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Bootstrap percolation on the hypercube

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Abstract. In the bootstrap percolation on the n-dimensional hypercube, in the initial position each of the 2^n sites is *occupied* with probability p and *empty* with probability $1 - p$, independently of the state of the other sites. Every occupied site remains occupied for ever, while an empty site becomes occupied if at least two of its neighbours are occupied. If at the end of the process every site is occupied, we say that the (initial) position *spans* the hypercube. We shall show that there are constants $c_1, c_2 > 0$ such that for $p(n) \geq \frac{c_1}{n^2}2^{-2\sqrt{n}}$ the probability of spanning tends to 1 as $n \to \infty$, while for $p(n) \leq \frac{c_2}{n^2}2^{-2\sqrt{n}}$ the probability tends to 0. Furthermore, we shall show that for each n the transition has a sharp threshold function.

1. Introduction

Cellular automata were introduced by von Neumann (see [11]) after a suggestion of Ulam [26]. A very popular cellular automaton is Conway's 'Game of Life' (see [18] and [9], Ch. 19); for an excellent description of a variety of cellular automata see Allouche, Courbage and Skordev [2].

In this paper we shall study a very special type of cellular automaton, bootstrap percolation on a finite graph G. As customary in percolation theory, we call the *vertices* of G *sites*; we shall also call G the *board* on which our process takes place. At every time step $t = 0, 1, \dots$, certain vertices (sites) of G are *occupied* (or *infected*) while the other vertices are *vacant* (or *healthy*). Putting it another way, at each time t, there is a function

$$\eta_t : V(G) \to \{0, 1\},$$

where $\eta_t(t) = 1$ iff the site x is occupied at time t. We call the function η_t the *configuration* at time t. Equivalently, the configuration at time t is the partition (V_0, V_1) of $V(G)$ into two sets, the set $V_0 = \eta_t^{-1}(0)$ of vacant or healthy sites and the set $V_1 = \eta_t^{-1}(1)$ of occupied or infected sites.

A *bootstrap percolation* on G with *(neighbourhood) parameter* r is a sequence $(\eta_t)_0^\infty$ of configurations such that the configuration at time t is determined by

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the configuration at time $t - 1$ according to the following rule. For a vertex x, $\eta_t(x) = 1$ iff either $\eta_{t-1}(x) = 1$ or x has at least r neighbours $y_1, \dots, y_r$ with $\eta_{t-1}(y_i) = 1, i = 1, \dots, r$. Note that the entire sequence $(\eta_t)_{t=0}^{\infty}$ is determined by η_0, the configuration at time 0. Clearly, $\eta_{t+1}(x) \geq \eta_t(x)$ for every t, so either there is a site x such that $\eta_t(x) = 0$ for every t or for every site x there is a time $t(x)$ such that $\eta_t(x) = 1$ for every $t \geq t(x)$. In the latter case we say that the starting configuration η_0 *spans* or *fills* the board G or simply that η *spanning* or *filling*.

A *random bootstrap percolation* on G with parameter r and *probability* p is a bootstrap percolation $\eta^p = (\eta_t)_0^{\infty}$ on G with parameter r in which for every site x we have $\eta_0(x) = 1$ with probability p, independently of the values of η_0 on $G \setminus \{x\}$. Ideally, we would like to determine the function $\phi_{G,r}(p) = \mathbb{P}(\eta^p \text{ spans})$. Unless G is very small or has a rather special structure, the determination of $\phi_{G,r}(r)$ appears to be out of reach. In view of this, we study spanning functions for sequences $(G_n)_1^{\infty}$ of graphs. We fix r, and look for *lower* and *upper threshold functions* $p_0(n)$ and $p_1(n)$, $0 < p_0(n) < p_1(n) < 1$, such that

$$\phi_{G_n,r}(p_0(n)) \to 0 \quad \text{as} \quad n \to \infty$$

and

$$\phi_{G_n,r}(p_1(n)) \to 1 \quad \text{as} \quad n \to \infty.$$

Needless to say, we would like to find a lower threshold that is as large as possible and an upper threshold that is as small as possible, so that if $p_0(n) < p(n) < p_1(n)$ and $p(n)$ is not close to either $p_0(n)$ or $p_1(n)$ then

$$0 < \liminf \phi_{G_n,r}(p(n)) \leq \limsup \phi_{G_n,r}(p(n)) < 1.$$

All this is rather vague, but in all the examples we shall encounter it will be clear whether a pair (p_0, p_1) is sufficient or not.

Ideally, we would like to find a pair (p_0, p_1) such that $\lim_{n\to\infty} p_1(n)/p_0(n) = 1$, i.e., $p_i(n) = (1+o(1))p(n)$ for $i = 0, 1$ and some function $p(n)$. In this case we call $(1 + o(1))p(n)$ the *threshold function*. Much of the time we cannot determine the threshold function (and, usually, we cannot even prove its existence), so we are happy to find a lower and upper threshold functions $p_0(n)$ and $p_1(n)$ with $\limsup_n p_1(n)/p_0(n) < \infty$; this is our aim in this paper as well. We are always interested in sequences (G_n) of "lattice-like" graphs, in fact, we shall restrict our attention to the case when G_n is the d-dimensional grid P_k^d or the d-dimensional torus C_k^d (both with k^d vertices), where $k = k(n)$ and $d = d(n)$ are functions of n. Here P_k is a path of length $k - 1$ and C_k is a cycle of length k. The case when G is the infinite graph P_∞^d is well studied in the literature.

Different versions of bootstrap percolation were investigated in a sequence of papers, including those of Schonmann [24], [25], Enter, Adler and Duarte [14], [15], Andjel [4], Mountford [21], [22], Gravner and McDonald [19], Cerf and Cirillo [12], and many others.

For bootstrap percolation with board $G = P_n^d$ and neighbourhood parameter 2, Aizenman and Lebowitz [3] proved the following fundamental result.

Theorem 1. *There are positive constants $c_1 < c_2$ such that for the bootstrap percolation on $G = P_n^d$ with neighbourhood parameter 2, the function $c_1/(\log n)^{d-1}$ is a lower threshold function and $c_2/(\log n)^{d-1}$ is an upper threshold function.*

Similar results were obtained by Balogh and Pete [7]. Recently Holroyd [20] proved that in two dimensions the threshold function is actually $(\pi^2/18+o(1))/\log n$. For higher dimensions Cerf and Manzo [13] have obtained good upper and lower threshold functions for the board $G = P_n^d$ and neighbourhood parameter $r \leq d$.

Theorem 2. *There are positive constants $c_1 < c_2$ such that for the bootstrap percolation on $G = P_n^d$ with neighbourhood parameter r, the function $c_1/(\log_{r-1} n)^{d-r+1}$ is a lower threshold function and $c_2/(\log_{r-1} n)^{d-r+1}$ is an upper threshold function, where the $\log_{r-1} n$ denotes the $r-1$ times iterated logarithm of n.*

These results concern bootstrap percolation on the board P_n^d, where n tends to infinity while d is fixed. In this paper we shall also study bootstrap percolation on P_n^d, but in a very different range of parameters: we keep n and the neighbourhood parameter fixed at 2 and let the dimension d tend to ∞. However, as in analogy with Theorems 1 and 2, we wish to let n tend to ∞ rather than d, we change the notation and consider bootstrap percolation on the hypercube $P_2^n = \{0, 1\}^n$ with neighbourhood parameter 2. Because of the high connectivity of the hypercube, as expected, the threshold functions tend to 0 as $n \to \infty$ fairly fast, much faster than in Theorems 1 and 2. Nevertheless, we can determine the order of the threshold functions.

Theorem 3. *For bootstrap percolation on $G = P_2^n = \{0, 1\}^n$ with neighbourhood parameter 2, the function $\frac{1}{150n^2}2^{-2\sqrt{n}}$ is a lower threshold function and $\frac{5000}{n^2}2^{-2\sqrt{n}}$ is an upper threshold function.*

Much of the paper will be devoted to the proof of Theorem 3.

The paper is organized as follows. In Section 2, we shall introduce our notation and prove some basic facts about bootstrap percolation. Our aim in Section 2 is to prove that if the initial configuration spans the hypercube then there is a so-called "internally spanned" subcube of appropriate dimension. In Section 3 we shall estimate the probability that one particular subcube of an appropriate dimension is internally spanned. Our estimate will be proved by induction on the dimension. In Section 4 we shall make use of this estimate to complete the proof of Theorem 3.

Finally, in Section 5, we shall make use of results of Friedgut and Kalai [17] to prove that the threshold function is sharp. Similar results about sharp threshold functions in bootstrap percolation appeared recently in [6].

2. Notation and basic observations

All the logarithms that we shall use will have base 2. In our calculations we shall use the following three basic inequalities valid for all integers $i \geq j > 0$:

$$i! > \sqrt{2\pi i}\left(\frac{i}{e}\right)^i > \left(\frac{i}{e}\right)^i, \tag{1}$$

$$\left(\frac{i}{j}\right)^j \leq \binom{i}{j} \leq \left(\frac{ei}{j}\right)^j, \tag{2}$$

and

$$\binom{i}{j} \le 2^i. \tag{3}$$

If $\ell \ge 5$ then

$$1 < 1.4 < \ell \log \ell - \ell \log(\ell - 1) < 1.65 < 2, \tag{4}$$

if $2 \le \ell$ then

$$2 \le \ell(\log(\ell + 2) - \log \ell), \tag{5}$$

if $4 \le k < k + 4 \le \ell$ then

$$4 \le k(\log \ell - \log k), \tag{6}$$

and if $m \ge 2$ then

$$m \log(m + 1) - m \log m \le 1.5. \tag{7}$$

From now on, as in Theorem 3, n will denote the dimension of the (large) hypercube that serves as our board. We shall write Q_ℓ for any of the $\binom{n}{\ell}2^{n-\ell}$ subcubes of dimension ℓ in Q_n. Similarly, we write $Q_{\le\ell}$ for a subcube of Q_n, with dimension at most ℓ. For $x = (x_i)_1^n \in \{0, 1, *\}^n$, let Q^x be the subcube $\{z = (z_i)_1^n \in \{0, 1\}^n : z_i = x_i \text{ if } x_i \ne *\}$. Clearly, $x \to Q^x$ gives a $1 - 1$ correspondence between $\{0, 1, *\}^n$ and the subcubes of Q_n; in particular we see that there are 3^n subcubes. This representation easily gives that the number of the ℓ-dimensional subcubes in an n-dimensional cube is $\binom{n}{\ell}2^{n-\ell}$. Let $d(0, 1) = 1$, $d(0, 0) = d(1, 1) = d(*, *) = d(0, *) = d(1, *) = 0$ be the distance of two coordinates. The distance of two subcubes Q^x, Q^y in Q_n is $d(Q^x, Q^y) = \sum_{i=1}^n d(x_i, y_i)$, where the vectors x, y represent the subcubes Q^x, Q^y. In the graph of the hypercube, the distance of the sets Q^x, Q^y is also $d(Q^x, Q^y)$. For a vertex $x \in Q_n$ the *neighbourhood* of x is $\Gamma(x) = \{y \in Q_n : d(x, y) = 1\}$.

