Lattice star and acyclic branched polymer vertex exponents in 3d

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Abstract
Numerical values of lattice star entropic exponents $\gamma_f$, and star vertex exponents $\sigma_f$, are estimated using parallel implementations of the PERM and Wang–Landau algorithms. Our results show that the numerical estimates of the vertex exponents deviate from predictions of the $\epsilon$-expansion and confirms and improves on estimates in the literature. We also estimate the entropic exponents $\gamma_G$ of a few acyclic branched lattice networks with comb and brush connectivities. In particular, we confirm within numerical accuracy the Duplantier scaling relation $\gamma_G - 1 = \sum_{f \geq 1} m_f \sigma_f$ for a comb and two brushes (where $m_f$ is the number of nodes of degree $f$ in the network) using our independent estimates of $\sigma_f$.

Keywords: lattice stars, vertex exponents, self-avoiding walk

(Some figures may appear in colour only in the online journal)

1. Introduction

Lattice self-avoiding walk models of star polymers have been studied since the 1970s [25] and remain of considerable interest in the statistical mechanics of polymeric systems. Numerical simulation of lattice stars stretches back decades [1, 19, 23, 41], and their properties and scaling exponents have been calculated numerically [1, 5, 13, 17, 18, 23, 28, 29, 41, 43] and by using field theoretic approaches [9, 10, 22, 26, 27, 33]. A general survey can be found in references [11, 21]. Recent results in reference [12] give predictions in models of confined branched and star polymers.

In this paper we revisit the numerical simulation of 3d lattice stars, using the parallel PERM algorithm [4, 13, 30]. Our aims are to update numerical estimates of the entropic exponent $\gamma_f$.
of lattice stars, and to test the scaling relation [9]

\[ \gamma_G - 1 = \sum_{f \geq 1} m_f \sigma_f, \]  

for lattice models of a few uniform branched structures with underlying graph or connectivity \( G \) (a comb and two brushes—see figure 1), where \( \gamma_G \) is the entropic exponent of the branched structure, and \( \sigma_f \) and \( m_f \) are the \( f \)-star vertex exponent and the number of nodes of degree \( f \) in \( G \), respectively. Conformational properties of these types of networks were studied in the Gaussian approximation in reference [31]. Networks with connectivities \( C, B_1 \) and \( B_2 \) are also examples of structures with two branching points (so-called ‘pom–pom structures’) and are of experimental and theoretical importance in modelling rheological and viscoelastic properties of long chain branched polymers [2, 3].

An \( f \)-star graph is an acyclic simple graph with one vertex of degree \( f \) (the central vertex), and \( f \) vertices of degree 1 (see figure 1). The \( f \)-star graph has \( f \) arms or branches which branch from the central node to their endpoints which are nodes of degree 1. A lattice \( f \)-star is a lattice embedding of an \( f \)-star graph such that each branch or arm is a self-avoiding walk from the central node (of degree \( f \)) to a node of degree 1 which is the endpoint of the arm. The arms of the embedded lattice star are mutually avoiding but do share the central node at their first vertices. A lattice \( f \)-star is strictly uniform if its \( f \) arms all have the exact same length. If the longest arm of a lattice star is exactly one step longer than its shortest arm, then it is almost uniform. We call lattice \( f \)-stars of arbitrary length \( n \) monodispersed if they are either strictly, or almost, uniform. The length of a lattice star is the total number of steps in all the arms of the star (that is, the sum of the lengths of the arms). In the simple cubic (SC) lattice \( 1 \leq f \leq 6 \), but it is possible to redefine the central node such that lattice stars with more than six arms can be embedded. In the face-centered cubic (FCC) lattice, \( 1 \leq f \leq 12 \), and in the body-centered cubic (BCC) lattice, \( 1 \leq f \leq 8 \).

Denote by \( c_n \) the number of self-avoiding walks in a lattice from the origin, and of length \( n \) steps. The growth constant \( \mu_d \) of self-avoiding walks is given by the limit [14–16]

\[ \lim_{n \to \infty} \frac{1}{n} \log c_n = \log \mu_d. \]
Asymptotically,

\[ c_n = C n^{\gamma - 1} \mu_d^n (1 + B n^{\Delta_1} + \cdots), \]

(3)

where \( \gamma \) is the \textit{entropic exponent}, and \( \Delta_1 \) is the leading confluent correction exponent. The best estimates of the entropic exponent in 3d are \( \gamma = 1.15698(34) \) [34] and \( \gamma = 1.15695300(15) \) [7]. The confluence correction exponent was estimated in reference [8] to be \( \Delta_1 = 0.528(8) \).

Denote by \( s_n^{(f)} \) the number of monodisperse lattice \( f \)-stars of length \( n \) counted with the central node fixed at the origin. The growth constant of monodisperse lattice \( f \)-stars is independent of \( f \) and is given by

\[ \lim_{n \to \infty} \frac{1}{n} \log s_n^{(f)} = \log \mu_d. \]

(4)

where \( \mu_d \) is given by equation (2) [37–39, 41, 42]. Notice that \( s_n^{(f)} \) is the number of strictly uniform \( f \)-stars and \( s_{n+f+k}^{(f)} \) is the number of almost uniform \( f \)-stars of length \( n f + k \) for each fixed \( k \in \{1, 2, \ldots, n - 1\} \). Similar to equation (3) for \( n = m f + k \) and \( k \) fixed in \( \{0, 1, 2, \ldots, f - 1\} \)

\[ s_n^{(f)} \equiv s_{n+f+k}^{(f)} = C_k^{(f)} n^{\gamma - 1} \mu_d^n (1 + B n^{\Delta_1} + \cdots). \]

(5)

The \textit{entropic exponent} \( \gamma_f \) is a function of the number of arms [9]. For values of \( k \in \{0, 1, \ldots, f - 1\} \) there are persistent parity effects in \( s_n^{(f)} \), so that the \textit{amplitudes} \( C_k^{(f)} \) are functions of \( k \) and corresponds to \textit{parity classes} of monodisperse lattice stars.

