Improved lower bounds on the connective constants for two-dimensional self-avoiding walks

Iwan Jensen

ARC Centre of Excellence for Mathematics and Statistics of Complex Systems, Department of Mathematics and Statistics, The University of Melbourne, Victoria 3010, Australia

E-mail: `I.Jensen@ms.unimelb.edu.au`

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Abstract. We calculate improved lower bounds for the connective constants for self-avoiding walks on the square, hexagonal, triangular, (4.8^2), and (3.12^2) lattices. The bound is found by Kesten's method of irreducible bridges. This involves using transfer-matrix techniques to exactly enumerate the number of bridges of a given span to very many steps. Upper bounds are obtained from recent exact enumeration data for the number of self-avoiding walks and compared to current best available upper bounds from other methods.

1. Introduction

The self-avoiding walk (SAW) on regular lattices is one of the most important and classic combinatorial problems in statistical mechanics [18]. An *n-step self-avoiding walk* $\boldsymbol{\omega}$ on a regular lattice is a sequence of *distinct* vertices $\omega_0, \omega_1, \ldots, \omega_n$ such that each vertex is a nearest neighbour of it predecessor. SAWs are considered distinct up to translations of the starting point ω_0. The fundamental problem is the calculation (up to translation) of the number of SAWs, c_n, with n steps. It is generally believed that c_n grows exponentially with power law corrections

$$c_n \sim A\mu^n n^{\gamma-1}, \tag{1}$$

where μ is called the *connective constant*, γ is a critical exponent and A a critical amplitude. Hammersley and Morton [10] were the first to prove the existence of the limit

$$\mu = \lim_{n\to\infty} c_n^{1/n} \tag{2}$$

The exact value of μ is known only on the hexagonal lattice, where Nienhuis [19, 20] showed, using non-rigorous methods, that $\mu_{\rm hex} = \sqrt{2+\sqrt{2}}$, and on the (3.12^2) lattice, where Jensen and Guttmann [15] found an exact and rigorous connection between the connective constant $\mu_{(3.12^2)}$ and the connective constant for the hexagonal lattice $\mu_{\rm hex} = \mu^3_{(3.12^2)}/(\mu_{(3.12^2)}+1)$. On the square lattice it has been observed [5] that $\mu_{\rm sq}$ is indistinguishable from the reciprocal of the unique positive root x_c of the simple polynomial $581x^4 + 7x^2 - 13 = 0$, and while this 'conjecture' has stood the test of time it remains a purely numerical observation.

Since finding the exact value of μ (let alone proving such results rigorously) is extremely difficult much effort has been devoted to more general methods for proving rigorous *bounds* on the connective constant. Brief overviews of some of the methods used can be found in [18, 7]. A systematic procedure for improving the lower bounds can be devised from a method due to Kesten [16]. It was used by Guttmann [7] to improve the lower bounds for the connective constant on the square and simple cubic lattices and more recently by Alm and Parviainen [4] to obtain improved lower bounds on the connective constant for the hexagonal lattice. In this paper we further refine these bounds and extend the work to the triangular, kagomé and (4.8^2) lattices.

Finally, we use recent exact enumeration data for c_n to obtain upper bounds for the connective constant on the square, hexagonal and triangular lattices. These bounds are then compared to better upper bounds obtained from other methods.

2. Lower bounds

Lower bounds for the connective constant can be found using a method due to Kesten [16]. The method utilises the fundamental result that certain restricted classes of self-avoiding walks have the same connective constant as the unrestricted problem.

