Three-dimensional terminally attached self-avoiding walks and bridges

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Abstract

We study terminally attached self-avoiding walks and bridges on the simple cubic lattice, both by series analysis and Monte Carlo methods. We provide strong numerical evidence supporting a scaling relation between self-avoiding walks, bridges, and terminally attached self-avoiding walks, and posit that a corresponding amplitude ratio is a universal quantity.

Keywords: self-avoiding walk; critical exponents; universal amplitude ratio; Monte Carlo; pivot algorithm

1 Introduction

A self-avoiding walk (SAW) on a lattice is an open, connected path on the lattice that does not revisit any previously visited vertex. Walks are considered distinct if they are not translates of one another. If we let the number of SAWs of \( n \) steps be \( c_n \), it is known that \( \lim_{n \to \infty} n^{-1} \log c_n = \log \mu \) exists \[18\], where \( \mu \) is the growth constant of self-avoiding walks on the lattice. This work will consider SAWs on the 3-dimensional simple cubic lattice \( \mathbb{Z}^3 \), with the vertices having integer coordinates \( \{x(i), y(i), z(i)\} \), for \( i = 0, 1, \ldots, n \).

The upper half-space \( \mathbb{H} \), is characterised by \( z \geq 0 \). An \( n \)-step bridge is a self-avoiding walk in the upper half-space that starts at the origin and is constrained so that \( z(0) < z(i) \leq z(n) \) for any \( 0 < i \leq n \). We denote the number of \( n \)-step bridges starting at the origin by \( b_n \). It is known that \( \lim_{n \to \infty} n^{-1} \log b_n = \log \mu \), where \( \mu \) is unchanged from the corresponding value for SAWs \[19\].

A terminally attached self-avoiding walk, or TAW, is a SAW with one end anchored in the surface, but with the rest of the walk free in the upper half-space. Terminally attached self-avoiding walks are also referred to as half-space self-avoiding walks in the literature. Clearly TAWs are a superset of bridges, and a subset of SAWs, so have the same growth constant. The number of \( n \)-step TAWs starting at the origin is denoted by \( t_n \).

The last subset of SAWs we wish to consider are arches, which are SAWs in the upper half-space with both the start- and end-point constrained to lie in the 2-dimensional surface \( z = 0 \). That is to say, \( z(0) = 0 = z(n) \). As the number of arches is bounded above by the number of SAWs and below by the number of self-avoiding polygons (SAPs), which are known to have the same growth constant as SAWs \[20\], it follows that arches

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also have the same growth constant as SAWs. The number of \( n \)-step arches starting at the origin is denoted by \( a_n \).

The results on growth constants are the only results that have been proved. Nevertheless, it is universally accepted that the asymptotic behaviour of the above objects is given by:

\[
\begin{align*}
c_n & \sim A \cdot \mu^n \cdot n^{\gamma - 1}, \\
b_n & \sim B \cdot \mu^n \cdot n^{\gamma_b - 1}, \\
t_n & \sim H \cdot \mu^n \cdot n^{\gamma_1 - 1}, \\
a_n & \sim C \cdot \mu^n \cdot n^{\gamma_{11} - 1},
\end{align*}
\]

for SAWs, bridges, TAWs and arches respectively. The existence of the various critical exponents has not been proved, but is universally accepted, and will be assumed hereinafter.

All the above definitions also hold for the two-dimensional square lattice, where the upper half-space referred to becomes the upper half-plane, and the originating surface is the line \( y = 0 \).

Another critical exponent that needs to be defined is that which characterises the length of a SAW. All standard measures of the square of the length, such as the mean-squared end-to-end distance, the radius of gyration, the squared caliper span etc., behave as \( \text{const} \times n^{2\nu} \), where in two dimensions it is accepted that \( \nu = 3/4 \). This exponent can also be understood as the reciprocal of the fractal dimension, \( d_f \).

In two dimensions, the exponents are known exactly (assuming existence). In that case it is believed that \( \gamma = 43/32, \gamma_1 = 61/64, \) and \( \gamma_{11} = -3/16 \). As far as we are aware, there are no published estimates for \( \gamma_b \), but as long ago as last millennium one of us (AJG) estimated the value of this exponent by series analysis to be \( 9/16 \). Subsequently, much longer series have been produced by Iwan Jensen, which enabled this estimate to be affirmed with much greater confidence. Somewhat later, Alberts and Madras (private communication) obtained the estimate \( \gamma_b = 9/16 \) for two-dimensional bridges through SLE arguments, subject to certain unproven assumptions, but this work was never published.

In \cite{[9]} both SAWs spanning a strip and bridges were discussed, and comparisons made with conjectured results from SLE\(_{8/3}\). The arguments given there allow one to predict \( \gamma_b \), and they are reproduced, in summary, here. In \cite{[28]} it was explained why the measure of bridges starting at the origin and ending at \( x + iy \) should be \( y^{-5/4} f(x/y) \) for an (explicit) function \( f \) that decays exponentially. Summing over all values of \( x \), it follows that the measure of bridges starting at the origin and ending at height \( h \) should be asymptotic to a constant times \( h^{-1/4} \). Then by integrating over height, the measure of bridges of height less than or equal to \( h \) should grow as \( h^{3/4} \).

Recall that for two-dimensional SAWs and bridges the exponent \( \nu = 1/d_f = 3/4 \). If we weight each bridge of length \( n \) by \( \mu^{-n} \), so that the normalised counts are given by \( b_n \mu^{-n} \), it follows that normalised bridges of height \( h \) typically have \( h^{d_f} = h^{4/3} \) steps. Hence the measure of bridges of \( n \) steps should be the same as the measure of bridges of height at most \( n^{3/4} \), which gives \( (n^{3/4})^{3/4} = n^{9/16} \) for the measure. Equivalently, the number of bridges of exactly \( n \) steps grows like \( b_n \sim \text{const} \times \mu^n \times n^{9/16 - 1} = \text{const} \times \mu^n \times n^{-7/16} \), so that \( \gamma_b = 9/16 \).

These exponents are not all independent. There is a scaling relation, due to Barber \cite{[1]}:

\[
2\gamma_1 - \gamma_{11} = \gamma + \nu,
\]
which holds independent of dimension. Very recently, Duplantier and Guttmann [10] have proposed the existence of another scaling relation giving the bridge exponent,

\[ \gamma_b = \gamma_{11} + \nu. \] (6)

As expected, the exponents given above for two-dimensional SAWs satisfy both these relations.

In three dimensions the most precise estimates we have are from the Monte Carlo work of one of us [4, 6], with \( \mu = 4.684039931 \pm 0.00000027, \gamma = 1.156957 \pm 0.000009 \) and \( \nu = 0.587597 \pm 0.000007 \), though the details of the Monte Carlo simulation for the estimation of \( \gamma \) have not yet been published. For \( \gamma_1 \) there are a few estimates in the literature based on rather short series. Some 30 years ago, Guttmann and Torrie [17] estimated \( \gamma_1 = 0.676 \pm 0.009 \), while the most recent Monte Carlo estimate is by Grassberger [23] who estimated \( \gamma_1 = 0.6786 \pm 0.0012 \). From Barber’s scaling relation this gives \( \gamma_{11} = -0.3874 \pm 0.0024 \).