1.1. Lattice star entropic and vertex exponents

The entropic exponent \( \gamma_f \) is related to \textit{vertex exponents} \( \sigma_f \) as shown in equation (1). That is,

\[ \gamma_f - 1 = \sigma_f + f \sigma_1. \]

(6)

If \( f = 1 \) or \( f = 2 \), then a monodisperse \( f \)-star is reduced to either a self-avoiding walk from the origin (when \( f = 1 \)), or a self-avoiding walk with a middle vertex at the origin. Thus, the number of one-stars of length \( n \) is equal to \( c_n \) so that \( \gamma_1 = \gamma \), and by equation (6), using the estimate for \( \gamma \) in reference [7],

\[ \sigma_1 = (\gamma - 1)/2 = 0.0784765(8). \]

(7)

The number of strictly uniform two-stars of length \( 2n \) is given by \( c_{2n}/2 \), and the number of almost uniform two-stars of length \( 2n + 1 \) is given by \( c_{2n+1} \). That is, \( s_2^{(2)} = c_{2n}/2 \) and \( s_{2n+1}^{(2)} = c_{2n+1} \). This shows that \( \gamma_2 = \gamma \) and by equation (1), \( \gamma_2 - 1 = \sigma_2 + 2 \sigma_1 \). This shows that \( \sigma_2 = 0 \), and that \( C_0^{(2)} = C/2 \) and \( C_1^{(2)} = C \).

Numerical estimates of \( \gamma_f \) can be found in references [1, 18, 28, 36, 43] and in this paper we verify and improve on some of those estimates. By combining estimates from our simulations in the SC, FCC and BCC lattices, we obtain the estimates in table 1.

Accurate estimates of \( \sigma_f \) in 3d can be obtained from the data in table 1, equation (6), and the estimate of \( \sigma_1 \) in equation (7). The results are shown for \( 3 \leq f \leq 6 \) in the last column of table 2,
Table 1. Estimates of $\gamma_f$ in 3d$^a$.

| $f$  | This work       | Models          | Older estimates                  |
|------|-----------------|-----------------|----------------------------------|
| 3    | 1.04282(11)     | SC, FCC, BCC    | 1.089(1)$^d$,1.0427(7)$^d$       |
| 4    | 0.8337(5)       | SC, FCC, BCC    | 0.879(1)$^d$,0.8355(10)$^d$      |
| 5    | 0.5412(8)       | SC, FCC, BCC    | 0.567(2)$^d$,0.5440(12)$^d$      |
| 6    | 0.1726(14)      | SC, FCC, BCC    | 0.16(1)$^d$,0.1801(20)$^d$       |
| 7    | −0.257(3)       | SC, FCC, BCC    | −0.2520(25)$^d$                  |
| 8    | −0.757(3)       | SC, FCC, BCC    | −1.00$^2$,−0.748(3)$^d$          |
| 9    | −1.309(4)       | SC, FCC         | −1.306(5)$^d$                    |
| 10   | −1.916(5)       | SC, FCC         | −1.922(7)$^d$                    |
| 11   | −2.588(6)       | SC, FCC         |                                  |
| 12   | −3.305(6)       | SC, FCC         | −3.35$^2$,−3.4(3)$^d$,−3.296(9)$^d$ |

$^a$References for older estimates: 1: [1], 2: [36], 3: [28], 4: [18]. SC-simple cubic, FCC-face-centered, BCC-body-centered.

Table 2. Vertex exponents $\sigma_f$ of $f$-stars in 3d.

| $f$  | [43]          | [1]           | [36]          | [18]          | This work       |
|------|---------------|---------------|---------------|---------------|-----------------|
| $\sigma_1$ | —           | 0.0855(5)     | —             | 0.07865(10)   | —               |
| $\sigma_3$ | −0.19(3)    | −0.1675(5)    | −0.216        | −0.1927(7)    | −0.19313(11)    |
| $\sigma_4$ | −0.44(3)    | −0.463(1)     | —             | −0.4784(10)   | −0.4802(5)      |
| $\sigma_5$ | −0.85(5)    | −0.8605(5)    | —             | −0.8484(12)   | −0.8512(8)      |
| $\sigma_6$ | −1.28(5)    | −1.353(7)     | −1.401        | −1.2908(20)   | −1.2983(14)     |

where earlier results (obtained from estimates of $\gamma_f$ in those references and equations (6) and (7)).

Studies using renormalization group methods and the $\epsilon$-expansion [9, 33] gives

$$\gamma_f = \sigma_f + f \sigma_1 = \nu(\eta_f - f \eta_2).$$

The numbers $\eta_f$ were calculated to $O(\epsilon^3)$ [33]. To second order in $\epsilon$,

$$\eta_f = -\frac{\epsilon}{8}f(f-1)\left(1 - \frac{\epsilon}{32}(8f-25) + O(\epsilon^3)\right).$$

These $\epsilon^2$ estimates are best for small values of $f \leq 4$, and has low fidelity for $f \geq 5$. A second order $\epsilon$-expansion for $\gamma$ [22] (and thus for $\sigma_1$) gives the following second order $\epsilon$-expansion for $\sigma_f$ [9, 10]:

$$\sigma_f = \frac{\epsilon}{16}f(2-f) + \frac{\epsilon^2}{512}f(2-f)(8f-21) + O(\epsilon^3).$$

In reference [35] equation (9) was extended by calculating terms up to order $\epsilon^4$. We list predictions using the $\epsilon$-expansion for $\sigma_f$ in three dimensions to order $\epsilon^k$ for $k = 1, 2, 3, 4$ in table 3; the order $\epsilon^1$ and $\epsilon^2$ approximations are obtained from equation (10), while the order $\epsilon^3$ and $\epsilon^4$ estimates follow from reference [35]. The $[3/2]$ Padé approximation was determined by a Borel resummation of the order $\epsilon^3$ expansion and then using the Padé approximant to recalculate the exponents. The results are shown in the sixth column. The Padé and $\epsilon^1$ results approximate the $\sigma_f$ reasonably for $f \leq 4$, but even these deviate from the numerical data for $f = 5$ and $f = 6$. 

