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Undergraduate Honors Thesis

Counting Clusters on a Grid

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Contents

COUNTING CLUSTERS ON A FINITE GRID

JACOB RICHEY

Abstract. We consider $p = 1/2$ site percolation on finite rectangles in the 2D square lattice. For $n, m \in \mathbb{Z}$, let $e(m, n)$ be the expected number of clusters - connected monochromatic components - over all two-colorings of $[0, m) \times [0, n) \cap \mathbb{Z}^2$, where points are connected orthogonally. We determine the values $e(m, n)$ explicitly for small values of m, and demonstrate connections between the expected number of clusters, expected cluster size, monochromatic cycles, and other plane animals. We show that the limit

$$\lambda = \lim_{m,n\to\infty} \frac{e(m, n)}{mn}$$

exists, and bound the constant by $\frac{29}{448} \leq \lambda \leq \frac{1}{12}$. We also give similar results for some related lattices, such as the 2D torus and hexagonal lattices, and extend the theory to some more general graphs.

1. Introduction

While the dynamics of site percolation on the 2D square lattice have been extensively studied, combinatorial properties of finite clusters have not been considered in this context. The question of bounding the expected number of clusters was inspired by a Putnam exam problem from 2005, which asked the following:

> "An $m \times n$ checkerboard is colored randomly: each square is independently assigned red or black with probability 1/2. We say that two squares, p and q, are in the same connected monochromatic region if there is a sequence of squares, all of the same color, starting at p and ending at q, in which successive squares in the same sequence share a common side. Show that the expected number of connected monochromatic regions is greater than $mn/8$."

We will show a number of ways this problem can be answered: determining the actual expectation is much more difficult, and will be our main task. For the most part we fix the

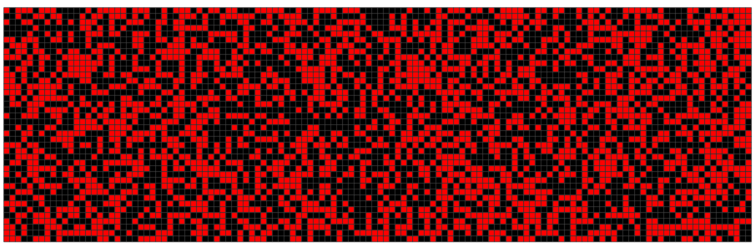

Figure 1. A coloring of the 40×128 square grid with 704 monochromatic regions.

probability of each color to be 1/2: however, we take as a more apt picture the chessboard with black and white squares rather than black and red squares on a checkerboard, checkers being less a mathematical game than chess. From the usual percolation viewpoint, a two coloring of an m by n grid is a $p = 1/2$ random site percolation process, and the number of connected monochromatic components is the number of clusters in the resulting subset of the grid. We will often take a hybrid of these viewpoints: for our main results, however, we take the percolation picture, where we only count clusters of one color (by convention, black).

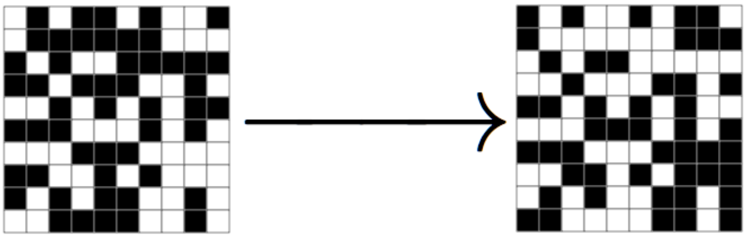

FIGURE 2. A coloring with 9 black clusters and 14 white clusters, and its dual coloring, with 14 black clusters and 9 white clusters.

For any two-coloring of the grid with b black clusters and w white clusters, the coloring obtained by switching the color of each square gives a grid with b white clusters and w black clusters. These two colorings have equal probabilities when $p = 1/2$, so the expected number of white clusters is equal to the expected number of black clusters. Therefore the expected number of clusters in the percolation picture is exactly half the expected number of clusters in the Putnam problem, so for our purposes these two viewpoints are equivalent.

We now make some formal definitions. By a coloring c of an m by n grid we mean a function

$$c : G_{m,n} := \mathbb{Z}^2 \cap [0, n) \times [0, m) \to \{0, 1\},$$

where a point p is black (or 'alive') if $c(p) = 1$, and white ('dead') if $c(p) = 0$. We will often think of coloring lattice squares rather than lattice points: this is the dual lattice of $\mathbb{Z}^2$, i.e. the set $\{(x + \frac{1}{2}, y + \frac{1}{2}) : x, y \in \mathbb{Z}\}$. We will call the colorings $c_0 = 0$ of all dead points, and $1 - c_0 = c_1 = 1$ of all alive points the empty and full colorings, respectively. Define the chessboard coloring c_a by $c_a(0, 0) = 0$, and $c_a(p) \neq c_a(q)$ if p and q are orthogonally adjacent.