There is renewed interest in the values of the exponents \( \gamma_1 \) and \( \gamma_b \) in this case, as the former exponent arises in recent tests for the conformal invariance of 3d SAWs [25, 26], and the latter has been predicted by the recent scaling argument [10] given above, and estimation of the exponent \( \gamma_b \) would be a useful test of that scaling relation. More precisely, Kennedy discusses the hitting density of a SAW in a connected domain when conformally mapped by a function \( f \) to another domain. The hitting densities with respect to arc length in the two domains are related by \( |f'(z)|^b \), where \( b \) is a critical exponent, identified by scaling arguments as

\[ b = \frac{\gamma - 2\gamma_1}{2\nu} + \frac{d}{2}, \] (7)

\[ = -\frac{\gamma_b}{2\nu} + \frac{d}{2}. \] (8)

Note that the above exponent estimates give the prediction \( b = 1.3296 \pm 0.0020 \), compared to Kennedy’s direct Monte Carlo estimate \( b = 1.3303 \pm 0.0003 \) [26]. For the bridge exponent the prediction from the pre-existing exponent estimates is \( \gamma_b = 0.2002 \pm 0.0024 \).

In this paper we will estimate critical exponents and amplitudes associated with bridges and TAWs via series and Monte Carlo methods.

### 1.1 Universal amplitude ratio

Combining the two scaling relations, (5) and (6), given in Sec. 1, we obtain

\[ 2\gamma_1 = \gamma + \gamma_b. \] (9)

This exact relation suggests that the relationship between amplitudes corresponding to the LHS and RHS of the equation must be lattice independent, which in turn leads to a universal amplitude ratio.

One interesting aspect of this ratio is that the objects involved are bridges and TAWs, which interact with a surface. Loosely speaking, the scaling relation (9) may be interpreted as saying that the exponent associated with the number of pairs of TAWs of length \( n \) (which together have 2 free ends, and two ends anchored to a surface) is the same as the exponent associated with the number of pairs made up of a SAW and a bridge, each of length \( n \).
In order for the lattice specific effects to cancel it is crucial that the boundary condition where the walk terminates on the surface is the same for the TAWs and both ends of the bridges.

Now, the TAWs are anchored to the surface, and must satisfy the rule that the entire walk lies above this surface. In contrast, for convenience the bridges are defined to be asymmetric, with an additional step prepended to one end to lift it completely out of the surface at one end.

Thus we need modify the definition of a bridge to make it symmetric between its two ends. The most natural way to do this is to remove the trivial edge from the start of the bridge. Conveniently, a straight-forward bijection exists between modified bridges of length $n$ which satisfy $z(0) \leq z(i) \leq z(n)$ for any $0 \leq i \leq n$, and the usual bridges of length $n + 1$ which satisfy $z(0) < z(i) \leq z(n+1)$ for any $0 < i \leq n + 1$. Hence the number of modified bridges of length $n$ is just $b_{n+1}$, and this is the coefficient that must be used in the definition of the amplitude ratio.

At the coefficient level, the above considerations lead to the following sequence of ratios

$$K_n = \frac{t_n^2}{c_n \cdot b_{n+1}} \sim \frac{H^2}{\mu A B} n^{2\gamma_1 - \gamma_6 - \gamma} (1 + o(1)),$$  
(10)

$$K \equiv \lim_{n \to \infty} K_n = \frac{H^2}{\mu A B},$$  
(11)

where the amplitudes $A$, $B$, and $H$ are from (1)–(3), and $K$ is a universal constant. That is to say, we expect this ratio $K$ to depend only on the spatial dimension of the lattice.

In terms of generating functions, the amplitude ratio is given as the limit

$$\lim_{x \to x_c^-} \frac{T(x)^2}{\mu \cdot C(x) \cdot B(x)} = \text{Universal constant.}$$  
(12)

### 1.2 Confidence intervals

We wish to highlight that the error estimates for the quantities calculated in this paper are not purely statistical, and hence there is a degree of subjectivity in obtaining them. In the analysis of relatively short series, which is the best that can be achieved for non-trivial 3d models such as SAWs, TAWs, and bridges, the interpretation of the results from series analysis can be quite subtle, and it is easy to be overly optimistic in interpreting the convergence (or lack thereof) of a sequence of improved estimates. For our Monte Carlo results we are approaching the large $n$ limit, and consequently there is a lesser (but non-zero) amount of subjectivity involved.

We have included plots where relevant to allow readers to judge for themselves how reliable our confidence intervals are. Loosely, one may think of the confidence intervals given in this paper as being roughly equivalent to a single standard deviation.
1.3 Outline

In Sec. 2 we describe the generation of the series data for simple cubic lattice TAWs and bridges, which is then analysed in the Sec. 3. Thereafter we describe the Monte Carlo computer experiment in Sec. 4 and analyse the resulting data in Sec. 5. Finally, we discuss possible extensions and conclude in Sec. 6.

2 Generation of series data

We directly enumerated bridges and TAWs via a straight-forward optimized backtracking algorithm, whose running time was roughly proportional to the number of items being computed.

To enumerate TAWs up to a certain length a recursive function was used that took the set of sites currently visited, the coordinates of the current site, and the maximum number of bonds left. The function first adds one to the tally of TAWs of the current length. It then, assuming there is at least one bond left, chooses each unused adjacent site (not allowing negative z coordinates) and calls the function again with that site as the current site, and one fewer sites remaining.

This algorithm clearly has the function called exactly once for each TAW enumerated. As each iteration of the recursive function contains a small amount of code, with only one loop over adjacent sites (maximum 6), its execution time is exactly proportional to the number of TAWs enumerated.

Enumerating bridges uses a very similar algorithm. In this case the recursive algorithm keeps track of an extra variable; the maximum z value reached ($Z_{\text{max}}$). Now instead of adding one to the TAW tally on each function call, a check is performed to see if the $z$ coordinate of the current site equals $Z_{\text{max}}$.

As described, this algorithm would have execution time proportional to the number of TAWs, as exactly the same function calls would be made as for the TAWs. The performance can be improved to be proportional to the (significantly smaller) number of bridges by pruning the search tree when the current TAW cannot ever result in a valid bridge. This can be prohibitively expensive to compute exactly; a fast and very effective heuristic is to prune any branches when the $z$ coordinate of the current point plus the number of remaining bonds is less than $Z_{\text{max}}$. This is somewhat conservative; it will not prune every dead branch as there might be an occupied site in the way; however in practice it works very well resulting in a runtime basically proportional to the number of bridges.

We can reduce the work required to determine $b_n$ by enumerating irreducible bridges instead, which are the set of bridges that cannot be decomposed into a sequence of more than one bridge. Irreducible bridges can also be characterised as the set of bridges which have at least 3 bonds between any two layers, other than the first layer, which must have precisely one bond. Each bridge can in fact be uniquely decomposed into a non-empty sequence of irreducible bridges, and so the generating function for bridges, $B(x)$, may be expressed in terms of the generating function for irreducible bridges, $I(x)$, as

$$B(x) = \frac{I(x)}{1 - I(x)}.$$ \hspace{1cm} (13)

Using this relation one may obtain $b_n$ from the series for the less numerous irreducible bridges.
Enumerating irreducible bridges requires a slight modification to the bridges algorithm. In this case yet another variable \( Z_{\text{irr}} \) is kept track of in the recursive function: \( Z_{\text{irr}} \) is the largest \( z \) value below which the TAW is irreducible (it has at least three bonds in the \( z \) direction at each layer). To see if it is a valid irreducible bridge one now checks that the current \( z \) value, \( Z_{\max} \), and \( Z_{\text{irr}} \) are all equal. \( Z_{\text{irr}} \) is easy to keep track of; \( Z_{\text{irr}} \) is incremented whenever a vertical step is made upwards from \( z = Z_{\text{irr}} \), as long as \( Z_{\text{irr}} < Z_{\max} \).