Particularly useful for our purposes is the class of walks known as *bridges*. Let x_j denote the x-coordinate of ω_j, then a bridge is a self-avoiding walk such that $x_0 < x_j \le x_n$ for all $j > 0$. We use b_n to denote the number of n-step bridges, and note Kesten showed that $b_n^{1/n}$ converges to μ as $n \to \infty$. Clearly concatenating two bridges of length n and m gives a bridge of length $n+m$ (we place the origin of the second walk on top of the end-point of the first walk). This means that any bridge can be decomposed into *irreducible bridges*, i.e., bridges which cannot be decomposed further, and we use a_n to denote the number of n-step irreducible bridges. It is now easy to see that the generating function $B(x)$ for bridges is simply related to the generating function for irreducible bridges $A(x)$

$$B(x) = \frac{1}{1 - A(x)}.$$

It then follows that $1/\mu$ is the solution to $A(x) = 1$. This relation also allows us to obtain lower bounds for μ. This relies on the observation that, if $0 \le \tilde{a}_n \le a_n$, for $n \ge 2$, then with x_c being the solution to

$$\sum_{n=1}^{\infty} \tilde{a}_n x^n = 1 \tag{3}$$

$1/x_c$ is a lower bound on μ. In particular we can set $\tilde{a}_n = 0$ for $n > N$ and thus truncate the series.

It is not easy to calculate the number of irreducible bridges directly. Thankfully they can easily be obtained from the number of bridges. Following Alm and Parviainen [4] we consider the number of bridges $b_{n,l}$ and irreducible bridges $a_{n,l}$ of length n and span l, that is bridges with $x_0 = 0$ and $x_n = l > 0$, with associated generating functions $B_l(x)$ and $A_l(x)$. Obviously $\sum_{l=1}^{\infty} a_{n,l} = a_n$, so if we truncate at some maximum span L and maximum walk length N then the reciprocal of the solution to

$$\sum_{n=1}^{N} \sum_{l=1}^{L} a_{n,l} x^n = 1 \tag{4}$$

is a lower bound on μ.

Since a bridge is either irreducible or the concatenation of a bridge with an irreducible bridge we get

$$B_l(x) = A_l(x) + \sum_{k=1}^{l-1} A_{l-k}(x) B_k(x)$$

and thus

$$A_l(x) = B_l(x) - \sum_{k=1}^{l-1} A_{l-k}(x) B_k(x),$$

which allows to obtain all generating functions $A_l(x)$ recursively from $B_l(x)$ for $1 \le l \le L$.

In this paper we also examine a second way of obtaining lower bounds. We again use irreducible bridges, but rather than using smallish L and very large N we calculate the exact series for irreducible bridges to order N (much lower than before) and use this truncated series to obtain a lower bound from the reciprocal of the solution to

$$\sum_{n=1}^{N} a_n x^n = 1, \tag{5}$$

that is in Eq. (3) we set $\tilde{a}_n = a_n$ for $n \leq N$ and $\tilde{a}_n = 0$ for $n > N$.

2.1. Enumeration of self-avoiding bridges

The number of self-avoiding bridges $b_{n,l}$ can easily be counted using the Transfer-Matrix (TM) methods we have developed for the unrestricted problems [12, 13, 14], which are devised to count the number of walks in a finite $l \times w$ rectangular sub-section of the underlying lattice. Here we shall only briefly outline the changes required to enumerate bridges. The most efficient implementation of the TM algorithm generally involves bisecting the rectangle with a boundary line and moving the boundary in such a way as to build up the lattice cell by cell. The sum over all contributing graphs is calculated as the boundary is moved through the lattice. For each configuration of occupied or empty edges along the intersection we maintain a generating function for partial walks cutting the intersection in that particular pattern. If we draw a SAW and then cut it by a line we observe that the partial SAW to the left of this line consists of a number of loops connecting two edges in the intersection, and at most two pieces connected to only one edge (these are the pieces from the end-points of the SAW). The computational complexity of the algorithm is essentially determined by the number of such configurations. So we must make the intersection as short as possible. Since we are looking to fix l and make N large it follows that w will be large as well (in fact proportional to $N - l$). So the boundary line must intersect the rectangle along the 'bridging' axis, e.g., along up to $l + 2$ edges. It is quite easy to demonstrate [5, 12] that the number of configurations grows like 3^l in the square lattice case. So the required CPU time will grow roughly as $(w + l)^2 3^l = N^2 3^l$, since there are $(w + l) = N$ updates and terms in the generating functions. Memory requirement will grow as $N3^l$. We note in passing that while the TM method can be used to study higher-dimensional lattices it quickly becomes inefficient because the boundary would be $(d - 1)$ dimensional and the number of edges in the intersection would grow ever more rapidly.

