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J. Phys. A: Math. Gen. **20** (1987) 1839-1854. Printed in the UK

On the critical behaviour of self-avoiding walks

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Received 9 July 1986

Abstract. For the self-avoiding walk problem the series expansions of the chain generating function and mean square end-to-end distance generating function have been extended to 27 steps for the square lattice and to 20 steps for the simple cubic lattice. We develop an analysis protocol based on the method of integral approximants. Using this protocol we find excellent agreement with Nienhuis' exact exponent values in two dimensions, $\gamma = 1.343\,75$ and $\nu = 0.750$. In three dimensions we find $\gamma = 1.162 \pm 0.002$ and $\nu = 0.592 \pm 0.002$. Accurate estimates of the critical point (reciprocal of the connective constant) for several two- and three-dimensional lattices are also obtained.

1. Introduction

We have extended the series for both the square lattice and simple cubic lattice self-avoiding walk chain generating function and mean square end-to-end distance series. For the square lattice we have obtained 27 terms, extended the existing series by two terms, while for the simple cubic lattice we have obtained 20 terms, an extension of one term for the chain generating function and five terms for the mean square end-to-end distance series.

The series extensions were performed on a dedicated DEC Micro Vax II, using a modified version of Torrie's dimerisation program (Torrie and Whittington 1975). The execution times were 30 d for the square lattice and 75 d for the simple cubic lattice! These enormous times nevertheless constitute cheap computing given the cost of the hardware.

The resulting series were carefully analysed by the method of integral approximants, using a protocol which we believe has widespread applicability. One difficulty in using integral approximants is that, in principle, a huge number of approximants are calculable and one must decide *which* approximants to calculate, and how to combine the results so obtained into a single estimate of the critical parameters, with associated error estimates.

In the next section we develop what we consider to be an appropriate protocol and demonstrate it on a variety of series with known critical behaviour. Subsequently, in § 3, we analyse the newly obtained series, and re-examine some existing series, in order to demonstrate the consistency of critical exponent estimates for a given space dimension and to obtain more precise values of the critical parameters. Section 4 comprises a discussion and conclusion.

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2. Method of analysis

The method of integral approximants (Fisher and Au-Yang 1979, Hunter and Baker 1979, Guttmann and Joyce 1972, Rehr *et al* 1980) consists of representing the power series under study by the integral of the kth-order linear differential equation

$$\sum_{i=0}^{K} Q_i(a)\mathscr{D}^i f(z) = P(z) \tag{2.1}$$

with

$$\mathscr{D} = z\,\mathrm{d}/\mathrm{d}z \tag{2.2}$$

and Q_i and P polynomials in z of degree N_i and L, respectively, so that

$$Q_i(z) = \sum_{j=0}^{N_i} Q_{i,j} z^j \qquad P(z) = \sum_{j=0}^{L} P_j z^j. \tag{2.3}$$

We choose $Q_{K,0} = 1$ and, in the homogeneous case when $P(z) \equiv 0$, $Q_{0,0} = 0$. This choice of differential equation is different from that used by Hunter and Baker (1979) and Fisher and Au-Yang (1979) in that we have forced the point at the origin to be a regular singular point. This choice is motivated by the fact that the Onsager (1944) solution of the zero-field free energy of the square lattice Ising model satisfies just such a differential equation. Further details of the method are discussed by Rehr *et al* (1980), Guttmann (1986b), Hunter and Baker (1979) and Fisher and Au-Yang (1979).

This differential equation is a 'natural' generalisation of the Dlog Padé representation. It is 'natural' in the sense that it generalises the class of functions representable by the differential equation to those functional forms we believe appropriate to the underlying thermodynamic functions.

To be more precise, if $K = 1$ in (2.1), we denote the approximants by $[L/N_0; N_1]$ and the differential equation can then represent functions with singularities of the form

$$f(z) \sim A(z) + B(z)(1 - z/z_i)^{-\gamma} \tag{2.4}$$

where A and B are regular in the neighbourhood of $z = z_i$. By comparison, the Dlog Padé approximants are appropriate to functions of the more restricted form,

$$f(z) \sim B(z)(1 - z/z_c)^{-\gamma}. \tag{2.5}$$

If $\gamma \geqslant 1$, then Dlog Padé's will usually do an acceptable job of representing functions of the form (2.4), as the additive term $A(z)$ is then negligible. Such is the case for the susceptibility of the two-dimensional Ising model, for which $\gamma = 1.75$. However, for the specific heat of the three-dimensional Ising model, with exponent $\alpha \approx 0.1$, the Dlog Padé's do a poor job, as now the additive term in (2.4) is *not* negligible compared to the singular term.

In the case of a confluent singularity, the $K > 1$ approximants would be expected to be appropriate, as (2.1) can then represent a singularity with $K - 1$ additional confluent terms, i.e.

$$f(z) \sim A(z) + B(z)(1 - z/z_c)^{-\gamma}[1 + C_1(z)(1 - z/z_c)^{\Delta_1} + C_2(z)(1 - z/z_c)^{\Delta_2} + \ldots + C_{K-1}(z)(1 - z/z_c)^{\Delta_{K-1}}] \tag{2.6}$$

where $\Delta_i < 0$, $\Delta_i \neq$ integer, $\Delta_i \neq \Delta_j$ and $C_i(z)$ is regular in the neighbourhood of z_c. Of course other types of singularity, such as confluent logarithms and even certain essential singularities, are also representable by the differential equation (2.1) (see Joyce and Guttmann 1973), but (2.4)-(2.6) are those commonly encountered in a variety of statistical mechanical models.

For the two-dimensional Ising model susceptibility, we expect singularities of the form (2.4), so a $K = 1$ differential approximant would be appropriate and we show that this is indeed the case. However, for both the two- and three-dimensional SAW problems, and the three-dimensional Ising problem, the representation (2.6) is believed to hold, and so we might expect that approximants with $K > 1$ are more appropriate in studying such functions than are approximants with $K = 1$. Somewhat surprisingly, we find that this is not usually so. In almost every case, including those where one or more confluent terms are expected, we find that the $K = 1$ approximants are more stable, and appear better converged, than their $K > 1$ counterparts. The only explanation we have for this is that the confluent terms are comparatively weak when compared to the leading singular term, and so can be adequately represented *numerically* by the additive analytic term $A(z)$. However, for the generating function of the mean square end-to-end distance, the confluent structure is more complex, as we show in § 3, and in that case higher-order ($K > 1$) approximants are more appropriate.

