

$$\begin{aligned} k = 4n + 2 - p = (4n+2) - (6n - e - 2|E|) \\ = e + 2|E| - 2n + 2 = e + 2r. \end{aligned}$$

2.2 Formulae for Defect $k = 0, 1, 2, 3$

PROPOSITION 2.2.
(1) $A_3(n, 4n+2) = 3$ for $n \geq 2$ (and 1 for $n = 1$);
(2) $A_3(n, 4n+1) = 12(n-2)$ for $n \geq 2$ (and 0 for $n = 1, 2$).

Proof. The formula $k = e + 2r$ allows us to identify all the possible shapes of polycubes with defect k. If the defect is either 0 or 1, then necessarily we have $r = 0$, and, hence, $k = e$. Therefore, $k = 0$ is possible only for *sticks*—the $1 \times 1 \times n$, $1 \times n \times 1$, and $n \times 1 \times 1$ cubes, and $k = 1$ is realizable only by paths with a single bend. The claims follow at once.

PROPOSITION 2.3. *$A_3(n, 4n) = 30n^2 - 222n + 456$ for $n \geq 6$ (and sporadic values for $n = 4, 5$).*

Proof. By Proposition 2.1(2), $k = 2$ implies either $\{e = 0, r = 1\}$ or $\{e = 2, r = 0\}$. This allows us to partition polycubes with defect $k = 2$ into several classes, shown in Figure 2. The general form of a member of such a class consists of *fixed cubes* (colored with red) and *legs*—sticks (colored with gray) of indeterminate, possibly 0, length.[1] We have the following cases.
Case (a): Non-trees. The combination $e = 0, r = 1$ is possible only for the $2 \times 2 \times 1$ block (possibly aligned in another way). Therefore, the count is 3 only for $n = 4$. In all other cases of $k = 2$, the polycubes are trees either with two perimeter cells of excess 1, or with one perimeter cell of excess 2.
Case (b): Paths with two coplanar bends in opposite directions. The number of such polycubes is $\binom{n-2}{2}$ (for $n \geq 4$), which is the number of decompositions of $n-4$ into three non-negative parts.
Case (c): Planar paths with two bends in the same direction, with at least two cells between the bends. Similarly to Case (b), except that here we have six fixed cells, the count is $\binom{n-4}{2}$ (for $n \geq 6$).
Case (d): T-like polycubes. The calculation is identical to that in Case (b).
Case (e): There is exactly one such polycube for each $n \geq 5$.
The last case is the only case of polycubes which span three dimensions.
Case (f): A 3-dimensional chain with two bends. Again, there are $\binom{n-4}{2}$ such polycubes (for $n \geq 6$).
These counts should be multiplied by a factor of 3 (Case (a)), 12 (Cases (b,c,d) and (e, $n = 5$), or 24 (Cases (e, $n \geq 6$) and (f)), depending on the symmetries of the shape. Summing up all cases completes the proof.

While the formulae for $A_3(n, 4n+2-k)$ for $k = 0, 1, 2$ are polynomials of degree k, the formula for $A_3(n, 4n-1)$ is a cubic *quasi-polynomial* with period 2.

[1] This coloring convention will be used throughout the paper.

PROPOSITION 2.4. $A_3(n, 4n-1) = \frac{103n^3}{2} - 623n^2 + \left(\frac{11681}{4} + \frac{15(-1)^n}{4}\right)n - \frac{10929}{2} - \frac{63(-1)^n}{2}$ *for* $n \geq 12$ *(and sporadic values for* $n \leq 11$*).*

Proof. The formula $k = e + 2r$ helps us to partition the set of such polycubes into 27 mutually-disjoint classes, shown in Figure 3. The full case analysis will be given in the full version of the paper; here we discuss in detail only Cases (xix) and (i).