As described, this algorithm would have the same execution time as the bridges algorithm. Again, pruning can improve the speed to close to the significantly smaller number of irreducible bridges. The following conservative heuristic is used:

- If \( z \leq Z_{\text{irr}} \leq Z_{\max} \), prune if the number of remaining steps is less than \( Z_{\max} - z \) (this is the same as the bridges pruning);
- If \( Z_{\text{irr}} < z \leq Z_{\max} \), prune if the number of remaining steps is less than \( Z_{\max} - z + 1 + 2(z - Z_{\text{irr}}) \) (this is due to the need to go back down to \( z = Z_{\text{irr}} \), take one step sideways, and then return to \( z = Z_{\max} \)).

We find that this heuristic works very well in practice, and so the running time is roughly proportional to the number of irreducible bridges.

There were a variety of other optimizations used to give constant improvements, such as assigning each conceivably reachable lattice point an integer index and pre-computing adjacencies so that points were represented by integers rather than a tuple of integers.

Symmetries were taken into account by enumerating all prefixes up to length roughly 8 (it varied somewhat depending on what computer the enumeration was run on), canonicalizing them to account for symmetries, and assigning to equivalence classes. Then the recursive algorithm described above was used on each equivalence class, and the results multiplied by the number of members of the equivalence class. The enumerations for each equivalence class were summed for the final result.

It was then straight-forward to make the algorithm parallel (to run on many different processors simultaneously). Each equivalence class can be computed independently, and so were parcelled out to multiple processors, with the only interaction being the final summation.

The algorithm as described above is in no way specific to three-dimensional systems, and indeed was made to also work in other dimensions. Different lattice types could also be used, but this may affect the heuristics used for pruning dead branches of the search tree.

The memory use is insignificant; execution time is the constraint.

### 3 Analysis of series

As usual, we assume that the critical behaviour of TAWs is given by

\[
T(x) = \sum_{n \geq 0} t_n \cdot x^n \sim A(1 - \mu \cdot x)^{-\gamma_1}(1 + A'(1 - \mu \cdot x)^{\Delta_1}),
\]

(14)
and that of bridges by

\[ B(x) = \sum_{n \geq 0} b_n \cdot x^n \sim C(1 - \mu \cdot x)^{-\gamma_h}(1 + C'(1 - \mu \cdot x)^{\Delta_1}). \]  

(15)

Here \( t_n \) (\( b_n \)) is the number of \( n \)-step TAWs (bridges), counted up to translations. \( \mu \) is the growth constant, for which we assume Clisby’s [6] estimate \( \mu = 4.684039931 \pm 0.000000027 \). Here \( \Delta_1 = 0.528 \pm 0.012 \) [4] is the leading correction-to-scaling exponent. \( A, A', C \) and \( C' \) are critical amplitudes (N.B., these are simply related to, but not the same as, the amplitudes for the series defined previously).

In analysing the data, we have of course assumed the existence of the various critical exponents (which has not been proved), and have also used the best available estimate of the growth constant, given above, and the estimate of the correction-to-scaling exponent \( \Delta_1 \). There are a number of estimates in the literature for this exponent, obtained by a variety of methods, including field theoretical methods, series methods and Monte Carlo methods. Estimates range from 0.47 up to 0.57, with non-overlapping error bars. The recent Monte Carlo work of one of us [4] gives \( \Delta_1 = 0.528 \pm 0.012 \), and it is this value that we will use in our Monte Carlo analysis. However our series work is less precise than the Monte Carlo work, and for that purpose taking \( \Delta_1 = 1/2 \) is sufficiently precise.

In Appendix A we give in Table 6 the series for TAWs up to length 26, and for bridges up to length 28. The bridge series is longer, as we actually counted the far less numerous irreducible bridges, and reconstructed the bridge generating function from the irreducible bridge generating function. We also recorded the heights of the irreducible bridges, and the full two-variable generating function for irreducible bridges, counting both length and height, is given in Table 7 in the appendix. The relationship between bridges and irreducible bridges is given in (13).

We first analysed both the TAW and bridge series by using the standard method of differential approximants [14]. We initially attempted unbiased analyses of both the TAW series and the bridge series. The results were disappointing imprecise, despite choosing to use third order differential approximants, which should, in principle, be able to accommodate the expected confluent singularity structure.

We had always intended to use biased differential approximants, as these are expected to give much more precise estimates of the exponents. But the disappointing lack of well-converged estimates in the unbiased case warns us not to be too hopeful of obtaining excellent results in the biased case. Despite this, the estimates appeared tolerably well converged, and for TAWs we estimated \( \gamma_1 = 0.683 \pm 0.005 \), while for bridges we estimated \( \gamma_h = 0.199 \pm 0.004 \). The estimate of \( \gamma_1 \) just overlaps the earlier Monte Carlo estimate of Grassberger [23], and also just overlaps our much more precise Monte Carlo estimate quoted below. We do not know why this estimate of \( \gamma_1 \) is not more accurate. It is possible that the amplitude of the correction-to-scaling exponent is quite large, but we were unable to confirm this from the available data. The corresponding estimate of the bridge exponent \( \gamma_h \) is in excellent agreement with our Monte Carlo estimate, given below, though that estimate is again significantly more precise. We do not give more details or tables of data here, as in the next subsection we give a more precise analysis.

A completely different method of analysis was also tried. We first calculated the ratios of alternate coefficients, \( r_n = \frac{t_{2n}}{t_{2n+1}} \), where we have used alternate coefficients to minimise the effect of the anti-ferromagnetic singularity located at \( x = -1/\mu \). Then by standard ratio method techniques [14], one expects
the ratios to behave as

\[ r_n \sim \mu \left( 1 + \frac{g}{n} + \frac{c}{n^{1+\Delta_1}} + \frac{d}{n^2} + \cdots \right). \tag{16} \]

Here, for TAWs \( g = \gamma_1 - 1 \), and \( c \) and \( d \) are constants, while for bridges \( g = \gamma_b - 1 \). Using the estimate of \( \mu \) given above, we can then estimate the exponent \( g \) as the limit of the sequence \( g_n \) defined by

\[ g_n = \left( \frac{r_n}{\mu} - 1 \right) n \sim g + \frac{\text{const.}}{n^{\Delta_1}} + \frac{\text{const.}}{n} + \cdots. \tag{17} \]

We used the inbuilt fitting function of Maple to fit the elements of the sequence \( g_n \) from \( n = n_{\min} \) to \( n = n_{\max} \), where \( n_{\max} = 28 \), to

\[ g_n = g + \frac{\text{const.}}{n^{\Delta_1}} + \frac{\text{const.}}{n}, \tag{18} \]

with \( n_{\min} \) varying from 10 up to 21. The estimates of \( g_n \) were reasonably well converged, and in this way we estimated \( g = -0.323 \pm 0.003 \), or \( \gamma_1 = 0.677 \pm 0.003 \). A similar analysis for the bridge series was less well converged. Fitting just to

\[ g_n = \left( \frac{r_n}{\mu} - 1 \right) n \sim g + \frac{\text{const.}}{n^{\Delta_1}} \tag{19} \]

gave a decreasing sequence of estimates of \( g_{\text{bridges}} \), while fitting to

\[ g_n = g + \frac{\text{const.}}{n^{\Delta_1}} + \frac{\text{const.}}{n} \tag{20} \]

as done for TAWs gave an increasing sequence of estimates of \( g_{\text{bridges}} \). Averaging corresponding entries gave a fairly stable sequence, from which we estimated \( g_{\text{bridges}} = -0.802 \pm 0.005 \), or \( \gamma_b = 0.198 \pm 0.005 \).

Combining our results from the two methods of analysis, we give as our series estimates from this data, \( \gamma_1 = 0.680 \pm 0.003 \) and \( \gamma_b = 0.1985 \pm 0.004 \). Again, we do not give more details or tables of data here, as in the next subsection we give a more precise analysis.

