Several Constants Arising in Statistical Mechanics

STEVEN R. FINCH

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Abstract. This is a brief survey of certain constants associated with
random lattice models, including self-avoiding walks, polyominoes, the Lenz-
Ising model, monomers and dimers, ice models, hard squares and hexagons,
and percolation models.

1. Introduction
Random lattice models give rise to combinatorial problems that are often easily-stated
but intractable. This article briefly presents several such problems, each involving the
numerical estimation of asymptotic growth constants. Emphasis is given to recent
developments. The author has been collecting and writing about various mathematical
constants for five years. His large evolving website [18] provides further discussion
and references; updates and corrections from readers are always welcome.

2. Self-Avoiding Walks
Let \( L \) denote the \( d \)-dimensional cubic lattice whose sites (vertices) are precisely all
integer points in \( d \)-dimensional space. An \( n \)-step self-avoiding walk \( \omega \) on \( L \), be-
ginning at the origin, is a sequence of sites \( \omega(0), \omega(1), \omega(2), \ldots, \omega(n) \) with \( \omega(0) = 0, \)
\(|\omega(j + 1) - \omega(j)| = 1 \) for all \( j \) and \( \omega(i) \neq \omega(j) \) for all \( i \neq j \).

The number of such walks \( \omega \) is denoted by \( c(n) \). For example, \( c(0) = 1, c(1) = 2d \)
and \( c(2) = 2d(2d - 1) \).

What can be said about the asymptotics of \( c(n) \)? It is known that
\[
\mu = \lim_{n \to \infty} \frac{c(n)^{\frac{1}{n}}}{}
\]
exists and is nonzero. The value \( \mu \) is called the connective constant and clearly
depends on \( d \). The current best rigorous lower and upper bounds for \( \mu \), plus the best
known estimates for \( \mu \), are given in the following table [18], [1], [37], [15], [23]:
The upper bounds were computed only recently \cite{37} via the Goulden-Jackson cluster method \cite{38}. Similar techniques can be used to estimate other constants associated with the combinatorics of words, e.g., the asymptotics of ternary square-free words and of binary cube-free words \cite{18}.

The connective constant values \( \mu \) given above apply not only to the growth of the number of self-avoiding walks, but also to the growth of numbers of self-avoiding polygons and of self-avoiding walks with prescribed endpoints \cite{27}.

For \( d = 2 \) and \( 3 \), there apparently is a positive constant \( \gamma \) such that

$$
\lim_{n \to \infty} \frac{c(n)}{\mu^n \cdot n^{\gamma-1}}
$$

exists and is nonzero \cite{33}, \cite{10}, \cite{12}. These constants are conjectured to be \( \frac{43}{92} \) if \( d = 2 \) and \( 1.1575... \) if \( d = 3 \).

Another interesting object of study is the mean square displacement

$$
s(n) = E \left\{ |\omega(n)|^2 \right\} = \frac{1}{c(n)} \cdot \sum_\omega |\omega(n)|^2
$$

where the summation is over all \( n \)-step self-avoiding walks \( \omega \) on \( L \), weighted with uniform probability. Like \( c(n) \), it’s believed for \( d = 2 \) and \( 3 \) that there is a positive constant \( \nu \) such that

$$
\lim_{n \to \infty} \frac{s(n)}{n^{2\nu}}
$$

exists and is nonzero; moreover \cite{33}, \cite{10}, \cite{33} it’s conjectured that \( \nu = \frac{3}{4} \) if \( d = 2 \) and \( \nu = 0.5877... \) if \( d = 3 \). The critical exponents \( \gamma \) and \( \nu \) are thought to be universal in the sense that they are lattice-independent (although dimension-dependent). No one has yet discovered a proof of their existence on \( L \), let alone a proof of universality.

3. Polyminoes

A domino is a pair of adjacent squares.

