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On two-dimensional self-avoiding random walks

A J Guttmann

Department of Mathematics, Statistics and Computer Science, University of Newcastle, New South Wales, 2308, Australia

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Abstract. Following Nienhuis' exact evaluation of the connective constant of the honeycomb lattice self-avoiding walk model, and the exact exponent values he has conjectured, we have re-examined the available data on all three regular two-dimensional lattices. In the case of the triangular lattice we have additionally corrected and extended the extant series.

We find support for Nienhuis' value $\gamma = 1\frac{11}{32}$ for all three lattices, and further find that $\alpha = \frac{1}{2}$ for all three lattices, as given by Nienhuis' result $\nu = \frac{3}{4}$ and the hyperscaling relation $d\nu = 2 - \alpha$. We are unable to find any consistent evidence of a 'correction-to-scaling' exponent $\Delta_1 < 1$ from the walk generating function, though other workers have found such an exponent for the mean square end-to-end distance series. We cannot however rule out an exponent $\Delta_1 > 1$.

For the connective constants we find $\mu = 2.6381 \pm 0.0002$ (square), $\mu = 4.150\,75 \pm 0.0003$ (triangular). We speculate on the form of the exact result for μ, and provide two mnemonics $\mu = 1 + \frac{1}{2}(9 + \sqrt{3})^{1/2} = 2.637\,990\ldots$ (square) and $\mu = 3 + (2\sqrt{10} - 5)^{1/2} = 4.150\,893\ldots$ (triangular).

1. Introduction

The recent exact results of Nienhuis (1982) for the connective constant and critical exponents of the self-avoiding walk (SAW) problem on the honeycomb lattice have prompted an extension and re-examination of available data pertaining to the square and triangular lattice SAW problem. As a result we have obtained new, sharper, numerical estimates of the connective constant on these lattices, but for a variety of reasons to be discussed, we have been unable to find exact results paralleling those of Nienhuis, though some possibly exact mnemonics are given.

A long-standing conjecture (Guttmann and Sykes 1973), that the sum of the connective constant of the SAW model on the triangular lattice (μ_T) and the corresponding quantity on the honeycomb lattice (μ_H) is exactly 6, is shown to be highly unlikely.

The generating functions for both the chains and the polygons (which are the analogues of the zero-field susceptibility and zero-field free energy respectively) appear to have a singularity structure similar to that of the two-dimensional Ising model, that is, a singular part plus an analytic component, with the apparent absence of any non-analytic 'correction-to-scaling' terms corresponding to any 'correction-to-scaling' exponent $\Delta_1 < 1$. This is in surprising contrast to the work of Majid *et al* (1983) and Privman (1983a, b) who analysed the mean square end-to-end distance series and found firm evidence for a 'correction-to-scaling' exponent $\Delta_1 \approx \frac{2}{3}$.

The chain and polygon generating functions are defined in the usual manner as

$$C(x)=\sum_{n\geq 0} c_n x^n, \qquad P(x)=\sum_{n\geq 0} p_n x^n$$

where $c_n(p_n)$ is the number of n-step self-avoiding walks (polygons) per site of an infinite lattice. To leading asymptotic order $c_n \sim \mu^n n^g$ and $p_n \sim \mu^n n^p$ where Nienhuis (1982) found $\mu_{\rm H}=(2+\sqrt{2})^{1/2}$, $g=\gamma-1=\frac{11}{32}$ and $p=\alpha-3=-\frac{5}{2}$. In fact, Nienhuis studied an N-vector model and obtained $\mu_{\rm H}(N)=(2+\sqrt{2-N})^{1/2}$, for $-2\leq N\leq 2$ which also reproduces the known Ising model result $\mu_{\rm H}(1)=\sqrt{3}$. Baxter (unpublished) has obtained Nienhuis' result for $\mu_{\rm H}$ by an alternative, and more direct, formulation.

The elegant simplicity of Nienhuis' result, particularly the N dependence of $\mu_{\rm H}(N)$, initially suggests that similar results may hold for the other regular two-dimensional lattices, or that, at the very least, some simple relation such as that produced by the Guttmann–Sykes conjecture should hold.

Unfortunately, all the evidence we have found points away from these conclusions. Nienhuis chooses a particular potential, defined by

$$\exp(-\beta V(s_i, s_j)) = 1 + x s_i \cdot s_j \tag{1.1}$$

where s_i are N-dimensional vectors located at site i. The usual nearest-neighbour interaction produces

$$Z(N)=\sum x^l N^c k(G) \tag{1.2}$$

for the zero-field partition function of the model *on a honeycomb lattice.* The sum is over the set of all disconnected polygons G with a total of l bonds and with weak lattice constant $k(G)$. c is the number of disconnected components. When $N=1$, (1.2) gives the Ising model partition function, while $Z(N)/N$ in the limit $N\rightarrow 0$ gives the polygon generating function. For $N=2$, the peculiar O(2) model discussed by Domany *et al* (1981) is recovered.

The significant aspect here is that as N changes, the class of graphs entering the sum (1.2) does not change. That is, for the Ising model partition function the contributory graphs are just polygons—as for the polygon generating function (PGF). For other regular lattices however, such as the square and triangular lattices, an infinite number of sets of graphs contribute to the Ising model specific heat but not to the PGF. This of course is a consequence of the low coordination number ($q=3$) of the honeycomb lattice, and it appears that the model (1.1) is only solvable on that lattice.

As a consequence, the simple N-dependence obtained by Nienhuis seems likely to be a feature of the uniquely low coordination number of the honeycomb lattice.