The choice of which approximants to use is suggested by the invariance properties of Padé approximants. The diagonal $[N/N]$ Padé approximants are known to be invariant under the homographic transformation

$$z = A\omega/(1 + B\omega) \tag{2.7}$$

which is the principal reason that one traditionally focuses on the diagonal and near-diagonal entries of the Padé table.

For the first-order integral approximants ($K = 1$), an analysis parallel to that given by Hunter and Baker (1979) shows that the $[L/L; L+1]$ approximants possess this same invariance property. For $K > 1$ the situation is more complex and is fully discussed by Baker (1984). In practice we have found that approximants *near to* the invariant approximants are equally good. Therefore we have chosen to use the following sequence of approximants, which, for the most part, are near to the invariant approximants. For $K = 1$ we use the $[L/N-1; N]$, $[L/N; N]$ and $[L/N+1; N]$ approximants with $1 \leqslant L \leqslant 8$ and $N \geqslant 2$. For $K > 1$ we use the $[L/N-1; N-1, \ldots, N-1, N]$, $[L/N; N, \ldots, N, N]$ and $[L/N+1; N+1, \ldots, N+1, N]$ approximants with $1 \leqslant L \leqslant 8$ and $N \geqslant 2$. Note too that biased approximants can also be defined, in which the position, or position and exponent, of one or more singularities may be specified—see Rehr *et al* (1980) and Guttmann (1987) for further details.

For our first example we take the high-temperature susceptibility series of the triangular lattice $S = \frac{1}{2}$ Ising model, for which only 16 terms are known. A section of the table of approximants is shown in table 1, corresponding to those approximants defined above with $K = 1$. Certain coefficients are marked as defective. These are defined as approximants in which there is a (spurious) singularity on the positive real axis closer to the origin than the physical singularity. This parallels standard practice with Padé approximants. Additionally, however, it has been observed that a singularity on the positive real axis *beyond*, but close to, the physical singularity has a seriously deleterious effect on the exponent estimate of the approximant. Accordingly, we denote as defective all approximants with singularities on the positive real axis in the range $0 < z < 1.15 z_c$, other than the physical singularity at $z = z_c$. (Rarely, we find singularities

Table 1. Triangular lattice Ising model susceptibility. Integral approximants $[L/N+\Lambda; N]$, $\Lambda = -1, 0, 1$, showing estimates of x_c and γ. Defective approximants (see text) are marked with an asterisk.

		N					
	Λ	2	3	4	5	6	7
$L=1$	−1	0.266 493	0.270 977*	0.268 993*	0.270 004*	0.267 986	0.267 922
		—	−1.927 0	−1.819 7	−1.891 2	−1.755 2	−1.745 0
	0	0.250 000	0.272 195*	0.268 523	0.269 723*	0.267 967	0.267 951
		−1.000 0	−1.994 2	−1.790 0	−1.897 7	−1.752 7	−1.750 3
	1	0.271 329*	0.269 020*	0.269 282*	0.268 051*	0.267 952	
		−1.946 9	−1.821 4	−1.902 0	−1.763 7	−1.750 5	
$L=2$	−1	0.264 516	0.268 555*	0.267 293*	0.267 989*	0.267 967*	0.268 274*
		−1.605 5	−1.792 2	−1.701 9	−1.755 7	−1.753 9	−1.784 2
	0	0.271 130*	0.268 678*	0.267 953*	0.267 983*	0.267 967*	
		−1.935 2	−1.799 4	−1.751 7	−1.755 1	−1.754 4	
	1	0.271 731	0.267 532*	0.267 937	0.267 967*	0.267 953	
		−1.970 1	−1.720 6	−1.749 5	−1.752 9	−1.750 7	
$L=3$	−1	0.295 532	0.268 689*	0.267 922*	0.267 983*	0.267 962*	
		−3.641 3	−1.800 2	−1.750 1	−1.755 0	−1.753 4	
	0	0.270 783*	0.267 355*	0.267 958*	0.267 988*	0.268 033*	
		−1.919 2	−1.707 0	−1.752 0	−1.755 7	−1.765 3	
	1	0.269 177*	0.267 960*	0.267 983*	0.267 983*		
		−1.831 1	−1.752 1	−1.755 0	−1.748 4		
$L=4$	−1	0.268 984	0.267 444	0.268 243*	0.267 964*	0.268 023*	
		−1.799 5	−1.700 5	−1.784 4	−1.752 5	−1.763 7	
	0	0.262 685	0.267 483	0.267 981*	0.267 934		
		−1.253 1	−1.697 7	−1.754 8	−1.747 8		
	1	0.267 469	0.267 948	0.267 971*	0.267 978*		
		−1.698 7	−1.750 7	−1.753 6	−1.755 4		
$L=5$	−1	0.267 400	0.268 349*	0.267 965	0.267 940		
		−1.717 9	−1.794 5	−1.750 9	−1.748 3		
	0	0.268 561*	0.268 077	0.267 990*	0.267 942*		
		−1.814 9	−1.765 3	−1.756 7	−1.748 4		
	1	0.268 133	0.267 979	0.267 944			
		−1.771 5	−1.754 2	−1.748 6			
$L=6$	−1	0.267 202	0.268 042	0.267 930	0.267 967*		
		−1.686 3	−1.761 2	−1.746 9	−1.753 5		
	0	0.268 444	0.267 828	0.267 952			
		−1.804 4	−1.734 9	−1.750 7			
	1	0.268 075	0.267 959	0.267 950			
	1	−1.765 0	−1.751 8	−1.750 1			
$L=7$	−1	0.268 176	0.267 933	0.267 974*			
		−1.772 9	−1.748 0	−1.755 2			
	0	0.269 152*	0.267 939	0.267 926			
		−1.867 4	−1.748 6	−1.744 6			
	1	0.267 952	0.267 953				
		−1.750 2	−1.751 0				
$L=8$	−1	0.267 935	0.267 941	0.267 987*			
		−1.746 9	−1.749 0	−1.757 3			
	0	0.267 837	0.268 834*				
		−1.734 5	−1.933 6				
	1	0.267 934	0.267 961				
		−1.747 7	−1.752 3				

in the complex plane close to this section of the real line. Such approximants are also considered to be defective.)