<FIGURE 1>

Generalizing, a polyomino or lattice animal of order \( n \) is a connected set of \( n \) adjacent squares, e.g., for \( n = 3 \),

<FIGURE 2>

Define \( A(n) \) to be the number of polyminoes of order \( n \), where it’s agreed that two polyminoes are distinct iff they have different shapes or different orientations. There
are different senses in which polyominoes are defined, e.g., free versus fixed, bond versus site, simply-connected versus not necessarily so, and others. For brevity’s sake, we focus only on the fixed, site, possibly multiply-connected case.

Redelmeier [43] computed $A(n)$ up to $n = 24$ and Conway and Guttmann [16] extended the sequence to $n = 25$. It is known that the limit

$$\alpha = \lim_{n \to \infty} A(n)^{\frac{1}{n}}$$

exists and is nonzero. The best known bounds on $\alpha$ are $3.791 \leq \alpha \leq 4.649551$ as discussed in [29], [12], [19], [21]. Improvements are possible using the new value $A(25)$. The best known estimate, obtained via series expansion analysis by differential approximants [16], is $\alpha = 4.06265...$ A more precise asymptotic expression [16] for $A(n)$ is

$$C \cdot n^{-1} \cdot \alpha^n$$

where $C = 0.316...$, but such an empirical result is far from being rigorously proved.

4. Lenz-Ising Model

Let $L_n$ denote the regular $d$-dimensional cubic lattice with $N = n^d$ sites. For example, in two dimensions, $L_n$ is the $n \times n$ square lattice with $N = n^2$. To eliminate boundary effects, $L_n$ is wrapped around to form a $d$-dimensional torus so that, without exception, every site has $2d$ nearest neighbors.

Let’s agree that a nonempty subgraph of $L_n$ is connected and contains at least one bond (edge). Suppose that several subgraphs are drawn on $L_n$ with the property that

- each bond of $L_n$ is used at most once
- each site of $L_n$ is used an even number of times (possibly zero).

Call such a configuration on $L_n$ an even polygonal drawing.

<FIGURE 3>

Note that an even polygonal drawing is the union of simple, closed, bond-disjoint polygons but need not be connected. Other names in the literature for these configurations include closed or Eulerian subgraphs. Let $B(r)$ be the number of even polygonal drawings for which there are exactly $r$ bonds. For example, when $d = 2$, it follows [13] that $B(4) = N$, $B(6) = 2N$ and $B(8) = \frac{1}{2}N(N + 9)$. When $d = 3$, it follows that $B(4) = 3N$, $B(6) = 22N$ and $B(8) = \frac{1}{2}N(9N + 375)$. Computing $B(r)$
for larger $r$ is quite complicated, especially considering that in $> 2$ dimensions, the drawings can intertwine and be knotted!

Define the **high temperature zero magnetic field free energy** for the **Ising model** to be the series

$$\beta(z) = \lim_{n \to \infty} \frac{1}{N} \cdot \ln(1 + \sum_{r} B(r) \cdot z^r) = \sum_{k=0}^{\infty} \beta_k \cdot z^k$$

where $z$ is called the **activity**. If $T$ denotes temperature, then $\tanh^{-1}(z) \propto 1/T$.

Coefficients $\beta_k$ of this series, as polynomials in $d$, are given here \[24\]:

- $k = 4$: $\beta_4 = \frac{1}{2}d(d - 1)$
- $k = 6$: $\beta_6 = \frac{1}{4}d(d - 1)(8d - 13)$
- $k = 8$: $\beta_8 = \frac{1}{8}d(d - 1)(108d^2 - 424d + 425)$
- $k = 10$: $\beta_{10} = \frac{3}{16}d(d - 1)(2976d^3 - 19814d^2 + 44956d - 34419)$

The radius of convergence \[22\], \[3\], \[36\], \[20\], \[10\] for $\beta(z)$ is

$$z_c = \lim_{k \to \infty} \beta_{2k}^{-\frac{1}{k}} = \left\{ \begin{array}{l}
\sqrt{2} - 1 = 0.414213562373095049... \text{ if } d = 2 \\
0.218094... \text{ if } d = 3 \\
0.14855... \text{ if } d = 4 \\
0.1134... \text{ if } d = 5 \\
0.0920... \text{ if } d = 6 \\
0.0775... \text{ if } d = 7
\end{array} \right.$$

which is important since knowledge of $z_c$ gives the **critical temperature** or **Curie point** $T_c$ of the model. The exact two dimensional result is a famous outcome of work by Kramers and Wannier and by Onsager.