Let

$$r(m, n, c) = \#\{\text{clusters in the coloring } c \text{ of the } m \text{ by } n \text{ grid}\},$$

so we can define the expected number of clusters

$$e(m, n) = \frac{1}{2^{mn}} \sum_{c:G_{m,n}\to\{0,1\}} r(m, n, c),$$

and mean cluster size

$$s(m, n) = \frac{1}{2^{mn} - 1} \sum_{c:G_{m,n}\to\{0,1\}} \sum_{p\in G_{m,n}} \frac{c(p)}{r(m, n, c)},$$

where by convention the empty coloring is not included (equivalently, clusters have positive size). In the context of the Putnam problem, $s(m,n)$ has the form

$$s(m,n) = \frac{1}{2^{mn}} \sum_{c:G_{m,n}\to\{0,1\}} \frac{mn}{\#\{\text{white clusters}\} + \#\{\text{black clusters}\}}.$$

Unlike the expected number of clusters, these two formulas for s are *not* compatible in any simple way: asymptotically, they are equal. Here $s(m,n)$ is the mean cluster size: note that this statistic differs from the mean cluster size *containing a particular point*, which we will denote by s_p. For large m and n, $s_p(m,n)$ has the simple formula

$$s_p(m,n) \sim \frac{mn}{2e(m,n)}.$$

We denote with subscripts T and H the same statistics on the torus and hexagonal 2D lattices: for example, $e_T(m,n)$ is the expected number of clusters over all colorings of the m by n torus grid. An m by n torus grid rectangle has all the same edges as the usual $\mathbb{Z}^2$ grid, only the top and bottom rows are connected, as are the leftmost and rightmost columns: that is, we add edges $((x,m-1),(x,0))$ and $((n-1,y),(0,y))$ for all $0 \le x < n, 0 \le y < m$. We think of an m by n rectangle of the hexagonal grid as a rectangle in the m by n square lattice, with an additional edge connecting each pair of points $((x,y),(x+1,y+1))$ for $0 \le x < n-1, 0 \le y < m-1$ (diagonals going in the direction $(1,1)$). We will investigate the limits

$$\lambda = \lim_{m,n\to\infty} \frac{e(m,n)}{mn},\ \lambda_T = \lim_{m,n\to\infty} \frac{e_T(m,n)}{mn},\ \text{and } \lambda_H = \lim_{m,n\to\infty} \frac{e_H(m,n)}{mn},$$

and in particular determine whether or not they exist.

More generally, if $G=(V,E)$ is any graph on the vertex set $[k] = \{1,2,\dots,k\}$, we can define

$$r_G(c) = \#\{\text{clusters in the coloring } c \text{ of G}\},$$

where c is any vertex coloring $c: V \to [0,1]$. Then

$$e(G) = \frac{1}{2^k} \sum_{c:G\to\{0,1\}} r_G(c)$$

is the expected number of clusters, and the mean cluster size can be defined analogously. It is often useful to have a generating function

$$M_G(z) = \sum_{c:G\to\{0,1\}} z^{r_G(c)}$$

from which the expected number of clusters and mean cluster size can be recovered. To get a feel for these objects, we consider the special case of finite tree graphs with undirected edges, and count both white and black clusters to make the calculations easier. We have the following proposition:

Prop 1.1 Let T be any tree on the vertex set $[n]$. Then $M_T(z) = 2z(1+z)^{n-1}$.

Proposition 1.1 follows from the lemma:

Lemma 1.2 Let $G = (V, E)$ be a nonempty finite graph, and let $H = (V \cup \{v\}, E \cup \{e\})$ be the union of G with a vertex $v \notin V$ of degree one, $e = (v, u)$ for some $u \in V$. Then

$$M_H(z) = (1+z)M_G(z).$$

Proof: Let $u \in V$ be the unique vertex with $(u, v) \in E$. Consider a coloring c of H. If $c(v) = c(u)$, then $r_H(c) = r_G(c)$. Otherwise, $c(v) \neq c(u)$, and $r_H(c) = 1 + r_G(c)$. Viewing c as a coloring of the graph G and of the vertex v, we can combine these two facts to obtain

$$M_H(z) = \sum_{\substack{c:G\to\{0,1\} \\ c(v)=c(u)}} z^{r_G(c)} + \sum_{\substack{c:G\to\{0,1\} \\ c(v)\neq c(u)}} z^{1+r_G(c)} = M_G(z) + zM_G(z) = (1+z)M_G(z),$$

as desired. □

We have the polynomial $M_{K_1}(z) = 2z$ for the graph with one vertex: since any tree can be obtained by attaching leaves (degree one vertices) one at a time, repeated application of the lemma yields proposition 1.1.

We can recover cluster data from this polynomial: for any tree T on the vertex set $[n]$, we have

$$2e(T) = \frac{1}{2^n} \sum_{0\leq k\leq n} k[z^k]M_T(z) = \frac{1}{2^n} \sum_{0\leq k\leq n} 2k\binom{n-1}{k-1} = \frac{n+1}{2}.$$

Thus the usual percolation-picture expectation is $e(T) = \frac{n+1}{4}$. A formula for the mean cluster size for any tree T also follows from proposition 1.1:

$$s(T) = \frac{1}{2^n} \sum_{1\leq k\leq n} \frac{n}{k} * [z^k]M_T(z) = \frac{1}{2^{n-1}} \sum_{1\leq k\leq n} \frac{n\binom{n-1}{k-1}}{k} = \frac{2^n - 1}{2^{n-1}} = 2 - \frac{1}{2^{n-1}}.$$

In particular, as $n \to \infty$ the mean cluster size on the tree T goes to 2. For the case where T is the 1 by n grid, we could have determined this without the generating function formalism: if k is a cluster, then starting from the leftmost point in k, there is a probability $1/2$ that the adjacent neighbor on the right is also alive. Continuing this way, the expectation of $|k|$, the size of the cluster, is

$$1 + \sum_{i\geq 1} 2^{-i} = 2,$$

or

$$\lim_{n\to\infty} s(1, n) = 2.$$

We can solve the same problem for the torus 1 by n grid, by considering a similar inductive process. We have the base cases $e_T(1,1) = 1/2, e_T(1,2) = e(1,2) = 3/4$, and for any 1 by n rectangle coloring with $n \geq 2$, we obtain a coloring of the 1 by $n+1$ rectangle by inserting a square between two existing ones: to get the new expectation, we measure how the expected number of clusters changes depending on the color of the new square.