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Asymptotically $\gamma_f$ and $\sigma_f$ scales with $f$ as [28, 44]

$$\gamma_f - 1 \sim \sigma_f + f\sigma_1 \sim -f^{3/2}.$$ (11)

Comparison to equation (10) suggests that the $\epsilon$-expansion should break down quickly with increasing $f$, as the order $\epsilon^n$ term is seen to grow as $O(f^{n+1})$. Moreover, it cannot be improved by calculating ever higher order corrections, as the coefficients increase quickly in magnitude with increasing $f$. Resummation techniques do give improved estimates, but are limited for large $f$, and by the increasing complexity of calculating higher order terms in longer $\epsilon$-expansions. See, for example, chapter 16 in reference [20].

1.2. Uniform acyclic branched structures (uniform trees)

Models of branched polymeric structures are lattice networks with connectivities or topologies denoted by $\mathcal{G}$. A lattice network consists of branches which are self-avoiding walks joining vertices of degrees equal to 1 or bigger than or equal to 3. The underlying connectivity of a lattice network is denoted by a graph. This may be, for example, one of the cases shown in figure 1. Lattice $f$-stars are examples of lattice networks of fixed connectivity, and so are the other cases shown in figure 1. These cases include a comb $\mathcal{C}$ (figure 2), and two brushes, $\mathcal{B}_1$ (figure 3) and $\mathcal{B}_2$ (figure 4).

A lattice network is strictly uniform if all the branches are self-avoiding walks of the same length. If a strictly uniform lattice network of connectivity $\mathcal{G}$ has $b$ branches, then the total number of such networks, equivalent under translations in the lattice, is denoted by $c_n(\mathcal{G})$, and

### Table 3. Vertex exponents: $\epsilon$-expansions in three dimensions.

| $f$  | $\epsilon$ [22] | $\epsilon^2$ [22] | $\epsilon^3$ [35] | $\epsilon^4$ [35] | Padé[3/2] | This work |
|------|----------------|-------------------|-------------------|-------------------|----------|-----------|
| $\sigma_1$ | 0.0625 | 0.0879 | 0.0556 | 0.1425 | 0.0798 | — |
| $\sigma_3$ | -0.1875 | -0.1699 | -0.2265 | -0.1094 | -0.2026 | -0.19313(11) |
| $\sigma_4$ | -0.5 | -0.3281 | -0.9037 | 0.9925 | -0.5079 | -0.4802(5) |
| $\sigma_5$ | -0.9375 | -0.3809 | -2.5321 | 6.0673 | -0.8964 | -0.8512(8) |
| $\sigma_6$ | -1.5 | -0.2344 | -5.8322 | 20.1822 | -1.3594 | -1.2983(13) |
it is generally accepted that
\[ c_n(G) = C_G n^{\gamma_G - 1} \mu_d (1 + o(1)). \]  
(12)

The growth constant \( \mu_d \) is equal to that of self-avoiding walks \([37–39, 42]\). The relation of the entropic exponent \( \gamma_G \) for a general network connectivity \( G \) and star vertex exponents \( \sigma_f \) is given by the relation
\[ \gamma_G - 1 = \sum_{f \geq 1} m_f \sigma_f - c(G) \nu, \]  
(13)

where \( m_f \) is the number of vertices of degree \( f \), and where \( c(G) \) is the cyclomatic index (the number of independent cycles) in the network \([9, 10]\) (see equation (1) for the case when \( c(G) = 0 \)). The models in figure 1 are acyclic, and by the above
Table 4. $\gamma - 1$ for lattice networks in the cubic lattice.

| $\mathcal{G}$ | $\epsilon^1$ | Padé[3/2] | Equation (14) | This work |
|---------------|--------------|------------|---------------|-----------|
| $\mathcal{C}$ | -0.1250      | -0.0860    | -0.07127(20)  | -0.0731(18) |
| $\mathcal{B}_1$ | -0.3750      | -0.3115    | -0.28000(32)  | -0.2896(69) |
| $\mathcal{B}_2$ | -0.6250      | -0.5370    | -0.48874(44)  | -0.5065(58) |

The underlying assumption is that the vertex exponents $\sigma_f$ are independent of the connectivity of the uniform branched polymer so that the presence of other nodes of given degree does not affect its value. For large $n$ this is a reasonable assumption since the distance between any two branch points in the lattice graph increases as $O(n^{\nu_d})$ (where $\nu_d$ is the self-avoiding walk metric exponent in dimension $d$).

Our results for lattice networks are shown in table 4. In three dimensions the predicted $\epsilon$-expansion results (at order $\epsilon^1$) deviate from the numerical results. Higher order $\epsilon$-expansion estimates do not improve these. The prediction using the Padé[3/2] estimates improves on the estimates $\epsilon^1$. The predictions by equation (14) are obtained by using our best estimates for $\sigma_f$ in table 3, while the estimates in the final column were obtained by analysing our data for networks in section 3.1.