### 3.1 Series extension and subsequent analysis

The analysis discussed above is based on the exact series coefficients given in Appendix A. We can however obtain accurate approximations to the next five to seven terms of the series, which can then be used in our ratio analysis. Because every differential approximant that uses all the available series coefficients implicitly predicts all subsequent coefficients, we realised that we could utilise this observation to calculate, approximately, all subsequent coefficients. Of course the number of significant digits decreases as the number of predicted coefficients increases, but as we show below, we can get useful estimates of the next six or seven coefficients.

For every approximant using all the known coefficients, we generated the subsequent six or seven coefficients. We observe that the predicted coefficients agree to a certain number of significant digits among all the approximants, and we take these as our estimates. That is to say, assume we know the coefficients \( a_n \),
for \( n \in [0, N_{\text{max}}] \). We then predict the coefficients \( a_{N_{\text{max}}+1}, a_{N_{\text{max}}+2}, \ldots, a_{N_{\text{max}}+7} \). Our estimate of each such coefficient is given by the average of the values predicted by the differential approximants. We reject obvious outliers, which are infrequent, and quote only those digits for which all approximants agree. So for example if the first 8 digits agree, and the coefficient is predicted to be a 20 digit integer, we will quote the coefficient as the 8 predicted digits followed by 12 zeros. Not surprisingly, we find the greatest number of digits are predicted for \( a_{N_{\text{max}}+1} \), with the number of digits slowly decreasing as we generated further coefficients.

These predicted coefficients are not suitable for including in our differential approximant analysis, as they were derived from lower order differential approximants. However for ratio type analyses they are very well suited, as discrepancies in say the seventh or eighth significant digits will not affect the ratio analysis in the slightest. This is particularly useful in those situations where we suspect there might be a turning point in the behaviour of ratios or their extrapolants with our exact coefficients, as these approximate coefficients are more than accurate enough to reveal such behaviour, if it is present.

As a demonstration of this method, assume we only have 23 terms in the bridge generating function, and we’ll predict the next 6 coefficients. In Table 1 we show the predicted and exact coefficients. (Note that the coefficient of \( x^{29} \) is not exact, but is as predicted from a longer series, as discussed below).

| \( n \) | Predicted bridges | Actual bridges |
|---|---|---|
| 24 | \( 7.115933 \times 10^{14} \) | \( 71153257794069 \) |
| 25 | \( 3.235637 \times 10^{15} \) | \( 323563407977801 \) |
| 26 | \( 1.472844 \times 10^{16} \) | \( 14728414578753489 \) |
| 27 | \( 6.71105 \times 10^{16} \) | \( 67110197685388181 \) |
| 28 | \( 3.06077 \times 10^{17} \) | \( 306074586987649389 \) |
| 29 | \( 1.39718 \times 10^{18} \) | \( 1.397156394 \times 10^{18} \) |

Table 1: Approximate, predicted coefficients of simple cubic lattice bridges of length \( n \), compared to exact values.

Note that in every case the predicted coefficient agrees with the exact coefficient to the order stated, with an uncertainty of a few parts in the last quoted digit. This demonstrates the utility of the method.

In Table 2 are the predicted coefficients from the full series, where, as explained above, we expect errors to be confined to the last quoted non-zero digit. (Of course it is possible that the last digit we are confident of is 0, but nothing is lost in glossing over this).

We repeated the basic ratio analysis described in the previous section, and show in Fig. 1 the estimators \( g_n \) of the exponent \( g \) for TAWs plotted against \( 1/\sqrt{n} \), as is appropriate, see (17). Strong oscillations can be seen, indicating the presence of a significant anti-ferromagnetic term.

We fitted the data using the curve-fitting features of Maple, simply by fitting the data points \( g_n \) from 12 up to \( N_{\text{max}} - k \) for \( k = 0 \ldots 9 \), where \( N_{\text{max}} = 35 \) in the case of bridges and is 34 in the case of TAWs, assuming \( g_n \) is quadratic in \( 1/\sqrt{n} \), as implied by (17). The sequence elements \( g_n \) are shown in Table 3 below.

These sequences have been simply extrapolated, using every alternate term in the case of TAWs, to give the limits below. Note that the extra, approximate, terms are (a) quite precise enough for this sort of analysis,
and (b) move the data into a regime where the extrapolations are much clearer than those using only the exact coefficients. The extrapolation method was based on the observation that the numerical gaps between successive (or alternate, as appropriate) coefficients apparently decrease as a geometric sequence, so this was summed.

As a result of this analysis we find $\gamma_1 = 0.676 \pm 0.002$, and $\gamma_b = 0.199 \pm 0.002$. These are consistent with, but more precise than, the results obtained in the previous section, using only the exactly known coefficients. In subsequent sections we discuss the Monte Carlo results, which are substantially more precise than the series results. However, as we show below, there is one property which is accessible from series analysis which is not easy to determine by Monte Carlo analysis, and that is the behaviour of spanning bridges in a

| $n$ | TAWs          | Bridges                  |
|-----|---------------|--------------------------|
| 27  | $6.99275590 \times 10^{17}$ | exact                   |
| 28  | $3.2418211 \times 10^{18}$  | exact                   |
| 29  | $1.5038283 \times 10^{19}$  | $1.397156394 \times 10^{18}$ |
| 30  | $6.9761657 \times 10^{19}$  | $6.38289508 \times 10^{18}$ |
| 31  | $3.237937 \times 10^{20}$   | $2.91825221 \times 10^{19}$ |
| 32  | $1.502907 \times 10^{21}$   | $1.33518243 \times 10^{20}$ |
| 33  | $6.979108 \times 10^{21}$   | $6.1129712 \times 10^{20}$ |
| 34  | $2.8005385 \times 10^{21}$  | $2.8005385 \times 10^{21}$ |
| 35  | $1.2837858 \times 10^{22}$  |                          |

Table 2: Approximate, predicted coefficients of simple cubic lattice TAWs and bridges of length $n$. 

Figure 1: Exponent sequence $g_n$ for TAWs
slab of given thickness, at the critical temperature, as the slab thickness increases. We discuss this in Sec. 3.3 below.

### 3.2 Universal amplitude ratio

From our series, and known series for 3d SAWs [8, 31], we have calculated $K_n$ for $n \leq 27$ using exact coefficients, and for $n \leq 34$ using the last seven approximate coefficients. From the asymptotic form of the
coefficients, we expect the asymptotic form of the amplitude to be

$$K_n \sim K \left(1 + \frac{k_1}{n^{\Delta_1}} + \frac{k_2}{n^2} + \cdots\right).$$

(21)

Accordingly, we extrapolated $K_n$ against $1/n^{\Delta_1}$, using our approximate value $\Delta_1 = 1/2$. As can be seen in Fig. 3 the sequence $\tilde{K}_n$ is monotone decreasing, as far as we have data, with the last entry being $K_{34} = 0.61601\ldots$, which suggests that this is an upper bound on $K$. The ratio plots against $1/\sqrt{n}$ exhibit significant curvature, consequently we could only form the estimate $K > 0.609$. Combining these numerical confidence bounds, our first estimate is $K = 0.6125 \pm 0.0035$. We also extrapolated $\tilde{K}_n$ against $1/n$, and those plots exhibited similar, though reduced curvature. The increased linearity when plotting against $1/n$ suggests that the amplitude of the leading correction-to-scaling term is rather weak, and that the sub-dominant behaviour for $n \leq 34$ is largely given by the $O(1/n)$ term. Accordingly, we eliminate this term by forming the estimators

$$\tilde{K}_n = \frac{n \cdot K_n - (n - 2) \cdot K_{n-2}}{2}.$$  

(22)

Note that alternate terms are used to reduce oscillations caused by the anti-ferromagnetic singularity present in all three generating functions at $x = -1/\mu$. We expect

$$\tilde{K}_n \sim K \left(1 + \frac{k_1}{n^{\Delta_1}} + o\left(\frac{1}{n}\right)\right).$$

(23)

We show in Fig. 3 a plot of $\tilde{K}_n$ against $1/\sqrt{n}$, and the importance of the extra estimated terms is now seen, as we are just getting the first clear indication of a turning-point in our estimates. If we plot the odd and even terms separately, this is even clearer. From this figure, and the separate odd-term and even-term plots (not shown), we can give the refined estimate $K = 0.6140 \pm 0.0020$, which is shown on the graph.