Given a spanning process on Q with initial occupied set $S \subset Q$, a subcube $Q_\ell \subset Q$ is said to be *internally spanned (i.s.)* if the restriction of the process to Q_ℓ spans Q_ℓ, i.e., if the process on Q_ℓ with initial position $S \cap Q_\ell$ spans Q_ℓ.

Furthermore, we say that the sites $R = \{P_1, \dots, P_t\} \subset Q_\ell$ *span* Q_ℓ if the bootstrap percolation process on Q_ℓ with initial occupied set R spans Q_ℓ. We also say that two subcubes $Q_k \subset Q_\ell$ and $Q_m \subset Q_\ell$ *span* Q_ℓ if $Q_k \cup Q_m$ spans Q_ℓ. An ordered $(t + 1)$-tuple $\{P_0, \dots, P_t\} \subset Q_{2t}$ is said to span Q_{2t} *sequentially* if for all i, $0 \le i \le t$, the sites $\{P_0, \dots, P_{i-1}\}$ internally span a $2i$-dimensional cube Q_{2i}. A set $S \subset Q_n$ is 2-*closed* or simply *closed*, if every site $x \in Q_n - S$ has at most one neighbour in S. The 2-*closure* $\overline{S}$ of a set S is the intersection of all closed sets containing S. As the intersection of two closed sets is again closed, the 2-closure of a set is 2-closed.

It is easy to see that, for a set $S \subset Q_n$, the 2-closure $\overline{S}$ is the set of finally occupied vertices when S is the starting configuration in the 2-neighbour bootstrap percolation. Note also that every subcube of a hypercube is closed.

Lemma 4. *If the hypercube Q_n contains a subcube Q_ℓ with $S \subset Q_\ell$, then $\overline{S} \subset Q_\ell$.*

Proof. Let $S \subset Q_\ell \subset Q_n$, where Q_ℓ is a subcube of Q_n. Since the subcube Q_ℓ is a closed set containing S, it contains the intersection of all closed sets containing S, hence it contains the closure of S. □

For vectors $x, y \in \{0, 1, *\}^n$ set $x \vee y = z = (z_i)$ where $z_i = x_i$ if $x_i = y_i$ and $*$ otherwise. It follows from the definition of $\vee$ that $Q^x, Q^y \subset Q^{x \vee y}$.

Sometimes we write Q^x_ℓ to emphasize that Q^x is an ℓ-dimensional cube (and the vector x contains ℓ stars). Similarly, $Q^x_{\le \ell}$ used when we know only that the cube has dimension at most ℓ.

Lemma 5. *Let x and y be vectors with $z = x \vee y$ and $d(x, y) \le 2$. If $S \subset Q^x_\ell \cup Q^y_k$, then $\overline{S} \subset Q^z_{\le \ell+k+2}$.*

Proof. Note that $S \subset Q^z$ since $S \subset Q^x_\ell \cup Q^y_m \subset Q^z$, and because the subcube Q^z is closed, we have $\overline{S} \subset Q^z$. Since the number of $*$ in the coordinates of z is at most $\ell+k+d(x, y)$, the dimension of the subcube Q^z is at most $\ell+k+d(x, y) \le \ell+k+2$. □

Note that if $d(x, y) \ge 3$, then there is no "interaction" between the two cubes Q^x and Q^y, or to be precise, $Q^x_\ell \cup Q^y_m = \overline{Q^x_\ell \cup Q^y_m}$ is a closed set, and we have $\overline{S} \subset Q^x \cup Q^y$.

Lemma 6. *For vectors $x, y \in \{0, 1, *\}^n$ with $d(x, y) \le 2$, the closure of $Q^x \cup Q^y$ is $Q^{x \vee y}$.*

Proof. By Lemma 5 we have $\overline{Q^x \cup Q^y} \subset Q^{x \vee y}$, since the subcube $Q^{x \vee y}$ is closed and contains the cubes $Q^x \cup Q^y$. Hence, our task is to show that $Q^{x \vee y} \subset \overline{Q^x \cup Q^y}$.

Note that there is a vector x' such that $d(x', y) = 2$, $Q^{x'} \subset Q^x$, and $x' \vee y = x \vee y$. Therefore, replacing x by x', if necessary, we may assume that $d(x, y) = 2$.

Write k and ℓ for the dimensions of the subcubes Q^x and Q^y, respectively. By interchanging some of the digits 0 and 1, if necessary, we may assume that there is an integer j such that $0 \le j \le k \le n - \ell + j - 2$, and the vectors $x = (x_i)$ and $y = (y_i)$ are of the form shown in Table 1. Putting it another way, the first k coordinates of x are $*$, all others are 0. Altogether ℓ coordinates of y are $*$, namely the first j coordinates and from the $(k + 1)$st to the $(\ell + k - j)$th, furthermore, the last two coordinates of y are 1 and the others are 0.

Table 1. The vectors x, y, z_0, z_i and $z_{k+\ell-2j}$.

	1	·	j	$j+1$	·	$i+j$	$i+j+1$	·	k	$k+1$	·	$k+\ell-j$	$k+\ell-j+1$	·	$n-2$	$n-1$	n
$x=$	*	.	*	*	.	*	*	.	*	0	·	0	0	·	0	0	0
$y=$	*	.	*	0	·	0	0	·	0	*	·	*	0	·	0	1	1
$z_0=$	*	.	*	0	·	0	0	·	0	0	·	0	0	·	0	*	*
$z_i=$	*	.	*	*	.	*	0	·	0	0	·	0	0	·	0	*	*
$z_{k+\ell-2j}=$	*	.	*	*	.	*	*	.	*	*	.	*	0	·	0	*	*

For $i = 0, 1, \ldots, k+\ell-2j$, let z_i be the vector with the first $i+j$ and the last two coordinates $*$, all other coordinates 0 for all integers i, $0 \le i \le k+\ell-2j$, again, as shown in Table 1. Note that $z_{k+\ell-2j} = x \vee y$.

In the arguments below, the following easy observation will be used several times.

($*$) *Let A and B be subsets of a cube such that $A \subset B \subset \bar{A}$. If u has at least 2 neighbours in B then $u \in \bar{A}$.*

We shall prove by induction on i that $Q^{z_i} \subset \overline{Q^x \cup Q^y}$ for $0 \le i \le k+\ell-2j$. Since $z_{k+\ell-2j} = x \vee y$, this will complete our proof of the lemma. To start the induction, note that each site of $Q^{z_0} \setminus (Q^x \cup Q^y)$ has one neighbour in Q^x and another in Q^y; hence, by ($*$), we have $Q^{z_0} \subset \overline{Q^x \cup Q^y}$. Assume now that $0 \le i < k+\ell-2j$ and $Q^{z_i} \subset \overline{Q^x \cup Q^y}$; our aim is to prove that $Q^{z_{i+1}} \subset \overline{Q^x \cup Q^y}$.

For a vertex $u = (u_1, \ldots, u_n)$ write u^{00} for $(u_1, \ldots, u_{n-2}, 0, 0)$, u^{01} for $(u_1, \ldots, u_{n-2}, 0, 1)$, u^{10} for $(u_1, \ldots, u_{n-2}, 1, 0)$ and u^{11} for $(u_1, \ldots, u_{n-2}, 1, 1)$. Let $u \in Q^{z_{i+1}} \setminus (Q^{z_i} \cup Q^x \cup Q^y)$. Then u has a neighbour in Q^{z_i}; in order to be able to apply ($*$), we hope to find another neighbour in $\overline{Q^x \cup Q^y}$.

First we take care of the case when $i \le k-j-1$. Since $u \notin Q^x$, the last two digits of u cannot be both 0. If exactly one of the last two digits of u is 0 then it has a (second) neighbour in Q^x and, by ($*$), $u \in \overline{Q^x \cup Q^y}$. If the last two coordinates of u are 1 then its two neighbours u^{01}, u^{10} are in $\overline{Q^x \cup Q^y}$, and ($*$) can be applied again.

Now assume that $i \ge k-j$. First we prove our claim when the last two digits of u are 1. Let r be the minimal value in the range $0 \le r \le k-j$ such that $u_{j+r+1} = \cdots = u_k = 0$. We apply induction on r to prove that $u \in \overline{Q^x \cup Q^y}$. To start the induction, note that if $r = 0$ then $u \in Q^y \subset \overline{Q^x \cup Q^y}$. Let us turn to the induction step. Thus $1 \le r \le k-j$, $u_{j+r} = 1$ and $u_{j+r+1} = \ldots = u_k = 0$. As $u \notin Q^{z_i}$, we have $u_{i+j+1} = 1$, and so switching u_{i+j+1} to 0 we obtain a neighbour of u in Q^{z_i}. Since $r \le k-j \le i$, we see that $j+r \ne i+j+1$. Therefore, if we change the $(j+r)$th digit of u to 0 then by the induction hypothesis we get a vertex in $\overline{Q^x \cup Q^y}$. Consequently, ($*$) implies that $u \in \overline{Q^x \cup Q^y}$. This completes our proof in the case when the last two digits of u are 1.

If exactly one of the last two digits of u is 0 then, by what we have just proved, we see that $u^{11} \in \overline{Q^x \cup Q^y}$, and so ($*$) can be applied.

If both of the last two digits of u are 0 then, as we have just seen, its two neighbours u^{01}, u^{10} are in $\overline{Q^x \cup Q^y}$, and so ($*$) can be applied again. □

Lemma 7. *(i) A subset of a hypercube is closed iff it is a union of a set of subcubes, any two of which are at distance at least 3 from each other.*
(ii) If a subcube Q_ℓ is the closure of a set $S \subset Q_\ell$ then $|S| \ge \ell/2 + 1$.

Proof. (i) Clearly the union of a set of cubes, with any two of them at distance at least 3, is closed. To prove the converse assertion, we shall study how the closure of a set can be obtained.

Let us recall how two cubes can span a third one. We say that a subcube Q_ℓ^z is spanned by internally spanned subcubes Q_k^x and Q_m^y if $d(x, y) \le 2$ and $z = x \vee y$. Note that, by Lemma 5, we have $\ell \le k+m+2$.