In § 2 we review the existing data for the connective constants on the square and triangular lattice. In § 3 we extend and correct the SAW series on the triangular lattice, and analyse the SAW and SAP series. The previously published series on the triangular lattice was known to be suspect in the 16th term due to the work of Grassberger (1982). We confirm Grassberger's corrected 16th coefficient, find corrections to the 17th coefficient and add the new 18th coefficient. Section 4 contains a brief discussion of our conclusions, while § 5 contains some speculations as to the exact value of μ.

2. Existing analyses

For many years it was believed that the critical exponent for the two-dimensional SAW problem was $g=\frac{1}{3}=0.333$, so that Nienhuis' result that $g=\frac{11}{32}=0.34375$ came as something of a surprise.

In 1975 Watts quoted unbiased estimates of the pair (μ, γ) obtained from a Padé approximant study as (1.8478, 1.342) for the honeycomb lattice, (2.6385, 1.335) for the square lattice and (4.1520, 1.330) for the triangular lattice.

These were in reasonable agreement with the earlier biased ratio estimates of Sykes *et al* (1972) who assumed $\gamma=\frac{4}{3}$ and estimated $\mu_{\rm H}=1.8481$, $\mu_{\rm S}=2.6385$ and $\mu_{\rm T}=4.1517$ with errors quoted as ± 1 in the last decimal place.

In a recent paper Derrida (1981) devised a phenomenological renormalisation scheme applicable to the SAW problem on the square lattice, and obtained $\mu_{\rm S}=2.638\,17\pm 0.0002$. This approach makes no assumption about the exponent, and so is expected to be a reliable unbiased estimate. At the same time Derrida estimated the mean square end-to-end distance exponent ν to be $0{\cdot}7503\pm 0.0002$, which lies outside the exact value of $\frac{3}{4}$ found by Nienhuis, so perhaps the error bounds on $\mu_{\rm S}$ should not be interpreted too rigidly.

As mentioned in the introduction, Grassberger (1982) obtained $c_{16}=24\,497\,330\,322$ while Martin *et al* (1967) give $c_{16}=24\,497\,321\,682$ and $c_{17}=103\,673\,881\,482$. To resolve this discrepancy, a FORTRAN program based on a back-tracking algorithm (similar in spirit to that discussed by Grassberger) was written. Running for a total of 100 hours on a VAX 11/780 we obtained $c_{16}=24\,497\,330\,322$, $c_{17}=103\,673\,967\,882$ and $c_{18}=438\,296\,739\,594$. These results confirm Grassberger's coefficient c_{16}, correct the coefficient of c_{17} (the error in which is due solely to the incorrect c_{16}, as Sykes' counting theorem gives our value of c_{17} using the corrected c_{16} and Martin *et al*'s value of c_{17}) and give one new term c_{18}. We have also verified the SAP's up to and including p_{17} as previously published (Martin *et al* 1967), and add one new term, $p_{18}=24\,852\,576$. To extend the series further would require an additional 450 hours on the VAX 11/780 for one extra term, or about 2000 hours for two extra terms. While further terms would be highly desirable, it is doubtful, given these timings, whether the above method can realistically be used for that purpose. After submission of this paper, Majid *et al* (1983) confirmed the new coefficient c_{18}.

3. Analysis

We have analysed the corrected and extended SAW series on the triangular lattice, and the existing series on the square and honeycomb lattices. In tables 1, 2 and 3 we show the poles and residues of Padé approximants to the logarithmic derivative of the SAW series. Table 1 displays results for the honeycomb lattice, and shows a trend that also holds for the square lattice results, that of steadily increasing estimates of both the pole (which estimates $1/\mu$) and the magnitude of the residue (which estimates $\gamma=-(1+g)$). By about the 14th row this trend seems to have converged, with the last eight estimates lying in the range $1/\mu=0.541\,19\pm 0.000\,03$ (cf the exact result of $1/\mu=0.541\,1961\ldots$) and $\gamma=1+g=1.342\pm 0.003$ (cf the 'exact' result $\gamma=1.343\,75$). We have ignored defective approximants in this assessment (see e.g. Gaunt and Guttmann (1974) for an expansion of this point).

Table 2 for the square lattice shows the same increasing trend, but there is no evidence that a region of stability has been reached. Ignoring defective approximants, the square lattice results have reached (0.379 01, −1.336) and are still increasing. The

Table 1. Dlog Padé approximants to honeycomb lattice SAW generating function.

N	$[N-1/N]$ Pole	(Residue)	$[N/N]$ Pole	(Residue)	$[N+1/N]$ Pole	(Residue)
8	0.546 96	(−1.719)	0.540 35	(−1.307)	0.542 38	(−1.417)
9	0.540 68	(−1.319)	0.541 62	(−1.364)	0.545 43	(−1.786)†
10	0.541 14	(−1.338)	0.541 02	(−1.332)	0.540 96	(−1.329)
11	0.540 88	(−1.324)	0.541 01	(−1.332)†	0.541 17	(−1.340)†
12	0.541 07	(−1.335)	0.541 08	(−1.336)	0.541 11	(−1.337)
13	0.541 14	(−1.339)	0.541 00	(−1.332)†	0.541 16	(−1.340)
14	0.541 22	(−1.345)	0.541 18	(−1.342)	0.541 17	(−1.341)
15	0.541 17	(−1.341)	0.541 17	(−1.341)†	0.541 18	(−1.342)
16	0.541 18	(−1.341)	0.541 18	(−1.341)	0.541 18	(−1.341)†
17	0.541 18	(−1.341)†				

† Pole—present closer to the origin than the displayed physical singularity.