Figure 3: Amplitude estimators $K_n$ and $\tilde{K}_n$ for universal amplitude $K$. Our best estimate from the series analysis $K = 0.6140 \pm 0.0020$ is also shown.

A similar analysis for the square lattice was also conducted. There we have much longer series available, and the dominant correction is $O(1/n)$, as in two dimensions $\Delta_1 = 1.5$. In that case we obtained $K_{2d} \approx 0.57280$ where we expect the error to be confined to the last digit.
### 3.3 Behaviour as strip width grows.

The data we have generated also allows us to estimate the exponent characterising the behaviour of the generating function of bridges, at the critical point, which span a strip of width $T$ as $T \to \infty$. For two-dimensional SAWs, under the assumption that these are describable in the scaling limit by SLE$_{8/3}$, one has [28]

$$B_T(x_c) \sim \frac{\text{const.}}{T^{1/4}}. \quad (24)$$

For the simple cubic lattice, we expect similar behaviour, so that

$$B_T(x_c) \sim \frac{\text{const.}}{T^\theta}. \quad (25)$$

From the data for simple cubic bridges, given in the appendix, we can construct the first 28 terms in the generating function for bridges in a strip of width $T$. Note that such generating functions have $xT$ as their first non-zero term, as one needs at least $T$-steps to span a strip of width $T$. Note too that the generating functions will diverge at a critical value $x_c > x_c$, where $x_c = 1/\mu$ is the bulk critical value. So evaluating $B_T(x_c)$ means we are evaluating these ordinary generating functions at a value inside their radius of convergence.

In order to do this as effectively as possible, we have used Padé approximants. For each width $T$, we have constructed a number of Padé approximants utilising all, or nearly all, of the coefficients, and evaluated these at $x_c$. As $T$ increases, the spread among the approximants for a given value of $T$ increases, and we found we could only get useful estimates for $T \leq 9$. These were $0.6967886, 0.5565774, 0.4720324, 0.4144, 0.3728, 0.3399, 0.3132, 0.2915, 0.273$ for $T = 1, \ldots, 9$. We do not quote errors, but expect the error in each case to be confined to the last quoted digit. A log-log plot of these data, which should have gradient $-\theta$, shows slight curvature. Accordingly, we calculate the local gradient given by

$$-\theta_T = \frac{\log B_T(x_c) - \log B_{T-1}(x_c)}{\log(T) - \log(T-1)}. \quad (26)$$

We plot $\theta_T$ against $T^{-1/2}$, reflecting the correction-to-scaling exponent around 0.5, which gives a straight line (with minor oscillations). Extrapolating this with a straight-edge, which is an appropriate level of sophistication given the paucity of data we have, gives a best estimate of $\theta = 0.7$. If the data is representative of the asymptotic behaviour, as it appears to be, quoting a confidence interval of $\pm 0.1$ is appropriately conservative.

We can also give an heuristic argument, based on the ideas given in Beaton et al. [3], as to the expected value of this exponent in terms of known exponents. We first argue that the measure of bridges of length $\leq n$ should scale as $n^{\gamma_b}$, where $\gamma_b$ is the bridge exponent introduced above. Now normalised bridges of height $T$ typically have $T^{1/\nu}$ steps. So the measure of bridges of height $\leq T$ behaves asymptotically as $(T^{1/\nu})^{\gamma_b}$. Then bridges of height exactly $T$ should scale as $(T^{\gamma_b/\nu-1}) \sim T^{-\theta}$, i.e.

$$\theta = 1 - \frac{\gamma_b}{\nu}. \quad (27)$$

In two dimensions $\nu = 3/4$, and $\gamma_b = 9/16$, so $\theta = 1/4$, as expected. In three dimensions we have $\nu = 0.587597 \pm 0.000007$, and our series estimate for $\gamma_b$ is $0.199 \pm 0.002$, so the above equation gives $\theta = 0.661 \pm 0.004$, which is consistent with the direct estimate.
4 Generation of Monte Carlo data

For our computer experiments we utilise the pivot algorithm, a Markov chain Monte Carlo scheme which allows for the efficient sampling of self-avoiding walks and related objects. The pivot algorithm was invented by Lal [27] but first studied in detail by Madras and Sokal [30]. In particular, we use the recent implementation of one of us [4, 5], which improved on earlier important work by Kennedy [24].

The pivot algorithm is a method to sample self-avoiding walks and TAWs of fixed length, which naturally gives estimates for quantities associated with the mean size and shape of a SAW, such as $\nu$. However, it is less obvious how to extend the method to calculate quantities which inherently depend on different lengths. We get around this difficulty by calculating ratios between different kinds of walks. The basic method is to efficiently sample walks in some larger set, and then at each time step test whether the walk belongs to some smaller set. For the sake of efficiency it is crucial that the ratio of the sizes of these two sets is not exponentially small; in practice the ratio is a negative power of the length $n$.

The two quantities we estimate are the probability that a self-avoiding walk is a TAW, and the probability that a TAW is a modified bridge which has had its first step removed. We choose to estimate this ratio for two reasons: it is more straight-forward for our implementation of the pivot algorithm to adapt it in this way$^1$ and also because it facilitates the estimation of the amplitude ratio $K$ from Sec. 3.2 that we anticipate is universal.

For the first computer experiment, we sampled self-avoiding walks via the pivot algorithm, and for each time step we tested whether the SAW is in fact also a TAW. Our observable is the indicator function $\chi_h(\omega)$, which is 1 if $\omega$ is a TAW, and zero otherwise. When we take the expectation of $\chi_h$ with respect to the uniform distribution on the set of SAWs of length $n$, from (1) and (3) we have

\[ \langle \chi_h \rangle_n = \frac{t_n}{c_n} \sim \frac{H \mu^n n^{\gamma_1 - 1}}{A \mu^n H^{\gamma - 1}} \sim \frac{H}{A} n^{\gamma_1 - \gamma}. \] (29)

Thus estimating the mean value of this observable for a variety of lengths allows us to estimate the difference between the exponent for TAWs, $\gamma_1$, and the exponent for SAWs, $\gamma$.

Similarly, for our other computer experiment we sampled TAWs via the pivot algorithm (N.B., the pivot algorithm is ergodic in this case, even though no proof has appeared in the literature as far as we know), and for each time step we tested whether the TAW is indeed a bridge with its first step removed. Our observable is the indicator function $\chi_b(\omega)$, which is 1 if $\omega$ is a bridge with its first step removed, and zero otherwise. When we take the expectation of $\chi_b$ with respect to the uniform distribution on the set of TAWs of length $n$.

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$^1$Technical aside: this is because we only need to check that the ends of the walk lie on opposite faces of the minimum bounding box, without needing to check if additional sites might lie on the faces.
(\mathcal{H}_n), from (2) and (3) we have

\[ \langle \chi_b \rangle_{\mathcal{H}_n} = \frac{b_{n+1}}{b_n} \]
\[ \sim \frac{B\mu^{n+1}(n+1)^{\gamma_b-1}}{H\mu^nn^{\gamma_1-1}} \]
\[ \sim \frac{B\mu}{H}n^{\gamma_b-\gamma_1}. \]  

This allows us to estimate the difference between the bridge exponent \( \gamma_b \) and the TAW exponent \( \gamma_1 \).