From this table we summarise the data by taking means of estimates of the critical parameters for fixed values of n, where n is the maximal order of the coefficients used in the construction of the approximant. For each value of n there are $l(n)$ non-defective approximants. These data are shown in table 2, together with an error, which is *twice* the standard deviation, corresponding to 99% confidence limits. (Occasional outliers being five standard deviations or more from the mean are also excluded.) Final estimates of the critical exponent γ and critical point v_c are obtained by taking all estimates with an error not exceeding four times the minimum error (which includes all entries in this case) and weighting them according to their associated error. Thus if we denote the entries for the critical exponent by $\gamma_i \pm \varepsilon_i$ $(i = 1, \ldots, M)$ we have

$$\langle \gamma \rangle = \sum_{i=1}^{M} (\gamma_i/\varepsilon_i) \left(\sum_{i=1}^{M} 1/\varepsilon_i \right)^{-1} \tag{2.8a}$$

with error given by

$$\langle \varepsilon \rangle = \sqrt{M} \left(\sum_{i=1}^{M} 1/\varepsilon_i \right)^{-1}. \tag{2.8b}$$

In this way we obtain

$$\begin{aligned} \gamma &= 1.7495 \pm 0.0024 \\ v_c &= 0.267\,945 \pm 0.000\,011 \end{aligned} \tag{2.9}$$

Table 2. Summary of results in table 1. The column labelled 'exponents' gives estimates of γ. The column labelled l gives the sample size used in calculating the means. Errors are *two* standard deviations. (*a*) Unbiased estimates, (*b*) biased estimates.

(*a*)

n	Exponent	Critical point	l
11			
12	1.7490 ± 0.0040	$0.267\,940 \pm 0.000\,014$	3
13	1.7512 ± 0.0059	$0.267\,963 \pm 0.000\,042$	5
14	1.7494 ± 0.0092	$0.267\,945 \pm 0.000\,029$	6
15	1.7488 ± 0.0042	$0.267\,942 \pm 0.000\,023$	7
16	1.7496 ± 0.0058	$0.267\,948 \pm 0.000\,026$	5

(*b*)

n	$K = 1$	l	$K = 2$	l
11	$1.750\,49 \pm 0.002\,38$	5	$1.748\,93 \pm 0.004\,09$	5
12	$1.750\,31 \pm 0.001\,91$	11	$1.749\,57 \pm 0.004\,39$	6
13	$1.750\,15 \pm 0.001\,15$	8	$1.749\,65 \pm 0.001\,68$	7
14	$1.750\,13 \pm 0.000\,67$	9	$1.750\,31 \pm 0.000\,32$	6
15	$1.749\,85 \pm 0.000\,84$	7	$1.750\,21 \pm 0.000\,21$	7
16	$1.749\,95 \pm 0.000\,43$	12	$1.749\,75 \pm 0.001\,45$	7

which can be compared to the exact values of 1.75 and 0.267 9491, . . . , respectively. Another calculation we did was a linear regression analysis of all entries corresponding to $n = 16$ (the highest-order coefficients). Then specifying the exact value of v_c gave $\gamma = 1.7499$.

Next we constructed biased approximants, utilising the known value of v_c, and obtained the results also shown in table 2 for both $K = 1$ and $K = 2$. Utilising the error analysis described above, we obtained the estimates

$$\begin{aligned} &\gamma = 1.750\,03 \pm 0.000\,35 \qquad K = 1 \\ &\gamma = 1.750\,19 \pm 0.000\,18 \qquad K = 2. \end{aligned} \tag{2.10}$$

Here we see that biased results ($K = 1$) are nearly an order of magnitude more accurate than their unbiased counterparts. Further, the results $K = 1$ are closer to the exact value than are those for $K = 2$. This is to be expected for this function, as there is no confluent singularity and so a $K = 1$ approximant is expected to be optimal. Both here and throughout this paper errors quoted in means are *two* standard deviations.

As a second example we turn to the series for the chain generating function of the honeycomb lattice SAW problem. In that case both the exponent ($\frac{43}{32}$) and the critical point $(2+\sqrt{2})^{-1/2} = 0.541\,1961\ldots$ are exactly known due to Nienhuis (1982, 1984). Furthermore, it is widely believed (though by no means settled) that this function *does* have one or more confluent terms, so that higher-order approximants might be expected to be more suitable than first-order approximants. We return to a discussion of the existence of a confluent singularity in § 4. For this problem we have repeated the previous analysis and show the results in table 3.

Table 3. Honeycomb lattice $C(x)$ series. Summary of exponent and critical point estimates from first- and second-order unbiased approximants. (*a*) $K = 1$ approximants, (*b*) $K = 2$ approximants.

(*a*)

n	Exponent	Critical point	l
26	1.349 47 ± 0.032 18	0.541 2481 ± 0.000 3122	8
27	1.349 18 ± 0.009 71	0.541 2366 ± 0.000 0756	7
28	1.344 12 ± 0.018 99	0.541 1736 ± 0.000 1423	11
29	1.345 07 ± 0.006 05	0.541 2448 ± 0.000 0405	10
30	1.344 61 ± 0.011 45	0.541 2128 ± 0.000 0771	10
31	1.343 87 ± 0.008 94	0.541 1961 ± 0.000 0571	5
32	1.343 03 ± 0.003 39	0.541 1899 ± 0.000 0228	7
33	1.341 20 ± 0.003 40	0.541 1776 ± 0.000 0247	8
34	1.341 30 ± 0.004 84	0.541 1776 ± 0.000 0298	11

(*b*)

n	Exponent	Critical point	l
23 and 24	1.345 45 ± 0.021 80	0.541 2562 ± 0.000 2976	16
25 and 26	1.346 36 ± 0.011 86	0.541 2189 ± 0.000 1332	14
27 and 28	1.347 19 ± 0.004 99	0.541 2201 ± 0.000 0443	9
29 and 30	1.346 88 ± 0.003 23	0.541 2162 ± 0.000 0297	12
31 and 32	1.344 32 ± 0.005 26	0.541 2004 ± 0.000 0265	7
33 and 34	1.345 23 ± 0.003 80	0.541 2039 ± 0.000 0249	6

We combine these as described above to give the estimates

$$\left.\begin{aligned}&\gamma = 1.3433 \pm 0.0021\\ &x_c = 0.541\,198 \pm 0.000\,014\\ &\langle x_c\rangle_{lr} = 0.541\,195\end{aligned}\right\} \quad K = 1$$
$$\left.\begin{aligned}&\gamma = 1.3460 \pm 0.0021\\ &x_c = 0.541\,209 \pm 0.000\,016\\ &\langle x_c\rangle_{lr} = 0.541\,192\end{aligned}\right\} \quad K = 2 \tag{2.11}$$

where $\langle x_c\rangle_{lr}$ is just the mean (averaged over n) of the estimates of x_c obtained by linear regression with fixed n *at* the exact value of γ.

