The dimension ladder: hollow polycubes in every dimension

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September 9, 2026

Abstract

A polycube in $\mathbb{Z}^d$ that encloses a cavity has at least $4d-1$ cells. The polycubes with exactly $4d-1$ cells and a cavity are, up to translation, in bijection with the spanning trees of the d-dimensional cross-polytope graph, so there are $(2d)^{d-2}(2d-2)^d$ of them: 4, 384, 82,944, 32,768,000, ... (OEIS A193130). The case $d=2$ is the classical seven-cell polyomino with a hole; the case $d=3$ is the first term of A396101.

1 Statement

Cells are the points of $\mathbb{Z}^d$, $d \geq 2$; two cells are adjacent when they differ by a unit vector $\pm e_i$. A *polycube* is a finite set of cells connected under adjacency. The complement of a polycube P splits into connected components; a bounded component is a *cavity* of P. Write $|c|$ for the ℓ_1 norm of a cell and $N(X)$ for the set of cells outside X adjacent to some cell of X.

The *cross-polytope graph* $\mathrm{CP}(d)$ has the $2d$ vertices $\pm e_1, \ldots, \pm e_d$, with two vertices adjacent unless they are opposite; it is the complete multipartite graph $K_{2,2,\ldots,2}$ with d parts. Its Laplacian has eigenvalues 0, $2d$ (multiplicity $d-1$) and $2d-2$ (multiplicity d), so by the matrix-tree theorem its number of spanning trees is

$$t(\mathrm{CP}(d)) \;=\; \frac{1}{2d}\,(2d)^{d-1}(2d-2)^d \;=\; (2d)^{d-2}(2d-2)^d.$$

Theorem 1. *Every polycube in $\mathbb{Z}^d$ with a cavity has at least $4d-1$ cells. A polycube with exactly $4d-1$ cells has a cavity if and only if, after a translation, it is*

$$P_T \;=\; \{\pm e_1, \ldots, \pm e_d\} \;\cup\; \{\, s + s' : \{s, s'\} \in T \,\}$$

for a spanning tree T of $\mathrm{CP}(d)$. Distinct trees give polycubes that are not translates of one another, so the number of minimal hollow polycubes up to translation is $t(\mathrm{CP}(d)) = (2d)^{d-2}(2d-2)^d$.

2 A cavity of one cell

Translate so that the cavity is the single cell 0. All $2d$ neighbours $\pm e_i$ of 0 lie in P; call them *sealers* and write S for their set. Group the remaining cells by norm: $L_k = \{c : |c| = k\}$. Changing one coordinate by ± 1 changes the norm by exactly ± 1, so adjacent cells lie in consecutive layers and no two cells of the same layer are adjacent. In particular the sealers are pairwise non-adjacent.

Lemma 2 (contacts)**.** (a) *A cell of* L_2 *is either a corner* $s+s'$ *with* s, s' *non-opposite sealers, adjacent among* S *exactly to* s *and* s'*, or a double* $2s$*, adjacent among* S *exactly to* s*.* (b) *A cell of* L_3 *is adjacent to at most three cells of* L_2*, and any two of those are adjacent to a common sealer.* (c) *A cell of norm at least* 4 *has no neighbour of norm at most* 2*.*

Proof. (a) and (c) are immediate from the norm rule. For (b), a cell of L_3 is $s+s'+s''$ with three sealers in distinct directions, whose L_2-neighbours are $s+s'$, $s+s''$, $s'+s''$; or $2s+s'$, with L_2-neighbours $2s$ and $s+s'$, both adjacent to s; or $3s$, with the single L_2-neighbour $2s$. □

Let $A = P \cap L_2$, with a corners and b doubles, let $C = P \cap L_{\geq 3}$, and let $B = S \cup A$. Form the graph M on the vertex set S whose edges are the corners of A, a corner $s+s'$ being the edge $\{s, s'\}$; a corner determines its pair, so distinct corners are distinct edges. A double $2s$ is attached to s alone. By Lemma 2(a) the connected components of B are exactly the components of M, so

$$\kappa(B) \;=\; \kappa(M) \;\geq\; 2d - a,$$

with equality if and only if M is a forest.

Now let $C_1, \ldots, C_p$ be the components of C. Contract each component of B and each C_r to a point; since P is connected, the resulting graph on $\kappa(B)+p$ vertices is connected, so it has at least $\kappa(B)+p-1$ edges, and by Lemma 2(c) every such edge joins some C_r to a component of B through a cell of $C_r \cap L_3$. By Lemma 2(b) all the L_2-neighbours of one cell of L_3 lie in a single component of B, so each cell of L_3 witnesses at most one edge. Hence $|C| \geq |C \cap L_3| \geq \kappa(B) + p - 1$, and

$$|P \setminus S| \;=\; a + b + |C| \;\geq\; a + b + (2d - a) + p - 1 \;=\; 2d - 1 + b + p.$$

So $|P| \geq 4d - 1$, with equality only when $b = 0$, $p = 0$ and M is a forest with $2d-1$ edges, that is, a spanning tree T of $\mathrm{CP}(d)$: then $P = P_T$.

Conversely each P_T is connected with $4d-1$ cells, and its only cavity is $\{0\}$: every cell of norm at least 3 lies outside P_T and walks to infinity by repeatedly increasing the magnitude of a nonzero coordinate; every cell of norm 2 outside P_T has a neighbour of norm 3; every cell of norm 1 is in P_T. Since P_T has exactly one cavity, a translation carrying P_T onto $P_{T'}$ carries cavity to cavity and is the identity, so $T = T'$.