In order to implement the first method for finding lower bounds, see Eq. (4), we count the number of bridges spanning rectangles of size $l \times w$, that is bridges starting at the bottom border and terminating at the top border. In addition the walks must also touch the left border of the rectangle (this takes care of the translational invariance) as illustrated in Figure 1. In all case bridges must terminate at a top most vertex in the top most row. Note in particular the implication of this restriction on the hexagonal, kagomé, and (4.8^2) lattices. For the hexagonal case this means that all bridges are of even length.

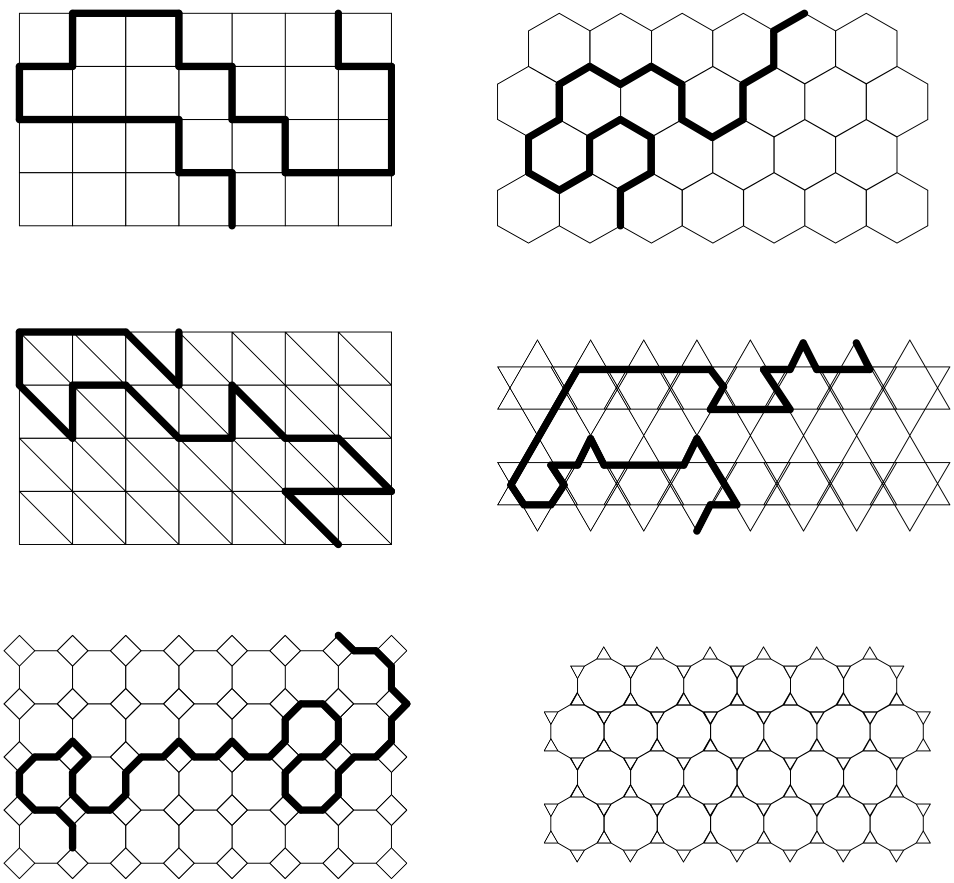

Figure 1. Examples of bridges on the square, hexagonal, triangular, kagomé and (4.8^2) lattices. In addition we also show a section of the (3.12^2) lattice.