Table 2. Dlog Padé approximants to the square lattice SAW generating function.

N	$[N-1/N]$ Pole	(Residue)	$[N/N]$ Pole	(Residue)	$[N+1/N]$ Pole	(Residue)
5	0.377 30	(−1.2765)	0.377 77	(−1.2881)	0.378 39	(−1.3064)
6	0.371 84	(−1.4353)†	0.378 63	(−1.3149)	0.379 51	(−1.3701)
7	0.378 82	(−1.3232)	0.378 85	(−1.3246)	0.378 86	(−1.3249)
8	0.378 86	(−1.3250)	0.378 85	(−1.3245)†	0.378 99	(−1.3338)
9	0.378 80	(−1.3224)†	0.378 97	(−1.3328)	0.378 98	(−1.3337)†
10	0.379 17	(−1.3564)	0.379 02	(−1.3375)†	0.379 01	(−1.3361)
11	0.379 00	(−1.3350)	0.379 01	(−1.3356)	0.379 01	(−1.3359)†
12	0.378 99	(−1.3337)†				

† Pole—present closer to origin than the displayed physical singularity.

Table 3. Dlog Padé approximants to the triangular lattice SAW generating function.

N	$[N-1/N]$ Pole	(Residue)	$[N/N]$ Pole	(Residue)	$[N+1/N]$ Pole	(Residue)
4	0.240 17	(−1.2926)	0.240 29	(−1.2971)	0.240 52	(−1.3062)
5	0.239 93	(−1.2880)†	0.240 61	(−1.3109)	0.241 44	(−1.4263)
6	0.240 70	(−1.3169)	0.240 79	(−1.3234)	0.240 83	(−1.3276)
7	0.240 90	(−1.3357)	0.240 87	(−1.3318)	0.240 89	(−1.3345)
8	0.240 88	(−1.3329)	0.240 88	(−1.3333)	0.240 88	(−1.3334)
9	0.240 88	(−1.3336)				

† Pole—present closer to the origin than the displayed physical singularity.

triangular lattice results do, however, seem to have settled down to the values (0.240 88, −1.333).

Looking at these results, it is easy to see why the earlier estimate of $\gamma=\frac{4}{3}$ was made, but a more systematic view, coupled with the hindsight of Nienhuis' exact results, clearly indicates a higher value of γ for both the square and honeycomb lattices, though the triangular lattice does not conform to this observation.

Discrepancies between series estimates of critical exponents and those obtained from renormalisation group studies—particularly for three-dimensional systems—have generally been resolved by allowing for confluent singularities. It seems plausible that such a mechanism is responsible for the slow convergence of the Padé estimates of the square and triangular lattices. We have exhaustively investigated this possibility, and have found no consistent evidence for a confluent singularity. The methods used included the Baker–Hunter transformation method (1973) using a range of values of μ including our central estimates, the method introduced by Saul *et al* (1975) in which one fits to the assumed confluent form, the method of Rehr *et al* (1980) based on differential approximants, and the method introduced by Roskies (1981) and generalised by Adler *et al* (1982). In this last method, a transformation is made so that if the old expansion variable is x, the new variable is

$$y = 1-(1-x/x_c)^{\Delta} \tag{3.1}$$

where x_c is the critical point, and in the new variable it is at $y = y_c = 1$. If the function under investigation behaves like

$$F(x) \sim (1-x/x_c)^{-\gamma}[a_1 + a_1(1-x/x_c)^{\Delta_1} + b_2(1-x/x_c)+\ldots] \tag{3.2}$$

then after transformation we have

$$f(y) = F(x(y)) \sim (1-y)^{-\gamma/\Delta}[b_1 + a_1(1-y)^{\Delta_1/\Delta} + b_2(1-y)^{1/\Delta}+\ldots]. \tag{3.3}$$

If Δ is chosen equal to Δ_1, the non-analytic correction-to-scaling term $(1-x/x_c)^{\Delta_1}$ becomes analytic in y, being transformed to $a_1(1-y)$. Of course, the analytic term $b_2(1-x/x_c)$ now becomes $b_2(1-y)^{1/\Delta}$ which is non-analytic unless $\Delta = 1/n$, where n is an integer. Even if Δ is not the reciprocal of an integer and $\Delta < 1$, then the effect of the transformation is still to reduce the effect of the term $b_2(1-x/x_c)$, changing it to $b_2(1-y)^{1/\Delta}$. However, it is clear that this transformation needs to be used with considerable care with values of $\Delta > 1$. Further, if $\Delta_1/\Delta = m > 1$ the original non-analytic term in F becomes an analytic term in f. This is the source of the resonances found by Privman (1983a) and discussed at greater length by him.

After transformation, the critical exponent γ is found by evaluating suitably formed Padé approximants to the logarithmic derivative of f. That is,

$$\Delta(1-y)(\mathrm{d}/\mathrm{d}y)\{\log f(y)\}|_{y=1} \sim \gamma + \mathrm{O}[(1-y)^{\Delta_1/\Delta}]. \tag{3.4}$$

We have applied this method to the honeycomb lattice SAW series, using the exact value for $x_c = 1/\mu_{\mathrm{H}} = (2+\sqrt{2})^{-1/2}$ found by Nienhuis and a range of values of Δ. For the purpose of comparison, we have performed similar calculations on the honeycomb lattice Ising model series, for which $x_c = 1/\sqrt{3}$, $\gamma = \frac{7}{4}$ and Δ_1 is known to be 1. For each value of Δ we have estimated γ by forming the mean of the last 15 diagonal and off-diagonal Padé approximants, and quoting an error of one standard deviation. In many cases, we have rejected one of the 15 entries in forming the mean, as this isolated 'outlier' differed from the mean by a factor of 5 or 10 more than did the remaining 14 entries.