There are some cases where the number of clusters will remain constant: if the inserted square is alive and not both of the neighboring squares are dead, or if the inserted square is dead and either of its neighbors is dead, then the cluster count doesn't change. If the inserted square is alive and both of its neighbors are dead, we increase the number of clusters by 1. Finally, there is a possible issue when the inserted square is dead, and its neighbors are both alive: it seems that we split a cluster into two distinct clusters. But if the two neighboring squares still belong to the same cluster, then the count will stay constant; otherwise it will increase by 1. Combining these cases, the new expectation is given by

$$e_T(1, n+1) = e_T(1, n) + \frac{1}{8} + \frac{1}{8}(1 - \frac{1}{2^{n-2}}) = e_T(1, n) + \frac{1}{4} - \frac{1}{2^{n+1}},$$

which yields

$$e_T(1, n) = \frac{n}{4} + 2^{-n}.$$

It should not come as a surprise that $e_T(1, n) \sim e(1, n)$ as $n \to \infty$, since the 1 by n grid differs from its torus counterpart in a single edge. It is often easier to consider the torus graph: in addition to being 4-regular, the torus grid looks the same from each vertex. We will see that statistically, the two are essentially identical, since they only differ on the (finite) boundary of the square lattice grid.

2. Preliminary Results

We now examine the limiting properties of the expectation $e(m, n)$. Proposition 1.1 gives immediately an infinite family of exact solutions for $m = 1$; we give similar exact solutions for $m \leq 3$ in the appendix. First, we summarize a few simple properties of the expectation in the following lemma.

Lemma 2.1 For all $m, n, n_1, n_2 \in \mathbb{Z}_{>0}$, we have:

i) $e(m, n) = e(n, m)$

ii) $0 < e(m, n) \leq \lceil mn/2 \rceil$

iii) (Subadditivity) $e(m, n_1 + n_2) \leq e(m, n_1) + e(m, n_2)$.

Proof: *i)* There is an obvious graph isomorphism between $G_{m,n}$ and $G_{n,m}$: since the expectation e depends only on the graph structure, it is preserved under graph isomorphism, so *i)* holds.

ii) The full coloring c_1 always has $r(m, n, c_1) = 1$, so being a finite sum the expectation $e(m, n)$ is positive. Consider the chessboard coloring c_a on $G_{m,n}$ by red and blue points. If c is any coloring, and p and q are two adjacent points in $G_{m,n}$, there cannot exist two distinct clusters k and k' with $p \in k$ and $q \in k'$, where we are considering clusters in the coloring c. Therefore, if any red (blue) point is contained in a cluster, its blue (red) neighbors are necessarily either contained in the same cluster or contained in no cluster. Hence there may only be as many

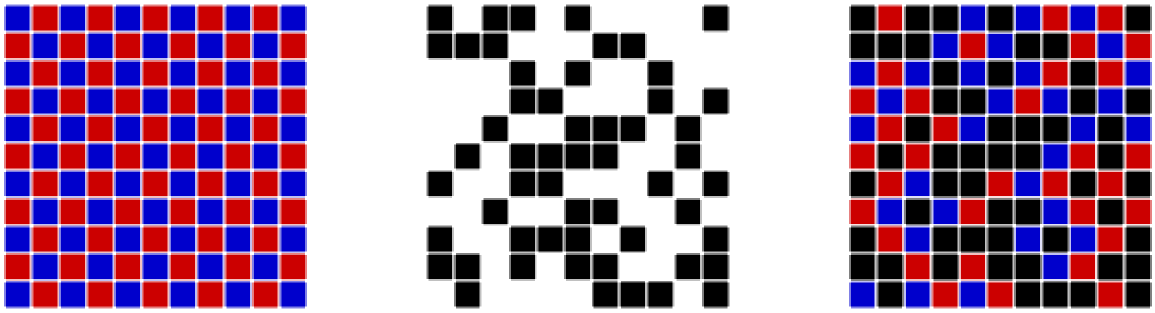

FIGURE 3. The chessboard coloring and an 'arbitrary' coloring laid over it, as in the proof of lemma 2.1 *ii*).

clusters as there are red or blue points: the extremal case is the chessboard coloring itself, where there are $\lceil mn/2 \rceil$ points of one color and $\lfloor mn/2 \rfloor$ of the other, so $e(m,n) \leq \lceil mn/2 \rceil$.

iii) Fix a coloring c of $G_{m,n}$, and let $R = r(m, n_1+n_2, c), R_1 = r(m, n_1, c_1)$, and $R_2 = r(m, n_2, c_2)$, where c_1 and c_2 are the restrictions of c to the subgrids $\mathbb{Z}^2 \cap [0, n_1) \times [0, m)$ and $\mathbb{Z}^2 \cap [n_1, n_1+n_2) \times [0, m)$, respectively. We claim that it suffices to show $R \leq R_1 + R_2$: then we would have

$$\begin{aligned} e(m, n_1+n_2) &= \frac{1}{2^{mn_1+mn_2}} \sum_{c:G_{m(n_1+n_2)} \to \{0,1\}} r(m, n_1+n_2, c) \\ &\leq \frac{1}{2^{mn_1+mn_2}} \sum_{c:G_{m(n_1+n_2)} \to \{0,1\}} r(m, n_1, c_1) + r(m, n_2, c_2) \\ &= \frac{1}{2^{mn_1+mn_2}} \Big(\sum_{c_1:G_{mn_1} \to \{0,1\}} 2^{mn_2} r(m, n_1, c_1) + \sum_{c_2:G_{mn_2} \to \{0,1\}} 2^{mn_1} r(m, n_2, c_2) \Big) \\ &= e(m, n_1) + e(m, n_2), \end{aligned}$$

as desired.