The number of polycubes of type (xix), as depicted, is equal to the number of decompositions of $n-7$ into four non-negative parts, which is $\binom{n-4}{3}$. To count the number of orientations, the polycubes of this type can be seen as a path P which spans all three dimensions plus a leg whose direction is determined by the middle part of P. There are 3! possibilities to embed P so as to span all three dimensions. In each direction, both positive and negative directions are possible, for a total of $3! \cdot 2^3 = 48$ options. Therefore, the total count of polycubes of this type is

$$48\binom{n-4}{3} = 8n^3 - 120n^2 + 592n - 960.$$

Refer now to Case (i) (drawn in Figure 4(a) in a two-dimensional view). The numbers a, b, c, d determine a polyomino in this class uniquely. Obviously, $c \geq 2$ and $a \geq c{+}1$; we do not need to care for upper bounds. Once a and c are chosen, we have $n{-}a{-}c{-}3$ cells for $b{+}d$. Moreover, $d \leq b{-}2$ and, therefore, $d \leq (n{-}a{-}c{-}5)/2$. Hence, the summation is

$$\sum_{c\geq 2}\ \sum_{a\geq c+1}\ \sum_{d=1}^{\lfloor\frac{n-a-c-5}{2}\rfloor} 1.$$

Due to the rounding in the upper bound for d, the explicit formula splits into two cases depending on the parity of n: For even n, we obtain

$$f_E(n) = (-10+n)(144-34n+2n^2)/48,$$

and for odd n, we obtain

$$f_O(n) = (-11+n)(126-32n+2n^2)/48.$$

Considering all possible orientations, the total count in this case is

$$24\left(\frac{f_E(n)+f_O(n)}{2} + (-1)^n\,\frac{f_E(n)-f_O(n)}{2}\right)$$
$$= n^3 - 27n^2 + \left(\frac{481}{2} + \frac{3(-1)^n}{2}\right)n - \frac{27(-1)^n}{2} - \frac{1413}{2}.$$

As we will see in Section 2.3, the formulae for Cases (i)–(iii) are non-polynomial due to the presence of parts whose (indeterminate) lengths are dependent. In all other cases, this phenomenon does not occur, hence, the formulae are polynomial. Summing up the formulae for all cases (see Table 1) completes the proof.

2.3 Generating Functions In this section we shall see how to obtain the same results in a uniform way by using generating functions. For each case, extracting the coefficient from the generating function provides the desired formula, and then we can sum up the generating functions of all cases and obtain the one of the total formula.

Let us return to Case (i) for defect $k = 3$ (redrawn in Figure 4(b)). In addition to twelve fixed cells which contribute x^{12} to the generating function, polycubes of this type contain two equal-length pairs of legs (of lengths c' and d'), and two independent legs (of lengths a' and b'). Each independent leg contributes the factor $\frac{1}{1-x}$, and each equal-length pair of legs contributes the factor $\frac{1}{1-x^2}$. Polycubes of this type can be aligned with either the xy, yz, or zx plane, and within each plane there are eight possible orientations. Hence, the generating function is

$$\frac{24x^{12}}{(1-x^2)^2(1-x)^2} = \frac{24x^{12}}{(1-x)^4(1+x)^2},$$

and its partial fraction decomposition is

$$3x^{12}\left(\frac{1}{1-x} + \frac{3}{2}\cdot\frac{1}{(1-x)^2} + 2\cdot\frac{1}{(1-x)^3} + 2\cdot\frac{1}{(1-x)^4} + \frac{1}{1+x} + \frac{1}{2}\cdot\frac{1}{(1+x)^2}\right).$$

The coefficient extraction from these basic generating functions yields

$$[x^n]\,\frac{24x^{12}}{(1-x)^4(1+x)^2} = 3\binom{n-12}{0} + \frac{9}{2}\binom{n-11}{1} + 6\binom{n-10}{2} + 6\binom{n-9}{3} + 3(-1)^n\binom{n-12}{0} + \frac{3}{2}(-1)^n\binom{n-11}{1},$$

which simplifies to the formula for Case (i) in Proposition 2.4.

