

Connective constant of the self-avoiding walk on the triangular lattice

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1986 J. Phys. A: Math. Gen. 19 2591

(<http://iopscience.iop.org/0305-4470/19/13/024>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 31/05/2010 at 10:01

Please note that [terms and conditions apply](#).

Connective constant of the self-avoiding walk on the triangular lattice

A J Guttmann[†], Thomas R Osborn[‡] and Alan D Sokal[§]

[†] Department of Mathematics, Statistics and Computer Science, The University of Newcastle, NSW, Australia 2308

[‡] School of Computing Sciences, New South Wales Institute of Technology, PO Box 123, Broadway 2007, Australia

[§] Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, NY 10012, USA

Received 13 September 1985, in final form 19 November 1985

Abstract. We use a recently developed Monte Carlo method to study the connective constant of the self-avoiding walk (SAW) on the triangular lattice. Assuming $\gamma = \frac{43}{32}$, we find $\mu_T = 4.150\,96 \pm 0.000\,10 \pm 0.000\,26$ (95% confidence limits) and $\mu_H = 4.150\,96 \pm 0.000\,20 \pm 0.000\,37$ (99% confidence limits), where the first error bar represents systematic error due to corrections to scaling and the second error bar represents statistical error. This rules out the conjecture $\mu_T + \mu_H = 6$ at the greater than 99% confidence level.

Nearly two decades ago, Sykes observed that the connective constants of the self-avoiding walk (SAW) on the triangular and honeycomb lattices appear to satisfy very closely the relation

$$\mu_T + \mu_H \stackrel{?}{=} 6 \quad (1)$$

and he conjectured that the relation (1) might be exact. Subsequent numerical studies by Guttmann *et al* (1968), Guttmann and Sykes (1973) and Watts (1975) gave strong support to this conjecture: they found $\mu_T + \mu_H = 5.999 \pm 0.006$, 5.9998 ± 0.0020 and 5.9998 ± 0.0012 , respectively.

The conjecture is a tantalising one. For the Ising model, the well known Kramers-Wannier duality (Syozzi 1972, Savit 1980, Baxter 1982) and star-triangle transformation (Syozzi 1972, Baxter 1982) actually give *two* relations between the triangular lattice and honeycomb lattice critical temperatures, allowing both to be determined exactly. The same occurs in bond percolation (Sykes and Essam 1964, Wierman 1981). However, for the self-avoiding walk, no exact duality or star-triangle transformation is known, only a 'star-triangle inequality' (Guttmann and Sykes 1973, but see also Watson 1974).

The conjecture takes on added interest in light of Nienhuis' (1982, 1984) exact value for the connective constant of the SAW on the honeycomb lattice, $\mu_H = (2 + \sqrt{2})^{1/2} = 1.847\,759 \dots$: one is led to the precise conjecture

$$\mu_T \stackrel{?}{=} 6 - (2 + \sqrt{2})^{1/2} = 4.152\,240 \dots \quad (2)$$

|| Though Nienhuis' argument is non-rigorous, his results are almost certainly correct. His argument in fact yields the exact critical temperature for a family of n -component spin models on the honeycomb lattice, as a function of n : $x_c(n) = (2 + \sqrt{2 - n})^{-1/2}$. For $n = 1$ (Ising model) and $n = 2$ (a modified plane-rotator model), this agrees with the known exact values; and for $n = 0$ (self-avoiding walk), it agrees splendidly with the best numerical estimate $\mu_H = 1.8478 \pm 0.0001$ (Watts 1975, Guttmann 1984). Baxter (1986) has obtained Nienhuis' result for μ_H by an alternative, and more direct, method.

Nienhuis' derivation is based on a combination of exact transformations and renormalisation group arguments; the exact transformations rely heavily on the fact that the honeycomb lattice has coordination number 3 (so that polygons without common bonds cannot touch), and have no apparent analogue for lattices of coordination number ≥ 4 . Thus, the conjectures (1) and (2), if true, could be explained only by radically new theoretical ideas.