For the second-order approximants, about half the approximants were defective. This, coupled with the fact that there are only eight possible approximants for each value of n under the scheme we have described, compared to 12 possible first-order approximants for each n value, meant that we had insufficient approximants at fixed n to make our analysis meaningful. (The mean and standard deviation of a sample of three or four items is clearly unsatisfactory.) Accordingly, for the $K = 2$ approximants we have combined the entries for n and $(n-1)$ and it is these we have shown in table 3 and summarised above.

It can be seen that the first-order approximants give a more accurate estimate of γ and first-order approximants also give a more accurate central estimate of x_c, both from the unbiased estimates and from the means of the biased linear regression estimates. Both sets of estimates have errors which are wide enough to include the exact values, and accordingly support Nienhuis' results.

In this example the critical point is exactly known, and so biased approximants can be formed. This has been done and the results are summarised in table 4 for $K = 1$ and $K = 2$ approximants biased both at x_c, and at $x_c(1-\varepsilon)$, where $\varepsilon = 9 \times 10^{-6}$. The purpose of this last biasing is to determine the sensitivity of exponent estimates to errors in the critical point.

Our results may be combined into a single estimate of γ utilising the procedure described above and we find

$$\begin{aligned}&\gamma(K=1, x=x_c) = 1.3440 \pm 0.0003 \qquad &&\gamma(K=1, x=x_c(1-\varepsilon)) = 1.3433 \pm 0.0003\\ &\gamma(K=2, x=x_c) = 1.3440 \pm 0.0006 \qquad &&\gamma(K=2, x=x_c(1-\varepsilon)) = 1.3434 \pm 0.0004.\end{aligned} \tag{2.12}$$

The results for $K = 1$ and $K = 2$ are in almost perfect agreement. However, the error bars are narrower for the first-order approximants. The exact result $\gamma = 1.343\,75$ is well supported by the approximants biased at x_c and is just excluded by the first-order approximants biased at $x_c(1-\varepsilon)$, while being just included by the corresponding second-order approximants. The change in γ induced by a change ε in x_c was approximately 50ε.

In summary then we find that the first-order approximants are marginally superior overall to the second-order approximants, even in the case of functions with confluent singularities. For functions of precisely the form (2.6) we would not expect this to be true indefinitely, but it appears to hold generally for most of the series one encounters in statistical mechanical systems. This complements the earlier observation of Hunter and Baker (1979) that first-order (inhomogeneous) approximants are usually superior to second-order *homogeneous* approximants.

Table 4. Honeycomb lattice $C(x)$ series. Summary of exponent estimates from first- and second-order biased approximants. Biasing is done at x_c and at $x_c(1-\varepsilon)$, $\varepsilon = 9\times10^{-6}$. (*a*) $K=1$ approximants, (*b*) $K=2$ approximants.

(*a*)

n	Exponent biased at x_c	l	Exponent biased at $x_c(1-\varepsilon)$	l
23	1.3434 ± 0.0118	9	1.3429 ± 0.0119	9
24	1.3424 ± 0.0114	10	1.3448 ± 0.0012	7
25	1.3454 ± 0.0016	12	1.3448 ± 0.0016	12
26	1.3447 ± 0.0023	11	1.3442 ± 0.0024	11
27	1.3437 ± 0.0033	8	1.3430 ± 0.0036	8
28	1.3439 ± 0.0013	6	1.3432 ± 0.0015	6
29	1.3440 ± 0.0005	7	1.3433 ± 0.0005	7
30	1.3437 ± 0.0009	10	1.3429 ± 0.0010	10
31	1.3440 ± 0.0006	8	1.3433 ± 0.0009	9
32	1.3440 ± 0.0012	9	1.3431 ± 0.0009	10
33	1.3439 ± 0.0012	6	1.3432 ± 0.0010	6
34	1.3442 ± 0.0008	8	1.3434 ± 0.0007	10

(*b*)

n	Exponent biased at x_c	l	Exponent biased at $x_c(1-\varepsilon)$	l
21 and 22	1.3426 ± 0.0196	13	1.3444 ± 0.234	14
23 and 24	1.3436 ± 0.0042	15	1.3432 ± 0.0036	15
25 and 26	1.3444 ± 0.0013	14	1.3439 ± 0.0011	13
27 and 28	1.3443 ± 0.0015	9	1.3437 ± 0.0009	7
29 and 30	1.3441 ± 0.0011	10	1.3435 ± 0.0014	10
31 and 32	1.3436 ± 0.0012	6	1.3430 ± 0.0017	8
33 and 34	1.3440 ± 0.0012	4	1.3431 ± 0.0005	4

We have now seen this to be true for inhomogeneous approximants also. We have carried out a similar analysis on the triangular lattice chain generating function, which is known to 19 terms (Rapaport 1985a). In order to save space we do not give details but simply quote the results of the analysis. We find

$$\begin{aligned} &\gamma = 1.3431 \pm 0.0010 \\ &x_c = 0.240\,916 \pm 0.000\,004 \\ &\langle x_c \rangle_{\mathrm{lr}} = 0.240\,920. \end{aligned} \tag{2.13}$$

These results were all obtained from first-order approximants. The higher-order approximants were consistent with, but more scattered than, the above values. The exponent estimate is in good agreement with the exact value of $\gamma = 1.343\,75$, while the critical point estimate is in excellent agreement with an earlier, and alternate, analysis (Guttmann 1984), in which we found $x_c = 0.240\,920 \pm 0.000\,017$.

In the next sections we apply this method to our newly extended series.