Now note that any nonempty cluster in the large grid can be written as the union of two clusters, one from each of the subgrids, by intersecting it with each subgrid (one intersection may be empty). Therefore each cluster in each subgrid contributes at most one cluster to the larger grid: it may contribute less if it meets a cluster from the other subgrid along the line $x = n_1$. Therefore R is at most $R_1 + R_2$, and the claim is proved. □

Corollary 2.2 Properties *i*), *ii*) and *iii*) also hold for the torus and hexagonal expectation functions e_T, e_H.

Proof: The proofs of properties *i*) and *iii*) are identical. Property *ii*) follows from the fact that the usual square lattice m by n grid is a subgraph of both the m by n torus and hexagonal rectangles. □

A number of other simple properties of the expectation e immediately follow from lemma 2.1. For example, the subadditivity property implies that $e(m_1, n_1) \leq e(m_2, n_2)$ whenever

$n_1 \leq n_2$ and $m_1 \leq m_2$. Note, however, that it is not necessarily true that $e(m,n) \leq e(k,l)$ if $mn \leq kl$. Asymptotically for large indices m,n,k,l, the inequality does hold, a corollary of our first main theorem:

Theorem 2.3 The limit

$$\lim_{n,m\to\infty} \frac{e(m,n)}{mn}$$

exists, and is finite.

Proof: By lemma 2.1, $0 \leq e(m,n) \leq \lceil mn/2 \rceil$, so we have $0 \leq \frac{e(m,n)}{mn} \leq 1 \ \forall m,n \in \mathbb{Z}_{>0}$. Therefore the limit is positive and finite if it exists.

Now write

$$\lim_{m,n\to\infty} \frac{e(m,n)}{mn} = \lim_{m\to\infty} \frac{1}{m} \left(\lim_{n\to\infty} \frac{e(m,n)}{n} \right).$$

Again by lemma 2.1, the sequence $\{e(m,n)\}_{n=1}^{\infty}$ is subadditive in each coordinate, so by Kingman's subadditive ergodic theorem [1], the limit

$$\lim_{n\to\infty} \frac{e(m,n)}{n} = \lambda_m$$

exists for all m. Therefore the limit reduces to

$$\lim_{m\to\infty} \frac{\lambda_m}{m},$$

and it suffices to show that the sequence $\{\lambda_m\}_{m=1}^{\infty}$ is subadditive: then by another application of Kingman's theorem, the limit would exist. For any $m_1, m_2, n \in \mathbb{Z}_{>0}$, the subadditivity condition in lemma 2.1 says

$$\frac{e(m_1+m_2,n)}{n} \leq \frac{e(m_1,n)}{n} + \frac{e(m_2,n)}{n},$$

so taking the limit in n on both sides yields

$$\lambda_{m_1+m_2} \leq \lambda_{m_1} + \lambda_{m_2},$$

i.e. the sequence of λ_m's is subadditive, the desired result. □

As an immediate consequence, we see that $e(m,n) \sim \lambda_m \cdot n$ for large n, and $e(m,n) \sim \lambda mn$ for both m and n large, so the expected number of clusters in a subgrid grows as a constant factor with the area of the subgrid: explicitly,

$$\forall \epsilon, m > 0 \ \exists N > 0 \ s.t. \ |\lambda mn - e(m,n)| < \epsilon \ \forall n > N.$$

Corollary 2.4 The limits

$$\lim_{m,n\to\infty} \frac{e_H(m,n)}{mn}, \lim_{n\to\infty} \frac{e_H(m,n)}{n},$$

[1] Kingman, John. *Subadditive Ergodic Theory.* Annals of Probability, Vol. 1, No. 6, December 1973, pp. (883-899).

$$\lim_{m,n\to\infty}\frac{e_T(m,n)}{mn} \text{ and } \lim_{n\to\infty}\frac{e_T(m,n)}{n}$$

exist for all positive integers m: we denote them by λ_H, $(\lambda_H)_m$, λ_T and $(\lambda_T)_m$, respectively.

Proof: Combining corollary 2.2 with the proof of theorem 2.3.

3. Main Results

Now that we have established that this limit exists, our next task will be to try and determine upper and lower bounds on the limit λ. We start by describing a simple but computationally difficult method to obtain lower bounds on λ, via a statistic of free polyominoes in the square lattice.