Unfortunately, we show in this paper that the conjectures (1) and (2) are almost certainly *false*. Previously, Guttmann (1984) reanalysed the series expansions for SAW on the regular two-dimensional lattices (square, triangular and honeycomb), in order to account for non-analytic corrections to scaling as predicted by renormalisation group theory (Wegner 1972, Brézin *et al* 1976): using 18 terms of the chain-generating-function series on the triangular lattice and assuming Nienhuis' (1982, 1984) exact critical exponent[†] $\gamma = \frac{43}{32}$, he estimated $\mu_T = 4.15075 \pm 0.00030$. A more recent analysis, based on 19 terms and using integral approximants (Rehr *et al* 1980), yields $\mu_T = 4.15081 \pm 0.00031$ if γ is unconstrained and $\mu_T = 4.15077 \pm 0.00004$ if $\gamma = \frac{43}{32}$ is assumed (Guttmann 1986a). The conjectured exact value for μ_T thus lies some 5–40 error bars distant from the current central estimates. However, series extrapolation is a notoriously tricky business (Nickel 1982, Guttmann 1986b): everything rests on the perhaps unjustified faith that the behaviour of N -step SAW for $N \leq 19$ is a reliable guide to their asymptotic behaviour as $N \rightarrow \infty$. Moreover, the error bars are subjective, and are based solely on criteria of internal consistency. It is thus of some interest to complement the series-extrapolation results with a Monte Carlo study: by using walks of length $N \approx 100$ –1000, the potential systematic errors due to unknown corrections to scaling are dramatically reduced (provided that the leading correction-to-scaling exponent Δ_1 is not too close to zero); one pays the price of statistical error, but this error can be quantified objectively as a statistical confidence interval.

We use the Monte Carlo algorithm and statistical methods of Berretti and Sokal (1985); details can be found in that paper, so we give here only a brief synopsis. The algorithm is a dynamic Monte Carlo algorithm which generates SAW in the grand canonical ensemble

$$\text{Prob}(\text{length} = N) = \text{constant} \times \beta^N c_N \quad (3)$$

where c_N is the number of distinct N -step SAW and β is a user-chosen parameter. The c_N are assumed to have the asymptotic behaviour

$$c_N = \mu^N N^{\gamma-1} A(1 + a_1/N + \dots) \quad (4)$$

as $N \rightarrow \infty$ (this assumption is discussed in more detail below), and we use maximum-likelihood estimation (MLE) to determine μ and γ . It can be shown that MLE is an optimal estimation method (Silvey 1975). The algorithm's autocorrelation time τ is of order $\langle N \rangle^2$, and is estimated numerically using standard methods of statistical time-series analysis (Priestley 1981); this plays an important role in the determination of error bars.

Our main run was performed at $\beta = 0.2397$, corresponding to

$$\langle N \rangle \approx \beta \mu \gamma / (1 - \beta \mu) \approx 265. \quad (5)$$

[†] In Nienhuis' original article (1982), $\mu_H = (2 + \sqrt{2})^{1/2}$ and $\nu = \frac{3}{4}$ were supported by a renormalisation group argument, but $\gamma = \frac{43}{32}$ had only the status of a promising numerical conjecture. Subsequently, Nienhuis (1984) gave the result for γ a comparable renormalisation group foundation.

We took the initial configuration to be the empty walk, and then performed 10.8×10^9 Monte Carlo iterations; this took approximately 500 h CPU time on the Perkin-Elmer 3220 minicomputer (using a rather inefficient FORTRAN compiler) at the University of Newcastle. Data were taken once every 10^5 MC iterations. In doing the statistical analysis we always skipped the data from the first 10^8 MC iterations; since this is $\approx 300 \tau$ (see below), the system has clearly reached equilibrium. We used a linear congruential pseudo-random-number generator (PRNG)

$$x_{n+1} = (ax_n + c) \bmod m \quad (6)$$

with $c = 1$ and $m = 2^{32}$; the multiplier was $a = 1566\ 083\ 941$ for the first third of the run and $a = 1664\ 525$ for the latter two-thirds†. Both generators are recommended by Knuth (1981, p 102). We verified that the results from the two parts of the run agree within statistical error; this provides an extra check against subtle defects in one or both of the PRNG.