3. Analysis of new series

In table 5 we give the series expansions for the chain generating function and the

Table 5. Coefficients of $C(x)$ and $R(x)$ series for the square and simple cubic lattices. $\langle R_n^2 \rangle$ is obtained from the quotient of the nth coefficient of the $R(x)$ series and the $C(x)$ series.

	Square lattice		Simple cubic lattice	
n	$C(x)$	$R(x)/4$	$C(x)$	$R(x)$
0	1		1	
1	4	1	6	6
2	12	8	30	72
3	36	41	150	582
4	100	176	726	4 032
5	284	679	3 534	25 566
6	780	2 452	16 926	153 528
7	2 172	8 447	81 390	886 926
8	5 916	28 120	387 966	4 983 456
9	16 268	91 147	1 853 886	27 401 502
10	44 100	289 324	8 809 878	148 157 880
11	120 292	902 721	41 934 150	790 096 950
12	324 932	2 777 112	198 842 742	4 166 321 184
13	881 500	8 441 319	943 974 510	21 760 624 254
14	2 374 444	25 398 500	4 468 911 678	112 743 796 632
15	6 416 596	75 744 301	21 175 146 054	580 052 260 230
16	17 245 332	224 156 984	100 121 875 974	2 966 294 589 312
17	46 466 676	658 855 781	473 730 252 102	15 087 996 161 382
18	124 658 732	1 924 932 324	2 237 723 684 094	76 384 144 381 272
19	335 116 620	5 593 580 859	10 576 033 219 614	385 066 579 325 550
20	897 697 164	16 175 728 584	49 917 327 838 734	1933 885 653 380 544
21	2 408 806 028	46 572 304 083		
22	6 444 560 484	133 556 779 740		
23	17 266 613 812	381 611 332 725		
24	46 146 397 316	1 086 759 598 120		
25	123 481 354 908	3 085 406 711 831		
26	329 712 786 220	8 735 073 410 100		
27	881 317 491 628	24 665 061 125 667		

series for the sum of mean square end-to-end distances. These are defined by

$$C(x) = \sum_{n \geq 0} c_n x^n$$
$$R(x) = \sum_{n \geq 0} \rho_n x^n \tag{3.1}$$

where

$$\rho_n = \sum_{c_n} r^2$$

and the mean square end-to-end distance is given by $\langle R_n^2 \rangle = \rho_n / c_n$ where c_n is the number of n step self-avoiding walks with a fixed origin and ρ_n is the sum of the squared end-to-end distances of the c_n SAW.

For the square lattice $C(x)$ series, our analysis was identical to the (unbiased) analysis carried out on the honeycomb lattice $C(x)$ series. The results are summarised in table 6 for first-order approximants. Combining the individual estimates as described

Table 6. Square lattice $C(x)$ series and $R(x)$ series. Unbiased first-order approximants for $C(x)$ and unbiased first- and second-order approximants for $R(x)$. (*a*) $K=1$ approximants, $C(x)$ series. (*b*) $K=1$ approximants, $R(x)$ series, (*c*) $K=2$ approximants, $R(x)$ series.

(*a*)

n	Exponent (γ)	Critical point	l
20	1.341 68 ± 0.024 44	0.379 0307 ± 0.000 3033	11
21	1.344 10 ± 0.010 28	0.379 0634 ± 0.000 0565	12
22	1.339 64 ± 0.015 95	0.379 0252 ± 0.000 0079	11
23	1.343 12 ± 0.003 51	0.379 0489 ± 0.000 0200	11
24	1.343 52 ± 0.000 89	0.379 0515 ± 0.000 0027	10
25	1.343 77 ± 0.000 51	0.379 0529 ± 0.000 0026	10
26	1.343 58 ± 0.000 21	0.379 0519 ± 0.000 0008	10
27	1.343 61 ± 0.000 10	0.379 0521 ± 0.000 0005	10

(*b*)

n	Exponent ($\gamma+2\nu$)	Critical point	l
21	2.831 44 ± 0.002 40	0.379 009 22 ± 0.000 013 63	11
22	2.833 56 ± 0.006 24	0.379 019 93 ± 0.000 032 39	4
23	2.836 96 ± 0.005 81	0.379 037 23 ± 0.000 029 00	3
24	2.835 40 ± 0.001 58	0.379 030 20 ± 0.000 009 22	2
25	2.835 38 ± 0.001 33	0.379 029 43 ± 0.000 008 45	4
26	2.836 55 ± 0.000 14	0.379 035 87 ± 0.000 000 38	2
27	2.837 12 ± 0.001 36	0.379 037 11 ± 0.000 007 56	8

(*c*)

n	Exponent ($\gamma+2\nu$)	Critical point	l
20 and 21	2.834 48 ± 0.002 26	0.379 021 42 ± 0.000 010 64	12
22 and 23	2.839 78 ± 0.004 17	0.379 043 51 ± 0.000 015 47	7
24 and 25	2.842 69 ± 0.004 91	0.379 054 01 ± 0.000 013 21	11
26 and 27	2.840 14 ± 0.006 38	0.379 045 97 ± 0.000 018 64	8

above gives

$$\gamma = 1.343\,61 \pm 0.000\,13$$
$$x_c = 0.379\,0520 \pm 0.000\,0006 \qquad (3.2)$$
$$\langle x_c \rangle_{lr} = 0.379\,052\,65 \pm 0.000\,000\,21 \qquad (\gamma = \tfrac{43}{32}).$$

These results are in excellent agreement with the exact value $\gamma = 1.343\,75$ and the estimate of x_c is also in excellent agreement with the previous estimate based on square lattice polygons of $x_c = 0.379\,0528$ obtained by Enting and Guttmann (1985). The results for $K = 2, 3$ approximants (not shown) are less precise but consistent with the above estimates. In order to determine the exponent ν, we can examine the series for $R(x)$, with exponent $(\gamma+2\nu)$ and the critical point at $x = x_c$, or the generating function for $\langle R_n^2 \rangle$ with exponent 2ν and critical point $x_c = 1.0$. This second series is clearly more appropriate when γ is not known, as in the case of three-dimensional models. Furthermore, for two-dimensional SAW models x_c is also unknown (except for the honeycomb lattice) and so this favours the analysis of the $\langle R_n^2 \rangle$ generating function.