2. Parallel PERM sampling of lattice stars

Our parallel PERM simulations of self-avoiding $f$-stars in the SC, FCC and BCC lattices were done by initialising $f$-stars with their central nodes at the origin and then growing branches by appending steps at the endpoints of arms one at a time while cycling through the $f$ arms of the star. For example, in figure 5 the steps in a three-star are labelled in the order they were appended. The steps along the arm labelled 1, were added first, fourth, seventh, tenth, and so on, giving the sequence of labels (1, 4, 7, 10, 13, 16, 19, 22, 25, 28) along this arm. The second arm is grown starting at step 2, and so on. Appending a step with label $fm$ gives a uniform $f$-star, while the other cases give almost uniform stars. That is, the algorithm samples in the state space of monodisperse $f$-stars producing approximate counts of the number of monodispersed $f$-stars. Using this implementation, $f$-stars were sampled in the SC to $f = 6$, the FCC to $f = 12$ and the BCC to $f = 8$.

There are $f!$ ways in which to grow a uniform $f$-star, and $k!(f - k)!$ ways to grow an almost uniform $f$-star of length $fm + k$. That is, PERM estimates the quantity $u^{(f)}_n = k!(f - k)!c^{(f)}_m$ if $n = fm + k$. By equation (5),

$$u^{(f)}_n = U^{(f)} n^{\sigma_f + \sigma_1 + \sigma_0}(1 + o(1)),$$

and $U^{(f)}$ is related to $C^{(f)}$ in equation (5) by

$$U^{(f)} = k!(f - k)C^{(f)}.$$
Figure 5. Growing a lattice three-star by PERM. The three branches are labelled by \{1, 2, 3\} and the growth point cycles with each step from one branch to the next. The first step is added to the origin to start growing the first arm, then the second step and third steps are added to initiate the second and third arms. The growth point is then situated at the endpoint of the first branch and the fourth step is added here. The growth point moves to the end point of the second branch, and the fifth step is added here, and so on. Eventually, step \(m\) is appended to arm \(k = m \mod f\). This elementary move is implemented using Rosenbluth dynamics [32], which with enrichment and pruning [13] gives the PERM algorithm for lattice stars. In some of our simulations this algorithm was implemented using the parallel implementation in reference [4]. Notice that only monodisperse (uniform or almost uniform) lattice stars are sampled.

The amplitudes of the parity classes of monodisperse \(f\)-stars, \(C^{(f)}_k\), can be estimated for each \(k\) by first estimating \(U^{(f)}\) from our data.

We also used parallel PERM to sample \(f\)-stars with \(f > 6\) in the SC lattice. These are grown by initiating each arm at a vertex with coordinates \((\pm a, \pm b, \pm c)\) where the signs are chosen and the coordinates permuted randomly. We used the values \((a, b, c) = (0, 1, 2)\) to sample \(f\)-stars with \(7 \leq f \leq 12\) (so that each arm is initiated on a sphere of radius \(\sqrt{3}\) centred at the origin in the SC lattice). In our simulations we used a 32 bit implementation of the Mersenne twister [24] to generate random numbers.

2.1. Results from lattice stars in the SC lattice

For cubic lattice \(f\)-stars equation (16) becomes

\[
\eta^{(f)}_n = U^{(f)} n^{-\gamma} \mu_n \eta^{(1)}_n (1 + B^{(f)} n^{-\Delta_1} + \cdots).
\]  

(17)
Dividing both sides by $n^{γ_f−1} μ_3^n$ and taking logarithms gives

$$Q_n = \log \left( \frac{μ_3^n}{μ_3^n} \right) \simeq S_f + \log(1 + B_f n^{−Δ_1}) + \cdots = S_f + B_f n^{−Δ_1} + \cdots. \quad (18)$$

Estimates of $γ_f$ are obtained using the best estimates $μ_3 = 4.684039931(27)$ [6] of the cubic lattice self-avoiding walk growth constant and $Δ_1 = 0.528(8)$ [8] in equation (18). If the correct value of $γ_f$ is inserted on the left-hand side, then $Q_n$ is to leading order a linear function of $n^{−Δ_1}$. Thus, we determine the best estimate for $γ_f$, assuming the model

$$Q_n = A_f + B_f n^{−Δ_1} + C n^{−1}, \quad (19)$$

where an analytic correction is included. Plotting $Q_n$ against $n^{−Δ_1}$ can be interpolated on the value of $γ_f$ to obtain that best estimate where the graph is a straight line, except perhaps at the smallest values of $n$. In figure 6 this is shown for cubic lattice four-stars by plotting $K_4 + Q_n$ against $n^{−Δ_1}$ and with $K_4$ chosen so that the curve passes through zero at $n = 500$. This simulation included $1.1334 \times 10^9$ realised parallel PERM tours along four parallel sequences of four-stars to total length $n = 12000$, and the graph straightens out when $γ_f = 0.83345(55)$. The confidence interval is determined by find those values of $γ_f$ where the top curve is clearly convex, and the bottom curve is clearly concave.

For $f$-stars in the SC lattice with $3 ≤ f ≤ 6$ the analytic correction in equation (19) proved to be negligible, even for small values of $n$, and so it could be ignored. In figure 7 our data are plotted for these $f$-stars using our best estimates of $γ_f$. Our results are collected in table 5, together with the parameters of our simulations.

A different approach was followed to extract $γ_f$ for $6 < f ≤ 12$. First note that arms of the stars were seeded at lattice points a distance $\sqrt{5}$ from the origin, increasing the length of each arm by this amount, resulting in a stronger correction term of order $n^{−2Δ_1}$ in equation (18).
Figure 7. $K_f + Q_n$ plotted against $1/n^{\Delta_1}$ with $K_f$ chosen such that the curves pass through zero when $n = 500$. In this curves straightened and gives the values for $\gamma_f$ shown in the legend of the plot.