One key detail of these simulations, which is similar to the calculation of the connective constant \( \mu \) in [6], is that if the pivot site is selected uniformly at random then this would result in an integrated autocorrelation time for the ratio which is \( \Omega(n) \). The reason that this is true for \( \chi_b \), in brief, is that a positive fraction of SAWs must have at their end a configuration which is of some fixed length \( k \) that cannot ever be attached to the surface. The shortest possible example for the beginning of a self-avoiding walk which can never be a TAW on the square lattice is shown in Fig. 4. Whenever the beginning of a walk assumes such a configuration, it must necessarily be the case that \( \chi_b(\omega) = 0 \).

![Figure 4](image-url)

**Figure 4**: Minimal walk beginning which can never be a TAW on the square lattice (solid line) with a possible extension (dashed line).

If we were to sample from the \( n \) possible pivot sites uniformly at random, then the probability of selecting one of the first \( k \) sites is \( k/n \). Thus we expect that it must take on average \( O(n) \) time steps before a pivot site is selected sufficiently closely to the end to have any chance in changing \( \chi_b \) from 0 to 1. A similar argument applies to the sampling of TAWs and the estimation of \( \chi_b \).

For each of the computer experiments, instead of sampling pivot sites uniformly at random on the \( n \)-step SAWs and TAWs we preferentially sample close to each of the ends, using the following three distributions for pivot sites \( i \in [0, n-1] \), each selected with probability 1/3:

- Integer \( i \) sampled uniformly from the interval \([0, n-1]\);
- Real \( x \) sampled uniformly from \([0, \log(n+1)]\), \( i = \lfloor e^x \rfloor - 1 \);
- Real \( x \) sampled uniformly from \([0, \log(n+1)]\), \( i = n - \lfloor e^x \rfloor \).

This choice of pivot site sampling distribution guarantees that all length scales with respect to the distance from each end are rapidly sampled. We sample uniformly from all symmetries of the simple cubic lattice, excluding the identity.
SAWs were initialised using the pseudo-dimerisation algorithm described in [5], followed by approximately $20n$ successful pivots, with pivot sites chosen uniformly at random, to equilibrate the Markov chain.

The TAWs were also initialised using pseudo-dimerisation, but an additional sequence of pivot moves was performed until the SAW was in the half-space. For further equilibration, we wanted to ensure that there was no bias due to the surface, and so instead of sampling pivot sites uniformly we sampled pivot sites $i \in [0, n−1]$ with probability 1/2 from the following two distributions:

- Integer $i$ sampled uniformly from the interval $[0, n−1]$;
- Real $x$ sampled uniformly from $[0, \log(n+1))$, $i = \lfloor e^x \rfloor − 1$.

We performed approximately $40n$ successful pivots in this case.

Each computer experiment was run for 21 different values of $n$, with $n = 2^k−1$ for $k = 9, 10, \cdots, 25$, with additional data for $n$ at $n = 723, 1447, 2895, 5791$, as we found that there was more information available for our estimates from smaller values of $n$. Approximately 20000 CPU hours were used in each experiment, divided equally between the different lengths, on SunFire X4600M2 machines with 2.3GHz AMD Opteron CPUs. These data are reported in Appendix B.

In addition, we invested a relatively small amount of computer time gathering data for shorter lengths. We do not report these result here, but show them in graphical form below in Fig. 9 to illustrate strong corrections-to-scaling.

5 Analysis of Monte Carlo data

For our analysis we used the method of direct fitting. We fitted our data from Appendix B with the asymptotic forms for each of the series, using in each case the term with the leading correction-to-scaling involving $\Delta_1$. We have also performed fits of the dominant term only, as an alternative, robust, but less accurate method for determining the values of critical parameters. These more robust fits confirm that it is reasonable to fit the $\Delta_1$ term in each case.

We used weighted least squares to fit all values for $n \geq n_{\text{min}}$, and plotted the fits against an appropriate power of $n_{\text{min}}$ which was of the same order as the first neglected correction-to-scaling term. We only required linear fits, and used the statistical programming language R as our tool. We performed fits with
The neglected next-to-leading correction-to-scaling terms have powers $-1$, $-2\Delta_1$, and $-\Delta_2$, which are all approximately $-1$ (which is why we write $O(1/n)$ as a shorthand). We chose not to attempt to fit these next-to-leading corrections, due to the competition between these terms which makes it difficult to sensibly interpret any fitting procedure. In addition, we neglected the anti-ferromagnetic singularity which we expect to be small for the values of $n$ considered here. Fortunately we have the luxury of being able to study the large $n$ regime where we expect all of these correction terms to be small compared to the leading $n^{-\Delta_1}$ correction.

As was the case for the series analysis, we biased the leading correction-to-scaling exponent $\Delta_1$. However, since our Monte Carlo estimates are more accurate, we used the best available estimate $\Delta_1 = 0.528 \pm 0.012$ \cite{4} rather than the approximate value $\Delta_1 = 0.5$. We performed fits for $\Delta_1 = 0.516, 0.528, 0.540$, but only plotted the confidence intervals for the central estimate. We did this to gain an understanding of the relative contributions of statistical error and the systematic error due to biasing the fits with an imprecise value for $\Delta_1$.

The parameters $\delta_b$ and $\delta_\ell$ were introduced by hand to reduce the slope of the fits in Figs. 5-8. We found that $\delta_b = 2$ and $\delta_\ell = 3$ do this job adequately, which made it easier to extrapolate our estimates to $n = \infty$. Effectively, this perturbation provides a crude method of approximately cancelling out the next-to-leading corrections to scaling. This trick is not useful for the fits involving the universal amplitude ratio, as in this case the leading exponent is zero which means the corrections introduced have small amplitude.

For the critical exponents corresponding to the amplitude ratio, we performed fits using (39) to verify that the combination of critical exponents is very nearly zero. For the amplitude ratio, we assumed that the combination of exponents in (9) is exactly zero, and used (38) to directly estimate the amplitude.

In each case we have confirmed that the goodness-of-fit is approximately 1 in the large $n$ regime, which indicates that the fitting form is sensible and that sub-leading terms are lost in the statistical noise.

In Figs. 5 and 6 we plot estimates of exponents and amplitudes from (35), obtaining estimates for $\gamma_1 - \gamma$ and $H_1$. In Figs. 7 and 8 we plot estimates of exponents and amplitudes from (37), obtaining estimates for $\gamma_b - \gamma_1$ and $B\mu H$. Note that the scaling relation in (9) implies that $\gamma_1 - \gamma = \gamma_b - \gamma_1$. 

$$n_{\min} \leq 16383,$$ as statistical noise for larger $n_{\min}$ rendered these fits useless. The fitting forms we used are:

$$\langle \chi_b \rangle_n = \frac{t_n}{c_n} \sim \frac{H}{A} n^{\gamma_1 - \gamma} \left( 1 + \frac{\text{const.}}{n^{\Delta_1}} + O\left( \frac{1}{n} \right) \right)$$

$$\log \langle \chi_b \rangle_n \sim (\gamma_1 - \gamma) \log(n + \delta_b) + \log \frac{H}{A} + \frac{\text{const.}}{(n + \delta_b)^{\Delta_1}} + O\left( \frac{1}{n} \right)$$

$$\langle \chi_b \rangle_{H_n} = \frac{b_{n+1}}{t_n} \sim \frac{B \mu}{H} n^{\gamma_b - \gamma_1} \left( 1 + \frac{\text{const.}}{n^{\Delta_1}} + O\left( \frac{1}{n} \right) \right)$$

$$\log \langle \chi_b \rangle_{H_n} \sim (\gamma_b - \gamma_1) \log(n + \delta_b) + \log \frac{B \mu}{H} + \frac{\text{const.}}{(n + \delta_b)^{\Delta_1}} + O\left( \frac{1}{n} \right)$$

$$\frac{\langle \chi_b \rangle_n}{\langle \chi_b \rangle_{H_n}} = \frac{t_n^2}{b_{n+1} c_n} \sim K n^{2\gamma_1 - \gamma_b - \gamma} \left( 1 + \frac{\text{const.}}{n^{\Delta_1}} + O\left( \frac{1}{n} \right) \right)$$

$$\log \frac{\langle \chi_b \rangle_n}{\langle \chi_b \rangle_{H_n}} \sim (2\gamma_1 - \gamma_b - \gamma) \log n + \log K + \frac{\text{const.}}{n^{\Delta_1}} + O\left( \frac{1}{n} \right)$$