The closure of a set S can also be defined as follows. Write S as a union of 0-dimensional cubes (sites):

$$S = Q^{(1)} \cup \cdots \cup Q^{(s)}. \tag{8}$$

Call this union a *cube partition* of S. If $d(Q^{(i)}, Q^{(j)}) \leq 2$ for some pair (i, j), $1 \leq i < j \leq m$, pick such a pair, and replace $Q^{(i)} \cup Q^{(j)}$ in the union (8) by $Q^{(i,j)} = Q^{(i)} \vee Q^{(j)}$; denote by $S^{(1)}$ the new union. (Note that, in general, $S^{(1)}$ is not unique: it depends on our choice of the pair (i, j).) Furthermore, the cubes occurring in the representation of $S^{(1)}$

$$\begin{aligned} S^{(1)} = {} & Q^{(1)} \cup \cdots \cup Q^{(i-1)} \cup Q^{(i+1)} \cup \cdots \cup Q^{(j-1)} \cup Q^{(j+1)} \\ & \cup \cdots \cup Q^{(s)} \cup Q^{(i,j)} \end{aligned} \tag{9}$$

are not necessary disjoint. It might even be the case that a new cube contains some of the old ones, and in that case, we simply omit the smaller cube as an unnecessary member of the union. If we keep repeating the replacement of two subcubes with a new one until each pair of the cubes has distance at least 3 then, in the end, the union of the subcubes gives the closure of S. Note that in (9) each site was in S so, by Lemma 6, every subcube appearing during the replacements will be a subset of $\overline{S}$. This union of the subcubes is the closure of S since it is closed and, according to Lemma 6, during the extension all new sites of the union are in the closure. This completes the proof of part (i).

(ii) Note that by replacing two subcubes of dimensions n_1, n_2 with a new cube during the process above, the new cube will have dimension at most $n_1 + n_2 + 2$.

Consider S as a union of $|S|$ 0-dimensional cubes in form (8). Then the sum of the dimensions of the "building blocks" in (8) is 0. At each replacement of two subcubes with one, this sum increases by at most 2, and there are at most $|S| - 1$ steps, hence, if $\overline{S}$ is an ℓ-dimensional cube, then $\ell \leq 2|S| - 2$. □

Lemma 8. *If a starting configuration spans the hypercube Q_n then for each $k \leq n$ there is an integer ℓ such that $k \leq \ell \leq 2k$ and the hypercube Q_n contains an internally spanned cube of dimension ℓ.*

Proof. Let S be a spanning set of occupied sites of the hypercube Q_n at time 0. Consider S in the form (8), i.e., as a union of 0-dimensional subcubes (sites). As in the proof of Lemma 7, let us "replace two subcubes with one subcube" as long as we can. Since S is a spanning set, when we stop the union consists of only one cube: the hypercube Q_n. As we noted earlier, in each step we have replaced two subcubes of dimension n_1 and n_2 by a subcube of dimension at most $n_1 + n_2 + 2$. Hence, in each step the maximal dimension of a subcube in the union increases from some integer m to at most $2m + 2$. Consequently, if before the step this maximum is at most $k - 1$, after the step it is at most $2(k - 1) + 2 = 2k$. □

Repeated applications of Lemma 8 give us a fairly precise description of the process starting from a spanning set; for sake of completeness we give all the details.

Theorem 9. *Let $S \subset Q_n$ be a spanning set of occupied sites at time* 0. *Then there is a nested sequence $Q_0 = Q_{i_1}^{x_1} \subset Q_{i_2}^{x_2} \subset \cdots \subset Q_{i_t}^{x_t} = Q_n$, of internally spanned subcubes (with respect to S), where $2i_j + 2 \geq i_{j+1}$ for all j, $0 \leq j \leq t-1$. Furthermore, for $j \geq 1$ each subcube $Q_{i_j}^{x_j}$ is spanned by two internally spanned cubes, namely by $Q_{i_{j-1}}^{x_{j-1}}$ and a subcube $Q_{m_{j-1}}$ of dimension $m_{j-1} \leq i_{j-1}$ which is not member of the sequence.*

Proof. Write S as the trivial union of the 0-dimensional subcubes formed by the sites in S. By assumption, $\overline{S} = Q_n$, so starting with the trivial union and successively replacing pairs of subcubes by the subcube they span internally, eventually we arrive at Q_n. If in this process Q_h replaces two subcubes Q_i and Q_j then $\max\{i, j\} \geq (h-2)/2$, i.e., at least one of the cubes Q_i, Q_j has dimension at least $(h-2)/2$ since $h \leq i + j + 2$. By considering the last step in the procedure differently, an internally spanned subcube H of dimension $h > 0$ contains an internally spanned proper subcube H^* of dimension at least $(h-2)/2$. Define a nested sequence $R_1 \supset R_2 \supset \cdots \supset R_t$ of internally spanned subcubes as follows. Set $R_1 = Q_n$. Having defined R_i, if R_i has dimension 0, set $i = t$ and stop the sequence; otherwise set $R_{i+1} = R_i^*$. The sequence $R_t \subset R_{t-1} \subset \cdots \subset R_1 = Q_n$ has the required properties. □

We call a longest nested sequence of internally spanned cubes as in Theorem 9 a *building sequence* of the hypercube.

3. Estimates for $P(\ell, p)$

Let us turn to the task of estimating various probabilities. Throughout the section we write p in the form $p = 2^{-s}$, and shall assume that s is large. Let $P(\ell, p)$ be the probability that a fixed ℓ-dimensional subcube is internally spanned if the initial density is p. Our aim in this section is to estimate $P(\ell, p)$ for $\ell < s$. Let us start with the small values of ℓ.

Lemma 10. *If s is large enough then*

$$P(0, p) = 2^{-s}, \quad P(1, p) = 2^{-2s},$$
$$2^{-2s} \leq P(2, p) = 2^{1-2s} - 2^{-4s} \leq 2^{1-2s},$$
$$2^{5-3s}(1 - 2^{-s})^5 \leq P(3, p) \leq 2^{5-3s},$$
$$3^2 \cdot 2^{4-3s}(1 - 2^{-s})^{13} \leq P(4, p) \leq 3^2 \cdot 2^{4-3s} + \binom{16}{4} 2^{-4s} < 2^{8-3s}. \quad (10)$$

Proof. The statements are trivial for $P(0, p)$ and $P(1, p)$. To span a Q_2, one of the pairs of vertices sitting in opposite corners needs to be occupied, implying the bounds for $P(2, p)$.

Let us turn to the bounds on $P(3, p)$. For the lower bound we shall count the spanning triplets in a Q_3. Observe that the spanning triplets are exactly those 3-sets that cannot be covered by a Q_2, hence the number of spanning triplets is

$$\binom{8}{3} - 6\binom{4}{3} = 32 = 2^5.$$

Indeed, there are $\binom{8}{3}$ triplets, the number of Q_2 is 6, and each Q_2 contains three points in $\binom{4}{3}$ different ways.

For the upper bound on $P(3, p)$ observe that every spanning configuration contains a spanning triplet.

Finally, we turn to $P(4, p)$. To establish the claimed lower bound it suffices to show that there are $3^2 \cdot 2^4 = 144$ spanning triplets. A spanning triplet in a Q_4 has the following structure: two vertices span a Q_2, and the third one is located in another Q_2 at distance two from the first cube. The number of Q_2 in a Q_4 is $\binom{4}{2}2^2 = 24$, and two spanning vertices in a Q_2 can be chosen 2 ways. The third vertex can be chosen in four ways, but two of them are counted twice, namely those in which the third vertex spans a Q_2 with one of the other two vertices.

To summarize, the number of spanning triplets is $24 * 2 * (2 + (1/2)2) = 144$. For the upper bound we note that if a spanning configuration does not contain a spanning triplet then it has at least 4 occupied sites. □

For $\ell > 4$ we shall use the following result concerning $P(\ell, p)$.

Theorem 11. *If s is large enough and $\ell < s$ then for $p = 2^{-s}$ we have*

$$2^{\ell^2/4-(\ell+3)s/2+\ell\log\ell-2\ell} \le P(\ell, p) \le 2^{\ell^2/4-(\ell+2)s/2+\ell\log\ell}. \qquad (11)$$

Proof. To give a lower bound for $P(\ell, p)$, first we consider the case when $\ell = 2t$ is even. Let $f(\ell)$ be the number of ordered $(t+1)$-tuples $(P_0, \dots, P_t)$ of sites of Q_ℓ such that for $1 \le i \le t$ the point P_i is at distance 2 from the subcube spanned by $\{P_0, \dots, P_{i-1}\}$. Clearly, every set $\{P_0, \dots, P_t\}$ internally spans Q_ℓ; in fact, these are precisely the $(t+1)$-sets of sites that span "sequentially". In a spanning sequence $\{P_0, \dots, P_t\}$ we have 2^ℓ choices for P_0 and, having chosen $\{P_0, \dots, P_i\}$, the site P_{i+1} has to be at distance 2 from the cube Q_{2i} spanned by $\{P_0, \dots, P_i\}$. Hence, we have $\binom{\ell-2i}{2}2^{2i}$ choices for P_{i+1}. Consequently,

$$f(\ell) = 2^\ell \prod_{i=0}^{t-1} \binom{\ell-2i}{2} 2^{2i} = \ell! 2^{\ell^2/4} \qquad (12)$$

and so there are at least

$$f(\ell)/(t+1)! = \ell! 2^{\ell^2/4}/(t+1)! \qquad (13)$$

$(t+1)$-sets of points $\{P_0, \dots, P_t\}$ that span Q_ℓ.

We shall count the number of sequentially spanning $(t+1)$-tuples, whose order is unique up to the interchange of the first two sites: in this way we can save a factor $2/(t+1)!$ in (13). (Trivially, if $(P_0, P_1, P_2, \dots P_t)$ is a sequentially spanning $(t+1)$-tuple, then so is $(P_1, P_0, P_2, \dots P_t)$, so we cannot hope to do better.)

In a spanning $(t+1)$-tuple $(P_0, P_1, \dots P_t)$, the order of the sites is unique (up to the interchange of the first two sites), if (P_0, P_1) is the unique pair of sites at distance 2 from each other, and for any $1 \le i < t$, the site P_{i+1} is at distance at least 3 from the subcube spanned by $P_0, P_1, \dots, P_{i-1}$. This ensures a unique start and at each step a unique continuation.