Here is a related problem. Suppose that several subgraphs are drawn on $L_N$ with the property that

- each bond of $L_N$ is used at most once
- all sites of $L_N$, except two, are even
- the two remaining sites are odd and must lie in the same (connected) subgraph.

Call this configuration an **odd polygonal drawing**. Note that an odd polygonal drawing is the bond-disjoint union of an even polygonal drawing and an (undirected) self-avoiding walk linking the two odd sites.

<FIGURE 4>
Enumerating odd polygonal drawings gives rise to what physicists call the high temperature zero field magnetic susceptibility

\[ \chi(z) = \sum_{k=0}^{\infty} \chi_k \cdot z^k \]

Coefficients \( \chi_k \) of this series, as polynomials in \( d \), are listed in [20]. The radius of convergence of \( \chi(z) \) is the same as that for \( \beta(z) \) for \( d > 1 \). Further, when \( d = 2 \),

\[ \lim_{T \to T_c} \left(1 - \frac{T_c}{T}\right)^{\frac{z}{T}} \cdot \chi(z) = 0.9625817322... \]

Wu, McCoy, Tracy, Barouch [52], [19] determined an exact formula for this coefficient in terms of the Painlevé III function. The expression is complicated: can a simpler formula in terms of other mathematical constants (e.g., Glaisher’s constant [18]) be found? An exact analog of this formula for \( d = 3 \) is also evidently not known.

5. Monomers and Dimers

Let \( L_N \) be as before, but without wraparound. Two sites of \( L_N \) are called adjacent if the distance between them is 1. A dimer consists of two adjacent sites of \( L_N \) and the (non-oriented) bond connecting them. A dimer arrangement is a collection of disjoint dimers on \( L_N \). Uncovered sites are called monomers, so dimer arrangements are also known as monomer-dimer coverings. A dimer covering is a dimer arrangement whose union contains all the sites of \( L_N \).

For \( d = 2 \), let \( g(n) \) denote the number of distinct monomer-dimer coverings of \( L_N \), then clearly \( g(1) = 1, g(2) = 7 \) and asymptotically [3], [25]

\[ \kappa = \lim_{n \to \infty} g(n)^{\frac{1}{n}} = 1.940215351... \]

No exact expression for the constant \( \kappa \) is known. Baxter’s approach for estimating \( \kappa \) was based on the corner transfer matrix variational approach. A natural way for physicists to discuss the monomer-dimer problem is to introduce an activity \( z \) for the number of monomers. The constant \( \kappa \) then corresponds to the situation in which \( z = 1 \). Values of \( g(n) \) were recently computed [26] up to \( n = 21 \).

The above contrasts with the special case of dimer coverings. An exact expression is known here for \( d = 2 \), due to Kastelyn, Fisher and Temperley. If \( f(n) \) is the number of distinct dimer coverings of \( L_N \), then \( f(n) = 0 \) if \( n \) is odd and asymptotically [40]

\[ \lim_{n \to \infty} f(n)^{\frac{1}{n}} = \exp\left(\frac{2G}{\pi}\right) = 1.79162281206959342... \]
a fascinating and unexpected occurrence of Catalan’s constant $G$. For $d = 3$, the number $h(n)$ of distinct dimer coverings \[^{32}\] of $L_N$ is $h(2) = 9$, $h(4) = 5051532105$ and asymptotically

$$\lim_{n \to \infty} h(n)^{\frac{1}{n}} = \exp(\lambda)$$

where the constant $\lambda$ is known only imprecisely. The current best rigorous bounds \[^{41}\], \[^{14}\], \[^{44}\] are $0.44007584 \leq \lambda \leq 0.463107$ and the best known estimate \[^{8}\] is $\lambda = 0.4466...$.