The results of this calculation are shown in table 4, where we have also shown the effect of a slight variation in the critical point.

Firstly, observe that the Ising model results point unerringly to the known exact results. As $\Delta \to 1$, the estimates of γ approach the exact value, and the standard deviation monotonically decreases. Further, at $\Delta = 1$, variations of the critical point

Table 4. Variation of critical exponent γ with the parameter Δ (equation (3.1)) for the honeycomb lattice SAW and Ising models.

Δ	Self-avoiding walks $\mu = 1.847\,759\ldots$ $\gamma = 1.343\,75$	Ising model $1/x_c = \mu = 1.732\,0508\ldots$ $\gamma = 1.7500$, $\Delta_1 = 1.0$
0.5	1.3392 ± 0.0050	1.7464 ± 0.0084
0.6	1.3439 ± 0.0023	1.7533 ± 0.0068
0.7	1.3457 ± 0.0017	1.7545 ± 0.0045
0.8	1.3454 ± 0.0017	1.7544 ± 0.0008
0.9	1.3454 ± 0.0003	1.7528 ± 0.0005
0.93	1.3445 ± 0.0001	1.7520 ± 0.0003
0.96	1.3439 ± 0.0001	1.7511 ± 0.0002
1.00	1.3432 ± 0.0005	1.7498 ± 0.0002
1.20	1.3400 ± 0.0031	1.7438 ± 0.0037
1.0	$\mu = 1.847\,65$ $\gamma = 1.3470 \pm 0.0031$	$\mu = 1.731\,95$ $\gamma = 1.7510 \pm 0.0020$
1.0	$\mu = 1.847\,85$ $\gamma = 1.3408 \pm 0.0002$	$\mu = 1.732\,15$ $\gamma = 1.7451 \pm 0.0019$

away from the exact value cause substantial changes in the estimates of γ, and a tenfold increase in the error estimate.

For the SAW series, the results are less clear. As Δ increases, estimates of γ at first increase, then decrease. The error decreases with increasing Δ, reaching a minimum around $\Delta \approx 0.95$. Even at $\Delta = 1$ however, the error is quite small, and the estimate of γ is quite close to Nienhuis' exact value of $\gamma = 1.343\,75$. There is insufficient evidence to conclude the presence of a confluent singularity for the SAW generating function with $\Delta \neq 1$. Even if such a term were present, with a value around $\Delta \approx 0.95$, as suggested by the very small error in that vicinity, its effect on the series is likely to be comparable to that of the analytic correction terms, and the other singularities believed to lie on the circle of convergence $|x| = x_c = 1/\mu$ (Guttmann and Whittington 1978). Note also that a small variation in the critical point changes the estimate of γ substantially, but that the associated error increases as x_c is increased while decreasing as x_c is decreased. Thus we see that this series is clearly less well behaved than its Ising counterpart. We nevertheless conclude that: (a) at the exact critical point the exponent estimates agree with Nienhuis' result that $\gamma = 1\frac{11}{32}$ exactly; (b) there is no compelling evidence for the presence of a confluent singularity with an exponent different from 1, though there is weak evidence for a confluent exponent just less than 1. After completing this section, we received a letter by Adler (1983), who analyses the honeycomb lattice SAW series similarly and also finds $\Delta_1 \approx 0.93$, as well as two additional correction-to-scaling exponents around $\Delta_2 = 1.25$ and $\Delta_3 = 1.55$. We believe that this interpretation is pushing the method beyond its region of applicability.

Turning now to the square lattice, the critical point is not known exactly. Table 2 implies $1/\mu > 0.379\,01$, and so we have formed Padé approximants as above for a range of values of μ, with $\Delta = 1$. In order to investigate further the possibility that there is a confluent singularity at a value of Δ around 0.95, we also estimated γ for $\Delta = 0.90$ and 0.95. It has been estimated from the mean of the last 11 Padé approximants, the error quoted being one standard deviation. As for the honeycomb results, one entry was generally rejected as an 'outlier'.

The results are summarised in table 5. Unlike the honeycomb lattice results there is no evidence to suggest a confluent singularity around $\Delta \approx 0.95$ for the square lattice. In the absence of a confluent singularity, the results for $\Delta = 1$ give the 'correct' values of $\gamma = 1.343\,75$ at $\mu \approx 2.637\,99$. Like the honeycomb lattice results, the error in γ is not minimised at this value of μ, but at a slightly higher value which does not, however, give the correct value for the exponent γ. For this lattice too, the Ising model series (of similar length) is much better behaved in that the error in γ is minimised at the correct value of x_c, and variations in x_c of ± 1 part in 40 000 produce a 10- to 50-fold increase in the standard deviation of the estimate of γ. We conclude that $\mu = 2.6380 \pm 0.0003$, subject to the assumptions that $\gamma = 1.343\,75$ and $\Delta_1 = 1$.