Table 5. Estimates of $\gamma_f$ in the SC lattice.

| $f$ | Length | Tours           | $\gamma_f$          |
|-----|--------|-----------------|----------------------|
| 3   | 12000  | $1.1303 \times 10^9$ | 1.0423(3)            |
| 4   | 12000  | $1.1334 \times 10^9$ | 0.8335(6)            |
| 5   | 12000  | $1.1505 \times 10^9$ | 0.5411(9)            |
| 6   | 12000  | $8.2231 \times 10^8$ | 0.1738(18)           |
| 7   | 12005  | $6.2800 \times 10^8$ | $-0.253(4)$          |
| 8   | 12000  | $6.0800 \times 10^8$ | $-0.754(4)$          |
| 9   | 12006  | $5.5200 \times 10^8$ | $-1.306(5)$          |
| 10  | 12000  | $6.0300 \times 10^8$ | $-1.912(6)$          |
| 11  | 13200  | $6.3100 \times 10^8$ | $-2.581(8)$          |
| 12  | 14400  | $6.3300 \times 10^8$ | $-3.301(9)$          |

Since $2\Delta_1 \approx 1$ the numerical effect is evident in a very strong analytic correction in our data. This effect was already noted in reference [18], and to compensate for this a modified approach was used to estimate of $\gamma_f$ from cubic lattice data with $f > 6$. Thus, we proceeded by writing equation (18) in the form

$$P_n = \log \left( \frac{\mu_n}{\mu_n^f} \right) = (\gamma_f - 1) \log n + a_f + b_f n^{-\Delta_1} + c_f n^{-1}. \quad (20)$$

Since parity effects in our data are of period $2f$, subtract $P_{n-2f}$ from $P_n$ and then expand the result in $n$ to obtain the model

$$R_n = P_n - P_{n-2f} = 2f(\gamma_f - 1)(n^{-1} + fn^{-2}) + b'_f n^{-1-\Delta_1} + c'_f n^{-2}. \quad (21)$$
Figure 8. $K_7 + Q_n$ plotted against $1/n^{3\gamma}$ with $\gamma_7 = -0.2526(35)$ using cubic lattice data for seven-stars with arms initiated on lattice sites on a sphere of radius $\sqrt{5}$ centred at the origin. Left panel: plot without taking account of the analytic correction in the data. Right panel: the same data but now with an analytic correction included and with $K_7$ chosen such that the middle curve passes through zero when $n = 500$. In the right panel the top and bottom curves correspond to the value of $\gamma_7$ at the limits of its error bars. The plots are for data with $n \geq 120$, and the estimate of $\gamma_7$ were extracted from data with $n \geq 200$.

Linear least squares analysis using this model for $n > n_{\text{min}} = 200$ gave good estimates of $\gamma_f$. For example, if $f = 7$ this gives $\gamma_7 = -0.2526 \ldots$ (this compares well with the estimate obtained from the Domb–Joyce model in reference [18]). In addition, we found that $c_7' = 35.57 \ldots$. The effect of the analytic correction can be checked by plotting $K_7 + Q_n$ against $1/n^{3\gamma}$ without the analytic correction. This is shown in the left panel of figure 8. The result is a strongly curved graph, which straightens when the correction is included (right panel). In the right panel we also determine an error bar on the estimate of $\gamma_7$ using the same approach as before. This gives $\gamma_7 = -0.2526(35)$. Estimates for $7 \leq f \leq 12$ are shown in table 5.

2.2. Results: FCC and BCC lattice stars

Simulations in the FCC and BCC lattices were performed similarly to those in the cubic lattice. In the FCC we are able to grow stars with central node at the origin for $3 \leq f \leq 12$, and in the BCC lattice for $3 \leq f \leq 8$. In each of these lattices good estimates of the growth constant $\mu_3$ were needed (see equation (18)). The most precise estimates (extrapolated from exact enumeration data) were obtained in reference [34] and are

$$\mu_3 = \begin{cases} 10.037075(20), & \text{(FCC)}; \\ 6.530520(20), & \text{(BCC)}. \end{cases}$$

(22)

Using these estimates in equation (18) proved that they are accurate enough to extract accurate estimates of the $f$-star exponents $\gamma_f$. Our analysis proceeded as in figures 6 and 7. Details of our results and estimates of $\gamma_f$ are shown in tables 6 and 7.

2.3. Amplitudes

Estimates of the amplitude $U_f$ in equation (15) can be made by using the results for $\gamma_f$. Noting that the $o(1)$ term is dominated by the confluent correction, it follows that

$$\log(s_n^{(f)}/\mu_3^f) - (\gamma_f - 1) \log n = \log U_f + B_f n^{-\Delta_1}. \quad (23)$$
Table 6. Estimates of $\gamma_f$ in the FCC lattice.

| $f$ | Length Tours | $\gamma_f$ (FCC) |
|-----|--------------|------------------|
| 3   | 12000 2      | $2.026 \times 10^8$ | 1.04290(12) |
| 4   | 12000 2      | $2.800 \times 10^8$ | 0.8343(15)   |
| 5   | 12000 2      | $2.150 \times 10^8$ | 0.5415(25)   |
| 6   | 12000 2      | $2.102 \times 10^8$ | 0.1712(28)   |
| 7   | 14000 2      | $2.866 \times 10^8$ | $-0.258(4)$  |
| 8   | 14000 2      | $2.836 \times 10^8$ | $-0.757(5)$  |
| 9   | 14400 2      | $2.712 \times 10^8$ | $-1.313(6)$  |
| 10  | 14000 2      | $2.764 \times 10^8$ | $-1.919(6)$  |
| 11  | 14300 2      | $2.898 \times 10^8$ | $-2.593(7)$  |
| 12  | 14400 2      | $2.840 \times 10^8$ | $-3.308(8)$  |

Table 7. Estimates of $\gamma_f$ in the BCC lattice.