6. Ice Models

Let $L_N$ be as before, with wraparound. An orientation of $L_N$ is an assignment of a direction (arrow) to each bond of $L_N$. Assume that $d = 2$ henceforth. What is the number, $\theta(n)$, of orientations of $L_N$ such that at each site there are exactly two inward and two outward pointing edges? (Such orientations are said to obey the ice rule and are also called Eulerian orientations.) Here is a sample configuration:

<FIGURE 5>

After intricate analysis, Lieb proved that \[^{40}\], \[^{45}\]

$$\lim_{n \to \infty} \theta(n)^{\frac{1}{n}} = \left(\frac{4}{3}\right)^{\frac{3}{2}} = 1.539600717839002039...$$

This constant is known as the residual entropy for square ice. Interestingly, $3\theta(n)$ is also the number of ways of coloring the square faces of $L_N$ with three colors so that no two adjacent faces are colored alike \[^{4}\]. Values of $\theta(n)$ were recently computed \[^{26}\] up to $n = 13$, and relevant computational complexity issues were discussed in \[^{35}\].

The residual entropy $W$ for ordinary hexagonal ice Ice-Ih and for cubic ice Ice-Ic (both complicated three-dimensional lattices) satisfy \[^{39}\]

$$1.5067 < W < 1.5070$$

and are equal within the limits of Nagle’s estimation error. These configurations are not the same as the simple models mathematicians tend to focus on. It would be interesting to see the value of $W$ for the customary $n \times n \times n$ cubic lattice $L_3$, either with the ice rule in effect (two arrows point out and four arrows point in) or with Eulerian orientation (three arrows point out and three arrows point in). No one appears to have done this.
7. Hard Squares and Hexagons

Consider the set of all \( n \times n \) binary matrices. What is the number \( F(n) \) of such matrices with no pairs of adjacent 1’s? Two 1’s are said to be adjacent if they lie in positions \((i, j)\) and \((i + 1, j)\), or if they lie in positions \((i, j)\) and \((i, j + 1)\), for some \( i, j \). Equivalently, \( F(n) \) is the number of configurations of non-attacking Princes on an \( n \times n \) chessboard, where a "Prince" attacks the four adjacent, non-diagonal places. Let \( N = n^2 \), then

\[
\xi = \lim_{n \to \infty} F(n)^{1/N} = 1.50304808247533226...
\]

is the hard square entropy constant \([1], [11], [34], [5]\). Essentially nothing is known about the arithmetic character of \( \xi \).

Instead of an \( n \times n \) binary matrix, consider an \( n \times n \) binary array which looks like:

\[
\begin{pmatrix}
a_{11} & a_{23} \\
a_{22} & a_{34} \\
a_{21} & a_{33} \\
a_{32} & a_{44} \\
a_{31} & a_{43} \\
a_{42} & a_{54} \\
a_{41} & a_{53} \\
a_{52} & a_{64}
\end{pmatrix}
\]

(here \( n = 4 \)). What is the number \( G(n) \) of such arrays with no pairs of adjacent 1’s? Two 1’s here are said to be adjacent if they lie in positions \((i, j)\) and \((i + 1, j)\), or in \((i, j)\) and \((i, j + 1)\), or in \((i, j)\) and \((i + 1, j + 1)\), for some \( i, j \). Equivalently, \( G(n) \) is the number of configurations of non-attacking Kings on an \( n \times n \) chessboard with regular hexagonal cells. It’s surprising that the hard hexagon entropy constant

\[
\eta = \lim_{n \to \infty} G(n)^{1/N} = 1.395485972479302735...
\]

is algebraic (in fact, is solvable in radicals \([28]\)) with minimal integer polynomial \([55]\):

\[
25937424601x^{24} + 2013290651222784x^{22} + 2505062311720673792x^{20} + 79772669866658379776x^{18} + 7449488310131083100160x^{16} + 295801503876958230528x^{14} - 72405670285649161617408x^{12} + 10715544815044388043264x^{10} - 71220809441400405884928x^8 - 73347491183630103871488x^6 + 97143135277377575190528x^4 - 32751691810479015985152
\]