Now, there are $2^{\ell-1}\binom{\ell}{2}$ pairs (P_0, P_1) at distance 2 from each other. Also, for a given sequence $(P_0, P_1, \dots P_i)$, the site P_{i+1} has to be at distance 2 from the cube Q_{2i} spanned by them, and at least at distance 3 from the subcube Q_{2i-2} spanned by $(P_0, P_1, \dots P_{i-1})$ and from P_i. Hence, there are $\binom{\ell-2i}{2}(2^{2i} - 2^{2i-2} - 1)$ ways of choosing P_{i+1}. This implies that the number of such $(t+1)$-tuples is

$$2^{\ell-1}\binom{\ell}{2}\prod_{i=1}^{t-1}\binom{\ell-2i}{2}(2^{2i} - 2^{2i-2} - 1) \geq 22 \cdot 2^{\ell/2-1} \cdot \ell! \cdot \prod_{i=3}^{t-1} 2^{2i-1/2}$$
$$= 22 \cdot \ell! \cdot 2^{\ell^2/4-\ell/4-5.5} > 2^{\ell^2/4+\ell\log\ell-\ell/4-\ell\log e+1.4} \geq 2^{\ell^2/4+\ell\log\ell-2\ell+3.2}, \tag{14}$$

where we made use of the facts that for $i \geq 3$ we have $2^{2i} - 2^{2i-2} - 1 \geq 2^{2i-1/2}$, that $\log 22 > 4.4$, that (1) for $\ell \geq 6$ implies $\ell! > 2^{2.5+\ell\log\ell-\ell\log e}$, and that for $\ell \geq 6$ we have

$$-\ell/4 - \ell\log e \geq -2\ell + 1.8. \tag{15}$$

Hence, if ℓ is even, then

$$P(\ell, p) \geq 2^{\ell^2/4+\ell\log\ell-2\ell+3.2-(\ell+2)s/2}(1-p)^{2^\ell} \geq 2^{\ell^2/4-(\ell+2)s/2+\ell\log\ell-2\ell}, \tag{16}$$

where the right hand side bounds the sum over all spanning $(t+1)$-sets of the probabilities of the event that exactly this $(t+1)$-set was originally occupied. (Recall that $t+1 = (\ell+2)/2$.) In (16), the factor $(1-p)^{2^\ell}$ stands for the probability of the empty sites, and we made use of the fact that for $\ell \leq -\log p > 1$ we have

$$(1-p)^{2^\ell} \geq 2^{-2}. \tag{17}$$

Now consider the case when $\ell \geq 7$ is odd. We claim that the following recursive inequality holds, as an ℓ-cube is internally spanned if it contains an internally spanned $(\ell-1)$-cube and exactly one additional occupied site in the "other half" of the hypercube:

$$P(\ell, p) \geq P(\ell-1, p)p(1-p)^{2^{\ell-1}}2^{\ell-1}. \tag{18}$$

Using the first inequality of (16) with $\ell - 1 \geq 6$, from the inequalities (17) and (4) we obtain

$$\begin{aligned} P(\ell, p) &\geq 2^{(\ell-1)^2/4-(\ell+1)s/2+(\ell-1)\log(\ell-1)-2(\ell-1)+3.2} \\ &\quad \times (1-p)^{2^{\ell-1}}2^{-s}(1-p)^{2^{\ell-1}}2^{\ell-1} \\ &\geq 2^{\ell^2/4-(\ell+3)s/2+\ell\log\ell-2\ell}2^{\ell/2-\log(\ell-1)+0.8}. \end{aligned} \tag{19}$$

For $\ell \geq 7$ we have $\ell/2 - \log(\ell-1) + 0.8 > 1$, proving the lower bound in our theorem.

Finally, for $\ell = 5$, we apply inequality (18) and the lower bound for $P(4, p)$ in Lemma 10 to obtain

$$P(5,p) \ge P(4,p)p(1-p)^{2^4}2^4 \ge 2^{5^2/4-4s+5\log 5-2\cdot 5}3^2 \cdot 2^{4-2+4-6.25-5\log 5+10} > 2^{5^2/4-4s+5\log 5-2\cdot 5}. \tag{20}$$

This completes our proof of the lower bound in Theorem 11.

Let us turn to the upper bound on $P(\ell, p)$. First we give a rather crude upper bound, and then we shall refine it. Set $t = \lceil \ell/2 \rceil$. By Lemma 7, if a subcube Q_ℓ is internally spanned, initially it contains at least $t+1$ occupied sites. Appealing to (2), this implies that

$$\begin{aligned} P(\ell,p) &\le \mathbb{P}(\text{number of occupied sites in } Q_\ell \ge t+1) \\ &\le \mathbb{E}(\text{number of occupied } (t+1)\text{-tuples in } Q_\ell) \\ &\le \binom{2^\ell}{t+1} p^{t+1} \le \left(\frac{e2^\ell p}{t+1}\right)^{t+1} = \left(\frac{e2^{\ell-s}}{t+1}\right)^{t+1} \\ &\le \left(\frac{2e}{\ell}\right)^{(\ell+1)/2} 2^{\ell^2/2-(\ell+2)s/2+3\ell/2}. \end{aligned} \tag{21}$$

If $\ell = \Omega(s)$, then there is a large gap between our upper and lower bounds for $P(\ell, p)$.

Our next aim is to improve the upper bound (21) on $P(\ell, p)$ to

$$P(\ell,p) \le R(\ell,p) = 2^{\ell^2/4-(\ell+2)s/2+\ell\log\ell}, \tag{22}$$

where the equality is the definition of $R(\ell, p)$. We shall prove (22) by induction on ℓ. For $\ell = 0, 1, 2, 3$ and 4 the inequality clearly holds by Lemma 10. Now let us turn to the induction step: let us assume that $\ell \ge 5$ and (22) holds for smaller values of ℓ. By Theorem 9, if a subcube Q_ℓ is internally spanned, then it contains internally spanned subcubes Q_k and Q_m (with $k \ge m$) such that together they span Q_ℓ. Let (Q_k, Q_m) be such a pair with k chosen as large as possible; having this k, choose m as small as possible. By Lemma 8, we have $k \ge \ell/2 - 1$.

We shall consider five (main) cases, according to the values of the pair (k, m) and the positions of the two subcubes in Q_ℓ. Denote by $P^1(\ell, p)$ the probability that $k = \ell - 1$ and $m = 0$; similarly let $P^2(\ell, p)$ be the probability that $k = \ell - 2$ and $m = 0$. For $d = 0$, 1, and 2, and $m \ge 1$, let $P^d_{k,m}(\ell, p)$ be the probability that $d(Q_k, Q_m) = d$. In each case we give upper bounds for these probabilities in terms of $R(\ell, p)$. Our goal is to prove that

$$P(\ell,p) \le P^1(\ell,p) + P^2(\ell,p) + \sum_{k\ge m\ge 1}\sum_{i=0}^{2} P^i_{k,m}(\ell,p) \le R(\ell,p). \tag{23}$$

First we make some observations for $m \ge 1$. If $m \ge 1$ (Cases 3, 4 and 5) then $k \le \ell - 4$. Indeed, if $k = \ell - 1$ then Q_k together with any occupied vertex outside of Q_k (which is a Q_0) spans Q_ℓ. If $k = \ell - 2$ then, as k was chosen maximal, there is no occupied vertex in the neighbourhood of Q_k, and any occupied vertex at distance 2 from Q_k spans Q_ℓ; therefore m could have been chosen as 0. Thus this case does not arise. In case $k = \ell - 3$, if there is an occupied vertex within distance 2 of Q_k then k can be chosen larger. The set of all sites at distance at least 3 from Q_k is a subcube; this subcube is a closed set hence together with Q_k cannot span Q_ℓ. Consequently, $k \le \ell - 4$ if $m \ge 2$.

Before we start to analyze our five cases, let us summarize what we have learned about the restrictions on k, ℓ and m. Either $m = 0$ and k is either $\ell - 1$ or $\ell - 2$, or else

$$k < \ell \le k + m + 2 \quad \text{and} \quad 2 \le m \le k \le \ell - 4. \tag{24}$$

Case 1: $m = 0, \quad k = \ell - 1, \quad d = 1.$
Since there are 2ℓ ways of choosing a subcube $Q_{\ell-1}$ in a cube Q_ℓ, and $2^{\ell-1}$ ways of choosing a subcube Q_0 disjoint from $Q_{\ell-1}$, we have by the induction hypothesis (i.e., $P(\ell-1, p) \le R(\ell-1, p)$) and by (7) that

$$\begin{aligned} P^1(\ell, p) &\le P(\ell-1, p) \cdot P(0, p) \cdot 2\ell \cdot 2^{\ell-1} \le R(\ell-1, p) \cdot 2^{\ell-s} \cdot \ell \\ &\le R(\ell, p) \cdot 2^{(\ell-s)/2 + (\ell-1)\cdot(\log(\ell-1) - \log \ell) + 1/4} \\ &\le R(\ell, p) \cdot 2^{-1.15} \le 0.46 \cdot R(\ell, p). \end{aligned} \tag{25}$$

The penultimate inequality in (25) is clear for $\ell < s - 4$. Otherwise, if $s \ge 104$ so that $\ell \ge s - 3 > 100$ then, since $(1 - 1/\ell)^{\ell-1}$ is monotone decreasing and $(1 - 1/101)^{100} < 0.37$, we have

$$(\ell - 1)(\log(\ell-1) - \log \ell) = \log(1 - 1/\ell)^{\ell-1} \le -1.4.$$

Since $\ell - s \le 0$, this implies the required inequality.

Case 2: $m = 0, \quad k = \ell - 2, \quad d = 2.$
In this case the subcubes Q_k and Q_m are at distance 2 from each other. There are $\binom{\ell}{2} 2^2 \le 2\ell^2$ ways to choose a subcube $Q_{\ell-2}$ in Q_ℓ, and $2^{\ell-2}$ ways to choose a subcube Q_0 at distance 2 from a given $Q_{\ell-2}$, so by the induction hypothesis $P(\ell-2, p) \le R(\ell-2, p)$, we obtain

$$\begin{aligned} P^2(\ell, p) &\le P(\ell-2, p) \cdot P(0, p) \cdot 2\ell^2 \cdot 2^{\ell-2} \le R(\ell-2, p) \cdot \ell^2 \cdot 2^{\ell-s-1} \\ &= R(\ell, p) \cdot 2^{(\ell-2)[\log(\ell-2) - \log \ell]} = R(\ell, p) \cdot \left(1 - \frac{2}{\ell}\right)^{\ell-2} \le 0.216 \cdot R(\ell, p), \end{aligned} \tag{26}$$

where we used that for $\ell \ge 5$

$$\left(1 - \frac{2}{\ell}\right)^{\ell-2} \le 0.216.$$

Case 3: $m \ge 2, \quad d = 2.$
Note that we have $k + m + 2 \ge \ell$. Our aim is to prove that

$$R(\ell, p)^{-1} \sum_{2 \le m \le k \le \ell-4} P^2_{k,m}(\ell, p) < \frac{1}{8}. \tag{27}$$