An autocorrelation analysis yielded $\tau = (3 \pm 1) \times 10^5$ MC iterations, i.e. $\tau \approx 5(N)^2$, in close agreement with the results of Berretti and Sokal (1985) for the square lattice self-avoiding walk problem.

We performed a two-parameter maximum-likelihood estimation of μ and γ , using the ansatz‡

$$c_N = \mu^N (N+3)^{\gamma-1} A [1 + a_1/(N+3)] \quad \text{for } N \geq N_{\min} \quad (4')$$

for a range of values of a_1 and N_{\min} ; the results are shown in table 1. The estimates for $N_{\min} = 0$ are clearly biased by strong systematic error due to higher-order corrections to scaling not included in (4'), and the estimates for $N_{\min} = 400, 800$ have huge statistical error due to the small sample size of such long walks; we thus concentrate on the remaining values of N_{\min} . It is somewhat difficult to apply the 'flatness criterion' (Berretti and Sokal 1985) to this table, because of the large statistical fluctuations; the 'glitch' at $N_{\min} = 100, 200$ makes analysis particularly difficult. We conclude that any value of a_1 in the range $-0.5 \leq a_1 \leq 2.0$ gives a reasonable degree of flatness (for $25 \leq N_{\min} \leq 200$), although the values $0.25 \leq a_1 \leq 1.0$ give a somewhat flatter plot for μ , and the values $0.5 \leq a_1 \leq 1.5$ give a somewhat flatter plot for γ . The fact that the 'good' values of a_1 do not coincide for μ and γ , contrary to what was observed by Berretti and Sokal (1985), is probably due, once again, to statistical fluctuation. We shall therefore quote a very conservative systematic error, by using *all* the values $0.25 \leq a_1 \leq 1.5$ for *both* μ and γ (estimates printed in boldface in table 1): following Berretti and Sokal (1985), we obtain

$$\begin{aligned} \mu &= 4.150\ 93 \pm 0.000\ 21 \pm 0.000\ 91 \\ \gamma &= 1.348 \pm 0.033 \pm 0.083 \end{aligned} \quad (7)$$

where the first error bar represents systematic error due to unincluded corrections to scaling (subjective 95% confidence limits), and the second error bar represents statistical error (classical 95% confidence limits, taken at $N_{\min} = 100$).

† Thus, the second PRNG cycled through its full period (2^{32}) nearly twice! It is perhaps slightly embarrassing that the same 'random numbers' were used more than once, but we do not consider it particularly serious: save for a possible (but highly improbable) fluke, the two cycles of the PRNG will have encountered the SAW in radically different configurations, so the responses will be 'unrelated' and the resulting data 'independent'.

‡ The constant 3 occurring in equation (4') has no special significance; it could be replaced by any small positive number. Provided that N_{\min} is reasonably large, a change in this constant is equivalent to a redefinition of a_1 , up to corrections of order $1/N_{\min}^2$ which can be ignored.

Table 1. Two-parameter maximum-likelihood estimates of μ and γ , assuming (4'). Error bars are 95% confidence intervals and include statistical error only.