This is a consequence of Baxter’s exact solution of the hard hexagon model \([1], [2]\) via theta elliptic functions and the Rogers-Ramanujan identities from number theory!
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Just as series for the Ising model were defined using counts of even polygonal drawings with exactly $r$ bonds, series for the hard hexagon model can be defined using counts of non-attacking configurations of exactly $r$ Kings (and likewise for the hard square model). The radius of convergence for the hexagon series

$$z_c = \frac{11 + 5\sqrt{5}}{2} = 11.0901699437494724...$$

possesses an exact expression. No similar theoretical breakthrough has occurred for the square model, hence the radius of convergence for the square series

$$z_c = 3.7962...$$

has no known analogous formula [4]. These values are important since they correspond to the critical activity (e.g., temperature or density) at which a phase transition occurs in the model.

If one replaces Princes by Kings on the chessboard with square cells, then the corresponding constant [34] is $1.342643951124...$. A related problem, that of enumerating the maximal configurations of $\frac{N}{4}$ nonattacking Kings, was discussed in [51], [30].

8. Percolation Models

Let $M$ be a random $n \times n$ binary matrix satisfying

- $m_{ij} = 1$ with probability $p$, 0 with probability $1 - p$ for each $i, j$
- $m_{ij}$ and $m_{kl}$ are independent for all $(i, j) \neq (k, l)$.

An s-cluster is an isolated grouping of $s$ adjacent 1’s in $M$, where adjacency means horizontal or vertical neighbors (not diagonal). For example, the $4 \times 4$ matrix

$$M = \begin{pmatrix}
1 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 \\
1 & 0 & 0 & 1
\end{pmatrix}$$

has one 1-cluster, two 2-clusters and one 4-cluster. The total number of clusters is 4 in this case. For arbitrary $n$, the total cluster count is a random variable with normalized expected value

$$K_n = \frac{E(C_n)}{n^2}$$

The limit $K_S(p)$ of $K_n$ exists as $n$ approaches infinity, and $K_S(p)$ is called the mean cluster count per site or the mean cluster density for the site percolation...
model. It’s known that $K_S(p)$ is twice continuously differentiable on $[0,1]$; further, $K_S(p)$ is analytic on $[0,1]$ except possibly at one point $p = p_c$. Monte Carlo simulation and numerical Padé approximants can be used to compute $K_S(p)$. For example [54], it’s known that $K_S(\frac{1}{2}) = 0.065770\ldots$

Instead of an $n \times n$ binary matrix $M$, consider a binary array $A$ of $2n(n-1)$ entries which looks like

$$A = \begin{pmatrix}
a_{12} & a_{14} & a_{16} 
a_{11} & a_{13} & a_{15} & a_{17} 
a_{22} & a_{24} & a_{26} 
a_{21} & a_{23} & a_{25} & a_{27} 
a_{32} & a_{34} & a_{36} 
a_{31} & a_{33} & a_{35} & a_{37} 
a_{42} & a_{44} & a_{46}
\end{pmatrix}$$