In table 6 we summarise the results of an unbiased analysis of the square lattice $R(x)$ series, and in table 7(a) we give the results of a *biased* analysis (at $x_c = 1.0$) of the generating function of $\langle R_n^2 \rangle$. From both analyses we see a tendency for the critical parameters to approach limiting value, though not a monotonic trend. For the $R(x)$ series, both $K = 1$ and $K = 2$ approximants give critical point estimates which are approaching the value of x_c found from the $C(x)$ series, while the exponent estimates are also approaching the expected value of $\gamma + 2\nu = 2.843\,75$, obtained from Nienhuis' exact results, $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$.

The generating function for $\langle R_n^2 \rangle$, biased at $x_c = 1.0$, gives even better results. Firstly, we observe that this generating function does not correspond to any physical thermodynamic quantity. It is just a mathematical construction of interest to this problem. Accordingly, a singularity on the positive real axis between the origin and x_c does not correspond to some non-physical critical point, and so we have no basis to reject such approximants, which comprise less than 10% of the total number of approximants. Accordingly we only reject those approximants with additional singularities in the range $x \in [0.9, 1.05]$, as it is these which are observed to cause a change in the exponent estimates at $x_c = 1.0$. Very occasionally, we will also reject an approximant if it lies well outside the scatter of all remaining approximants (more than five or six standard deviations from the mean). Such outliers occur for only 1 or 2% of the approximants.

Another feature of the generating function for $\langle R_n^2 \rangle$ is that if $R(x)$ and $C(x)$ have a confluent singularity structure, the generating function for $\langle R_n^2 \rangle$ will have a more complex confluent singularity structure. To be precise, if $C(x)$ is of the form (2.6),

Table 7. Square lattice and triangular lattice $\langle R_n^2 \rangle$ analysis. Biasing the approximants at $x_c = 1$, first-, second- and third-order approximants are constructed. (a) Square lattice $\langle R_n^2 \rangle$ analysis, (b) triangular lattice $\langle R_n^2 \rangle$ analysis.

(a)

n	$K = 1$	l	$K = 2$	l	$K = 3$	l
18	2.4906 ± 0.0034	12	2.4910 ± 0.0016	8	2.4897 ± 0.0094	6
19	2.4917 ± 0.0024	12	2.4913 ± 0.0056	7	2.4939 ± 0.016	6
20	2.4929 ± 0.0047	11	2.4926 ± 0.0112	7	2.4984 ± 0.0088	6
21	2.4934 ± 0.0018	11	2.4895 ± 0.0036	8	2.4946 ± 0.0074	5
22	2.4946 ± 0.0035	11	2.4963 ± 0.0107	5	2.4978 ± 0.0018	6
23	2.4955 ± 0.0021	12	2.4979 ± 0.0044	7	2.4987 ± 0.0012	6
24	2.4956 ± 0.0022	12	2.4975 ± 0.0019	6	2.4987 ± 0.0021	6
25	2.4960 ± 0.0017	11	2.4983 ± 0.0028	8	2.4984 ± 0.0008	5
26	2.4968 ± 0.0016	12	2.4981 ± 0.0010	8	2.4980 ± 0.0013	6
27	2.4971 ± 0.0012	10	2.4984 ± 0.0010	8	2.4985 ± 0.0012	6

(b)

n	$K = 1$	l	$K = 2$	l	$K = 3$	l
12	2.4872 ± 0.0019	10				
13	2.4891 ± 0.0042	12				
14	2.4903 ± 0.0048	11	2.4929 ± 0.0239	5	2.4884 ± 0.0173	3
15	2.4936 ± 0.0068	11	2.4921 ± 0.0074	2	2.4869 ± 0.0102	2
16	2.4953 ± 0.0212	11	2.4928 ± 0.0066	4	2.4930 ± 0.0139	4
17	2.4951 ± 0.0045	11	2.4948 ± 0.0069	7	2.4933 ± 0.0091	3
18	2.4951 ± 0.0009	12	2.4956 ± 0.0045	5	2.4961 ± 0.0014	6
19	2.4955 ± 0.0009	12	2.4973 ± 0.0022	7	2.4975 ± 0.0019	4

and $R(x)$ is of the same form—but of course with γ replaced by $(\gamma+2\nu)$ and different values of the amplitudes A, B and C_i, then $\langle R_n^2 \rangle$ will have additional confluent singularities with exponents $2\Delta_1, 3\Delta_3, 4\Delta_1, \ldots$, and $2\Delta_2, 3\Delta_2, 4\Delta_2, \ldots$. Indeed, unless a totally improbable cancellation of amplitudes occurs, such a complication will always arise unless the only correction terms are analytic. That is, unless the functions $C(x)$ and $R(x)$ are of the simpler form (2.4).

The conclusion one may draw from these observations is that higher-order approximants would seem to be appropriate for the generating function of $\langle R_n^2 \rangle$, due to the additional confluent terms it contains. This expectation is borne out by the results shown in table 7(a), where the $K=2$ approximants appear to be better converged than their $K=1$ counterparts, and the $K=3$ approximants appear to be still better converged.

In all cases, $K=1$, 2 and 3, exponent estimates are increasing, almost monotonically and are entirely consistent with a limit of 2.500. We have no theoretical results for the expected rate of convergence of such sequences (see Guttmann (1987) for a fuller discussion), but empirically we expect the series to have reached the asymptotic regime by $n=33$ or 34. Unfortunately this represents six or seven additional series coefficients, which is quite unattainable by current methods.

We have also studied the triangular lattice $\langle R_n^2 \rangle$ generating function given by Rapaport (1985a) biased at $x_c=1.0$. The results are shown in table 7(b). Again we observe a steady increase of exponent estimates with n. The last entry of the $K=1$ approximants is some 0.005 away from the expected limit, while for $K=2$ and 3 the limit is about 0.003 away from the last entries. We use this behaviour as a guide to extrapolating the simple cubic lattice $\langle R_n^2 \rangle$ generating function results. These are shown in table 8 and again a quasi-monotone trend of exponent estimates is apparent. Assuming the approach to the limit occurs at a comparable rate to the triangular lattice data—an assumption that is entirely consistent with the two sets of data—allows us to make the estimate $1+2\nu=2.184\pm0.004$ or $\nu=0.592\pm0.002$. This is precisely the value of ν obtained by Rapaport (1985b) based on Monte Carlo analysis of SAW on the simple cubic and body-centred cubic lattices. The field theoretic results of Le Guillou and Zinn-Justin (1980) of $\nu=0.588\pm0.001$ lie just outside our value.