$a \backslash N_{\min}$	0	25	50	100	200	400	800
-0.50	4.150 890	4.151 037	4.150 998	4.151 061	4.150 853	4.151 019	4.152 147
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.341 950	1.330 094	1.333 564	1.326 395	1.355 784	1.330 116	0.958 396
-0.25	$\pm 0.027 209$	$\pm 0.039 784$	$\pm 0.052 963$	$\pm 0.083 375$	$\pm 0.170 879$	$\pm 0.520 743$	$\pm 3.045 829$
	4.150 804	4.151 014	4.150 983	4.151 053	4.150 849	4.151 017	4.152 147
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
0.00	1.350 039	1.333 267	1.335 865	1.327 997	1.356 853	1.330 799	0.958 813
	$\pm 0.027 146$	$\pm 0.039 782$	$\pm 0.052 965$	$\pm 0.083 378$	$\pm 0.170 883$	$\pm 0.520 749$	$\pm 3.045 836$
	4.150 722	4.150 990	4.150 969	4.151 045	4.150 845	4.151 015	4.152 146
0.25	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.357 902	1.336 418	1.338 157	1.329 594	1.357 921	1.331 482	0.959 229
	$\pm 0.027 085$	$\pm 0.039 782$	$\pm 0.052 967$	$\pm 0.083 380$	$\pm 0.170 885$	$\pm 0.520 753$	$\pm 3.045 844$
0.50	4.150 612	4.150 967	4.150 955	4.151 037	4.150 841	4.151 013	4.152 145
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.365 553	1.339 548	1.340 438	1.331 186	1.358 987	1.332 165	0.959 645
0.75	$\pm 0.027 030$	$\pm 0.039 780$	$\pm 0.052 969$	$\pm 0.083 384$	$\pm 0.170 889$	$\pm 0.520 756$	$\pm 3.045 851$
	4.150 561	4.150 944	4.150 941	4.151 029	4.150 837	4.151 012	4.152 145
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
1.00	1.373 003	1.342 655	1.342 709	1.332 774	1.360 052	1.332 846	0.960 061
	$\pm 0.026 977$	$\pm 0.039 780$	$\pm 0.052 971$	$\pm 0.083 388$	$\pm 0.170 892$	$\pm 0.520 762$	$\pm 3.045 858$
	4.150 489	4.150 922	4.150 927	4.151 021	4.150 833	4.151 010	4.152 144
1.25	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 704$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.380 263	1.345 742	1.344 970	1.334 357	1.361 113	1.333 526	0.960 177
	$\pm 0.026 928$	$\pm 0.039 778$	$\pm 0.052 973$	$\pm 0.083 390$	$\pm 0.170 896$	$\pm 0.520 766$	$\pm 3.045 866$
1.50	4.154 416	4.150 899	4.150 913	4.151 013	4.150 829	4.151 008	4.152 143
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 706$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.387 342	1.348 807	1.347 220	1.335 936	1.362 174	1.334 206	0.960 890
1.75	$\pm 0.026 879$	$\pm 0.039 778$	$\pm 0.052 975$	$\pm 0.083 394$	$\pm 0.170 900$	$\pm 0.520 770$	$\pm 3.045 877$
	4.150 345	4.150 877	4.150 899	4.151 006	4.150 825	4.151 006	4.152 143
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 706$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
2.00	1.394 250	1.351 852	1.349 461	1.337 510	1.363 232	1.334 886	0.961 305
	$\pm 0.026 836$	$\pm 0.039 776$	$\pm 0.052 977$	$\pm 0.083 396$	$\pm 0.170 904$	$\pm 0.520 774$	$\pm 3.045 883$
	4.150 276	4.150 855	4.150 885	4.150 998	4.150 821	4.151 005	4.152 142
2.00	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 706$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.400 996	1.354 876	1.351 691	1.339 079	1.364 288	1.335 565	0.961 720
	$\pm 0.026 793$	$\pm 0.039 776$	$\pm 0.052 979$	$\pm 0.083 400$	$\pm 0.170 908$	$\pm 0.520 780$	$\pm 3.045 891$
2.00	4.150 209	4.150 833	4.150 871	4.150 990	4.150 817	4.151 003	4.152 141
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 706$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
	1.407 585	1.357 880	1.353 911	1.340 644	1.365 343	1.336 241	0.962 134
2.00	$\pm 0.026 754$	$\pm 0.039 774$	$\pm 0.052 981$	$\pm 0.083 404$	$\pm 0.170 910$	$\pm 0.520 784$	$\pm 3.045 899$
	4.150 144	4.150 811	4.150 858	4.150 983	4.150 813	4.151 001	4.152 141
	$\pm 0.000 494$	$\pm 0.000 604$	$\pm 0.000 706$	$\pm 0.000 909$	$\pm 0.001 411$	$\pm 0.002 973$	$\pm 0.010 988$
2.00	1.414 027	1.360 864	1.356 122	1.342 205	1.366 395	1.336 919	0.962 548
	$\pm 0.026 715$	$\pm 0.039 774$	$\pm 0.052 983$	$\pm 0.083 406$	$\pm 0.170 914$	$\pm 0.520 788$	$\pm 3.045 907$