(here $n = 4$). One should associate $a_{ij}$ not with a site of the $n \times n$ square lattice (as one does for $m_{ij}$) but with a bond. An $s$-cluster here is an isolated, connected subgraph of the graph of all bonds associated with 1’s. For example, the array

$$A = \begin{pmatrix}
1 & 0 & 0 
1 & 0 & 0 & 0 
0 & 1 & 0 
0 & 1 & 1 & 0 
0 & 1 & 0 
1 & 0 & 0 & 0 
0 & 0 & 0
\end{pmatrix}$$

has one 1-cluster, one 2-cluster and one 4-cluster. For bond percolation models such as this, one often includes 0-clusters in the total count as well, that is, isolated sites with no attached 1’s bonds. In this case there are seven 0-clusters, hence the total number of clusters $C_4$ is 10. The limiting mean cluster density $K_B(p) = \lim_{n \to \infty} K_n = \lim_{n \to \infty} \frac{E(C_n)}{n^2}$ exists as $n$ approaches infinity and similar smoothness properties hold. Remarkably, however, an exact integral expression exists at $p = \frac{1}{2}$ for the limiting mean cluster density [47], [17]

$$K_B(\frac{1}{2}) = -\frac{1}{8} \cot(y) \cdot \frac{d}{dy} \left\{ \frac{1}{y} \cdot \int_{-\infty}^{\infty} \operatorname{sech}\left(\frac{\pi x}{2y}\right) \cdot \ln \left( \frac{\cosh(x) - \cos(2y)}{\cosh(x) - 1} \right) dx \right\} \bigg|_{y = \frac{\pi}{8}}$$
which Adamchik [54] recently simplified to

\[ K_B\left(\frac{1}{2}\right) = \frac{3\sqrt{3} - 5}{2} = 0.09807621135331594... \]

An analogous expression for the limiting variance of cluster density was computed in [54]. In the same way, the bond percolation model on the triangular lattice gives a known limiting mean cluster density at a specific value of \( p \) (discussed below), but the relevant variance is not known here.

Let’s turn attention away from mean cluster density \( K(p) \) and instead toward mean cluster size \( S(p) \). In the examples given earlier, \( S_4 = (1 + 2 + 2 + 4)/4 = 9/4 \) for the site case, \( S_4 = (1 + 2 + 4)/3 = 7/3 \) for the bond case, and \( S(p) \) is the limiting value of \( E(S_n) \) as \( n \) approaches infinity. The critical probability or percolation threshold \( p_c \) is defined to be [46], [27]

\[ p_c = \inf_{0<p<1} \frac{S(p)}{S(p)=\infty} \]

that is, the concentration at which an infinite cluster appears in the infinite lattice.

For site percolation on the square lattice, there are rigorous bounds [50], [48]

\[ 0.556 < p_c < 0.679492 \]

and an estimate [53] \( p_c = 0.5927460... \) based on extensive simulation. Ziff [54] has additionally calculated that \( K_S(p_c) = 0.0275981... \) via simulation.

In contrast, for bond percolation on the square and triangular lattices, there are exact results due to Sykes and Essam. Kesten [27] proved that \( p_c = \frac{1}{2} \) on the square lattice, corresponding to the expression \( K_B\left(\frac{1}{2}\right) \) above. On the triangular lattice, Wierman [27] proved that

\[ p_c = 2 \cdot \sin\left(\frac{\pi}{18}\right) = 0.347296355333860698... \]

corresponding to another exact expression [7], [54]

\[ K_B(p_c) = \frac{35}{4} - \frac{3}{2} \cdot \csc\left(\frac{\pi}{18}\right) = \frac{23}{4} - \frac{3}{2} \cdot \left\{ \frac{\sqrt{4 \cdot (1 + i\sqrt{3})}}{4} + \frac{\sqrt{4 \cdot (1 - i\sqrt{3})}}{4} \right\} = 0.111842752845497... \]

Similar results apply for the hexagonal lattice by duality.

Much energy has been placed into the computation of universal exponents for random lattice models in \( d \)-dimensional space (akin to what we briefly mentioned for self-avoiding walks). The existence of such exponents is hypothesized on the basis of both theoretical procedures (finite size scaling and renormalization group methods) and experimental data. We shall not attempt to discuss this important subject, but instead refer readers to [33], [46], [27].
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Steven R. Finch
MathSoft Inc., 101 Main Street
Cambridge, MA, USA 02142
sfinch@mathsoft.com
\[ \Lambda(2) = 2 \]