For the square lattice we calculated the number of bridges to $L = 15$ and $N = 250$, for the hexagonal lattice to $L = 15$ and $N = 500$, for the triangular lattice to $L = 12$ and $N = 150$, for the kagomé lattice to $L = 10$ and $N = 300$,and for the (4.8^2) lattice to $L = 12$ and $N = 500$. Because of the exact connection between the connective constants $\mu_{(3.12^2)}$ and $\mu_{\rm hex}$, $\mu_{\rm hex} = \mu^3_{(3.12^2)}/(\mu_{(3.12^2)}+1)$, any bounds for the hexagonal lattice yields corresponding bounds for the (3.12^2) lattice. So we don't actually count bridges on the (3.12^2) lattice and have thus not shown an example of one in Figure 1.

The integer coefficients occurring in the series expansions become very large. The calculations were therefore performed using modular arithmetic [17]. This involves performing the calculation modulo various integers p_i and then reconstructing the full integer coefficients at the end. The p_i are called moduli and must be chosen so they are mutually prime. The Chinese remainder theorem ensures that any integer has a unique representation in terms of residues. If the largest value occurring in the final expansion is m, then we have to use a number of moduli k such that $p_1 p_2 \cdots p_k > m$. We used moduli which are prime numbers of the form $p_k = 2^{30} - r_k$.

Naturally the calculation for each l and moduli are completely independent. It is evident from the exponential growth in the computational complexity most of the CPU time is spent on the largest value of L, where up to 16 moduli were required to represent the coefficients. Typically each run (at the maximal span L) required up to 24 CPU hours on a 1GHz Alpha processor and could use up to 2.5Gb of memory. In all we used about 3000 CPU hours on the calculations. Our method is much more efficient than that used by Alm and Parviainen [4], who report using more than 20000 CPU hours calculating the number of bridges on the hexagonal lattice with $L = 10$ and $N = 58$. A similar calculation using our method takes no more than a couple of minutes!

The second method for finding lower bounds, see Eq. (5), uses the exact data for the number of irreducible bridges up to length N. Again the first step is the calculation of the relevant data for bridges. We illustrate the method in the square lattice case. An irreducible bridge of width L has length at least $3L$. This is because each row (apart from the bottom most) must have more than one occupied edge (otherwise we could cut the walk into two bridges) and the walk must thus go up, come down, and go up again. We also have the first step and at least two horizontal steps for a grand total of at least $3L$ steps. So if we require the number of irreducible bridges to order N we must count the number of bridges with span up to $L = N/3$. That is we have to count the number of bridges on rectangles of size $w \times l$, where $1 \leq l \leq L = N/3$ and $1 \leq w \leq N - l$. Note that this calculation gives the number of bridges correctly only to order L. However, by first extracting the series for $A(x)$ we can also get $B(x) = 1/(1 - A(x))$ correct to order $3L$. The efficient calculation of the bridge generating function is in many aspects more complicated and time consuming than for the first method. Details of the properties of the bridge generating function will appear in a separate paper. Suffice to say that we have obtained generating functions to order 72 on the square lattice and 122 on the hexagonal lattice.

The series for the problems studied in this paper can be obtained by request from the author or at http://www.ms.unimelb.edu.au/∼iwan/ by following the relevant links.

2.2. Results

Lower bounds are obtained by forming the polynomials of Eq. (4). It is thus possible to obtain ever improved lower bounds by increasing N and L. In Table 1 we use the hexagonal lattice data to illustrate the method. Note that for this problem the minimal number of steps for an irreducible bridge of span L is $6L - 2$. From this data we observe first of all, that for $N = 100$ little is gained by going beyond span $L = 12$. This is somewhat surprising since $A_{13}(x)$ contributes already at order 76, but obviously the influence of these terms is almost negligible. Likewise with fixed L and increasing N it is a case of rapidly diminishing returns. If we are interested in optimising the procedure, that is, getting a decent bound, but with as little wasted effort possible, it appears that for given L we should choose N larger than twice the order of the first non-zero contribution to $A_L(x)$ (otherwise the calculation of $A_L(x)$ is largely wasted)

Table 1. Lower bounds for the connective constant for the hexagonal lattice. The supposed exact value is $\mu = \sqrt{2+\sqrt{2}} = 1.847759065\ldots$.