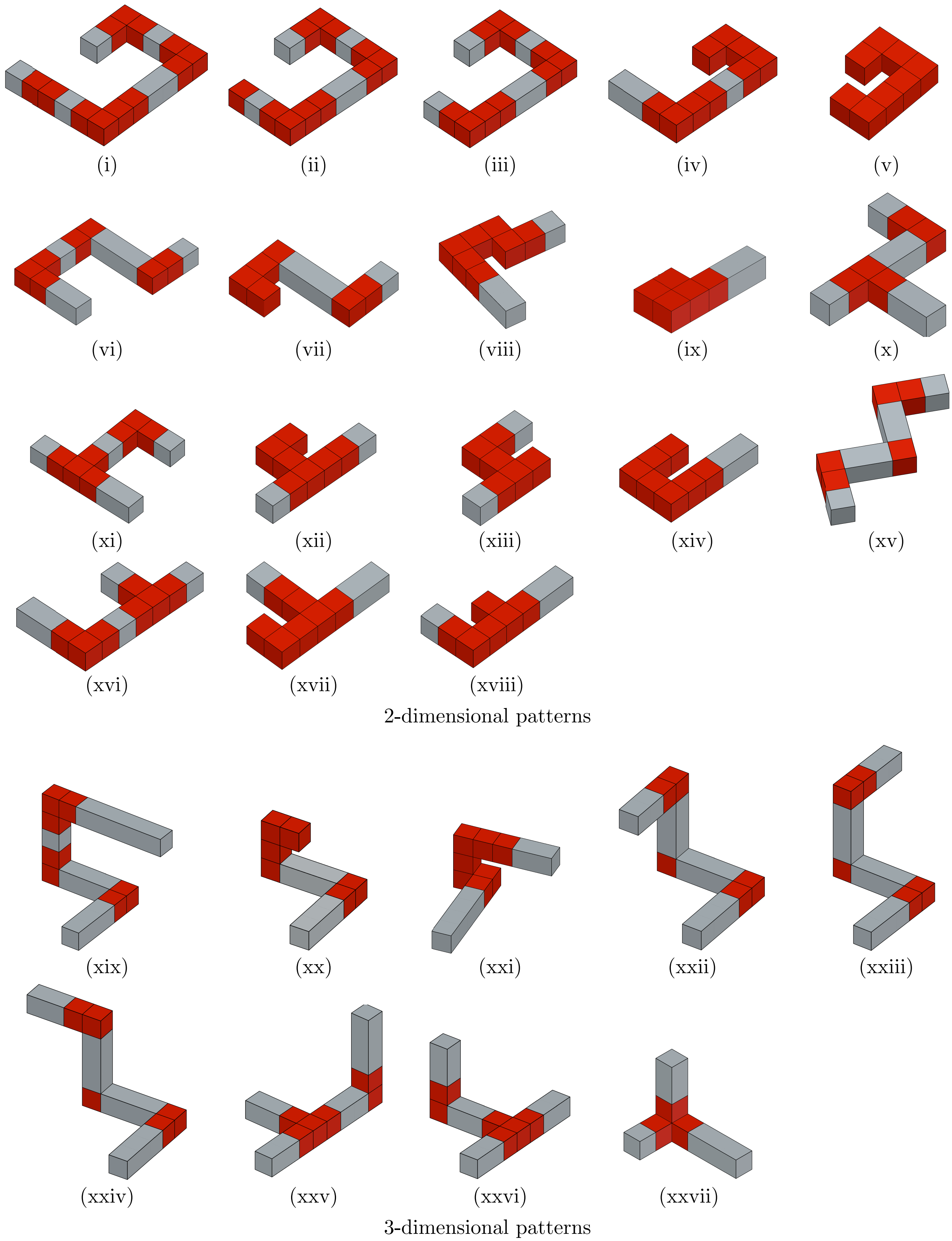
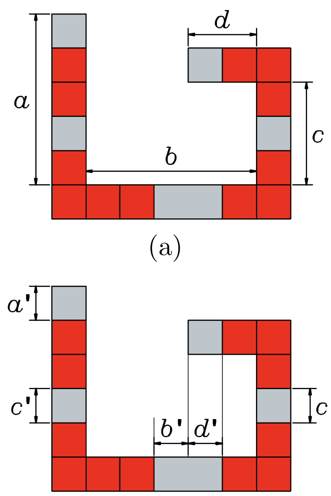