For the FCC lattice, 14 terms of the chain generating function are known (McKenzie 1979), but only 12 terms of the $R(x)$ series are known (Majid *et al* 1983). For the BCC and diamond lattices both the $C(x)$ and $R(x)$ series are significantly shorter than for the simple cubic and FCC lattices, so we do not attempt an analysis of the data for

Table 8. Simple cubic lattice $\langle R_n^2 \rangle$ analysis. Biased approximants of first, second and third order, with $x_c=1$.

n	$K=1$	l	$K=2$	l	$K=3$	l
12	2.1962 ± 0.0076	9	2.1969 ± 0.0011	4	2.1967 ± 0.0110	2
13	2.1955 ± 0.0018	12	2.1962 ± 0.0028	6	2.1957 ± 0.0	2
14	2.1947 ± 0.0014	10	2.1951 ± 0.0117	6	$2.1973\pm\infty$	1
15	2.1953 ± 0.0058	8	2.1967 ± 0.0092	6	2.1972 ± 0.0158	2
16	2.1908 ± 0.0045	9	2.1917 ± 0.0037	6	2.1997 ± 0.0144	3
17	2.1923 ± 0.0019	11	2.1930 ± 0.0028	8	2.1928 ± 0.0032	3
18	2.1904 ± 0.0048	12	2.1928 ± 0.0048	8	2.1926 ± 0.0060	6
19	2.1904 ± 0.0042	11	2.1892 ± 0.0076	8	2.1889 ± 0.0044	5
20	2.1891 ± 0.0026	12	2.1874 ± 0.0010	7	2.1840 ± 0.0038	5

those lattices. For the FCC $\langle R_n^2 \rangle$ generating function, the exponent estimates, summarised in table 9, are rapidly decreasing with increasing n. It is difficult to extrapolate these sequences, but they are clearly entirely consistent with the simple cubic lattice result of $1+2\nu = 2.184 \pm 0.004$.

Table 9. Face-centred cubic lattice $\langle R_n^2 \rangle$ analysis. Biased approximants of first and second order, with $x_c = 1$.

n	$K=1$	l	$K=2$	l
7	2.1939 ± 0.0019	3		
8	2.1979 ± 0.0052	3		
9	2.1967 ± 0.0033	7	2.1993 ± 0.0	2
10	2.1966 ± 0.0031	7	2.1976 ± 0.0002	2
11	2.1948 ± 0.0018	10	2.1954 ± 0.0063	4
12	2.1930 ± 0.0015	9	2.1912 ± 0.0081	5

Turning now to the chain generating function data for three-dimensional lattices, our analyses of the $C(x)$ series for the SC and FCC lattices were the same as for the square lattice data. The results of our analysis for the SC lattice are shown in table 10(a) and may be summarised as

$$\begin{aligned} \gamma &= 1.1613 \pm 0.0021 \\ x_c &= 0.213\,497 \pm 0.000\,010 \end{aligned} \tag{3.3}$$

from the $K=1$ approximants. The $K=2$ approximants are more widely scattered than their $K=1$ counterparts. Only the last entry ($n=19$ and 20) has an associated error of comparable size to the $K=1$ approximants, and the estimates given there of $\gamma = 1.1621 \pm 0.0034$ and $x_c = 0.213\,500 \pm 0.000\,017$ are in complete agreement with the $K=1$ results. We have performed a similar analysis for the FCC lattice. For the chain generating function 14 series terms are known and the results, shown in table 10(b), may be summarised as follows:

$$\begin{aligned} \gamma &= 1.1623 \pm 0.0018 \\ x_c &= 0.099\,635 \pm 0.000\,005 \end{aligned} \qquad K=1$$

$$\begin{aligned} \gamma &= 1.1633 \pm 0.0011 \\ x_c &= 0.099\,638 \pm 0.000\,002 \end{aligned} \qquad K=2. \tag{3.4}$$

We combine these to give our final estimate of

$$\begin{aligned} \gamma &= 1.1629 \pm 0.0020 \\ x_c &= 0.099\,637 \pm 0.000\,006. \end{aligned} \tag{3.5}$$

Combining this estimate of γ with that obtained for the SC lattice, assuming that they are equal, gives

$$\gamma = 1.1620 \pm 0.0020. \tag{3.6}$$

The field theoretic result (Le Guillou and Zinn-Justin 1980) of $\gamma = 1.1615 \pm 0.0015$ is in excellent agreement with this value, though their more recent value (Le Guillou and Zinn-Justin 1985) of $\gamma = 1.160 \pm 0.004$ is not quite as consistent.

Table 10. Simple cubic and face centred cubic $C(x)$ series. Unbiased analysis using first- and second-order approximants. (*a*) Simple cubic lattice, (*b*) face-centred cubic lattice.

(*a*)

	n	Exponent	Critical point	*l*
$K=1$	13	1.171 44 ± 0.035 46	0.213 5693 ± 0.000 2702	11
approximants	14	1.163 69 ± 0.012 84	0.213 5149 ± 0.000 0871	9
	15	1.154 77 ± 0.016 17	0.213 4550 ± 0.000 1008	10
	16	1.162 70 ± 0.006 92	0.213 5037 ± 0.000 0380	6
	17	1.162 81 ± 0.005 69	0.213 5055 ± 0.000 0279	7
	18	1.160 96 ± 0.004 29	0.213 4971 ± 0.000 0258	11
	19	1.158 97 ± 0.003 96	0.213 4867 ± 0.000 0160	7
	20	1.161 96 ± 0.003 69	0.213 4993 ± 0.000 0146	11
$K=2$	13 and 14	1.165 88 ± 0.008 04	0.213 5280 ± 0.000 0474	11
approximants	15 and 16	1.164 11 ± 0.009 08	0.213 5177 ± 0.000 0907	13
	17 and 18	1.168 60 ± 0.016 50	0.213 5345 ± 0.000 0824	16
	19 and 20	1.162 12 ± 0.003 35	0.213 4998 ± 0.000 0168	14