L	$N = 100$	$N = 200$	$N = 300$	$N = 400$	$N = 500$
2	1.787760	1.787760	1.787760	1.787760	1.787760
3	1.808678	1.808678	1.808678	1.808678	1.808678
4	1.819369	1.819370	1.819370	1.819370	1.819370
5	1.825750	1.825767	1.825767	1.825767	1.825767
6	1.829869	1.829984	1.829984	1.829984	1.829984
7	1.832546	1.832950	1.832951	1.832951	1.832951
8	1.834182	1.835137	1.835140	1.835140	1.835140
9	1.835061	1.836802	1.836814	1.836814	1.836814
10	1.835448	1.838094	1.838132	1.838132	1.838132
11	1.835574	1.839101	1.839191	1.839193	1.839193
12	1.835602	1.839878	1.840058	1.840063	1.840063
13	1.835606	1.840464	1.840775	1.840788	1.840789
14	1.835606	1.840890	1.841372	1.841400	1.841402
15	1.835606	1.841184	1.841868	1.841921	1.841925

but not much larger than four times this order. Similar considerations apply to the other problems as well though the optimal cut-off varies from problem to problem.

Here we briefly summarise our results for the lower bounds. For the hexagonal lattice we find the lower bound, $1.841925 < \mu_{\rm hex}$, which is less than 0.32% lower than the exact value $\mu_{\rm hex} = \sqrt{2+\sqrt{2}} = 1.847759065\ldots$. The previous best lower bound was $1.833009 < \mu_{\rm hex}$ [4]. For the square lattice we obtain the lower bound, $2.625622 < \mu_{\rm sq}$, which is within 0.48% of the best estimate for the connective constant $\mu_{\rm sq} = 2.63815853031(3)$ [11]. This should be compared to the previous bound $2.62006 < \mu_{\rm sq}$ [6]. For the triangular lattice the lower bound is, $4.118935 < \mu_{\rm tri}$, within 0.77% of the best estimate $\mu_{\rm tri} = 4.150797226(26)$ [13], whereas the previous best bound was $4.03333 < \mu_{\rm tri}$ [3]. The Kagomé lattice lower bound is, $2.548497 < \mu_{\rm kag}$, within 0.48% of the estimate $\mu_{\rm kag} = 2.560576765(10)$ (based on our unpublished enumerations of self-avoiding polygons), while the previous best bound was $2.50967 < \mu_{\rm kag}$ [3]. For the (4.8^2) lattice we found the lower bound, $1.804596 < \mu_{(4.8^2)}$, which is just 0.24% lower that the estimate $\mu_{(4.8^2)} = 1.80883001(6)$ [15], which improves on the bound $1.78564 < \mu_{(4.8^2)}$ [3]. Finally, for the (3.12^2) lattice we get the lower bound, $1.708553 < \mu_{(3.12^2)}$, which is just 0.15% from the exact value $\mu_{(3.12^2)} = 1.711041296\ldots$ [15], and again improves on the previous bound $1.705263 < \mu_{(3.12^2)}$ [4].

As stated earlier we also used a second approach to obtain lower bounds for the connective constant. This entails the calculation of an exact series expansion for the generating function for irreducible bridges up to some maximal order N (this was also the method employed by Guttmann [7, 8]). Lower bounds are then obtained from the truncated series in Eq. (5). Obviously we could truncate at any order $n < N$ and obtain a sequence of lower bounds $\mu(n)$. In Table 2 we have listed the lower bounds obtained from this method for the hexagonal and square lattice cases. Clearly this method

Table 2. Lower bounds for the connective constant for the hexagonal and square lattices.