Figure 3: Cases for $k = 3$ (Proposition 2.4)

Case	Volume	Count	Case	Vol.	Count
(i)	≥ 12	$-\frac{1413}{2}-\frac{27(-1)^n}{2}+\left(\frac{481}{2}+\frac{3(-1)^n}{2}\right)n-27n^2+n^3$			
(ii)	≥ 10	$\frac{333}{2}-\frac{45(-1)^n}{2}+\left(-45+3(-1)^n\right)n+3n^2$			
(iii)	≥ 9	$-\frac{201}{2}+\frac{9(-1)^n}{2}+\left(\frac{211}{4}-\frac{3(-1)^n}{4}\right)n-9n^2+\frac{n^3}{2}$			
(iv)	≥ 9	$-192+24n$	Case	Vol.	Count
(v)	8	24	(xvi)	≥ 7	$-480+296n-60n^2+4n^3$
(vi)	≥ 5	$-480+296n-60n^2+4n^3$	(xvii)	≥ 7	$-144+24n$
(vii)	≥ 6	$-120+24n$	(xviii)	≥ 6	$-120+24n$
(viii)	≥ 7	$-144+24n$	(xix)	≥ 7	$-960+592n-120n^2+8n^3$
(ix)	≥ 5	24	(xx)	≥ 6	$-240+48n$
(x)	≥ 5	$-96+104n-36n^2+4n^3$	(xxi)	≥ 7	$-288+48n$
(xi)	≥ 7	$-480+296n-60n^2+4n^3$	(xxii)	≥ 5	$-96+104n-36n^2+4n^3$
(xii)	≥ 7	$-144+24n$	(xxiii)	≥ 5	$-96+104n-36n^2+4n^3$
(xiii)	≥ 6	$-120+24n$	(xxiv)	≥ 5	$-192+208n-72n^2+8n^3$
(xiv)	7	12	(xxv)	≥ 6	$-240+188n-48n^2+4n^3$
	≥ 8	24	(xxvi)	≥ 6	$-240+188n-48n^2+4n^3$
(xv)	≥ 5	$-48+52n-18n^2+2n^3$	(xxvii)	≥ 4	$24-20n+4n^2$

Table 1: Counts of cases for $k=3$ (Proposition 2.4)



(a)

(b)

Figure 4: Case (i) for $k=3$ (two drawings)

In a similar manner, we obtain the generating function for Case (xix). Seven fixed cells contribute the factor x^7 to the generating function, and each of the four independent legs contributes to it a factor of $\frac{1}{1-x}$. There are $3!\cdot 2^3 = 48$ different orientations as explained above, thus, the generating function is

$$48\cdot\frac{x^7}{(1-x)^4}=\frac{48x^7}{(1-x)^4}.$$

k	Characteristic Polynomial
0	$x-1$
1	$(x-1)^2$
2	$(x-1)^3$
3	$(x-1)^4(x+1)^2$

Table 2: Characteristic polynomials for $0 \leq k \leq 3$

A standard coefficient extraction gives

$$[x^n]\,\frac{48x^7}{(1-x)^4}=48\binom{n-4}{3}=8n^3-120n^2+592n-960.$$

Similar reasoning shows that the characteristic polynomials (equivalently, the denominator of the rational generating functions) for all other cases consists of $(x-1)$ to the power at most 4, and $(x+1)$ to the power at most 2. In other words, they all divide $(x-1)^4(x+1)^2$. Therefore, when we sum up the formulae of all cases in order to obtain the resulting formula for $k=3$, the denominator of the generating function is the least common multiple of the denominators of all the cases, that is, $(x-1)^4(x+1)^2$. Consequently, the characteristic polynomial for defect $k=3$ is $(x-1)^4(x+1)^2$. A similar, but simpler, reasoning leads to the characteristic polynomials for $k=0,1,2$, summarized in Table 2.