The neglected next-to-leading correction-to-scaling terms have powers $-1$, $-2\Delta_1$, and $-\Delta_2$, which are all approximately $-1$ (which is why we write $O(1/n)$ as a shorthand). We chose not to attempt to fit these next-to-leading corrections, due to the competition between these terms which makes it difficult to sensibly interpret any fitting procedure. In addition, we neglected the anti-ferromagnetic singularity which we expect to be small for the values of $n$ considered here. Fortunately we have the luxury of being able to study the large $n$ regime where we expect all of these correction terms to be small compared to the leading $n^{-\Delta_1}$ correction.
In Fig. 5 we plot the universal amplitude ratio as a function of \( n \), to illustrate the grave difficulty in extracting reliable estimates from short series. In this case no fits are performed, we simply plot the amplitudes against the leading correction to scaling which corresponds to \( \Delta_1 \). One can see that the sub-leading corrections to scaling are extremely large, and overwhelm the leading \( \Delta_1 \) corrections to scaling until \( n \) is of the order of 500 or so. To be able to extract reliable estimates from the low order coefficients one must therefore take into account the next-to-leading corrections.

In Fig. 6 we show our estimates of \( 2\gamma_1 - \gamma_b - \gamma \) from fitting (39). The fits strongly suggest that this
combination of exponents is indeed identically zero. In Fig. 11 we show our fits of (38) with $2\gamma_1 - \gamma_b - \gamma$ biased to be zero, i.e. we assume that the scaling relation (9) is correct. By doing this we can obtain far more accurate fits of this putative universal amplitude ratio than we were able to for the other amplitude ratios.

Figure 9: Plot of $K_n = t_n^2/(b_{n+1}c_n)$ for $n \geq 20$ to show the strong next-to-leading corrections to scaling. It is impossible to reliably extrapolate these data for $n \lesssim 500$ without taking the next-to-leading corrections into account.

Figure 10: Estimates of $2\gamma_1 - \gamma_b - \gamma$ from fits to Monte Carlo estimates of ratios $K_n = t_n^2/(b_{n+1}c_n)$, with correction-to-scaling exponent $\Delta_1 = 0.516, 0.528, \text{ and } 0.54$. Our extrapolated estimate is $2\gamma_1 - \gamma_b - \gamma = 0.000025(30)$.

Figure 11: Plot of amplitude estimates from fits to Monte Carlo estimates of $K_n = t_n^2/(b_{n+1}c_n)$, biased to have $2\gamma_1 - \gamma_b - \gamma = 0$, and with correction-to-scaling exponent $\Delta_1 = 0.516, 0.528, \text{ and } 0.54$. Our extrapolated estimate is $K = 0.614730(30)$. 

$\Delta_1 = 0.540$
$\phi \Delta_1 = 0.528$
$\sigma \Delta_1 = 0.516$
5.1 Summary of results

We summarise our Monte Carlo results in Table 4, providing comparisons between different estimates of $2\gamma_1 - \gamma_b - \gamma$ and $K$ from fitting data from the two computer experiments separately, and together. Reassuringly, we find in each case that the confidence intervals overlap. Note that the direct estimate of $K$ is an order of magnitude more accurate than the combined estimate, due to the biasing of the exponents to satisfy (9).

| Quantity          | Estimate          | Source       |
|-------------------|-------------------|--------------|
| $\gamma_1 - \gamma$     | -0.479290(15)   | Fig. 5       |
| $\gamma_b - \gamma_1$  | -0.479315(20)   | Fig. 7       |
| $2\gamma_1 - \gamma_b - \gamma$ | 0.000025(25) | Fig. 5 and Fig. 7 |
| $2\gamma_1 - \gamma_b - \gamma$ | 0.000025(30) | Fig. 10      |
| $\frac{H}{A}$         | 1.38431(41)      | Fig. 6       |
| $\frac{\mu B}{T'}$    | 2.25286(68)      | Fig. 8       |
| $K$                  | 0.61447(26)      | Fig. 6 and Fig. 8 |
| $K$                  | 0.614730(30)     | Fig. 11      |

Table 4: Summary of estimates made via analysis of Monte Carlo data.

In addition, we combine our direct Monte Carlo estimates with previous exponent estimates $\gamma = 1.156957 \pm 0.000009$ [7] and $\nu = 0.587597 \pm 0.000007$ [4]. We then obtain estimates for the TAW exponent $\gamma_1 = (\gamma_1 - \gamma) + \gamma = -0.479290(15) + 1.156957(9) = 0.677667(17)$, and the bridge exponent $\gamma_b = (\gamma_b - \gamma_1) + (\gamma_1 - \gamma) + \gamma = -0.479315(20) - 0.479290(15) + 1.156957(9) = 0.198352(27)$. N.B., we combine the confidence intervals as if they were independent statistical estimates of a single standard deviation.

The Monte Carlo estimates are consistent with the series analysis estimates of Sec. 3.1 ($\gamma_1 = 0.676 \pm 0.002$ and $\gamma_b = 0.199 \pm 0.002$) but are dramatically more precise.

From the scaling relation (6), we calculate $\gamma_{11} = \gamma_b - \nu = 0.198352(27) - 0.587597(7) = -0.389245(28)$.

From the scaling relation (8), we calculate $b = -\gamma_b/(2\nu) + d/2 = 1.331218(23)$, which may be compared with the direct estimate due to Kennedy of $b = 1.3303(3)$ [26].

For the exponent $\theta$, the hand-waving argument in Sec. 3.3 gave us the scaling relation (27), from which we obtain $\theta = 1 - \gamma_b/\nu = 0.662435(46)$. This indirect estimate of $\theta$ should be compared with the direct estimate of $\theta = 0.7 \pm 0.1$ and the indirect estimate of $\theta = 0.661 \pm 0.004$ from the series analysis in Sec. 3.3.

We summarise these results in Table 5. In each case, our estimates improve significantly on those previously available in the literature.
| Quantity | Estimate       |
|----------|---------------|
| $\gamma_1$ | 0.677667(17)  |
| $\gamma_b$ | 0.198352(27)  |
| $\gamma_{11}$ | -0.389245(28) |
| $b$       | 1.331218(23)  |
| $\theta$ | 0.662435(46)  |

Table 5: Summary of estimates for critical exponents from Monte Carlo.

6 Discussion and conclusion

6.1 Possible improvements and extensions

For the enumerations, we utilised a straightforward backtracking algorithm despite the fact that some improved algorithms have been developed in recent years for self-avoiding walks for $d = 3$. The three innovations are the use of the lace expansion and the two-step method [8], and the length-doubling algorithm [31].

Of these methods, it is unlikely that the lace expansion would help as this works by enumerating configurations like self-avoiding polygons instead of SAWs, and there would not be as much of a gain for TAWs and bridges.