Hexagonal		Square	
N	Bound	N	Bound
32	1.812833	30	2.583704
38	1.817977	33	2.588448
44	1.821786	36	2.592419
50	1.824722	39	2.595794
56	1.827055	42	2.598698
62	1.828955	45	2.601224
68	1.830532	48	2.603442
74	1.831863	51	2.605405
80	1.833002	54	2.607155
86	1.833987	57	2.608726
92	1.834847	60	2.610143
98	1.835606	63	2.611428
104	1.836279	66	2.612599
110	1.836882	69	2.613671
116	1.837424	72	2.614656

is inferior to the previous one (the bounds are not as good) particularly considering that the computational effort is significantly greater. However, this approach allows us to study the convergence of the lower bounds $\mu(n)$ to the connective constant as a function of the truncation order n. We find that $\mu - \mu(n) \sim a/n$, this behaviour can be seen directly in Fig. 2 where we have plotted $\mu - \mu(n)$ vs. $1/n$. We also formed the generating function $D(x) = \sum_n d_n x^n$, where $d_n = \mu - \mu(n)$, analysed this using differential approximants and found a logarithmic singularity at $x_c = 1$, as expected if $d_n \sim a/n$.

3. Upper bounds

The best current method for obtaining upper bounds is due to Alm [2] and it essentially requires one to enumerate the number of walks according to length n and a specified head and tail each of length m. More precisely Alm showed that

$$\mu \leq (\lambda(G(m,n)))^{1/(n-m)}, \tag{6}$$

where λ is the largest eigenvalue of the matrix $G(m,n)$. The entries g_{ij} of this matrix are equal to the number of n-step self-avoiding walks starting with a walk $\boldsymbol{\omega}_i$ and ending with a translation of a walk $\boldsymbol{\omega}_j$. Each walk $\boldsymbol{\omega}_i$, $i = 1, \ldots, K_m$, is one of the K_m possible m-step self-avoiding walks (up to all possible symmetries). While this method can yield quite sharp upper bounds (within 1.1% for the hexagonal lattice [4]) it is unfortunately not suited for a transfer-matrix enumeration.

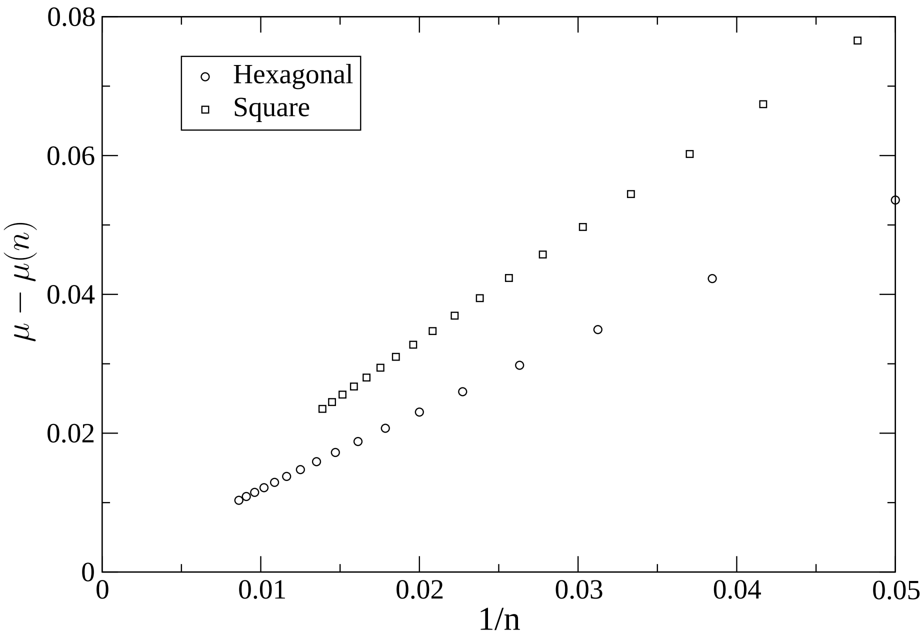

Figure 2. The difference between the connective constant μ and the lower bound $\mu(n)$ vs. $1/n$. Data is plotted for the hexagonal and square lattices.