More importantly, generating functions give us insight into the general case of fixed k. We saw that for $k\leq 3$, the sequence satisfies a linear recurrence because the generating function is rational, and its characteristic polynomial factors into powers of $1\pm x$ (see the table above). In Section 3, we show that for each fixed k, the sequence satisfies a linear recurrence whose characteristic polynomial factors into *cyclotomic polynomials*. In order to find the generating function for polycubes with a fixed defect k, we systematically partition them into finitely-many classes whose generating functions are routine.

3 The General Form

In this section we show that the generating function for polycubes of a fixed defect k is always rational.

THEOREM 3.1. $\sum_{n\geq 0} A(n, 4n+2-k)x^n$, *the generating function that enumerates polycubes with a fixed defect k with respect to their volume, is rational. Moreover, its denominator is a product of cyclotomic polynomials. Equivalently, from a certain position, the enumerating sequence of such polycubes satisfies a linear recurrence, and its characteristic polynomial is a product of cyclotomic polynomials (all of which roots are therefore roots of unity).*

Proof. The proof consists of the following three steps.

1. First, we partition the set of polycubes with defect k into mutually-disjoint subsets, to be called "pattern classes." Informally, a pattern class consists of polycubes which have a "similar shape" (in some precise sense detailed below);
2. Next, we show that for each pattern class, its generating function has the form as stated in the Theorem;
3. Then, we prove that the number of pattern classes is bounded.

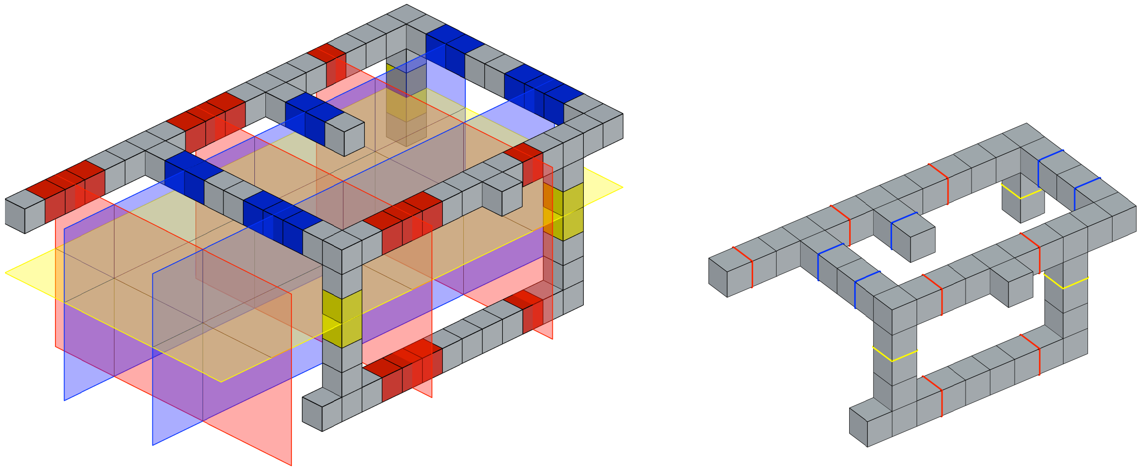
Finally, the combination of (2) and (3) implies the Theorem.