The length-doubling algorithm is extremely promising, but would be challenging to adapt to the present problem. If this could be done, then it may be possible to extend the series past the existing $n = 36$ for SAWs [31].

Finally, the two-step method could be adapted quite easily and used to increase the length of the series for the same computational effort, perhaps by a few terms.

Unfortunately it is unlikely that the extent of the improvement would be sufficient to be competitive with Monte Carlo, even in the case of the length-doubling algorithm.

To improve the Monte Carlo results it would be possible to perform the same computer experiment with weakly self-avoiding walks (also known as the Domb-Joyce model) where the weight factor is chosen so that the leading correction-to-scaling term corresponding to $\Delta_1$ has small amplitude.

In future we will perform further Monte Carlo computer experiments for a variety of two- and three-dimensional lattices to test our hypothesis that $\tilde{K}$ is indeed a universal amplitude ratio. We have some preliminary numerical evidence that this ratio is the same for the simple cubic, face-centred cubic, and body-centred cubic lattices.
6.2 Conclusion

We have obtained high precision estimates of a variety of exponents and amplitudes associated with terminally attached self-avoiding walks and bridges in three dimensions. In particular, we have confirmed to high precision that the scaling relation in (9) holds, and estimated the corresponding amplitude ratio $K$ which we believe to be universal.

A Enumerations

| $n$ | TAWs | Bridges |
|-----|------|---------|
| 0   | 1    | 0       |
| 1   | 5    | 1       |
| 2   | 21   | 5       |
| 3   | 93   | 21      |
| 4   | 409  | 89      |
| 5   | 1853 | 369     |
| 6   | 8333 | 1553    |
| 7   | 37965| 6573    |
| 8   | 172265| 28197  |
| 9   | 787557| 122093 |
| 10  | 3593465| 533369 |
| 11  | 1647784| 2345429|
| 12  | 7548110| 10366677|
| 13  | 346960613| 46013585|
| 14  | 1593924045| 204927833|
| 15  | 7341070889| 915448621|
| 16  | 33798930541| 4100092693|
| 17  | 155915787353| 18407472565|
| 18  | 719101961769| 82815889677|
| 19  | 3321659652529| 373321398437|
| 20  | 15341586477457| 1685838489629|
| 21  | 70944927549085| 7625255897889|
| 22  | 328054694768261| 34541044018277|
| 23  | 1518490945278377| 156678876463321|
| 24  | 7028570356547189| 711593257794069|
| 25  | 32560476643826933| 3235634079777801|
| 26  | 150838831585499069| 14728414578753489|
| 27  | 67110197685388181| 67110197685388181|
| 28  | 306074586987649389| 306074586987649389|

Table 6: Simple cubic lattice TAWs and bridges of length $n$. 
| $n$  | height 1 | height 2 | height 3 | height 4 | height 5 | height 6 | height 7 | height 8 | height 9 |
|------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1    | 1        |          |          |          |          |          |          |          |          |
| 2    | 4        |          |          |          |          |          |          |          |          |
| 3    | 12       |          |          |          |          |          |          |          |          |
| 4    | 36       |          |          |          |          |          |          |          |          |
| 5    | 100      |          |          |          |          |          |          |          |          |
| 6    | 284      | 12       |          |          |          |          |          |          |          |
| 7    | 780      | 144      |          |          |          |          |          |          |          |
| 8    | 2172     | 1104     |          |          |          |          |          |          |          |
| 9    | 5916     | 6744     | 12       |          |          |          |          |          |          |
| 10   | 16268    | 35484    | 252      |          |          |          |          |          |          |
| 11   | 44100    | 170344   | 3332     |          |          |          |          |          |          |
| 12   | 120292   | 760656   | 33188    | 12       |          |          |          |          |          |
| 13   | 324932   | 3240024  | 272056   | 360      |          |          |          |          |          |
| 14   | 881500   | 13266260 | 1944216  | 6708     |          |          |          |          |          |
| 15   | 2374444  | 52897744 | 12469228 | 92040    | 12       |          |          |          |          |
| 16   | 6416596  | 206110864| 73725500 | 1032008  | 468      |          |          |          |          |
| 17   | 17245332 | 790696704| 407848052| 9733040  | 11232    |          |          |          |          |
| 18   | 464666767| 2990802868| 2141811776| 81770392| 195756    | 12       |          |          |          |
| 19   | 124658732| 11206740432| 10770243016| 62267708| 2739436   | 576      |          |          |          |
| 20   | 335116620| 41617757096| 5231025276| 4368861352| 32483296 | 16904    |          |          |          |
| 21   | 897697164| 153655478264| 246718702580| 28658873096| 337104536| 356792   | 12       |          |          |
| 22   | 2408806028| 563984887964| 1136186599756| 177561158756| 3140961204| 6011640 | 684      |          |          |
| 23   | 6444560484| 2062508494408| 5126606123704| 1048578720568| 26724562112| 85255000| 23724    |          |          |
| 24   | 17266613812| 7512897046320| 22746305294180| 5942315016020| 210656680128| 1052099212| 587604   | 12       |          |
| 25   | 46146397316| 27302951014488| 99466683163980| 32513181993504| 1554742879184| 11586414632| 11569024| 792      |          |
| 26   | 123481354908| 98952488047860| 429730858249952| 172562782519172| 10843077619792| 115848555164| 190791832| 31692    |          |
| 27   | 329712786220| 358096887158816| 1837073895696056| 892191489850824| 71975965355296| 1066811813096| 2726830756| 900648   | 12       |
| 28   | 881317491628| 1293405464647968| 7784187577745060| 4508562016424432| 457618567787368| 9145657703324| 34630365164| 20280096| 900      |

Table 7: Simple cubic lattice irreducible bridges of length $n$ and various heights.
B Monte Carlo data

| $n$   | $\langle \chi_h \rangle_n$        | $\langle \chi_b \rangle_{H_n}$       |
|-------|----------------------------------|--------------------------------------|
| 511   | 0.06923625(26)                   | 0.1128060(11)                        |
| 723   | 0.05870409(26)                   | 0.0956331(11)                        |
| 1023  | 0.04975890(24)                   | 0.08104698(73)                       |
| 1447  | 0.04217388(24)                   | 0.0686814(10)                        |
| 2047  | 0.03573665(22)                   | 0.05818965(67)                       |
| 2895  | 0.03028231(23)                   | 0.04930093(93)                       |
| 4095  | 0.02565517(21)                   | 0.04176450(63)                       |
| 5791  | 0.02173570(21)                   | 0.03538056(85)                       |
| 8191  | 0.01841284(19)                   | 0.02996852(60)                       |
| 16383 | 0.01321296(18)                   | 0.02150202(57)                       |
| 32767 | 0.00948020(16)                   | 0.01542623(53)                       |
| 65535 | 0.00680166(15)                   | 0.01106585(50)                       |
| 131071| 0.00487920(13)                   | 0.00793876(47)                       |
| 262143| 0.00350038(12)                   | 0.00569498(44)                       |
| 524287| 0.00251118(12)                   | 0.00408485(40)                       |
| 104875| 0.001801345(94)                  | 0.00293075(36)                       |
| 2097151| 0.001292118(84)                  | 0.00210227(34)                       |
| 4194303| 0.000926791(74)                  | 0.00150794(30)                       |
| 8388607| 0.000665041(66)                  | 0.00108145(26)                       |
| 16777215| 0.000477001(60)                  | 0.00077565(24)                       |
| 33554431| 0.000342261(50)                  | 0.00055642(23)                       |

Table 8: Estimates of $\langle \chi_h \rangle_n$ and $\langle \chi_b \rangle_{H_n}$ from Monte Carlo computer experiments.

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