However, we have recently obtained greatly extended series for the number of SAWs on the square, hexagonal and triangular lattices [12, 13, 14]. This allows us to use a special case of Alm's work [2] which states that if $K_m = 1$ then

$$\mu \leq \mu_m(n) = (c_n/c_m)^{1/(n-m)}. \tag{7}$$

On all lattices $K_1 = 1$ so $\mu \leq \mu_1(n) = (c_n/c_1)^{1/(n-1)}$ as proven earlier by Ahlberg and Janson [1] while $K_2 = 1$ for the hexagonal and L lattices yielding sharper bounds $\mu \leq \mu_2(n) = (c_n/c_2)^{1/(n-2)}$ as proven by Guttmann [8]. Ahlberg and Janson also proved that an upper bound $\mu_a(n)$ can be obtained from the positive root of the equation

$$zx^{n-1} = [c_n - (z-2)c_{n-1}]x + (z-2)[(z-1)c_{n-1} - c_n], \tag{8}$$

where $z = c_1$ is the coordination number of the lattice. An upper bound is then found as $\min(\mu_m(n), \mu_a(n))$.

For the square lattice we have $c_{71} = 4190893020903935054619120005916$ and $c_{70} = 1580784678250571882017480243636$, which gives us the upper bounds $\mu_1 = 2.684484$ and $\mu_a = 2.681360$. These bounds are sharper than the one obtained by Alm [2], $\mu_{\text{sq}} < 2.695759$, using $n = 24$ and $m = 8$. An improved upper bound, $\mu_{\text{sq}} < 2.679193$, has been obtained by Pönitz and Tillmann [21], by counting walks with finite memory.

For the triangular lattice we have $c_{40} = 2261091167257542651065322 6$ and $c_{39} = 5401678666643658402327390$, which gives us the upper bounds $\mu_1 = 4.267349$ and $\mu_a = 4.263713$. These bounds are sharper than the one obtained by Alm [2], $\mu_{\text{tri}} < 4.277799$, using $n = 16$ and $m = 6$ (Alm has since improved this to $\mu_{\text{tri}} < 4.25152$ [3]).

Table 3. Summary of results for the connective constant μ with the current best lower and upper bounds

Lattice	Lower Bound	μ	Upper Bound
Square	2.625622	2.63815853031(3) [11]	2.679193 [21]
Hexagonal	1.841925	1.847759065 . . . [19]	1.868832 [4]
Triangular	4.118935	4.150797226(26) [13]	4.25152 [3]
Kagomé	2.548497	2.560576765(10)	2.590301 [9]
(4.8^2)	1.804596	1.80883001(6) [15]	1.82926 [3]
(3.12^2)	1.708553	1.711041296 . . . [15]	1.719254 [4]

For the hexagonal lattice we have $c_{100} = 2585241775338665938539885252$ and $c_{99} = 1394474897269109512317080364$, which gives us the upper bounds $\mu_1 = 1.871004$, $\mu_2 = 1.869731$ and $\mu_a = 1.869836$. This should be compared with the sharper bound $\mu_{\rm hex} \leq 1.868832$ obtained in [4] using the method of [2] with $n = 45$ and $m = 17$.

It is clear that sharper upper bounds can be obtained for square and triangular lattices by Alm's method if carried out to higher values of n and m. Judging from the computational resources (928 CPU hours) required to obtain the bounds in [4] this should not be a very demanding calculation (compare this to the 25000 CPU hours used for the enumeration of the hexagonal lattice SAWs).

4. Summary

We have used Kesten's method of irreducible bridges to obtain improved lower bounds on the connective constant for self-avoiding walks on several planar lattices. The number of irreducible bridges is obtained by enumerating exactly the number of bridges using transfer-matrix techniques. In one approach we calculate the number of bridges of limited span but to great lengths while in a second approach we obtain an exact series expansion for the number of irreducible bridges. The first approach turns out to yield the sharpest lower bounds. The second approach allows us to study the convergence of the lower bounds $\mu(n)$ to the connective constant as a function of the truncation order n. We find that the limit is approached linearly in $1/n$. In addition we use recent exact data for the number of SAWs c_n to obtain some upper bounds on the connective constant. The upper bounds are generally much poorer than the lower bounds and also worse than those already obtained by other methods. We have summarised the results in Table 3.

5. Acknowledgments

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