We emphasise that the ansatz (4') ignores a possible non-analytic correction to scaling with exponent $\Delta_1 < 1^\dagger$, as well as higher-order corrections to scaling. However, it appears to us unfeasible at present to distinguish reliably between $0.5 \leq \Delta_1 < 1.0$ and $\Delta_1 \approx 1.0$, because of the relatively large *statistical* errors at large N_{\min} (and N_{\min} must be large if the leading correction to scaling is to dominate all the others); any effect of $\Delta_1 \neq 1$ could for all practical purposes be absorbed into a slightly changed value of a_1 . As more powerful computers become available for Monte Carlo work, a more sophisticated analysis of corrections to scaling will become important. In any case, the errors resulting here from the approximation $\Delta_1 \geq 1$, as well as from the neglected higher-order corrections to scaling, are included in the quoted systematic error. This estimate of the systematic error should be reliable (and indeed conservative) provided only that Δ_1 is not too close to zero, e.g. $\Delta_1 \geq 0.5$. There have been several estimates of Δ_1 in the literature (see references cited below), and all are ≥ 0.67 .

The result (7) for γ is consistent with Nienhuis' (1982, 1984) exact value $\gamma = \frac{43}{32} = 1.34375$, but the error bars are clearly too large for the estimate to be of much interest! The estimate for μ is not bad—it already rules out conjecture (2) at the 95% confidence level—but we can do much better by *assuming* $\gamma = \frac{43}{32}$ and performing a one-parameter maximum-likelihood analysis. The results are shown in table 2. We ignore the values $N_{\min} = 0, 800$ for the reasons noted previously. The 'glitch' at $N_{\min} = 100, 200$ is still present, but it is weaker than in table 1. The flattest plots are found for $a_1 = 0.75, 1.0$, but a reasonable degree of flatness can be obtained for any value in the range $0.25 \leq a_1 \leq 1.5$; using these latter values (estimates printed in boldface), we obtain

$$\mu = 4.15096 \pm 0.00010 \pm 0.00032 \quad (95\% \text{ confidence limits}) \quad (8a)$$

and‡

$$\mu = 4.15096 \pm 0.00020 \pm 0.00042 \quad (99\% \text{ confidence limits}). \quad (8b)$$

The conjecture (2) is thus ruled out at the greater than 99% confidence level. We do not attempt to specify the exact level of confidence (e.g. 99.999%), since to do so would require a detailed analysis of the small deviations from normality in the MLE, as well as prolonged (and probably fruitless) introspection to determine the extreme tails of our subjective probability distribution for the systematic error. We prefer to leave well enough alone.

The estimates and error bars in tables 1 and 2 were computed by using all the data as if they were independent, and then multiplying the MLE theory error bars by a factor $\approx (2\tau)^{1/2}$ with $\tau = 3 \times 10^5$ to adjust for the effects of autocorrelations. As a check, we performed an alternate analysis: we split the run (or rather, almost all of it) into 15 equal-sized blocks, each one large enough ($\approx 2000\tau$) to be considered effectively independent and for the block MLE to be normally distributed; we then determined confidence intervals using the standard *t* test. Typical results are shown in table 3. The two methods give nearly identical central estimates; the slight discrepancies are

† Evidence for such an exponent in the two-dimensional SAW is highly contradictory: compare Le Guillou and Zinn-Justin (1980), Grassberger (1982), Nienhuis (1982), Havlin and Ben-Avraham (1983), Majid *et al* (1983), Adler (1983), Djordjevic *et al* (1983), Privman (1984), Guttmann (1984, 1985), Rapaport (1985a, b) and Kremer and Lyklema (1985).

‡ Note that our systematic error bar for 99% confidence is *twice* as wide as that for 95% confidence, while the statistical error bar is only $2.58/1.96 = 1.31$ times as wide. This is because our subjective probability distribution for the systematic error has 'heavy tails' (reflecting our uncertainty about the true form of corrections to scaling), while the statistical error in the MLE is approximately normally distributed.