Step 1. Let us start with some definitions. We label the grid cells by three coordinates, (x_1, x_2, x_3). A *grid slice* is the set of all unit cubes with one coordinate fixed. Specifically, the grid slice that contains all the cells with $x_j = p$ (the jth coordinate equal to p) will be denoted by $C_{j,p}$. A *j-orthogonal cut* of a polycube P is a maximal set $\mathcal{C}$ of consecutive grid slices, $C_{j,p}, C_{j,p+1}, \ldots, C_{j,q}$, such that the projection of $P \cap (C_{j,p-1} \cup C_{j,p} \cup \ldots \cup C_{j,q+1})$ on the plane spanned by all the coordinates except j is a non-empty finite set A of (2-dimensional) cells that do not neighbor each other and have no common neighbors. That is, this intersection consists of one or several legs with the same orientation, that extend to all the width of $\mathcal{C}$ augmented by two neighboring slices and have maximal possible perimeter, and $\mathcal{C}$ is a maximal set with such property. As a special case, we consider a *trivial* (or *empty*) cut, corresponding to the case $q = p - 1$. See Figure 5(a) for an illustration. The polycube shown on this figure has three x-orthogonal cuts (indicated by red), two y-orthogonal cuts (indicated by blue), and one z-orthogonal cut (indicated by yellow). (In addition to coloring the cubes that belong to cuts, we indicate each cut by a transparent plane.)

The key property of cuts is the following obvious fact. Suppose that P has a nontrivial cut $\mathcal{C}$. Then, if one removes the slices of $\mathcal{C}$ and glues the remaining parts of the plane together, a new valid polycube **with the same defect** is obtained, and the removed cut "shrinks" into a trivial cut. Applying this *shrinking procedure* to all nontrivial cuts, one eventually obtains a polycube without nontrivial cuts: such polycubes will be called *reduced*. Notice that shrinking a cut never produces new cuts: indeed, two cuts of the same orientation are always disjoint, and the intersection of two cuts of different orientations never contains cells of P. Therefore, all the cuts are independent in the sense that successive shrinking of nontrivial cuts in any order is equivalent to their simultaneous shrinking. In particular, exactly one irreducible polycube can be obtained in this way from a given polycube P. Figure 5(b) shows the irreducible polycube obtained by reducing the polycube shown in Figure 5(a).

A *pattern class* is the set of all polycubes that produce the same irreducible polycube by the shrinking procedure. Since, as explained above, each polycube produces a unique reduced polycube, pattern classes form a partition of the set of polycubes with defect k.

Step 2. Given an irreducible polycube R, all the members of the class of R can be easily reconstructed. Indeed, if R has trivial cut(s), then any polycube from the class of R can be obtained from R by expanding the cuts, that is, inserting some number of grid slices with appropriately oriented legs, to replace some trivial cuts by nontrivial cuts. In other words, for each trivial cut of R and for any non-negative integer ℓ, we can insert a *bundle* of legs $\ell\times 1\times 1$, $1\times\ell\times 1$, or $1\times 1\times\ell$ (depending on the orientation of the trivial cut) between all the *ports*—pairs of the cells where this trivial cut intersects R. The contribution of this bundle of legs to the generating function of the pattern class is clearly $1/(1-x^s)$, where s is the number of ports of this cut. Therefore, the generating function of the pattern class of R is x^b (where b is the size of R) multiplied by a product of some terms of the form $1/(1-x^s)$. For example, for the reduced polycube R shown in Figure 5(b), the three red cuts contribute $1/(1-x) \cdot 1/(1-x^3)^2$, the two blue cuts contribute $1/(1-x^3) \cdot 1/(1-x^2)$, and the yellow cut contributes $1/(1-x^3)$. In total, the generating function



(a) A polycube P (b) The polycube R obtained by reducing P

Figure 5: A polycube and the reduced representative of its pattern class

for the class of R is $x^{51}/((1-x)(1-x^2)(1-x^3)^4)$, since 51 is the number of cubes in R.

If R has no trivial cuts, then R is the only element in its class, and the generating function is simply x^b.