Polyominoes as Clusters

Given a coloring of the square grid, the possible shapes clusters can take are the free plane polyominoes. Indeed, the expected number of clusters $e(m,n)$ is the sum of the expected number of clusters of each polyomino shape. To obtain a lower bound, then, we can write down all possible polyominoes of small sizes, and determine the expected number of clusters of that shape over all colorings. The calculation can be done for any fixed m and n, but we will only be interested in the limiting case for $m,n\to\infty$. For any free polyomino P of size i, write $|P|=i$; for a cluster k in the m by n grid of shape P, write $\mathrm{sh}(k)=P$. Then we can define

$$b_{m,n}(k)=b(k)=\#\{\text{lattice points bordering } k \text{ inside } G_{m,n}\},$$

and

$$N_{m,n}(P)=\#\{\text{distinct positions of a shape } P \text{ cluster in } G_{m,n}\}.$$

For example, the size one polyomino has four bordering lattice points, and can occupy mn different positions in the m by n grid; the domino has six bordering points, and can occupy $2mn-(m+n)$ positions in the m by n grid. In general, the probability that a cluster k has shape P in a fixed position is $2^{-|P|}2^{-b(k)}$, since each point in the cluster must be alive, and each square bordering the cluster must be dead. Therefore we have the formula for $e(m,n)$:

$$e(m,n)=\sum_{1\le|P|\le mn}\ \sum_{\mathrm{sh}(k)=P}\frac{N(P,m,n)}{2^{|P|}2^{b(k)}}.$$

We can recover exactly the formula for $e(1,n)$ from this summation: the possible polyominoes are all the 1 by j blocks, each of which have two bordering squares, except in the special cases $j=n$, or when the block is at one end of $G_{1,n}$. We obtain

$$e(1,n)=\frac{1}{2^n}+\sum_{1\le j\le n-1}\frac{n-j-1}{2^2*2^j}+\frac{2}{2*2^j}=\frac{1}{2^n}+(\frac{n}{4}+\frac{1}{2^n}-\frac{3}{4})+(1-\frac{1}{2^{n-1}})=\frac{n+1}{4},$$

the same result. This is the only case where an exact calculation is feasible: enumerating polyominoes is a difficult task in general, even in a fixed finite grid.

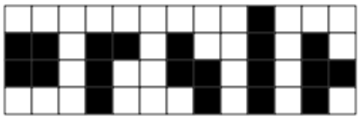

FIGURE 4. A 4×13 grid with five clusters, one for each of the five free tetromino shapes.

To make the calculation a bit easier, we can work on the torus lattice instead, where there are no boundary restrictions about where polyominoes of certain shapes can be placed. In fact, we do not concede any power of this method in working over the torus lattice, a consequence of the following proposition:

Proposition 3.1 $\lambda = \lambda_T$.

Proof: We claim that for each $m, n \in \mathbb{Z}_{>0}$,

$$e(m,n) \geq e_T(m,n) \geq e(m,n) - \frac{m+n}{2} \tag{1}$$

The first inequality follows from the fact that the m by n grid is a subgraph of the m by n torus grid, so $r_T(m,n,c) \leq r(m,n,c)$ for any coloring c. Now observe that the grid and torus grid structures only differ on the border points, along the lines $x = 0, y = 0, x = n-1$ and $y = m-1$, where the torus grid has extra edges connecting the top and bottom rows, and leftmost and rightmost columns. There are at most $2(m+n)$ such bordering edges. Now imagine we start with a coloring of the usual square lattice, and add the torus edges. Then each bordering edge decreases the cluster count by at most 1, if it connects two black points: looking over all possible colorings, the expectation decreases by at most $\frac{1}{4} * 2(m+n) = \frac{m+n}{2}$, so (1) holds.

Now since $e(m,n) \sim \lambda mn$ for large m and n, the linear correction for the torus grid becomes negligible: dividing by mn and taking the limit yields

$$\lambda \geq \lambda_T \geq \lim_{m,n\to\infty} \frac{e(m,n)}{mn} - \frac{m+n}{2mn} = \lambda,$$

i.e. $\lambda = \lambda_T$. □

Corollary 3.2 For all positive integers $m, \lambda_m = (\lambda_T)_m$.

The numbers $N(P,m,n)$ are much easier to calculate for the torus grid, using its invariance under orthogonal translations: indeed, for a fixed shape P, the number of positions P can fit in the m by n grid is some multiple of mn, depending on how many rotational symmetries the polyomino P has. The allowable rotations are by $\pi/2$ radians in the plane, or π through the third dimensional axis: these operations form a group of order 8, so any polyomino P has 1, 2, 4 or 8 different plane incarnations, each of which takes exactly mn distinct positions on the torus grid. Thus, writing $N(P,m,n) = z_P \cdot mn$, where $z_P \in \{1,2,4,8\}$ is the number of distinct plane positions of P, we obtain the following formula for λ:

$$\lambda = \sum_P \frac{z_P}{2^{|P|+b(P)}}.$$

This sum can be taken over any subset of all free plane polyominoes to give a lower bound for λ: for example, summing over all polyominoes of rectangular shape yields

$$\sum_{i\geq 1}\sum_{j\geq i}\frac{2}{2^{ij+2i+2j}}\approx 0.0404558.$$

Unfortunately, this formulation does not offer an efficient method for determining the constant λ. If large clusters were rare, we could take the summation out to some small polyomino sizes and obtain a good lower bound. However, this doesn't seem to be the case: indeed, we have computed the sum for all polyominoes P with $|P|\leq 8$, obtaining the value

$$\sum_{|P|\leq 8}\frac{z_P}{2^{|P|+b(P)}}=0.0540994.$$

We note here a connection with the expected cluster size statistic introduced earlier. We have seen the asymptotic formula $s_q(m,n)\sim\frac{mn}{2e(m,n)}$ for the expected size of a cluster containing a fixed point on the grid. This formulation gives an easy algorithm to compute $1/2\lambda$, and hence λ, via calculating the value s_q directly for large m and n. We can look over colorings of the infinite lattice (either square or hexagonal), and compute the size of the cluster containing the origin; equivalently, we can consider random self-avoiding walks on the $p=1/2$ site-percolated lattice starting from the origin, and compute the average length of such a walk. Indeed, we can write down a sum over all such walks:

$$\frac{1}{2\lambda}=\sum_{w}P(w)\cdot|w|,$$

where w is as above, $P(w)$ is the probability that the path w consists of all black points, and $|w|$ is the length of the path. These walks are really polyominoes in disguise: the sum gives the expected size of a plane polyomino, in the context of lattice percolation.