Table 2. One-parameter maximum-likelihood estimates of μ , assuming (4') with $\gamma = \frac{43}{32}$. Error bars are 95% confidence intervals and include statistical error only.

$a_1 \backslash N_{\min}$	0	25	50	100	200	400	800
-0.50	4.150 862 ±0.000 267	4.150 853 ±0.000 276	4.150 874 ±0.000 288	4.150 883 ±0.000 318	4.150 948 ±0.000 392	4.150 942 ±0.000 617	4.150 769 ±0.001 584
-0.25	4.150 901 ±0.000 267	4.150 872 ±0.000 276	4.150 887 ±0.000 288	4.150 892 ±0.000 318	4.150 953 ±0.000 392	4.150 944 ±0.000 617	4.150 770 ±0.001 584
0.00	4.150 939 ±0.000 267	4.150 891 ±0.000 274	4.150 901 ±0.000 288	4.150 900 ±0.000 318	4.150 957 ±0.000 392	4.150 946 ±0.000 617	4.150 771 ±0.001 584
0.25	4.150 977 ±0.000 265	4.150 911 ±0.000 274	4.150 915 ±0.000 288	4.150 908 ±0.000 318	4.150 962 ±0.000 392	4.150 949 ±0.000 617	4.150 772 ±0.001 584
0.50	4.151 015 ±0.000 265	4.150 930 ±0.000 274	4.150 928 ±0.000 288	4.150 917 ±0.000 318	4.150 966 ±0.000 392	4.150 951 ±0.000 615	4.150 772 ±0.001 584
0.75	4.151 052 ±0.000 265	4.150 949 ±0.000 274	4.150 941 ±0.000 288	4.150 925 ±0.000 318	4.150 971 ±0.000 392	4.150 953 ±0.000 615	4.150 773 ±0.001 584
1.00	4.151 089 ±0.000 265	4.150 968 ±0.000 274	4.150 955 ±0.000 286	4.150 934 ±0.000 318	4.150 975 ±0.000 392	4.150 955 ±0.000 615	4.150 774 ±0.001 584
1.25	4.151 126 ±0.000 265	4.150 986 ±0.000 274	4.150 968 ±0.000 286	4.150 942 ±0.000 318	4.150 979 ±0.000 392	4.150 957 ±0.000 615	4.150 775 ±0.001 584
1.50	4.151 163 ±0.000 263	4.151 005 ±0.000 274	4.150 981 ±0.000 286	4.150 950 ±0.000 318	4.150 984 ±0.000 392	4.150 959 ±0.000 615	4.150 776 ±0.001 584
1.75	4.151 199 ±0.000 263	4.151 024 ±0.000 274	4.150 995 ±0.000 286	4.150 958 ±0.000 318	4.150 988 ±0.000 392	4.150 961 ±0.000 615	4.150 776 ±0.001 584
2.00	4.151 235 ±0.000 263	4.151 042 ±0.000 274	4.151 008 ±0.000 286	4.150 967 ±0.000 318	4.150 993 ±0.000 392	4.150 963 ±0.000 615	4.150 777 ±0.001 584

Table 3. Comparison of autocorrelation-adjusted MLE analysis with 'blocking'/*t*-test analysis. Both analyses use the whole run minus the first 10^8 MC iterations and the last 2×10^8 iterations; both are one-parameter maximum-likelihood estimates of μ assuming $\gamma = \frac{43}{32}$. Error bars are 95% confidence intervals.

	$a_1 = 1.0$ $N_{\min} = 0$	$a_1 = 1.0$ $N_{\min} = 100$	$a_1 = 1.0$ $N_{\min} = 200$
Autocorrelation-adjusted MLE	4.151 100 ±0.000 267	4.150 941 ±0.000 319	4.150 980 ±0.000 396
'Blocking'/ <i>t</i> test	4.151 091 ±0.000 257	4.150 928 ±0.000 264	4.150 960 ±0.000 302