For a fixed k, there are $\binom{\ell}{k} 2^{\ell-k}$ ways to choose a subcube Q_k in a cube Q_ℓ. Given a subcube Q_k in a cube Q_ℓ, there are $2^{\ell-m-2}\binom{\ell-k}{2}\binom{k}{\ell-m-2}$ subcubes Q_m at distance 2 from Q_k so that they internally span Q_ℓ. Hence in this case, using the induction hypothesis $P(i, p) \le R(i, p)$ for every $i < \ell$, we have

$$\begin{aligned}P^2_{k,m}(\ell, p) &\le P(k, p)P(m, p)\binom{\ell}{k}2^{\ell-k}\binom{\ell-k}{2}\binom{k}{\ell-m-2}2^{\ell-m-2}\\ &\le R(k, p)R(m, p)\binom{\ell}{k}\binom{\ell-k}{2}\binom{k}{\ell-m-2}2^{2\ell-k-m-2} = h(\ell, k, m),\end{aligned} \tag{28}$$

where the function $h(\ell, k, m)$ on the right-hand side stands for

$$2^{(k^2+m^2)/4-(k+m+4)s/2+k\log k+m\log m+2\ell-k-m-2}\binom{\ell}{k}\binom{\ell-k}{2}\binom{k}{\ell-m-2}.$$

First we shall prove that for $m \le s - 6\log s$, $h(\ell, k, m)$ is a decreasing function of m. For this we can use that for $m \le k \le \ell - 4 < s$ the following holds:

$$\frac{h(\ell, k, m+1)}{h(\ell, k, m)} \le 2^{m/2+3/4-s/2+\log(m+1)}\,\frac{\ell-m-2}{k+m-\ell+3}, \tag{29}$$

where we used (7). The right-hand side of (29) is clearly less than $1/s$ if $m \le s - 6\log s$, hence in that case for $s > 11$

$$\begin{aligned}\sum_{m,\ 2\le m\le k,\ \ m\le s-6\log s} h(\ell, k, m) &< \frac{1}{1-s}\cdot h(\ell, k, \ell-k-2)\\ &< 1.1\cdot h(\ell, k, \ell-k-2).\end{aligned} \tag{30}$$

Now, first we give a bound on $h(\ell, k, m)$ when $m \ge s - 6\log s$. Note that this part of the calculation is robust enough to be applied in Cases 4 and 5, without any significant change.:

$$\begin{aligned}h(\ell, k, m) &\le 2^{\ell^2/2-(2s-12\log s+4)s/2+2s\log s+2s+3s} \le 2^{-s^2/2+o(s^2)}\\ &\le R(\ell, p)\cdot 2^{-s^2/4+o(s^2)}.\end{aligned} \tag{31}$$

When $m \le s - 6\log s$, we have to be more careful. By (30) it is sufficient estimate $h(\ell, k, \ell-k-2)$. Note that

$$\begin{aligned}&h(\ell, k, \ell-k-2)\\ &\quad= 2^{k^2/4+(\ell-k-2)^2/4-(\ell+2)s/2+k\log k+(\ell-k-2)\log(\ell-k-2)+\ell}\cdot\binom{\ell}{k}\binom{\ell-k}{2}\binom{k}{k}\\ &\quad= R(\ell, p)2^{-\ell\log\ell+k(k+2-\ell)/2+k\log k+(\ell-k-2)\log(\ell-k-2)+1}\binom{\ell}{\ell-k}\binom{\ell-k}{2}\\ &\quad= R(\ell, p)S(\ell, k),\end{aligned} \tag{32}$$

where the last equality defines the factor $S(\ell, k)$. Our next task is to bound this factor $S(\ell, k)$. For small values of ℓ we compute $S(\ell, k)$ explicitly.
If $\ell = 6$ then $k = 2$ and $S(6, 2) = 15\cdot 6\cdot 6^{-6}\cdot 2^{-2+2+2+1} < 0.02$.
If $\ell = 7$ then $k = 3$ and $7^{-7}\cdot 2^{-3}\cdot 3^3\cdot 2^3\cdot 35\cdot 6 < 0.007$.

If $\ell = 8$ then there are two possible values for k, namely 3 and 4, and $S(8,3) = 2^{-24-9/2+3\log 3+3\log 3+1} \cdot 560 < 0.003$ and $S(8,4) = 2^{-17} \cdot 420 < 0.005$.
Finally, if $\ell = 9$ then there are again two possible values for k, namely 4 and 5, and $S(9,4) = 3^{-15} \cdot 2^3 \cdot 1260 < 0.001$ and $S(9,5) = 9^{-9} \cdot 2^{-2} \cdot 5^5 \cdot 756 < 0.002$.

In conjunction with inequalities (28) and (30), these calculations imply (27) for $s > 100$. Hence, from now on we may and shall assume that $\ell \geq 10$ and so $4 \leq k < k+4 \leq \ell$.

Using

$$\log\left(\binom{\ell}{\ell-k}\right) \leq (\ell-k)\cdot(\log\ell + \log e - \log(\ell-k)), \tag{33}$$

(5), (6), $\binom{\ell-k}{2} \leq 2^{2\log(\ell-k)-1}$ and $(k-2\log e)(k-\ell) \leq -2k+4\log e$ we find that

$$\begin{aligned} S(\ell,k) &\leq 2^{k(\log k-\log\ell)+(\ell-k-2)(\log(\ell-k-2)-\log(\ell-k))+(k-2\log e)(k-\ell)/2+k} \\ &< 2^{-6+k+(k-2\log e)(k-\ell)/2} < 2^{-k-0.2}. \end{aligned} \tag{34}$$

Now (27) follows from (28), (30), (31), (32) and (34):

$$\begin{aligned} &R(\ell,p)^{-1} \sum_{2\leq m\leq k\leq \ell-4} P^2_{k,m}(\ell,p) \\ &= R(\ell,p)^{-1}\Big(\sum_{s-6\log s\leq m\leq k\leq\ell-4} P^2_{k,m}(\ell,p) \\ &\quad + \sum_{2\leq m\leq k\leq\ell-4,\ m<s-6\log s} P^2_{k,m}(\ell,p)\Big) \\ &\leq 2^{-s^2/4+o(s^2)} + 1.1\cdot \sum_{4\leq k\leq\ell-4} h(\ell,k,\ell-k-2) \\ &\leq o(1) + 1.1\cdot 2^{-0.2}\sum_{4\leq k} 2^{-k} < \frac{1}{8}. \end{aligned} \tag{35}$$

Case 4: $m \geq 2$, $d(Q_k, Q_m) = 1$.
We shall apply the same method as in Case 3. Now we have $k+m+1 \geq \ell$, together which with $k \leq \ell-4$, implies $3 \leq m$. There are $\binom{\ell}{k}2^{\ell-k}$ ways to choose a subcube Q_k in a cube Q_ℓ. Given a subcube Q_k of a cube Q_ℓ, there are $2^{\ell-m-1}(\ell-k)\binom{k}{\ell-m-1}$ subcubes Q_m at distance 1 from Q_k (so that these subcubes internally span Q_ℓ). Hence, in this case (as in Case 3) we have

$$\begin{aligned} P^1_{k,m}(\ell,p) &\leq P(k,p)P(m,p)\binom{\ell}{k}2^{\ell-k}(\ell-k)\binom{k}{\ell-m-1}2^{\ell-m-1} \\ &\leq R(k,p)R(m,p)\binom{\ell}{k}(\ell-k)\binom{k}{\ell-m-1}2^{2\ell-k-m-1} = h_1(\ell,k,m), \end{aligned} \tag{36}$$

where $h_1(\ell,k,m)$ stands for

$$2^{(k^2+m^2)/4-(k+m+4)s/2+k\log k+m\log m+2\ell-k-m-1}\binom{\ell}{\ell-k}(\ell-k)\binom{k}{\ell-m-1}. \tag{37}$$

We claim that $h_1(\ell, k, m)$ is a decreasing function of m for $m \le s - 6\log s$. Indeed, using (7),

$$\frac{h_1(\ell, k, m+1)}{h_1(\ell, k, m)} \le 2^{m/2+3/4-s/2+\log(m+1)} \frac{\ell - m - 1}{k + m - \ell + 2}. \tag{38}$$

Clearly, for $m \le s - 6\log s$ the right hand side of (38) is less than $1/s$, and so if $s > 11$ then

$$\begin{aligned}\sum_{m,\ 3\le m\le k,\ \ m\le s-6\log s} h_1(\ell, k, m) &< \frac{1}{1-s} \cdot h_1(\ell, k, \ell - k - 1)\\ &< 1.1 \cdot h_1(\ell, k, \ell - k - 1).\end{aligned} \tag{39}$$

Note that

$$\frac{4}{\ell^2} < \frac{h_1(\ell, k, m)}{h(\ell, k, m)} = 2 \cdot \frac{(\ell - k)\cdot \binom{k}{\ell-m-1}}{\binom{\ell-k}{2}\binom{k}{\ell-m-2}} = 2^2 \cdot \frac{k - \ell + m + 2}{(\ell - k - 1)\cdot(\ell - m - 1)} < 4\ell; \tag{40}$$

hence, for $m \ge s - 6\log s$, by (31) we have

$$h_1(\ell, k, m) \le 2^{-s^2/2+o(s^2)} \le R(\ell, p)\cdot 2^{-s^2/4+o(s^2)}. \tag{41}$$

Because of (39), it is sufficient to bound $h_1(\ell, k, \ell - k - 1)$ when $m \le s - 6\log s$:

$$\begin{aligned}&h_1(\ell, k, \ell - k - 1)\\ &\le 2^{k^2/4+(\ell-k-1)^2/4-(\ell+3)s/2+k\log k+(\ell-k-1)\log(\ell-k-1)+\ell}\binom{\ell}{\ell-k}(\ell-k)\binom{k}{k}\\ &\le R(\ell, p)\cdot 2^{(k+1-\ell)k/2+(\ell-s)/2+(\ell-k)\log e+k(\log k-\log\ell)+(\ell-k-1)(\log(\ell-k-1)-\log(\ell-k))+1/4}\\ &< R(\ell, p)\cdot 2^{(k+1-\ell)k/2+(\ell-s)/2+(\ell-k)\log e+1/4} < R(\ell, p)\cdot 2^{-s/25},\end{aligned} \tag{42}$$

where we used (33). To see that the last inequality of (42) holds, consider three cases.

If $\ell < s/5$ then the exponent of 2 is clearly at most $-s/10$. If $\ell - k \le 10$ and $\ell \ge s/5$ then $(\ell - k)\log e < 15$ and $k(k+1-\ell)/2 \le -3k/2 \le -3\ell/5 \le -3s/25$.

Finally, if $\ell - k > 10$ and $\ell \ge s/5$, then $k(k-\ell+1)/2 \le -5k \le -2\ell \le -2s/5$.