| $f$ | Length Tours | $\gamma_f$ (BCC) |
|-----|--------------|------------------|
| 3   | 12000 2      | $2.142 \times 10^8$ | 1.0429(5)   |
| 4   | 12000 2      | $2.106 \times 10^8$ | 0.8340(8)   |
| 5   | 12000 3      | $3.034 \times 10^8$ | 0.5405(20)  |
| 6   | 12000 2      | $2.720 \times 10^8$ | 0.1715(25)  |
| 7   | 12005 5      | $5.262 \times 10^8$ | $-0.259(4)$ |
| 8   | 12000 6      | $6.230 \times 10^8$ | $-0.762(6)$ |

Table 8. Estimated amplitudes $U(f)$.

| $f$ | SC lattice | FCC lattice | BCC lattice |
|-----|------------|-------------|-------------|
| 3   | 1.142(7)   | 1.189(25)   | 1.161(12)   |
| 4   | 0.952(10)  | 1.25(4)     | 1.147(18)   |
| 5   | 0.631(10)  | 1.36(6)     | 1.09(5)     |
| 6   | 0.247(8)   | 1.53(8)     | 0.95(5)     |
| 7   | —          | 1.58(11)    | 0.62(5)     |
| 8   | —          | 1.66(15)    | 0.26(3)     |
| 9   | —          | 1.56(17)    | —           |
| 10  | —          | 1.20(13)    | —           |
| 11  | —          | 0.80(10)    | —           |
| 12  | —          | 0.28(4)     | —           |

Thus, by taking $\gamma_f$ at its best value, and by plotting the left-hand side against $n^{-\Delta_1}$, the y-intercept would be equal to $\log U(f)$. To avoid bias due to corrections at small $n$, data with $n \leq 30f$ were discarded, and the remaining data plotted and extrapolated using a linear model against $n^{-\Delta_1}$. This gives the estimates in table 8.

The error bars were estimated by exploring the values of the amplitudes at the limits of the confidence intervals on $\gamma_f$, as shown in tables 5–7, for the SC, FCC and BCC lattices respectively. Notice that the amplitudes $C_k^f$ in equation (5) can be obtained using the symmetry factors relating $U(f)$ and $C_k^f$. For example, in the cubic lattice the relation is given by equation (16) for $3 \leq f \leq 6$ and $0 \leq k < f$. This relation similarly generalises to the FCC and BCC, but for $3 \leq f \leq 12$ and $3 \leq f \leq 8$, respectively.
3. Sampling branched structures

In this section the consistency of vertex exponents is examined by considering the scaling of more general branched structures. That is, we calculate the entropic exponents of the acyclic branched structures in figure 1 to show that they satisfy the relations in equation (14) within the numerical accuracy obtained in this paper.

As in section 1.2, define the length or size $n$ of a lattice network to be the total number of steps or edges. A lattice network with connectivity $G$ is monodisperse or strictly uniform if all branches have the same length. The underlying connectivities of networks in this study are shown in figure 1, and are $C$ (a comb) and two kinds of brushes, namely $B_1$ and $B_2$. Examples of these networks are shown in figures 2–4. The scaling of $C$, $B_1$ and $B_2$ are given by equation (12), and the entropic exponents are given in terms of the vertex exponents in equation (14).

There is a repulsion between vertices of higher degree in networks like combs and brushes which stretches the self-avoiding walks joining them. This effect is more difficult to simulate using the PERM algorithm, and motivated us to use the Wang–Landau algorithm [40] instead. In this study we used a parallel implementation of this algorithm.

This Wang–Landau algorithm efficiently approximates the density of states in the presence of a cost function. In this case the cost function is the energy of the states. The sampling is from a probability distribution that becomes asymptotically uniform. If $E_{\text{old}}(g(E_{\text{old}}))$ is the energy (respectively density) of the current configuration and $E_{\text{new}}(g(E_{\text{new}}))$ is the energy (respectively density) of the proposed configuration, a proposed move to the new state is accepted with probability $\min \left\{ \frac{g(E_{\text{new}})}{g(E_{\text{old}})}, 1 \right\}$. Each time a state is visited, the density of states is updated by a modification factor $f$ such that $g(E) \leftarrow g(E) \cdot f$. A histogram $H(E)$ recording each visit is kept and a flatness criterion for the histogram is used to update the modification factor $f$. That is, when the histogram achieves the flatness criterion it is reset and $f$ is reduced in a predetermined fashion. This must be done with care, since if $f$ is decreased too rapidly this can lead to saturation errors. In our implementation there are four parallel streams that are used to control the update of $f$ common to all parallel streams.

For branched structures the algorithm first grows a central uniform star and then grows the additional branches from the endpoint of that star. To grow a star with $f$ arms the central vertex is fixed and at each stage $f$ steps are sampled uniformly at random to be appended to the end-vertices of the star. If there are no intersections in the proposed steps and the state change is accepted then the new configuration is kept. Otherwise, the original configuration is re-read and the density is updated accordingly. When the star is fully grown the branch vertex is chosen uniformly at random from the $f$ candidates. Once chosen the remaining branches are grown from the branch vertex analogously to the arms of the star.

Let $b$ denote the number of total branches (including the original star arms), each of length $\ell$, of the comb or brush under consideration. The process of first growing a star and then growing the remaining branches is iterated so that each structure of uniform length $n = b\ell$ is independently sampled via the Wang–Landau algorithm for $\ell = 1, \ldots, 200$. For each $\ell$, on the order of $10^9$ configurations were sampled. A more explicit formulation of the Wang–Landau algorithm used for sampling stars is provided below for reference.

**Wang–Landau algorithm**

This algorithm samples $M$ stars with $s$ arms, each of length 0 to $\ell$ and returns the approximate counts $\hat{c}_\ell$ at each length $\ell$. Define $d_\ell = \ln(\hat{c}_\ell)$
(a) Let \( d_f = 0 \) for all \( \ell \), set \( f = 1 \) and let \( v_{0} \) be the vertex at the origin. Set checkpoint \( c \) to test for histogram flatness and \( o_{\ell} \) the number of observations of length \( \ell \) for each \( \ell \). Let \( t = 1 \) be the number of checks.