k-Expectations

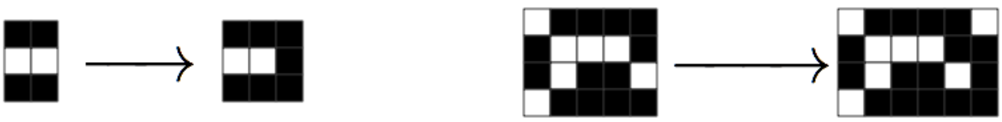

FIGURE 5. Two examples of loops: when a new column is added, the cluster count may decrease, as clusters are connected via the new column.

We now present the main method for obtaining arbitrarily high precision bounds on the limiting constant λ. Recall our derivation of the exact formula for $e(1,n)$: we proved the formula inductively, by appending a point to the end of a 1 by n grid and keeping track of how the expected cluster count changed. We can think of doing this for any value of m: starting with a m by n grid with some coloring, we append an m by 1 column with a fixed coloring to the end, and observe how the cluster count changes. In the cases $m=1,2$, adding an extra m by 1 column with some coloring cannot decrease the cluster count: in general, this is not the case, as some pair of previously distinct clusters may become connected via the new column, as in the two examples shown in figure 5, where the cluster count decreases by

1. Our approach will be to estimate the expected change in the cluster count after appending an m by 1 column to the end of an m by n grid for each fixed m: by convention, we will think of appending on the right.

Fix $m \in \mathbb{Z}_{>0}$, let $n \in \mathbb{Z}_{>0}$, and choose a (small) integer $2 < k < n$. We consider all colorings of the rightmost m by k subgrid of the m by $(n+1)$ grid to estimate the expected change in cluster count. Note that there are many colorings where the change in cluster count is easy to calculate. For example, if no cluster has points on both the rightmost and leftmost columns of this m by k subgrid, we have all the information we need to determine the change in the cluster count: it is the number of clusters in the m by k grid less the number of clusters in the m by $(k-1)$ subgrid excluding the rightmost column, or in our previous notation, $r(m,k,c) - r(m,k-1,c')$, c' the restriction of c to the smaller subgrid. This works because the clusters of the new column dont 'see' the clusters beyond the k columns we are keeping track of. We will refer to these cases and this difference calculation as the 'simple part' of the k-expectation.

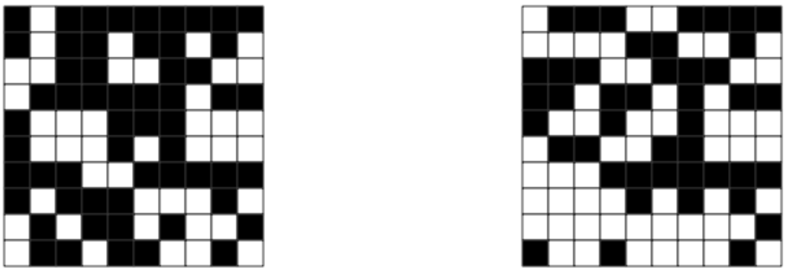

FIGURE 6. Two colorings of a 10×10 grid with the same rightmost 10×3 subgrid ($k = 3$), in a loop case (left) and a simple case (right).

There are some colorings where this is not the complete picture: if two distinct clusters meet both the rightmost and leftmost columns of the m by k subgrid, we may not have enough information to decide how many clusters to add or subtract from the count. These scenarios will be referred to as the 'loop part' of the k-expectation; the loop part will be dealt with by bounding the change in expectation from below and from above in the simplest possible way.

To obtain a lower bound on the change in cluster count for a loop case, we make the assumption that no pair of clusters disconnected in the m by k subgrid connect somewhere in the remaining m by $(n-k)$ grid: this way, if there is any possibility that the cluster cound should decrease, we assume it does. Similarly, an upper bound can be obtained by, for each loop scenario, assuming each pair of clusters *do* connect in the m by $(n-k)$ subgrid: then we overcount the change in the number of clusters, since each possible loop adds a 0 instead of a -1.