Now, similarly to (35), using (39), (41) and (42) we have

$$\begin{aligned}R(\ell, p)^{-1}\cdot \sum_{3\le m\le k\le \ell-4} P^1_{k,m}(\ell, p) &< (6\log s)^2 2^{-s^2/4+o(s^2)}\\ &+1.1\cdot\sum_{3\le k\le\ell-4} h_1(\ell, k, \ell-k-1)\\ &\le (6\log s)^2 2^{-s^2/4+o(s^2)} + 1.1\cdot\ell\cdot 2^{-s/25} < \frac{1}{100}\end{aligned} \tag{43}$$

if s is large enough.

Case 5: $m \ge 2,\ \ d(Q_k, Q_m) = 0$.

In this case the subcubes Q_k and Q_m are intersecting. We shall show that the choice of (k, m) implies that the internally spanned cubes Q_k and Q_m are "disjointly reached", meaning that the occupied sites guaranteeing that Q_m is internally spanned are not in Q_k. We shall make use of the following simple assertion. (This simple but useful idea was used in earlier versions of this paper and in a write-up of our results in [5]; later it was also discovered independently by Holroyd [20].)

Lemma 12. *Let Q_k and Q_m be subcubes of Q_ℓ, and let E be the event that there are disjoint subsets S_k and S_m of the initial p-random set of occupied sites, $S_k \subset Q_k$ and $S_m \subset Q_m$, such that S_k guarantees that Q_k is internally spanned and S_m guarantees that Q_m is internally spanned. Then the probability of E is at most $P(k, p)P(m, p)$.*

The lemma is immediate from the van den Berg-Kesten lemma (see [8]) for monotone properties. For a proof of the van den Berg-Kesten conjecture, which is a considerable extension of the van den Berg-Kesten lemma, see Reimer [23].

Let us see how we can apply Lemma 12. Let R_m be the set of initially occupied vertices in Q_m, and let us study the closure $\overline{R_m - Q_k}$. The set $R_m - Q_k$ is not empty since $\overline{R_m} = Q_m \not\subset Q_k$. The set $\overline{R_m - Q_k}$ is the union of internally spanned cubes which are at distance at least 3 from each other. (It is possible that $\overline{R_m - Q_k}$ consists of only one cube.) If all of the subcubes of this union are at least at distance 3 from Q_k, then $\overline{(R_m - Q_k) \cup Q_k} \neq Q_\ell$, so this cannot be the case. If a subcube, say Q_r, is within distance 2 from Q_k, then $\overline{Q_r \cup Q_k} = Q_\ell$, since otherwise $\overline{Q_r \cup Q_k}$ would have been chosen instead of Q_k, as k was as large as possible. If $\overline{Q_r \cup Q_k} = Q_\ell$ then, by the minimality of m, we have $Q_r = Q_m$. This means that Q_m was internally spanned by occupied sites disjoint from the cube Q_k.

There are $\binom{\ell}{k}2^{\ell-k}$ ways to choose a subcube Q_k in a cube Q_ℓ. Given a subcube Q_k in a cube Q_ℓ, there are $2^{\ell-m}\binom{k}{\ell-m}$ subcubes Q_m intersecting Q_k so that they internally span Q_ℓ. Hence, similarly to Cases 3 and 4, and using the induction hypotheses that $P(k, p) \le R(k, p)$ and $P(m, p) \le R(m, p)$, and applying Lemma 12, we have

$$\begin{aligned} P^0_{k,m}(\ell, p) &\le P(k, p)P(m, p)2^{2\ell-k-m}\binom{\ell}{k}\binom{k}{\ell-m} \\ &\le R(k, p)R(m, p)2^{2\ell-k-m}\binom{\ell}{k}\binom{k}{\ell-m} = h_0(\ell, k, m), \qquad (44) \end{aligned}$$

where $h_0(\ell, k, m)$ stands for

$$2^{(k^2+m^2)/4-(k+m+4)s/2+k\log k+m\log m+2\ell-k-m}\binom{\ell}{k}\binom{k}{\ell-m}. \qquad (45)$$

We proceed as in Cases 3 and 4. Note that

$$\begin{aligned} \frac{8}{\ell^4} < \frac{h_0(\ell, k, m)}{h(\ell, k, m)} &= \frac{\binom{k}{\ell-m}}{2^{-2}\binom{\ell-k}{2}\binom{k}{\ell-m-2}} \\ &= \frac{8(k+m+2-\ell)(k+m+1-\ell)}{(\ell-k)(\ell-k-1)(\ell-m)(\ell-m-1)} \le 8\ell^2. \end{aligned}$$

Combining this inequality with (31), we obtain that, for $m \geq s - 6\log s$,

$$h_0(\ell, k, m) \leq 2^{-s^2/2+o(s^2)} \leq R(\ell, p) \cdot 2^{-s^2/4+o(s^2)}. \tag{46}$$

We claim that $h_0(\ell, k, m)$ is a decreasing function of m for $m \leq s - 6\log s$. Indeed, by (7) we have that

$$\begin{aligned}\frac{h_0(\ell, k, m+1)}{h_0(\ell, k, m)} &= 2^{m/2+1/4-s/2+(m+1)\log(m+1)-m\log m-1}\frac{\binom{k}{\ell-m-1}}{\binom{k}{\ell-m}}\\ &\leq 2^{(m-s)/2+\log(m+1)+3/4}\cdot\frac{\ell-m}{k+m-\ell+1}.\end{aligned} \tag{47}$$

For $m \leq s - 6\log s$ the right-hand side of (47) is less than $1/s$, so for $s > 11$

$$\sum_{m\leq s-6\log s} h_0(\ell, k, m) < \frac{1}{1-s}\cdot h_0(\ell, k, \ell-k) < 1.1\cdot h_0(\ell, k, \ell-k). \tag{48}$$

It remains to give an upper bound on $h_0(\ell, k, \ell-k)$. Using (33),

$$\begin{aligned}h_0(\ell, k, \ell-k) &= 2^{k^2/4+(\ell-k)^2/4-(\ell+4)s/2+k\log k+(\ell-k)\log(\ell-k)+\ell}\binom{\ell}{\ell-k}\binom{k}{k}\\ &\leq R(\ell, p)\cdot 2^{k^2/2-k\ell/2+\ell-s+k(\log k-\log\ell)+(\ell-k)\log e}\\ &\leq R(\ell, p)\cdot 2^{(k-\ell)(k-2\log e)/2+\ell-s} \leq R(\ell, p)\cdot 2^{-s/5}.\end{aligned} \tag{49}$$

Only the last inequality in (49) needs any justification. This time it suffices to consider two cases. If $\ell < s/3$ then $(k-\ell)(k-2\log e)/2+\ell-s \leq 4-2s/3 < -s/5$. If $\ell \geq s/3$ then $(k-\ell)/2 \leq -2$ and $k - 2\log e > \ell/2 - 3 \geq s/6 - 4 > s/10$, implying (49).

Combining (46), (48) and (49) we have for s large enough

$$\begin{aligned}&\sum_{1\leq m\leq k} P^0_{k,m}(\ell, p)\\ &\quad\leq \sum_{2\leq m\leq k\leq \ell-4} h_0(\ell, k, m)\\ &\quad\leq \left((6\log s)^2\cdot 2^{-s^2/4+o(s^2)} + 2\ell 2^{-s/10}\right)\cdot R(\ell, p) < 2^{-s/10}\cdot R(\ell, p).\end{aligned} \tag{50}$$

Now after handling the five cases, we can prove, using (25), (26), (35), (43) and (50) that

$$\begin{aligned}P(\ell, p) &\leq P^1(\ell, p) + P^2(\ell, p) + \sum_{k\geq m\geq 2}\sum_{i=0}^{2} P^i_{k,m}(\ell, p)\\ &\leq R(\ell, p)(2^{-1.15} + 0.216 + 0.125 + 1/100 + 2^{-s/10}) < R(\ell, p),\end{aligned} \tag{51}$$

for s large enough (independently of ℓ). □

4. The threshold

Theorem 11 gives a rather good estimate for $P(\ell, p)$ when ℓ is small. As in this section we "reset" the constants, we restate this theorem as follows.

For $\ell < -\log p$ we have

$$2^{\ell^2/4+\ell\log\ell-2\ell}\, p^{(\ell+3)/2} \le P(\ell, p) \le 2^{\ell^2/4+\ell\log\ell}\, p^{(\ell+2)/2}. \tag{52}$$

Proof of Theorem 3. First we shall prove that for $p(n) = \frac{5000}{n^2} 2^{-2\sqrt{n}}$ the probability that the cube Q_n percolates tends to 1 as $n \to \infty$. We shall use the standard second moment method, which is useful when the square of the expectation has larger magnitude than the variance (see [10] (p 2. (1.2'')).

Lemma 13. *Let X_n be a random variable with*

$$\mathbb{E}(X_n) \to \infty \text{ and } Var(X_n)/(\mathbb{E}(X_n))^2 \to 0,$$

where $Var(X_n)$ denotes the variance of X_n. Then

$$\mathbb{P}(|X_n - \mathbb{E}(X_n)| \le \varepsilon|\mathbb{E}(X_n))|) \to 1,$$

for every $\varepsilon > 0$.

In the estimates below we shall always suppose that n is large, in particular that $\sqrt{n} > 1000 \log^2 n$ holds. Set $p_0(n) = p_0 = n^{-2} \cdot 2^{12-2\sqrt{n}}$ and $\ell = \lfloor 2\sqrt{n} + \log n \rfloor$, i.e., let ℓ be the unique integer such that

$$2\sqrt{n} + \log n - 1 < \ell \le 2\sqrt{n} + \log n < \sqrt{5n}. \tag{53}$$

Let us show first that if the initial density is p_0, then the probability of the existence of an internally spanned ℓ-subcube Q_ℓ in the hypercube Q_n tends to 1. Writing X_n for the number of such cubes, by (52) we have

$$\begin{aligned} E_{p_0}(X_n) &:= \mathbb{E}_{p_0}(\text{number of i.s. } Q_\ell) = 2^{n-\ell}\binom{n}{\ell} P(\ell, p_0) \\ &\ge 2^{n-\ell}\, \frac{n^\ell}{\ell^\ell}\, 2^{\ell^2/4+\ell\log\ell-2\ell}\, p_0^{(\ell+3)/2} \\ &= 2^{n-3\ell+\ell\log n+\ell^2/4} \cdot 2^{(-2\sqrt{n}+12-2\log n)(\ell+3)/2} \\ &= 2^{n+\ell^2/4-\ell\sqrt{n}+3\ell-3\sqrt{n}+18-3\log n} \\ &\ge 2^{2\sqrt{n}+0.25\log^2 n-0.5\log n+15.25} > 2^{2\sqrt{n}}, \end{aligned} \tag{54}$$

for n large enough. In the estimate (54) we have used (52), (2), $\log p = 2\sqrt{n} + 2\log n - 12$, and the fact that there are $2^{n-\ell}\binom{n}{\ell}$ ℓ-dimensional subcubes in Q_n.