(b) Suppose \( \ell > m \geq 0 \). Choose uniformly among the nearest neighbours of \( \{v_{m}^{1}, \ldots, v_{m}^{f}\} \), unoccupied or otherwise, to propose the next steps of the star.

(c) If the proposed move is \( \{v_{m-1}^{1}, \ldots, v_{m-1}^{f}\} \) then step back with probability \( \min\{1, \exp(\Delta d_m - \Delta d_{m-1})\} \). Set \( d_{m-1} = d_{m-1} + f \) and \( o_{m-1} = o_{m-1} + 1 \). Otherwise reread the current location and set \( d_{m} = d_{m} + f \) and \( o_{m} = o_{m} + 1 \). Else check for intersections with previously visited vertices \( \{v_{i}^{1}, \ldots, v_{i}^{f}\} \) for \( i = 0, \ldots, m-1 \) and among the proposed vertices. If there are no intersections set \( \{v_{m+1}^{1}, \ldots, v_{m+1}^{f}\} \) to be the new vertices with probability \( \min\{1, \exp(\Delta d_{m} - \Delta d_{m+1})\} \). Set \( d_{m+1} = d_{m+1} + f \) and \( o_{m+1} = o_{m+1} + 1 \). Otherwise if the proposed vertices are rejected or there is an intersection, reread the current location and set \( d_{m} = d_{m} + f \) and \( o_{m} = o_{m} + 1 \).

(d) Suppose \( m = \ell \). Then perform the steps as in step 3 but step forward with probability 0.

(e) Repeat steps 2 to 4 until \( c \) iterations are performed. Test for histogram flatness by considering the \( o_{\ell} \). If the desired flatness is reached set \( t = t + 1 \) and update \( f \).

(f) Repeat steps 2 to 5 until \( M \) observations have been reached.

Data were collected and analysed similarly to the analysis done in section 2. In determining the approximate counts for lattice networks, there are (similarly to the case for lattice stars) symmetry factors which should be taken into account when calculating amplitudes \( C_G \).

The symmetry factors are determined as follows: let the root star of the network have \( f \) arms, and \( b - f \) branches are grown on the endpoint of one of the root star arms. The symmetry factor is then equal to the number of ways to colour these arms, namely \( (f - 1)! (b - f)! \). This is seen by noting that the arm from which the branching occurs is coloured in one way, and the remaining arms in \( (f - 1)! \) ways. The last \( b - f \) arms can be coloured in \( (b - f)! \) ways.

In addition, the counts also have to be normalised by counting the number of ways the same network can be grown by the algorithm. Each network of length \( n \) is grown by first growing a star of length \( \ell f \) and then growing the addition arms comprising \( (b - f) \ell \) steps. In \( d \) dimensions the sample space of each step in the \( f \)-star is \( (2d)^{\ell f} \) and for the addition branches is \( (2d)^{b - f} \). In flat histogram sampling these factors are accounted for in the relative weights of stars-to-network. Since stars are grown first and the empty walk of unit weight is the root of the star, if the normalization is done in this way, there is systematic under-counting by a factor of \( (2d)^{\ell f - (b - f)} \). Taken together, in order to account for these factors we must divide the original counts by \( \frac{(f - 1)! (b - f)!}{(2d)^{\ell f - (b - f)}} \).

### 3.1 Estimating vertex exponents from lattice networks

In this section we will follow closely the procedure for stars in order to estimate the entropic exponent of branched lattice networks. These estimates can then be used to recover the vertex amplitudes and corroborate the estimates of the preceding sections alongside the scaling relation (13). As with stars we expect

\[
c_d(\mathcal{G}) = C_d n^{\gamma_{d-1} - 1} \mu_{d}^{n},
\]

(24)
Table 9. Estimates of $\sigma_f$ from $\gamma_G$ in 3d.

| Exponent | Table 2 | This work |
|----------|---------|-----------|
| $\sigma_3$ (via $C$) | $-0.19313(11)$ | $-0.19350(91)$ |
| $\sigma_4$ (via $B_1$) | $-0.4802(5)$ | $-0.4885(78)$ |
| $\sigma_4$ (via $B_2$) | $-0.4802(5)$ | $-0.4887(29)$ |

and so, to estimate $\gamma_G$ from the data we search for $x = \gamma_G - 1$ such that

$$Q_n(x) = \log \left( \frac{c_n(G)}{n^{\gamma_G}} \right) \approx \text{constant},$$

as $n \to \infty$. These networks have $b \in \{5, 6, 7\}$ branches and were sampled for $n = b\ell$ where $\ell = 1, 2, \ldots, 200$ (that is, 200 steps per branch) giving a maximum size $n_{\max} \in \{1000, 1200, 1400\}$. To account for corrections due to small networks we perform the analysis for $\ell \geq \ell_{\min}$. By plotting $Q_n(x)$ against $\log(n)$ for $\ell \geq \ell_{\min}$ and different values of $x$ we can calculate the slope by way of a linear fit and interpolate to find the optimal value of $x$. Since we have less data for branched structures we let $\ell_{\min}$ range over $\{2, \ldots, 15\}$ and then similarly extrapolate the estimate via a fit against $\frac{1}{\sqrt{n_{\min}}} = \frac{1}{\sqrt{b\ell_{\min}}}$. To arrive at a final estimate for $\gamma_G$ we first take independent samples of 90% of our data to estimate the slope for each $\ell$. Note that for each $\ell$ the counts were generated completely independently so there is no serial correlation in the estimates introduced by the simulation. When this is done we have several data sets with estimates at each $\ell_{\min}$ and we subset each data set by sampling half of the $\ell_{\min}$ values at random. Iterating this several times gives us a large set of estimates from which we can calculate the variance. The error bars are given by three standard deviations to account for unknown corrections due to the size of the networks and the best estimate is taken to be the average. In total we sample the count data 10 times and perform the extrapolation procedure 100 times. In all, this gives us a final set of 1000 estimates and the final estimates of this analysis are

$$\gamma_C - 1 = -0.0731(18), \quad \gamma_{B_1} - 1 = -0.2896(69), \quad \gamma_{B_2} - 1 = -0.5065(58).$$