The results of a similar analysis of the 18-term triangular lattice series is given in table 6. An additional column corresponding to $\Delta_1 = 0.84$ is also given, because it was found that estimates of γ were very stable there. While this might point to a confluent exponent with a value around $\Delta = 0.84$, we consider this unlikely as there is no evidence of such a value for the other two lattices, and such exponents are expected to be universal. Fortunately, however, even if such a confluent singularity were present it would not affect our estimate of the connective constant μ significantly, as the estimates of γ with $\Delta_1 = 0.84$ are very close to those with $\Delta_1 = 1.0$. The estimate $\mu = 4.1507 \pm 0.0004$ thus encompasses both possibilities.

Before analysing these same series by ratio techniques, we turn to the SAP series, which are analogues of the free energy. Nienhuis' result $\nu = \frac{3}{4}$ gives $\alpha = \frac{1}{2}$ *via* the scaling relation $d\nu = 2 - \alpha$. Thus we write the free energy as

$$F(x) \sim F_0(x) + (1 - x/x_c)^{2-\alpha}[f_0 + f_1(1 - x/x_c)^{\Delta_1} + \ldots] \tag{3.5}$$

Table 5. Variation of critical exponent γ with the parameter Δ (equation (3.1)) and the connective constant μ for the square lattice SAW series.

μ	$\Delta = 0.9$	$\Delta = 0.95$	$\Delta = 1.00$
2.637 84	1.3498 ± 0.0019	1.3484 ± 0.0018	1.3468 ± 0.0018
2.637 99	1.3460 ± 0.0009	1.3449 ± 0.0010	1.3437 ± 0.0011
2.638 10	1.3436 ± 0.0005	1.3424 ± 0.0009	1.3417 ± 0.0007
2.638 20	1.3416 ± 0.0003	1.3407 ± 0.0003	1.3399 ± 0.0004
2.638 30	1.3392 ± 0.0002	1.3390 ± 0.0002	1.3383 ± 0.0002
2.638 40	1.3381 ± 0.0002	1.3374 ± 0.0002	1.3367 ± 0.0001

Table 6. Variation of critical exponent γ with the parameter Δ (equation (3.1)) and the connective constant μ for the triangular lattice SAW series.

μ	$\Delta = 0.84$	$\Delta = 0.90$	$\Delta = 0.95$	$\Delta = 1.000$
4.150 41	1.3461 ± 0.0010	1.3434 ± 0.0020	1.3371 ± 0.0097	1.3471 ± 0.0091
4.150 55	1.3446 ± 0.0007	1.3423 ± 0.0013	1.3374 ± 0.0070	1.3445 ± 0.0068
4.150 65	1.3435 ± 0.0005	1.3415 ± 0.0010	1.3375 ± 0.0053	1.3429 ± 0.0055
4.150 755	1.3424 ± 0.0004	1.3407 ± 0.0007	1.3375 ± 0.0037	1.3412 ± 0.0042
4.150 85	1.3415 ± 0.0004	1.3399 ± 0.0005	1.3374 ± 0.0025	1.3398 ± 0.0032
4.150 95	1.3404 ± 0.0004	1.3390 ± 0.0005	1.3371 ± 0.0016	1.3384 ± 0.0023

where $F_0(x)$ is a background term analytic near x_c, while f_0, f_1 etc are constants arising in the expansion of the singular part of the free energy. Δ_1 is, as before, the correction-to-scaling exponent. Consider now the special case of $\Delta_1 - \alpha =$ integer. Then the 'confluent' term $f_1(1-x/x_c)^{2-\alpha+\Delta_1}$, being analytic, would merge with the background analytic term. Or, more pertinently, with

$$F(x) \sim F_0(x) + (1-x/x_c)^{2-\alpha} F_1(x) \tag{3.6}$$

where both F_0 and F_1 are analytic near x_c, and $0<\alpha<1$, then if $\Delta_1 \geqslant \alpha$ the method of analysis we have used would suggest an apparent confluent exponent $\Delta_1 = \alpha$. In this case, with $\alpha = \frac{1}{2}$, the series might therefore be expected to display an *apparent* confluent exponent of $\Delta = \frac{1}{2}$, and this is precisely what is observed.

In order to analyse these series by the Padé method we must first differentiate them twice (thus converting them to specific heat analogues) in order to get a divergent singularity, as the Padé method cannot resolve non-factorisable zeros (see Gaunt and Guttmann 1974). Another point is that for the loose-packed lattices the SAP generating function is a power series in v^2, so only half the number of coefficients are available for this series compared with the SAW series. Thus for the honeycomb lattice the specific heat series has only 13 non-zero coefficients. Analysing this series as for the walk series, we show in table 7 the average of the last six diagonal and off-diagonal Padé approximants, with a quoted error of one standard deviation. The exact critical point $1/\mu = (2+\sqrt{2})^{-1/2}$ has been used. The correct value of α ($\frac{1}{2}$) is given for a range of values of Δ around 0.5–0.55, in reasonable agreement with the expected value of $\Delta = \alpha = \frac{1}{2}$.

Table 7. Estimates of the 'specific-heat' exponent α obtained by averaging the last six (honeycomb) or eight (square) Padé approximants to the transformed self-avoiding-polygon series.

Δ	Honeycomb lattice $\mu = 1.847\,759\ldots$ α	Square lattice $\mu = 2.638\,14$ α
0.3	0.217 ± 0.035	0.326 ± 0.252
0.4	0.367 ± 0.023	0.457 ± 0.070
0.45	0.427 ± 0.026	0.463 ± 0.020
0.50	0.473 ± 0.029	0.502 ± 0.003
0.55	0.524 ± 0.035	0.500 ± 0.074
0.60	0.564 ± 0.035	0.553 ± 0.021

For the square lattice we are in possession of a much longer series, due to the work of Enting (1980), whose finite lattice calculation gives the series to powers of x^{38}, compared with x^{24} for the SAW series. In the specific heat, 16 non-zero coefficients remain, and an analysis of this series identical to the analysis of the honeycomb lattice series above (though with a non-exact value of μ) produced the results shown in the third column of table 7. The decrease in the error in the estimate of α as $\Delta \to \frac{1}{2}$ is quite dramatic, and shows the sort of improvement that can be expected from longer series.