We have to prove that various internally spanned ℓ-cubes arise almost independently. Fix an ℓ-cube Q_ℓ^1. For $0 \le j \le \ell - 1$, there are $\binom{\ell}{j} 2^{\ell-j} \binom{n-\ell}{\ell-j}$ ℓ-cubes intersecting Q_ℓ^1 in a j-dimensional subcube. If Q_ℓ^1 is internally spanned and an internally spanned Q_ℓ^2 intersects it in a j-dimensional subcube, then $Q_\ell^2 \setminus Q_\ell^1$ contains at least $\lceil (\ell - j)/2 \rceil$ initially occupied sites. Hence we have the following estimates for the expected number of *intersecting* internally spanned (i.i.s.) ℓ-cubes $Q_\ell^2 \neq Q_\ell^1$, conditioned on Q_ℓ^1 being internally spanned:

$$\begin{aligned}&\mathbb{E}_{p_0}(\text{number of i.i.s. } Q_\ell^2 \neq Q_\ell^1 | Q_\ell^1 \text{ is i.s.})\\&\quad = \sum_{j=0}^{\ell-1} \binom{\ell}{j}\binom{n-\ell}{\ell-j} 2^{\ell-j} \binom{2^\ell}{\lceil \frac{\ell-j}{2} \rceil} p_0^{\lceil (\ell-j)/2 \rceil}. \end{aligned} \tag{55}$$

There are ℓ terms: we shall show that each of them is at most $2^{\sqrt{n}}$. This will enable us to apply Lemma 13.

Using (2), (53) and $\binom{\ell}{j} = \binom{\ell}{\ell-j}$ we have

$$\begin{aligned}&\binom{\ell}{j}\binom{n-\ell}{\ell-j} 2^{\ell-j} \binom{2^\ell}{\lceil \frac{\ell-j}{2} \rceil} p_0^{\lceil (\ell-j)/2 \rceil}\\
&\leq \left(\frac{e\ell}{\ell-j}\right)^{\ell-j} \left(\frac{e(n-\ell)}{\ell-j}\right)^{\ell-j} 2^{\ell-j} \left(\frac{e2^\ell}{\lceil \frac{\ell-j}{2} \rceil}\right)^{\lceil \frac{\ell-j}{2} \rceil} p_0^{\lceil \frac{\ell-j}{2} \rceil}\\
&\leq \left(\frac{e^2\ell^2}{(\ell-j)^2} \cdot \frac{e^2(n-\ell)^2}{(\ell-j)^2} \cdot \frac{4e2^\ell}{\lceil \frac{\ell-j}{2} \rceil} \cdot \frac{2^{12-2\sqrt{n}}}{n^2}\right)^{\lceil \frac{\ell-j}{2} \rceil}\\
&\leq \left(\frac{2^{15} \cdot e^5 \cdot (n-\ell)^2 \cdot 2^{\log n} \cdot \ell^2}{(\ell-j)^5 n^2}\right)^{\lceil \frac{\ell-j}{2} \rceil} \leq \left(\frac{5 \cdot 2^{15} \cdot e^5 \cdot (n-\ell)^2}{(\ell-j)^5}\right)^{\lceil \frac{\ell-j}{2} \rceil}\end{aligned} \tag{56}$$

We have to consider two cases according to the size of j. First let us suppose that $\ell - j \geq 100 n^{2/5}$. Then the base on the the right-hand side of (56) is less than 1. If $\ell - j \leq 100 n^{2/5}$, then the base is $O(n^2)$, hence the whole expression is at most $2^{O(n^{2/5} \log n)}$. Consequently,

$$\mathbb{E}_{p_0}(\text{number of i.i.s. } Q_\ell^2 \neq Q_\ell^1 | Q_\ell^1 \text{ is i.s.}) \leq n 2^{O(n^{2/5} \log n)} < 3^{\sqrt{n}}, \tag{57}$$

for n large enough. If two ℓ-cubes Q_ℓ^1 and Q_ℓ^2 do not intersect then

$$\mathbb{P}(Q_\ell^1 \text{ and } Q_\ell^2 \text{ are i. s.}) = \mathbb{P}(Q_\ell^1 \text{ is i.s})^2.$$

Therefore (57) and (55) imply that

$$\mathbb{E}_{p_0}(X_n^2) \leq \mathbb{E}_{p_0}(X_n)^2 + \mathbb{E}_{p_0}(X_n) \cdot 2^{\sqrt{n}},$$

i.e., $Var_{p_0}(X_n) \leq \mathbb{E}_{p_0}(X_n) \cdot 2^{\sqrt{n}}$. Consequently, by (54)

$$\frac{Var_{p_0}(X_n)}{(\mathbb{E}_{p_0}(X_n))^2} \leq \frac{2^{\sqrt{n}}}{2^{2\sqrt{n}}} \to 0.$$

Hence, by Lemma 13, $\mathbb{P}_{p_0}(X_n \geq 1) \to 1$ as $n \to \infty$.

For $1 \leq j \leq \sqrt{n}$, set $p_j = \frac{8}{n^2} 2^{-2\sqrt{n}-j}$ and, for $j > \sqrt{n}$, set $p_j = 2^{-3\sqrt{n}}$ (and recall that $p_0 = \frac{4096}{n^2} 2^{-2\sqrt{n}}$). Our strategy is that first we consider the occupied sites with density p_0, then we find an internally spanned Q_ℓ using only these sites, and we extend that Q_ℓ to a $Q_{\ell+2}$ using a new set of occupied sites with density p_1. In general, for $1 \le j \le (n-\ell)/2$ we extend $Q_{\ell+2j-2}$ to a $Q_{\ell+2j}$ using only a new set of occupied sites with density p_j, and if $n-\ell$ is odd then use the new set of occupied sites with density $p_{(n+1-\ell)/2}$ to extend Q_{n-1} to Q_n. Clearly, the event that Q_n is spanned the way described above has smaller probability than the event that Q_n is internally spanned if the density is p, as $\sum_j p_j < p$.

First consider the case when $0 \le j \le \sqrt{n}$. A subcube $Q_{\ell+2j}$ extends to a subcube $Q_{\ell+2j+2}$ in the hypercube Q_n using occupied sites at density $p_{j+1} = \frac{8}{n^2} 2^{-2\sqrt{n}-j-1}$, if there is an occupied point at distance 2 from $Q_{\ell+2j}$. The cardinality of the set of points at distance 2 from a subcube $Q_{\ell+2j}$ in the hypercube Q_n is $\binom{n-\ell-2j}{2} 2^{\ell+2j} \ge n^2 2^{\ell+2j-2}$. Hence the probability that an extension is possible is

$$\begin{aligned} P(Q_{\ell+2j} \to Q_{\ell+2j+2}, p_{j+1}) &\ge 1-(1-p_{j+1})^{n^2 2^{\ell+2j-2}} \\ &\ge 1-\exp(-p_{j+1} n^2 2^{\ell+2j-2}) \\ &= 1-\exp(-2^{\ell_j - 2\sqrt{n}}) \ge 1-\exp(-n2^{j-1}), \end{aligned} \tag{58}$$

where we used (53). The case $\sqrt{n} < j < (n-\ell-2)/2$ can be dealt with similarly. Note that there are at least $2^{\ell+2j}$ sites in $Q_{\ell+2j+2}$ that are at distance 2 from $Q_{\ell+2j}$. Hence,

$$P(Q_{\ell+2j} \to Q_{\ell+2j+2}, p_{j+1}) \ge 1-(1-p_{j+1})^{2^{\ell+2j}} \ge 1-\exp(-2^{\sqrt{n}+j}). \tag{59}$$

If $n-\ell$ is odd, then we have to estimate the probability of an extension from Q_{n-1} to Q_n. The probability that $Q_n - Q_{n-1}$ contains an occupied point at density $2^{-3\sqrt{n}}$ is

$$1-(1-2^{-3\sqrt{n}})^{2^{n-1}}.$$

Putting these together, we find that

$$\begin{aligned} P(Q_\ell \to Q_n) &\ge (1-(1-2^{-3\sqrt{n}})^{2^{n-1}})(1-\exp(-n/2))^{\sqrt{n}} \\ &\times \prod_{j=\sqrt{n}}^{(n-\ell)/2} (1-\exp(-2^{\sqrt{n}+j-1}) \to 1, \end{aligned} \tag{60}$$

so this completes the proof of that part.

Now we shall prove that for $p = p(n) = \frac{1}{150n^2} 2^{-2\sqrt{n}}$ the probability of spanning Q_n tends to 0. Set $\ell = \lfloor 2\sqrt{n} \rfloor$. Let S be a p-dense set of occupied sites in the hypercube Q_n. We call a sequence of nested internally spanned subcubes $Q_0 \subset Q_{t_1} \subset \cdots \subset Q_{t_r} = Q_n$ *finest* if for any two $Q_{t_i} \subset Q_{t_{i+1}}$ consecutive elements there is no internally spanned Q_k which internally spans $Q_{t_{i+1}}$ with a Q_m where $k > t_i$. If S, the set of occupied sites at time 0, spans Q_n then, by Theorem 9, there is a finest sequence of internally spanned nested cubes. For each such sequence, there is a smallest $t > \ell$ such that a Q_t and its predecessor Q_k, with $k \le \ell$, are members of the sequence. By Theorem 9, there is a subcube $Q_m \subset Q_t$, which together with Q_k spans the cube Q_t. We shall show that the expected number of such cube-triples (Q_t, Q_k, Q_m) is $o(1)$, which implies that the probability that they exist is $o(1)$ and hence the probability that there is a sequence of internally spanned nested cubes is also $o(1)$. Therefore $P(n, p) = o(1)$.

Fix a triple (t, k, m). The number of the choices of a subcube Q_t in the hypercube Q_n is $2^{n-t}\binom{n}{t}$. In a given subcube Q_t for given k and m the number of choices of pairs of internally spanned subcubes Q_k, Q_m such that Q_k and Q_t are neighbours in a building sequence of the hypercube Q_n, is at most $2^{t-k}\binom{t}{k}2^{t-m}\binom{t}{m}$. Recall that the probability that Q_k and Q_m are both internally spanned is at most $P(k, p)P(m, p)$ (either the two cubes are disjoint, or "disjointly spanned", see Lemma 12). Hence the expected number of such triples is at most

$$2^{n+t-k-m}\binom{n}{t}\binom{t}{k}\binom{t}{m}P(k, p) \cdot P(m, p). \tag{61}$$

To give upper bound on (61), we shall use Theorem 11, where $s = -\log p = 2\sqrt{n} + 2\log n + \log 150 \geq 2\sqrt{n} + 2\log n + 7.2$. Let

$$f(n, t, k, m) := 2^{(k^2+m^2)/4-(k+m+4)s/2+k\log k+m\log m+n+t-k-m}\binom{n}{t}\binom{t}{k}\binom{t}{m}.$$

Note that the parameters satisfy $k+m+2 \geq t > \ell \geq k \geq m$ and the restrictions above. By Theorem 11, the function $f(n, t, k, m)$ is an upper bound on (61).