Using the best estimate of $\sigma_1$ in the square and cubic lattices allows us to recover the vertex exponents $\sigma_f$ for $f = 3$ and $f = 4$ from the estimates of $\gamma_G$ via the relations in equation (14). For $B_1$ we use the estimate of $\sigma_3$ from $\gamma_C$ to get a second estimate of $\sigma_4$. The results are compiled in table 9 alongside our estimates from stars in the cubic lattice. The estimates of $\sigma_4$ slightly overestimate the results from the star data (in particular the estimate from $B_2$ which is roughly three error bars from the star estimate). This may be due to the shorter branches in our network models. We investigated this possibility by re-analysing our data for four-stars, but using a maximum cut-off of 200 on the length of branches (so that four-stars have length at most 800). This gives the estimate $-0.4875(17)$, which is consistent with the estimates obtained from $B_1$ and $B_2$ in table 9, showing that estimates obtained from the lattice networks are systematically under-estimated. Taking this into account show that our network results for $\sigma_3$ and $\sigma_4$ are in good agreement (for $C$ and $B_1$), or at worst marginal (for $B_2$), when compared to our results from lattice stars.

Finally, comparing the results for $\gamma_G$ with the predicted values from our star data via equation (14) shows very good agreement (see table 4), and confirms for these networks the predictions from relation (1).
Table 10. Estimates of $C(G)$ in the cubic lattice.

| Network | $C_G$  | $C$   |
|---------|--------|-------|
| $G = C$ | 0.29(4) | 1.19(6) |
| $G = B_1$ | 0.094(5) | 1.196(6) |
| $G = B_2$ | 0.0304(12) | 1.2013(16) |

3.2. Estimating amplitudes for lattice networks

Taking logarithms of the ratio $c_n(G)/c_n$, and using equations (3) and (12) gives the models

$$\log \left( \frac{c_n(G)}{c_n} \right) = \log \left( \frac{C_G}{C} \right) + \left( \gamma_G - 1 - 2\sigma_1 \right) \log n, \quad (26)$$

$$\log \left( \frac{c_n(G)}{\sqrt{c_{2n}}} \right) = \log \left( \frac{C_G}{\sqrt{2^\sigma_1}} \right) + \left( \gamma_G - 1 - \sigma_1 \right) \log n. \quad (27)$$

Fitting the model to our data allows us to get estimates for the amplitude ratios $C_G/C$ where $C$ is the self-avoiding walk amplitude (see equation (3)). By considering the results for $\ell_{\text{min}} = 1, 2, \ldots, 50$ we extrapolate using

$$\log \left( \frac{C_G}{C} \right) \bigg|_{n_{\text{min}}} \approx \beta_0 + \frac{\beta_1}{n_{\text{min}}} + \frac{\beta_2}{n_{\text{min}}^2},$$

$$\log \left( \frac{C_G}{\sqrt{2^\sigma_1}} \right) \bigg|_{n_{\text{min}}} \approx \delta_0 + \frac{\delta_1}{n_{\text{min}}} + \frac{\delta_2}{n_{\text{min}}^2}. \quad (28)$$

A systematic error is estimated by comparing the results to that of a three parameter regression adding the term $c/n$ to the right-hand side of equations (26) and (27). Due to data limitations, to avoid over fitting in this three parameter fit we perform the extrapolation for $\ell_{\text{min}} \in \{1, \ldots, 15\}$. The estimated systematic error is taken to be the absolute difference between these estimates. Then, by using the best estimate of $\sigma_1$ we can solve simultaneously for $C_G$ and $C$. Our results are collected in table 10. The final reported errors are computed by carrying through the errors computed in the original fits. Once again, we see good agreement between the values of $C$ for each network structure.

4. Conclusion

In this paper we have given an account of sampling lattice stars and acyclic lattice networks using implementations of parallel PERM [4, 13, 17] and a parallel implementation of the Wang–Landau algorithm [40]. Our simulations produced a large set of data in the form of approximate counts, which we analysed to extract estimates of the entropic exponents $\gamma_f$, and the vertex exponents $\sigma_f$, of lattice stars, as well as lattice networks.

Our final estimates of the entropic exponents are listed in table 1 (these are weighted averages of the estimates obtained in tables 5–7). Our best estimates of the vertex exponents are shown in tables 2 and 3 for $3 \leq f \leq 6$. These results are consistent with, and in some cases improve on, estimates in other studies.

The estimates obtained from the $\epsilon$-expansion are shown in table 3. For the exponents $\sigma_1$ and $\sigma_3$ the $\epsilon$-expansion gives reasonable results at the order $\epsilon$ level, but breaks down at higher orders. The $\epsilon$ expansions for $\sigma_4$, $\sigma_5$ and $\sigma_6$ deteriorate for higher order expansions, and there
appears little prospect at this time, even with resummation techniques, of finding better values for the vertex exponents in this way.

Our results for the entropic exponents for the lattice networks $C$, $B_1$ and $B_2$ are listed in table 4. Our results deviate from predictions of first order $\epsilon$-expansion, and higher order expansions does not improve this. Our predictions of the entropic exponent for lattice networks from our vertex exponent data are shown in table 4, and compares well with the direct estimates obtained from our simulations. This serves as an independent confirmation of the earlier results and presents evidence affirming the theorized scaling relation (14) for these branched structures.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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