Accepting the value $\Delta = 0.5$—which we emphasise corresponds to an additive, analytic term rather than a square root correction-to-scaling exponent—we show in table 8 the variation in estimates of α obtained by varying the connective constant μ over the same range as for the SAW series. Table 8 also displays corresponding results for the triangular lattice, where the series is known up to the same length as the SAW series, that is, 18 terms. Thus while the triangular lattice SAP series is as long as the square lattice SAP series when measured in terms of coefficients, it represents significantly less configurational information, corresponding as it does to only 18-step polygons, compared with 38-step polygons on the square lattice. Among the three lattices, it is the honeycomb lattice that gives the most badly behaved SAP series—reflecting the small number of polygons embeddable on this lattice up to order v^{34}. At the correct value of μ and with $\Delta = 0.5$, the honeycomb lattice series gives $\alpha = 0.473 \pm 0.029$—just consistent with the 'exact' value of $\frac{1}{2}$. For the square lattice, the requirement that $\alpha = \frac{1}{2}$ gives $\mu = 2.6382 \pm 0.0002$, while for the triangular lattice we estimate similarly $\mu = 4.1509 \pm 0.0005$.

Table 8. Variation of specific heat exponent α with connective constant μ for the square and triangular lattice.

Square lattice		Triangular lattice	
μ	α	μ	α
2.637 84	0.5101 ± 0.0036	4.150 41	0.5050 ± 0.0075
2.637 99	0.5061 ± 0.0019	4.150 58	0.5034 ± 0.0077
2.638 10	0.5030 ± 0.0024	4.150 65	0.5026 ± 0.0078
2.638 20	0.4998 ± 0.0035	4.150 755	0.5017 ± 0.0079
2.638 30	0.4957 ± 0.0062	4.150 80	0.5013 ± 0.0080
2.638 40	0.4890 ± 0.0165	4.150 90	0.5004 ± 0.0081
		4.151 00	0.4994 ± 0.0082
		4.151 10	0.4984 ± 0.0083

Turning now to ratio type methods, we have repeated the analysis of Sykes *et al* (1972) for the square and triangular lattices with the following differences. (i) We have used the exponent value $\gamma = 1\frac{11}{32}$ rather than $\frac{4}{3}$; (ii) we have used the extended and corrected triangular lattice SAW series; and (iii) for the triangular lattice we have calculated an additional column of extrapolants.

For the triangular lattice we assume that

$$C(x) = \sum c_n x^n \sim (1 - \mu x)^{-g-1} \Phi(x) + \Psi(x) \tag{3.7}$$

where Φ and Ψ are regular in the disc $|\mu x| \leq 1$, while for the square lattice we assume that

$$C(x) = \sum c_n x^n \sim A(x)(1 - \mu x)^{-g-1} + B(x)(1 + \mu x)^{-h-1} + D(x) \tag{3.8}$$

where A, B and D are regular in the disc $|\mu x| \leq 1$. Further, we assume that $g = \frac{11}{32}$ and $h = -\frac{3}{2}$, as discussed by Sykes *et al.* The form of these equations thus tacitly assumes the absence of confluent singularities. For both lattices we investigate the sequences $\{\beta_n | \beta_n = (nc_n/c_{n-1})/(n+g)\}$. For the triangular lattice we form sequences $\{\mu_{1,n}\}$ and $\{\mu_{2,n}\}$ corresponding to solutions of $\beta_n = \mu_{1,n}\{1 + a/n^2\}$ and $\beta_n = \mu_{2,n}\{1 + b/n^2 + c/n^3\}$ obtained from successive pairs or triples of β_n's. For the square lattice we form sequences $\{\mu_{1,n}\}$, $\{\mu_{2,n}\}$ and $\{\mu_{3,n}\}$ corresponding to solutions of $\beta_n = \mu_{1,n}\{1 + a/n^2\}$, $\beta_n = \mu_{2,n}\{1 + (-1)^n b/n^\theta\}$ with $\theta = g - h$ and $\beta_n = \mu_{3,n}\{1 + c/n^2 + (-1)^h d/n^\theta\}$ where successive *alternate* values of β_n are used.

The results are shown in tables 9 and 10. In table 9 we see the triangular lattice results. The estimators $\{\mu_{1,n}\}$ imply $\mu \gtrsim 4.1505$ while the $\{\mu_{2,n}\}$ sequence is quite stable, and implies $\mu = 4.150\,75 \pm 0.0002$.

In table 10 the estimators $\{\mu_{1,n}\}$ imply $2.6379 < \mu < 2.6383$ while the estimators $\{\mu_{2,n}\}$ imply $\mu \approx 2.638\,17$, a value that is supported by the combined estimators $\{\mu_{3,n}\}$.

Combining all analyses reported, we conclude

$$\mu\ (\text{triangular}) = 4.150\,75 \pm 0.0003, \qquad \mu\ (\text{square}) = 2.6381 \pm 0.0002. \tag{3.9}$$

The sum μ (triangular) + μ (honeycomb) = 5.9985 ± 0.0003 would seem to rule out the conjecture that this sum is precisely 6.