To give the upper bound on $f(n, t, k, m)$, in addition to relations (2) and (3), we shall use the following simple inequalities:

$$\begin{aligned}
\binom{n}{t}\binom{t}{k}\binom{t}{m} &\leq 2^{2t}\left(\frac{en}{t}\right)^t \leq (2e\sqrt{n})^t, \\
t-k-m &\leq 2, \\
2^{-3.6(k+m+2)} &\leq 2^{-3.6t}, \\
2^{-(k+m)\log n+k\log k+m\log m} \leq 2^{\log(k/n)^{k+m}} &\leq 2^{\log(\frac{2.1}{\sqrt{n}})^{k+m}} \leq \frac{n}{4}(\sqrt{n})^{-t}2^{1.1t}, \\
(\frac{k}{2}-\sqrt{n})^2 + (\frac{m}{2}-\sqrt{n})^2 - n &\leq \log^2 n.
\end{aligned} \tag{62}$$

To see the last inequality, it needs some case analysis. It clearly holds when $m \geq 2\sqrt{n}$. Otherwise, the left hand side of the inequality is maximized (for fixed k), when m is minimized, i.e. $k+m = \ell - 2$, and now fixing $k+m$ it is maximized when $m = 0$, and the inequality clearly holds.

By making use of these inequalities, straightforward calculations give that

$$\begin{aligned}
&f(n, t, k, m) \leq 2^{(k^2+m^2)/4-(k+m+4)(\sqrt{n}+\log n+3.6)+k\log k+m\log m+n+2}(2e\sqrt{n})^t \\
&\leq 2^{(k/2-\sqrt{n})^2+(m/2-\sqrt{n})^2-n-4\sqrt{n}-(k+m)\log n+k\log k+m\log m-4\log n-3.6(k+m+2)-5.2}(2e)^t(\sqrt{n})^t \\
&\leq 2^{\log^2 n-4\sqrt{n}-4\log n-5.2+t(\log e-2.6)} \cdot (\sqrt{n})^t \cdot \frac{n}{4}2^{1.1t}(\sqrt{n})^{-t} \\
&\leq 2^{\log^2 n-4\sqrt{n}-3\log n-7.2+t(\log e-1.5)} < 2^{-2\sqrt{n}}.
\end{aligned} \tag{63}$$

The number of triples (t, k, m) is at most $(4\sqrt{n})^3 \leq 64n^{3/2}$, so (63) implies our claim. □

More careful calculations would give better estimates for the constants in the threshold functions. We have chosen the approach above in order to give a reasonably clean presentation that suffices to determine the order of the main term.

5. A sharp threshold

For a set S, the power set of S is naturally identified with the cube $\{0, 1\}^S$. A *property* of subsets of S is a collection $\mathcal{A}$ of subsets, i.e., a subset of $P(S) = \{0, 1\}^S$. The properties $\mathcal{A} = \emptyset$ and $\mathcal{A} = \{0, 1\}^S$ are *trivial*; in what follows, we shall consider only non-trivial properties. A property $\mathcal{A} \subset \{0, 1\}^S$ is *increasing* or *monotone* if $x, y \in \{0, 1\}^S, x \in \mathcal{A}$ and $x_s \leq y_s$ for every $s \in S$ imply that $y \in \mathcal{A}$. Since our properties are assumed to be non-trivial, if $\mathcal{A}$ is monotone increasing then the identically 1 sequence is in $\mathcal{A}$ and the identically 0 sequence is not in $\mathcal{A}$.

A property $\mathcal{A}$ is *symmetric* if for all $t, u \in S$ there is a permutation π of S such that $\pi(t) = u$ and $\mathcal{A}$ is invariant under the permutation induced by π: if for $x \in \{0, 1\}^S$ the element $\pi(x) \in \{0, 1\}^S$ is given by $\pi(x)_s = x_{\pi(s)}, s \in S$, then $\pi(\mathcal{A}) = \mathcal{A}$. For $0 \leq p \leq 1$, let us define a random subset of S by picking the elements of S independently, with probability p. Thus the *p-probability* (or simply *probability*) of a subset X of S is $\mathbb{P}_p(X) = p^{|X|}(1 - p)^{|S \setminus X|}$. Equivalently, for $x \in \{0, 1\}^S$, set $|x| = \sum |x_s|$; then the *p-probability* of x is

$$\mathbb{P}_p(x) = \prod_{x_s=1} p \prod_{x_s=0} (1 - p) = p^{|x|}(1 - p)^{|S|-|x|},$$

and the *p-probability* of $\mathcal{A}$ is

$$\mathbb{P}_p(\mathcal{A}) = \sum_{x \in \mathcal{A}} \mathbb{P}_p(x).$$

For a (non-trivial) monotone property $\mathcal{A} \subset \{0, 1\}^S$ and $0 \leq p \leq 1$, the *probability function* $\mathbb{P}_p(\mathcal{A})$ is continuous and strictly increasing from 0 to 1. Hence, for every $0 \leq r \leq 1$, there is a unique probability $p(r, \mathcal{A})$ such that $\mathbb{P}_{p(r,\mathcal{A})}(\mathcal{A}) = r$. Now, let $S_1, S_2, \ldots$ be a sequence of ground sets with $|S_n| \to \infty$ and, for $n \geq 1$, let $\mathcal{A}_n \subset \{0, 1\}^{S_n}$ be a monotone property. Although, strictly speaking, for $n < m$, the property $\mathcal{A}_n$ and $\mathcal{A}_m$ have nothing to do with each other, we view the sequence $(\mathcal{A}_n)$ as a single "property". We are interested in the speed that the probability function $\mathbb{P}_p(\mathcal{A}_n)$ grows from "very small" to "very large". More precisely, for $0 < c < 1/2$, we wish to give bound on $p(1 - c, \mathcal{A}_n) - p(c, \mathcal{A}_n)$. In fact, just this difference does not tell us much about the nature of the transition: what matters is how large this difference is compared to the *critical probability* $p(1/2, \mathcal{A}_n)$.

To give a formal definition of the speed of transition, set $p^{(n)} = p(1/2, \mathcal{A}_n)$. We say that a sequence $(\mathcal{A}_n)$ of properties has a *sharp threshold* if for every c, $0 < c < 1/2$, we have

$$\lim_{n\to\infty} \frac{p(1 - c, \mathcal{A}_n) - p(c, \mathcal{A}_n)}{p(1/2, \mathcal{A}_n)} = 0.$$

For bootstrap percolation on the cube $\{0, 1\}^n$ the ground set is $S_n = \{0, 1\}^n$, and we consider the monotone property $\mathcal{B}_n$ of subsets X of S_n such that if X is the set of occupied sites at time 0 then complete occupation takes places. By Theorem 3 we know that if c is a positive constant, $c < 1$ and n is large enough (depending only on c) then

$$\frac{2^{-2\sqrt{n}}}{150n^2} < p(c, \mathcal{B}_n) < 5000 \cdot \frac{2^{-2\sqrt{n}}}{n^2}; \tag{64}$$

in particular, (64) holds for $c = 1/2$ and n large enough. Our main aim in this section is to show that bootstrap percolation has a sharp threshold, i.e., we have transition from probability at most c to probability at least $1 - c$ when the probability p of open sites increases by $o(\frac{2^{-2\sqrt{n}}}{n^2})$. As we shall see, this result is an easy consequence of the following fundamental theorem of Friedgut and Kalai [17].

Theorem 14. *There is an absolute constant $C > 0$ such that if $\mathcal{A} \subset \{0, 1\}^m$ is monotone increasing and symmetric, $0 < \varepsilon < 1/2$, $0 < p < q < 1$, and $p(p, \mathcal{A}) > \varepsilon$ then*

$$q \geq p + \frac{C \log(1/2\varepsilon) p \log(1/p)}{\log m}$$

implies that $p(q, \mathcal{A}) \geq 1 - \varepsilon$.

Theorem 14 was the starting point of much research on sharp threshold functions: see Friedgut [16] and Achlioptas and Friedgut [1] for several deep results. Now we are ready to state and prove our result.

Theorem 15. *There is constant $C > 0$ and a function $c(n)$, $1/150 < c(n) < 5000$, such that if $0 < \varepsilon < 0.5$ then with $\delta(n) = 3C \cdot \log(1/2\varepsilon)/\sqrt{n}$ and $p(n) = c(n)\frac{2^{-2\sqrt{n}}}{n^2}$ we have for n large enough that*

$$\mathbb{P}_{(1-\delta(n))p(n)}(\mathcal{B}_n) < \varepsilon \quad \textit{and} \quad \mathbb{P}_{(1+\delta(n))p(n)}(\mathcal{B}_n) > 1 - \varepsilon. \tag{65}$$

Proof. Fix any $0 < \varepsilon < 0.5$. Define $c(n)$ by the equation $p(n) = p(\varepsilon, \mathcal{B}_n) = \frac{c(n)}{n^2} 2^{-2\sqrt{n}}$, so that for n large enough $1/150 < c(n) < 5000$ by Theorem 3. It is sufficient to prove that

$$p(1 - \varepsilon, \mathcal{B}_n) - p(\varepsilon, \mathcal{B}_n) < \delta(n)p(n).$$

By Theorem 14, if n is sufficiently large,

$$\begin{aligned} p(1 - \varepsilon, \mathcal{B}_n) - p(\varepsilon, \mathcal{B}_n) &\leq C \cdot \log\Big(\frac{1}{2\varepsilon}\Big) \frac{-p(n) \log(p(n))}{\log 2^n} \\ &\leq C \cdot \log\Big(\frac{1}{2\varepsilon}\Big) p(n) 3\frac{\sqrt{n}}{n} = 3C \cdot \log\Big(\frac{1}{2\varepsilon}\Big) \frac{1}{\sqrt{n}} p(n), \end{aligned} \tag{66}$$

implying (65). Note that we had $m = 2^n$ and we have used that for n large enough

$$\log\Big(\frac{1}{p(n)}\Big) = \log\Big(\frac{n^2 2^{2\sqrt{n}}}{c(n)}\Big) = 2 \log n + 2\sqrt{n} - \log(c(n)) \leq 3\sqrt{n}.$$

□

Note that although the threshold function is sharp, we do not know that the function $c(n)$ in Theorem 15 tends to a limit, i.e., that

$$\lim_{n\to\infty} c(n) = \lim_{n\to\infty} P(1/2, B_n)n^2 2^{2\sqrt{n}}$$

exists. There is no doubt that the limit exists, but this fact is likely to be very difficult to prove.

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