It remains to compute these upper and lower bounds on the k-expectation. Define upper and lower '$k-$ expectations' $\Delta_k^u(m)$ and $\Delta_k^l(m)$ as follows:

$$\Delta_k^u(m) = e^u(m,k) - e^u(m,k-1),$$
$$\Delta_k^l(m) = e(m,k) - e(m,k-1),$$

where $e^u(m,n)$ is the expected number of clusters in the m by $n+1$ grid whose (conventionally) leftmost column is all black points. (Define $r^u(m,n,c)$ analagously.) Note that unlike the usual expectation, the 'upper expectation' e^u is not symmetric: $e^u(m,n) \neq e^u(n,m)$. We summarize this discussion with the following proposition:

Proposition 3.3 For any positive integers m and n, and $2 \leq k \leq n$, the following inequality holds:

$$\Delta_k^l(m) \leq e(m,n) - e(m,n-1) \leq \Delta_k^u(m).$$

Proof: We have already seen that this inequality holds in the simple cases, where there is no error in the upper and lower bounds. Explicitly, suppose c is a coloring of the m by n grid, c' its restriction to the leftmost m by $(n-1)$ subgrid, d the coloring c restricted to the rightmost m by k subgrid, and d' the restriction of d to the rightmost m by $(k-1)$ subgrid, and suppose no two distinct clusters k, k' of the coloring c' both contain points on the line $x = n-k$ *and* are subclusters of the same cluster K in the coloring c. (This is the definition of a simple case.) Then there are no potential loops, since the change in cluster count $r(m,n,c) - r(m,n-1,c')$ depends only on the rightmost k columns of the grid, and we have equality with the lower bound. For the upper bound, we either have

$$r^u(m,k,d) = r(m,k,d) + 1 \text{ and } r^u(m,k-1,d') = r(m,k-1,d') + 1, \text{or}$$

$$r^u(m,k,d) = r(m,k,d) \text{ and } r^u(m,k-1,d') = r(m,k-1,d'),$$

depending on whether the leftmost (all black) column is a disjoint cluster or not. In either case equality holds:

$$r(m,n,c) - r(m,n-1,c) = r(m,k,d) - r(m,k-1,d') = r^u(m,k,d) - r^u(m,k-1,d').$$

Now suppose we are in a loop case, so that the colorings c, c', d, d' are so that some clusters k, k', K exist with the properties described above. Then the inequalities

$$r(m,k,d) - r(m,k-1,d') \leq r(m,n,c) - r(m,n-1,c') \leq r^u(m,k,d) - r^u(m,k-1,d')$$

hold, since for each such pair of clusters k, k', the actual cluster count changes by either 0 or -1, while the lower difference adds a -1 and the upper difference adds 0. Summing over all colorings gives

$$e(m,k) - e(m,k-1) \leq e(m,n) - e(m,n-1) \leq e^u(m,k) - e^u(m,k-1),$$

the desired result. □

Corollary 3.4 The same inequality holds for the hexagonal lattice: for all positive integers m and n, and $2 \leq k \leq n$,

$$e_H(m,k) - e_H(m,k-1) \leq e_H(m,n) - e_H(m,n-1) \leq e_H^u(m,k) - e_H^u(m,k-1).$$

As a corollary, these upper and lower simple expectations translate directly to upper and lower bounds on the limiting constants λ, λ_H:

Corollary 3.5 For any positive integer $k > 1$, the following inequality holds:

$$\lambda_k - \lambda_{k-1} \leq \lambda \leq \lambda_k^u - \lambda_{k-1}^u,$$

and similarly for the hexagonal case, where

$$\lambda_k^u = \lim_{m\to\infty} \frac{e^u(m,k)}{m}.$$

Note that unlike the limit values λ_m, the values λ_k^u are different from those taking the limit in the other coordinate:

$$\lim_{n\to\infty} \frac{e^u(k,n)}{n}.$$

Proof: Dividing through by m and taking the limit $m \to \infty$ in the inequality of proposition 3.3 gives

$$\lim_{m\to\infty} \frac{\Delta_k^l(m)}{m} \leq \lambda_n - \lambda_{n-1} \leq \lim_{m\to\infty} \frac{\Delta_k^u(m,k)}{m},$$

or

$$\lambda_k - \lambda_{k-1} \leq \lambda_n - \lambda_{n-1} \leq \lambda_k^u - \lambda_{k-1}^u.$$

Taking the limit $n \to \infty$ now yields

$$\lambda_k - \lambda_{k-1} \leq \lambda \leq \lambda_k^u - \lambda_{k-1}^u$$

since $e(m,n) \sim \lambda_n \cdot m \sim \lambda mn \implies \lambda_n \sim \lambda n$, the desired result. □

This inequality turns out to give us significant mileage, even for small values of k:

Corollary 3.6 In the case $k = 3$, we have the bounds

$$\frac{29}{448} \leq \lambda \leq \frac{1}{12}$$

and

$$\frac{1}{112} \leq \lambda_H \leq \frac{1}{24}.$$

Proof: These values are obtained by determining closed forms for the expectations on the $3 \times m$ and $2 \times m$ grids: the formulas used are given in the appendix. □

4. Related Results

Monochromatic Loops

The k-expectation method relies on estimating from above and below the number of 'loop' scenarios that occur in building up a lattice grid one column at a time. We can ask about these loops more generally: for example, how many are there? For the hexagonal grid, loops are easy to handle, since the set of squares bordering any monochromatic component is also a monochromatic component (of the opposite color): we define a loop as a cluster that is the set of bordering squares of another cluster. Call the expected number of such loops in the $m \times n$ hexagonal grid $\chi_H(m,n)$.