Table 9. Generalised ratio analysis of triangular SAW series. Each column should converge to μ.

n	β_n	$\mu_{1,n}$	$\mu_{2,n}$
10	4.144 46	4.148 88	4.149 39
11	4.145 37	4.149 75	4.152 37
12	4.146 07	4.149 75	4.149 78
13	4.146 66	4.150 02	4.151 01
14	4.147 14	4.150 17	4.150 74
15	4.147 54	4.150 26	4.150 69
16	4.147 88	4.150 36	4.150 79
17	4.148 17	4.150 42	4.150 74
18	4.148 42	4.150 47	4.150 76

Table 10. Generalised ratio analysis of square lattice SAW series. Each column should converge to μ.

n	β_n	$\mu_{1,n}$	$\mu_{2,n}$	$\mu_{3,n}$
13	2.642 99	2.637 79	2.637 27	2.637 81
14	2.629 09	2.637 72	2.638 57	2.637 75
15	2.641 82	2.638 28	2.637 93	2.638 00
16	2.631 09	2.637 62	2.638 25	2.637 94
17	2.641 05	2.638 34	2.638 08	2.637 99
18	2.632 48	2.637 74	2.638 24	2.638 03
19	2.640 50	2.638 31	2.638 10	2.638 03
20	2.633 50	2.637 82	2.638 23	2.638 06
21	2.640 10	2.638 30	2.638 13	2.638 07
22	2.634 26	2.637 87	2.638 21	2.638 08
23	2.639 80	2.638 29	2.638 15	2.638 09
24	2.634 84	2.637 91	2.638 20	2.638 10

4. Discussion

Our principal results are the estimates (3.9) above. We find strong evidence to support Nienhuis' result that $\gamma = 1\frac{11}{32}$, and that $\alpha = \frac{1}{2}$ which follows from the hyperscaling relation $d\nu = 2 - \alpha$ and Nienhuis' result that $\nu = \frac{3}{4}$.

We find no consistent evidence for the presence of a confluent singularity with exponent $\Delta_1 < 1$. Our methods cannot reliably detect confluent exponents $\Delta_1 > 1$, though these have been predicted both by ε expansions, where Le Guillou and Zinn-Justin (1980) gave $\Delta_1 \approx 1.15$, and by Monte Carlo calculations (Havlin and Ben-Avraham 1983) as $\Delta_1 = 1.2 \pm 0.1$. In previous work, Grassberger (1982) also reports the absence of any detectable confluent singularity with $\Delta_1 < 1$. Nienhuis (1982) obtains $\Delta_1 = \frac{3}{2}$, though the status of this exponent is not clear. Most recently, Privman (1983b) estimated $\Delta_1 = 0.65 \pm 0.08$ using both series analysis and a finite-size scaling renormalisation technique, while Adler (1983) reports $\Delta_1 \approx 0.93$ for the honeycomb lattice data, as discussed in § 3, and Majid *et al* (1983) find $\Delta_1 < 1$ in their analysis of the mean square end-to-end distance series.

Our analysis cannot comment on the estimates of $\Delta_1 > 1$. We find no evidence of a universal exponent $\Delta_1 < 1$, though it follows from renormalisation group theory that if such a singularity is present in the mean square end-to-end distance series, it should also be present in the SAW generating function.

It seems pertinent that the two-dimensional Ising model has no correction-to-scaling exponent $\Delta_1 < 1$ (Aharony and Fisher 1980), and our series analysis suggests a similar conclusion for the two-dimensional SAW generating function series. On the other hand, Privman (private communication) has discussed the possibility of a number of background terms combining together to give a large number of distinct 'correction' exponents, making the leading correction exponent hard to detect, and also providing a plausible explanation for the apparent exponent value $\gamma \approx \frac{4}{3}$ found for the triangular lattice.

5. Speculation

In this section we speculate on some possibly exact values of the connective constant of the square and triangular lattice SAW models.

For the Ising model we write $\nu = 1/v_c = 1/\tanh(J/kT_c)$ as the analogue of the SAW connective constant μ. The following exact results are well known:

$$\begin{aligned} &\nu(\mathrm{H}) = \sqrt{3}, && \text{honeycomb,} \\ &\nu(\mathrm{K}) = \tfrac{1}{2}(1 + \sqrt{3} + \sqrt{2\sqrt{3}}), && \text{Kagomé,} \\ &\nu(\mathrm{S}) = 1 + \sqrt{2}, && \text{square,} \\ &\nu(\mathrm{T}) = 2 + \sqrt{3}, && \text{triangular.} \end{aligned} \tag{5.1}$$

Note that the square and triangular results are of a more complex form than the honeycomb result. That is, they are not just square roots. Nevertheless, the honeycomb square and triangular results are connected by Onsager's relation $\mathrm{gd}(2K_c) = \pi/q$ where gd is the Gudermanian function $\mathrm{gd}(x) = \tan^{-1}(\sinh x)$, q is the coordination number of the lattice and $K_c = J/kT_c$. This relation can be rewritten $1/\nu = \tan(\pi/2q)$. The Kagomé lattice, being a non-regular lattice, is not part of this pattern. Another feature of (5.1) is that all three regular lattices have critical points ν given by the solution of quadratic equations with integer coefficients, while the Kagomé lattice ν is given by the solution of a quartic equation with integer coefficients.