3 A cavity of two or more cells

Lemma 3. *For a finite nonempty* $X \subset \mathbb{Z}^k$, $|N(X)| \geq 2k$*.*

Proof. If x is the lexicographically largest cell of X then $x + e_j \notin X$ for each j; if x' is the smallest, $x' - e_j \notin X$. These $2k$ cells are distinct: $x + e_i = x' - e_j$ would put $x' = x + e_i + e_j$ above x. □

Lemma 4. *Let* $W \subset \mathbb{Z}^d$ *be connected with* $|W| \geq 2$*. Then* $|N(W)| \geq 4d - 2$*, with equality only when* W *is a domino (two adjacent cells). If* $|W| \geq 3$ *and* $d \geq 3$ *then* $|N(W)| \geq 6d - 5$*; if* $|W| \geq 3$ *and* $d = 2$ *then* $|N(W)| \geq 7$*, with equality only for an L-tromino.*

Proof. Choose a coordinate, say x_1, on which W is not constant, with minimum α and maximum β. Let $T = W \cap \{x_1 = \beta\}$ and $B = W \cap \{x_1 = \alpha\}$, and regard each layer $\{x_1 = m\}$ as a copy of $\mathbb{Z}^{d-1}$. The following sets lie in $N(W)$ and in distinct layers: $T + e_1$; $B - e_1$; the neighbours of T inside its layer; the neighbours of B inside its layer; and, for each middle layer $\alpha < m < \beta$, the neighbours of $W \cap \{x_1 = m\}$ inside that layer (a connected W meets every middle layer). By Lemma 3 in dimension $d-1$,

$$|N(W)| \;\geq\; |T| + |B| + 2(d-1) + 2(d-1) + 2(d-1) \cdot \#\{\text{middle layers}\} \;\geq\; 4d - 2,$$

with equality only if $|T| = |B| = 1$ and there is no middle layer, so W is two cells in adjacent layers, hence a domino. If $|W| \geq 3$, either a middle layer exists and $|N(W)| \geq 2 + 6(d-1) = 6d-4$, or $|T| + |B| \geq 3$, say $|T| \geq 2$; for $d \geq 3$ the first part of this lemma in dimension $d-1$ gives at least $4(d-1)-2$ in-layer neighbours of T, so $|N(W)| \geq 3 + (4d-6) + (2d-2) = 6d-5$. For $d = 2$ the layers are lines, in-layer neighbours number 2 each, and $|N(W)| \geq 3+2+2 = 7$, with equality only when $|T| + |B| = 3$ and there is no middle layer: two adjacent columns holding a vertical domino and a cell adjacent to it, an L-tromino. $\square$

Now let P have a cavity W with $|W| \geq 2$; then $N(W) \subseteq P$.

Domino. Translate $W = \{0, e_1\}$. Then $N(W) = \{-e_1, 2e_1\} \cup \{\pm e_j,\ e_1 \pm e_j : j \geq 2\}$ has $4d-2$ cells in $2d$ components: $\{-e_1\}$, $\{2e_1\}$, and the $2(d-1)$ pairs $\{\pm e_j, e_1 \pm e_j\}$. A direct enumeration of the cells at distance 2 from W shows that every cell outside $W \cup N(W)$ is adjacent to at most two cells of $N(W)$: the cells $-e_1 \pm e_j$, $2e_1 \pm e_j$, $\pm e_j \pm e_k$, $e_1 \pm e_j \pm e_k$ touch two, and $\pm 2e_j$, $e_1 \pm 2e_j$, $-2e_1$, $3e_1$ touch one. So a single extra cell leaves at least $2d-1 \geq 3$ components, P needs at least two extra cells, and $|P| \geq 4d$.

Three or more cells, $d \geq 3$. By Lemma 4, $|P| \geq |N(W)| \geq 6d-5 \geq 4d+1$.

Three or more cells, $d = 2$. By Lemma 4, $|N(W)| \geq 7$, with equality only for an L-tromino, whose seven neighbours are not connected (the cell beyond the foot of the L is isolated among them), so $P \supsetneq N(W)$ and $|P| \geq 8$.

In every case a cavity of two or more cells costs at least $4d$ cells, one more than the bound of Section 2. Together with Section 2 this proves Theorem 1. $\square$

4 Up to symmetry

The symmetries of $\mathbb{Z}^d$ that fix the cavity form the hyperoctahedral group of order $2^d\, d!$, and they act on the sealers exactly as the symmetry group of the d-cube acts on its facets; $\mathrm{CP}(d)$ is the facet-adjacency graph of the d-cube. An edge unfolding of a convex polytope is determined by a spanning tree of its facet-adjacency graph, and its nets are counted up to the symmetry of the polytope. So the minimal hollow polycubes up to symmetry correspond to the nets of the d-dimensional hypercube: 1, 11, 261, 9694, ... (OEIS A091159). Counting the orbits of the spanning trees of $\mathrm{CP}(d)$ under the hyperoctahedral group directly gives 1, 11, 261 for $d = 2, 3, 4$.

5 Checks

Exhaustive search over all connected supersets of the sealers, and over every cavity shape that could fit in the budget, confirms the theorem directly for $d = 2, 3, 4$: no hollow polycube has fewer than 7, 11, 15 cells, and exactly 4, 384, 82,944 have that many, all of the form P_T. The same search with cells restricted to norm at most 3 reproduces 32,768,000 for $d = 5$. The values agree with A193130, the number of spanning trees of the cocktail-party graphs.

References

[1] OEIS Foundation, Sequence A193130, Numbers of spanning trees of the cocktail party graphs, `https://oeis.org/A193130`.

[2] OEIS Foundation, Sequence A091159, Number of distinct nets for the n-hypercube, `https://oeis.org/A091159`.

[3] S. J. Pursey, Sequence A396101, Number of fixed polycubes with n cells that have cavities, `https://oeis.org/A396101`, 2026.