For the square lattice, the picture is not so simple: the set of bordering squares of a cluster is not necessarily a cluster itself. Given a coloring of the square lattice grid G_{mn}, consider the set of alive points $p = (x,y)$ whose left and lower neighbors $p_l = (x-1,y)$ and $p_d = (x,y-1)$ are

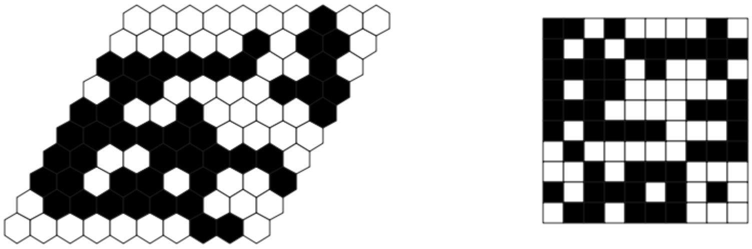

FIGURE 7. Two 10×10 grids, one hexagonal and one square. The hexagonal grid has two monochromaic loops; the square grid has three.

also alive. We say that p represents a loop if there is a path of points $p_0 = p_l, p_1, \ldots, p_r = p_d$ where the points $p_i = (x_i, y_i)$ have the properties $0 \leq y_i \leq y$ and $0 \leq x_i \leq n$ unless $y_i = y$ in which case $0 \leq x_i < x$. We can define the expected number of loops $\chi(m,n)$, the expected number of such points p over all colorings of the $m \times n$ square grid. We have the following theorem:

4.1 Theorem $\chi(m,n) = e(m,n) - \frac{m+n+2}{4}$.

Proof: We proceed by using a naive algorithm to try and calculate $e(m,n)$. Fix a coloring c of $G_{m,n}$, and for each point $p = (x,y) \in G_{m,n}$, assign a partial sum value s_p, which is recursively defined as follows:

$$s_{(0,0)} = 1;$$

$$s_{p_r} = \begin{cases} s_p + 1 & c(p) = 1, c(p_l) = c(p_d) = 0 \\ s_p - 1 & c(p) = c(p_l) = c(p_d) = 1, \text{ and } p \text{ does not represent a loop} \\ s_p & \text{otherwise} \end{cases}$$

where $p_r = (x+1, y)$ is the right neighbor. When p_d or p_l is undefined, say $c(p_d) = 0$ or $c(p_l) = 0$, respectively. This occurs on the bottom row $[0,n) \times \{0\}$ and the left column $\{0\} \times [0,m)$.

The values s_p keep track of the cluster count as we go along: if a point p is alive and its lower and left neighbors are dead, it adds a new cluster; if p and its lower and left neighbors are alive, and p doesn't represent a loop, then it subtracts a cluster; if p represents a loop, or in any other coloring situation, it doesn't do anything to the cluster count. Therefore the number of clusters in the subgraph with vertices $\left(\mathbb{Z}^2 \cap [0,n) \times [0,y]\right) \cup ([0,x] \times \{y\})$ is exactly s_p: in particular, $r(m,n,c) = s_{(n-1,m-1)}$. Summing the expectation values for the partial sums s_p, we obtain the formula

$$e(m,n) = 1 + \frac{m-1}{4} + \frac{n-1}{4} + \frac{(m-1)(n-1)}{8} - \frac{(m-1)(n-1)}{8} + \chi(m,n),$$

or

$$\chi(m,n) = e(m,n) - \frac{m+n+2}{4}$$

proving the claim. □

Corollary 4.2 For large m and n, $\chi(m,n) \sim e(m,n)$ and $\chi_H(m,n) \sim e_H(m,n)$.

Proof: As in theorem 4.1, a similar formula can be obtained for the hexagonal grid expectation. Since the boundary cases contribute a part linear in m and n in both lattices, the result follows from 2.3-2.4. □

This theorem shows that our definition of loops in the square lattice actually makes sense: for example, theorem 4.1 shows that it is symmetric in m and n, which is not obvious from the definition. This analysis shows that the expected number of loops also grows like λmn, so they are just as populous as monochromatic clusters.

5. Appendix

We have the following exact solutions for the expectations $e(m,n), e^u(m,n), e_H(m,n)$, and $e^u_H(m,n)$:

n	$e(m,n)$	$e^u(m,n)$	$e_H(m,n)$	$e^u_H(m,n)$
1	$\frac{m+1}{2}$	1	$\frac{m+1}{2}$	1
2	$\frac{5n+7}{16}$	$\frac{3m+41+4^{1-m}}{36}$	$\frac{m+2}{4}$	$\frac{3m+83-4^{2-m}}{72}$
3	$\frac{1183m+1945+8^{m-2}}{3136}$		$\frac{203m+573+8^{2-m}}{784}$	

These formulas are obtained by exactly calculating the expected change in cluster count when a $n \times 1$ column is appended to an existing $n \times m$ grid, which is managable for $n \leq 3$. The difficulty in the $n = 3$ case comes from the unique loop scenario pictured in figure 5: all possible loop scenarios in the $n \times (m+1)$ grid with rightmost three columns as in that coloring must be accounted for. For $n = 4$, there are two loop cases to consider, but determining the possible loop shapes is considerably more difficult: they can be put in bijection with a certain type of lattice path, but these are already too difficult to write down completely.

High precision estimations of Δ^u_k and Δ^l_k for large k have been computed on the Dartmouth computer science department cluster: the best bounds obtained were

$$0.067105 \leq \lambda \leq 0.0677055$$

in the case $k = 10$.

The polyomino sums as in section 3 up to size 8 have all been computed: they are

n	$p(n)$
1	$1/32$
2	$1/2^7$
3	$5/2^{10}$
4	$27/2^{13}$
5	$157/2^{16}$
6	$953/2^{19}$
7	$6133/2^{22}$
8	$79362/2^{26}$

where $p(n) = \sum_{|P|=n} \frac{z_P}{2^{|P|+b(P)}}$ is the sum over all size n polyominoes. (These values were painstakingly computed by hand.)

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