We have

$$\begin{aligned} &\nu(\mathrm{H})^2 - 3 = 0, && \nu(\mathrm{S})^2 - 2\nu(\mathrm{S}) - 1 = 0, \\ &\nu(\mathrm{T})^2 - 4\nu(\mathrm{T}) + 1 = 0, && \nu(\mathrm{K})^4 - 2\nu(\mathrm{K})^3 - 2\nu(\mathrm{K}) + 1 = 0. \end{aligned} \tag{5.2}$$

For the honeycomb lattice SAW series, the corresponding result is $\mu(\mathrm{H})=(2+\sqrt{2})^{1/2}$, which satisfies the quartic equation

$$\mu(\mathrm{H})^4-4\mu(\mathrm{H})^2+2=0. \tag{5.3}$$

Arguing in analogy with the Ising model results, it seems reasonable to speculate that $\mu(\mathrm{S})$ and $\mu(\mathrm{T})$ are also given by the solution of quartic equations with integer coefficients. We mention in passing that there are no solutions of the form $\mu=(a+\sqrt{b})^{1/2}$ for reasonable integer values of a and b that give our estimates (3.9) for the square and triangular lattices.

A systematic search for solutions of quartic equations with (a) integer coefficients and (b) solutions of the form

$$\tfrac{1}{2}[a\pm\sqrt{b}\pm\sqrt{c\pm\sqrt{d}}] \tag{5.4}$$

was undertaken, for reasonable integral values of a, b, c, d. While (5.4) is not the *most* general form for the solution of a quartic, it seemed reasonable in view of the essential simplicity of other results to assume that no more complex form would prevail. Pragmatically, a search using the most general form for the solution of a quartic would have been computationally unfeasible. As it was, we generated about 2×10^7 distinct quartics, and found only ten likely contenders.

For the triangular lattice we find six possible contenders:

$$\begin{aligned}
&\text{(i)} && \mu=-3+\sqrt{7}+\sqrt{15+2\sqrt{7}}=4.150\,360\ldots,\\
&\text{(ii)} && \mu=-2+\sqrt{35+2\sqrt{2}}=4.150\,481\ldots,\\
&\text{(iii)} && \mu=\tfrac{1}{2}[5+\sqrt{6+2\sqrt{6}}]=4.150\,680\ldots,\\
&\text{(iv)} && \mu=3+\sqrt{2\sqrt{10}-5}=4.150\,893\ldots,\\
&\text{(v)} && \mu=1+\sqrt{3+4\sqrt{3}}=4.150\,905\ldots,\\
&\text{(vi)} && \mu=\tfrac{1}{2}[1+\sqrt{15}+\sqrt{4+2\sqrt{15}}]=4.150\,111\ldots,
\end{aligned} \tag{5.5}$$

which correspond to integer coefficient quartics with no particularly compelling feature. We note that result (5.5) (iii) is closest to the series estimate, though (iv) and (v) are almost as close.

For the square lattice, the only plausible solutions we found were:

$$\begin{aligned}
&\text{(i)} && \mu=\tfrac{1}{2}[2+\sqrt{9+\sqrt{3}}]=2.637\,990\ldots,\\
&\text{(ii)} && \mu=1+\sqrt{6-\sqrt{11}}=2.638\,101\ldots,\\
&\text{(iii)} && \mu=\sqrt{11+\sqrt{5}}-1=2.638\,140\ldots,\\
&\text{(iv)} && \mu=\tfrac{1}{2}[\sqrt{13+2\sqrt{7}}+1]=2.638\,428\ldots.
\end{aligned} \tag{5.6}$$

Solution (ii) lies closest to the estimated value (3.9), but contains an unlikely looking $\sqrt{11}$. (It is amusing to note, however, that the surd $11+5\sqrt{5}$ arises in Baxter's exact solution of the hard hexagon problem.) Solution (i) looks the most likely from the point of view of square roots of small numbers. The Ising model solutions contain only $\sqrt{2}$'s and $\sqrt{3}$'s, while the honeycomb SAW result contains a $\sqrt{2}$. This suggests that, other things being equal, it is reasonable to choose a solution for the SAW model on the other two lattices that also contains only $\sqrt{2}$'s and $\sqrt{3}$'s. For this reason we consider solution (i) slightly more likely than the other two.

One way to immeasurably strengthen our confidence in the correctness of these results would be to find some connection between the results on the three lattices paralleling the result $\nu = 1/\tan(\pi/2q)$ that holds for the Ising model. To date we have been unable to find such a connection. However, for ordinary random walks, the parameter $\sigma = q-1$ enters the equation for the connective constant. Nienhuis' exact result $\mu(\mathrm{H}) = (2+\sqrt{2})^{1/2}$ contains $\sqrt{2} = \sqrt{\sigma}$ which arises from trigonometric functions with argument $(\pi/2\sigma)$. For the square and triangular lattices, $(\pi/2\sigma) = \pi/6$ and $\pi/10$ respectively. Trigonometric functions of these arguments contain factors $\sqrt{3}$ and, for $\pi/10$, $\sqrt{2}$ and $\sqrt{5}$. These highly speculative considerations provide a plausible means of distinguishing between the possible results (5.5) and (5.6), and suggest (5.5)(iv) for the triangular lattice and (5.6)(i) for the square lattice.

In summary then we find that

$$\begin{aligned} \mu &= 1+\tfrac{1}{2}\sqrt{9+\sqrt{3}} = 2.637\,990\ldots\ \text{(square)}, \\ \mu &= 3+\sqrt{2\sqrt{10}-5} = 4.150\,893\ldots\ \text{(triangular)}, \end{aligned} \tag{5.7}$$

are at least useful mnemonics.

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