(*b*)

	n	Exponent	Critical point	*l*
$K=1$	9	1.174 68 ± 0.026 00	0.099 6781 ± 0.000 1289	5
approximants	10	1.176 51 ± 0.025 40	0.099 6911 ± 0.000 0992	7
	11	1.161 28 ± 0.002 63	0.099 6317 ± 0.000 0090	4
	12	1.159 61 ± 0.009 99	0.099 6279 ± 0.000 0285	10
	13	1.163 14 ± 0.003 26	0.099 6374 ± 0.000 0078	10
	14	1.163 43 ± 0.003 06	0.099 6383 ± 0.000 0063	9
$K=2$	11	1.163 00 ± 0.002 86	0.099 6367 ± 0.000 0096	3
approximants	12	1.163 37 ± 0.003 70	0.099 6379 ± 0.000 0109	5
	13	1.163 19 ± 0.001 63	0.099 6376 ± 0.000 0032	5
	14	1.163 45 ± 0.001 72	0.099 6383 ± 0.000 0032	6

4. Discussion

Our analysis of the data for the square and triangular SAW problem strongly supports the values proposed for the critical exponents by Nienhuis (1982, 1984) as exact, i.e. $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$. Accepting these as exact, linear regression on unbiased integral approximants gives the following estimates of the critical points:

$$\begin{aligned} x_c &= 0.541\,1935 \pm 0.000\,0045 \quad \text{(honeycomb)} \\ x_c &= 0.379\,0528 \pm 0.000\,0015 \quad \text{(square)} \\ x_c &= 0.240\,920 \pm 0.000\,003 \quad \text{(triangular).} \end{aligned} \tag{4.1}$$

These estimates are in good agreement with the exact value (Nienhuis 1982) of 0.541 1961 ... on the honeycomb lattice, the estimate based on square lattice polygons of 0.379 0528 ± 0.000 0040 (Enting and Guttmann 1985) and the Monte Carlo estimates for the triangular lattice (Guttmann *et al* 1986) of 0.240 91 ± 0.000 02 and the previous series analysis estimate (Guttmann 1984) of 0.240 920 ± 0.000 017.

Turning to the question of the existence, and value, of the correction-to-scaling exponent for the two-dimensional SAW problem, it is fair to say that the situation is confused! For a review of the numerous opinions until the end of 1983 see Guttmann (1984), while more recent views are discussed in Rapaport (1985a, b). In those papers, Rapaport argues that there is no need to assume the presence of a correction-to-scaling exponent, and that indeed his Monte Carlo data favours an exponent of 1—corresponding to an analytic correction—in both two and three dimensions. While we are unable to provide an analysis for all three two-dimensional lattice SAW models that points to the *same* correction-to-scaling exponent for all lattices, we *are* able to provide strong evidence, both numerically and theoretically, for the existence of non-analytic corrections in the two-dimensional case. If they are present in the two-dimensional case, it is then most reasonable to expect their presence in the three-dimensional case.

The theoretical evidence for the presence of such a term follows from Nienhuis' (1982) work, where he successfully identifies the critical point (for the honeycomb lattice model) and the critical exponents γ and ν. The same theory also predicts a correction-to-scaling term with an exponent of 1.50. Weaker evidence for a non-analytic correction to scaling term comes from the field theory calculations of Le Guillou and Zinn-Justin (1980), who obtain an exponent of 1.15. Their results are not terribly accurate for two-dimensional models however. Recent conformal invariance arguments by Saleur (1987) suggest the presence of at least one correction-to-scaling exponent, with a value of $\frac{11}{16}$ and Saleur (1987) also suggests the presence of a second such term with exponent $\frac{1}{2}$. The arguments for the latter are somewhat suspect and evidence for the first such correction-to-scaling exponent from series analysis is scant.

Turning now to the numerical evidence, we point out that, if only analytic corrections were present, then we could write $\langle R_n^2 \rangle$ as

$$\langle R_n^2 \rangle \sim A n^{2\nu}(1 + C_1/n + C_2/n^2 + C_3/n^3 + \dots). \tag{4.2}$$

Then the sequence $\{R_n^2/n^{2\nu}\}$ should be well fitted by a polynomial in $1/n$, with the quality of the fit improving with the degree of the polynomial. This is precisely the observed behaviour for the analogous quantity in the two-dimensional Ising problem, which is the second moment of the correlation function M_2. However, for the SAW data the estimates of the amplitudes C_1, C_2, C_3 show highly erratic behaviour as the degree of the polynomial in (4.2) is increased. Thus we conclude that the sequence is *not* well fitted by (4.2) and hence that non-analytic correction terms exist. We consider their value to be an open question, but note that there is no compelling series evidence to suggest a value different from Nienhuis' value $\Delta = 1.5$.

Turning now to our analysis of the three-dimensional data, we find $\nu = 0.592 \pm 0.002$ from the simple cubic lattice data, while our analysis of the chain generating functions of the FCC and SC lattices gave

$$\begin{aligned} &x_c = 0.213\,497 \pm 0.000\,010 && \text{SC} \\ &x_c = 0.099\,637 \pm 0.000\,006 && \text{FCC} \\ \text{and} \quad &\gamma = 1.1613 \pm 0.0021 && \text{SC} \\ &\gamma = 1.1629 \pm 0.0020 && \text{FCC.} \end{aligned} \tag{4.3}$$

Assuming lattice independence of the exponents leads to our final estimate of $\gamma = 1.162 \pm 0.002$, in good agreement with field theory predictions previously cited. In a

subsequent paper (Guttmann 1987a) we apply this method of analysis to the high-temperature susceptibility series of the three-dimensional Ising model and obtain exponent estimates consistent with lattice independence. However in that paper we point out that, for the spin-$\frac{1}{2}$ Ising model data, the results of this analysis are slightly misleading, and that trends in the data must also be accounted for. It might be asked whether the same effect might not be present in the cases considered here. We think this is unlikely as it is clearly easier to reach the asymptotic regime for the SAW problem than for the Ising problem. For the latter, new classes of magnetic graph enter at higher and higher order in the series, whereas for the SAW problem we are considering, only one class of graph contributes, so the approach to asymptotia should be smoother.

Acknowledgments

I would like to thank Dr Glenn Torrie for the use of his dimerisation counting program on which these enumerations were based. Programming assistance from Alan Hargreaves, Scott Merillees and Kevin Wallace is gratefully acknowledged. The support of the Australian Research Grants Committee is also gratefully acknowledged. Finally I wish to thank Professor Colin J Thompson for the hospitality of the Department of Mathematics, University of Melbourne, where much of this work was carried out.

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