Step 3. Now we prove that, for a fixed value of k, the number of pattern classes is finite. The central argument of our proof is the following claim:

> *In a polycube with fixed defect k, only a finite number of slices (among those which intersect P) do not belong to cuts. More precisely: For a fixed k, there exists a constant $\gamma = \gamma(k)$, such that for each coordinate j, in each polycube P with defect k, at most γ many j-orthogonal slices, which intersect P, do not belong to j-orthogonal cuts.*

In order to show that, we analyze what can prevent from a slice to be a part of a cut. First, we define three kinds of *special cells*:

- An occupied cell with at least one pair of occupied non-opposite neighbors (such cells will be referred to as *L-cells*[2]);
- An excess cell (defined as above, recall that an excess cell is free); and
- An occupied cell of degree 1.

Suppose that three consecutive j-orthogonal slices, C_{p-1}, C_p, and C_{p+1} (we omit j from the notation), intersect P. We show that if C_p is not a part of a nontrivial cut, then at least one of the slices C_{p-1}, C_p, and C_{p+1} contains a special cell. Indeed, suppose for contradiction that C_{p-1}, C_p, and C_{p+1} do not contain any special cells. First, C_p does not contain two adjacent cells of P, otherwise the connected component of $P \cap C_p$, that contains such two cells, necessarily contains a degree-1 cell or an L-cell. Thus, $P \cap C_p$ consists of isolated cells, and no pair of such cells has a common neighbor, otherwise C_p contains an excess cell. The same is true for C_{p-1} and C_{p+1}. That is, each one of C_{p-1}, C_p, and C_{p+1} has individually a shape that fits a slice that belongs to a cut. We need to prove that these three slices have occupied cells in exactly the same positions. Assume for contradiction and without loss of generality that $j = 1$, and that the projection of $P \cap C_{p-1}$ on the plane spanned by x_2 and x_3 is not equal to that of $P \cap C_p$. Assume also, without loss of generality, that for some q, r we have $(p-1, q, r) \in P$, $(p, q, r) \notin P$. But then $(p-1, q, r)$ is a degree-1 cell: only $(p-2, q, r)$ can be its neighbor. All this means that C_p belongs to a cut, which is a contradiction.

Next, for each kind of special cells, we prove that the number of its occurrences in a polycube with a fixed defect k is bounded from above by a constant number. Recall the formula $k = e + 2r$. Since each excess cell contributes at least 1 to e, it follows directly that the number of excess cells is bounded. Consider now the L-cells—the corners of L-shapes embedded in P. If the fourth cell of the L-shape is free, then it is an excess cell, and thus the L-cell contributes to the count of e; and if the fourth cell of the L-shape is occupied, then we have a 2×2 block, that is, a loop, and thus the L-cell contributes to the count of r. Therefore, if we have an unbounded number of L-cells, then either e or r is

[2] That is, in a polycube of size at least 2, any cell Z is an L-cell unless Z has degree 1, or Z has degree 2 and its two neighbors are attached to opposite faces of Z.

unbounded too, which is a contradiction. For degree-1 cells, we consider the dual graph of P. Denote by V_1, V_2, and $V_{\geq 3}$ the sets of cells of degree 1, 2, and at least 3, respectively. Since the maximum possible vertex-degree is 6, we have

$$1|V_1| + 2|V_2| + 6|V_{\geq 3}| \geq 2|E| \geq 2(|V| - 1) = 2|V_1| + 2|V_2| + 2|V_{\geq 3}| - 2,$$

which implies $|V_1| \leq 4|V_{\geq 3}| + 2$. However, cells with degree at least 3 are necessarily L-cells. Since we already know that the number of L-cells is bounded, it follows from the last relation that the number of degree-1 cells is bounded as well.

In summary, we showed that each j-orthogonal slice, which does not belong to a cut, or at least one of its neighbors, contains a special cell; and that the number of special cells is bounded. Therefore, the number of j-orthogonal slices, which do not belong to the cuts, is bounded.

It follows directly from this claim that all the irreducible polycubes with defect k are contained in the grid cube $\gamma \times \gamma \times \gamma$, where γ is a constant number. Therefore, the number of irreducible polycubes, and, consequently, that of pattern classes, is finite.

This means that we can simply sum up the generating functions for all patterns. Since each of them has a product of cyclotomic polynomials in the denominator, the same is true for their sum, and the proof is now complete.

4 Conclusion

In this paper, we provided formulae enumerating 3-dimensional polycubes with a small defect. We proved that for any defect, the generating function is rational, and that the characteristic polynomial is a product of cyclotomic polynomials.

Our next goal is to extend these results to the higher dimension. For any dimension d, the maximum possible perimeter of a polycube of volume n is

$$M_d = 2dn - 2(n-1) = 2(d-1)n + 2,$$

and the formula $k = e + 2r$ holds in any dimension. Denote by $B(n,d,k)$ the number of d-dimensional polycubes of volume n and with defect k (that is, perimeter $M_d - k$). It is easy to see that $B(n,d,0) = d$ and $B(n,d,1) = \binom{d}{2}4(n-2) = d(d-1)(n-2)/2$. Then, it is also easy to verify that patterns of defect k can span at most $k+1$ dimensions. Equivalently, patterns that span d dimensions have defect at least $d-1$. Hence, in order to compute the formula for $B(n,d,k)$, we need to sum up only the formulas for patterns that span $1 \leq i \leq k-1$ dimensions, multiplying the respective formulae by $\binom{d}{i}$. Our goal will be, then, to characterize $B(n,d,k)$ more precisely.

In addition, Theorem 3.1 generalizes to any dimension, that is, the generating function of $B(n,d,k)$ is rational, and its denominator is a product of cyclotomic polynomials, for any value of d. We will attempt to prove this formally.

Another direction for future study is the asymptotics. We conjecture that in any dimension d and for any fixed k, the highest-degree factor of the characteristic polynomial will be $(x-1)^{k+1}$, contributed, in particular, by patterns that consist of $k+1$ independent legs. This would imply that the asymptotics of $(B(n,d,k))_{n\geq 0}$ is γn^k, where γ is some constant.

Finally, we plan to analyze possible dependencies between legs in pattern classes, as functions of d and k. This will enable us to set bounds on the maximum q, such that the factor $(1-x^q)$ appears in the generating function of some pattern. In its turn, this will make possible to estimate the characteristic polynomial without actual calculations.

References

[1] *The On-Line Encyclopedia of Integer Sequences*, `http://oeis.org` .

[2] A. Asinowski, G. Barequet, and Y. Zheng, *Enumerating polyominoes with fixed perimeter defect*, Proc. 9th European Conf. on Combinatorics, Graph Theory, and Applications, Vienna, Austria, August-September 2017, Electronic Notes in Discrete Mathematics, 61 (2017), pp. 61–67.

[3] G. Aleksandrowicz and G. Barequet, *Counting d-dimensional polycubes and nonrectangular planar polyominoes*, Int. J. of Computational Geometry and Applications, 19 (2009), pp. 215–229.

[4] A. Blecher, C. Brennan, A. Knopfmacher, and T. Mansour, *The site-perimeter of words*, Trans. on Combinatorics, 6 (2017), pp. 37–48.

[5] S. R. Broadbent and J. M. Hammersley, *Percolation processes: I. Crystals and mazes*, Proc. Cambridge Phil. Society, 53 (1957), pp. 629–641.

[6] S. W. Golomb, *Polyominoes*, Scribners, New York, 1965 (2nd ed., Princeton Univ. Press, 1996).

[7] W. F. Lunnon, *Symmetry of cubical and general polyominoes*, in: Graph Theory and Computing (R. C. Read, ed.), Academic Press, New York, 1972, pp. 101–108.

[8] W. F. Lunnon, *Counting multidimensional polyominoes*, The Computer Journal, 18 (1975), pp. 366–367.

[9] S. Luther and S. Mertens, *Counting lattice animals in high dimensions*, J. of Statistical Mechanics: Theory and Experiment, 9 (2011), pp. 546–565.

[10] D. H. Redelmeier, *Counting polyominoes: Yet another attack*, Discrete Mathematics, 36 (1981), pp. 191–203.