attributable to the differing biases of the full-run and block MLE (since bias $\sim 1/\text{sample size}$). For this reason we consider the central estimates based on full-run MLE to be more accurate (their bias is $< 0.000\ 002$ for all $N_{\min} \leq 200$). The two methods give nearly identical error bars for $N_{\min} = 0$, but for $N_{\min} = 100, 200$ the error bars based on the autocorrelation-adjusted MLE are significantly larger than those based on the *t* test. This can be explained as follows: as N_{\min} increases, fewer data points contribute (so the MLE theory error bars increase correspondingly); but this also means that the average spacing in time between contributing data points grows, so they are probably less strongly autocorrelated; if so, it is an overcorrection to multiply the MLE theory error bars by $(2\tau)^{1/2}$ with $\tau = 3 \times 10^5$. We conclude that the error bars based on the

autocorrelation-adjusted MLE (tables 1 and 2) are overly conservative†, and that those based on the t test are probably more accurate. Our final estimates are therefore

$$\mu = 4.150\,96 \pm 0.000\,10 \pm 0.000\,26 \quad (95\% \text{ confidence limits}) \quad (9a)$$

and

$$\mu = 4.150\,96 \pm 0.000\,20 \pm 0.000\,37 \quad (99\% \text{ confidence limits}). \quad (9b)$$

These estimates agree well with (but are slightly higher than) the series-extrapolation estimates; they have, however, larger error bars.

Finally, we remark on the theoretical justification of the 'flatness criterion' in the maximum-likelihood estimation of μ and/or γ . Suppose that the *true* asymptotic form of c_N is

$$c_N = \mu^N (N+3)^{\gamma-1} A [1 + a_1^{\text{true}}/(N+3) + O(N^{-\Delta})] \quad (10)$$

with $\Delta > 1$, but that we use the ansatz (4') to compute our maximum likelihood estimates. Then, if $a_1 \neq a_1^{\text{true}}$, our estimates of μ and γ will be afflicted by a systematic error of order $1/N_{\min}^2$ and $1/N_{\min}$, respectively (with amplitude proportional to $a_1 - a_1^{\text{true}}$); but if $a_1 = a_1^{\text{true}}$, then the systematic error will be of order $1/N_{\min}^{\Delta+1}$ and $1/N_{\min}^{\Delta}$, respectively. That is, the plot of $\hat{\mu}$ or $\hat{\gamma}$ against N_{\min} will be *asymptotically flatter* as $N_{\min} \rightarrow \infty$ if a_1 is chosen equal to the 'correct' value a_1^{true} . (If $\Delta < 1$, then the systematic error will be of order $1/N_{\min}^{\Delta+1}$ and $1/N_{\min}^{\Delta}$ no matter what value is chosen for a_1 ; that is, the flatness criterion does asymptotically no good at all, but neither does it do any harm.) In practice, of course, the flatness criterion is not applied asymptotically as $N_{\min} \rightarrow \infty$, but rather for some range of intermediate N_{\min} for which the statistical error is not too large. In that case the 'optimum' value of a_1 will be that 'effective' amplitude which best simulates the true *combination* of correction-to-scaling terms in that range of N_{\min} . We have tested the flatness criterion on a sample of 1.2×10^7 independent *ordinary* random walks of average length ≈ 100 , generated by simple sampling; the results point unerringly to the correct value $a_1^{\text{true}} = 0$.

In summary: assuming $\mu_H = (2 + \sqrt{2})^{1/2}$ and $\gamma = \frac{43}{32}$, our Monte Carlo data rule out the conjecture $\mu_T + \mu_H = 6$ at the greater than 99% confidence level. Instead, we find

$$\mu_T + \mu_H = 5.998\,72 \pm 0.000\,36 \quad (11)$$

as our 95% confidence bounds. Such coincidences do happen.

Acknowledgments

One of us (ADS) wishes to thank the Department of Mathematics, Statistics and Computer Science at the University of Newcastle for their gracious hospitality during two visits. This research was supported in part by ARGS grant B-8416060 and NSF grant DMS-8400955.

References

- Adler J 1983 *J. Phys. A: Math. Gen.* **16** L515
 Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (New York: Academic)

† This was also observed by Berretti and Sokal (1985), although they did not give any explanation for it.

- 1986 to be published
- Berretti A and Sokal A D 1985 *J. Stat. Phys.* **40** 483
- Brézin E, Le Guillou J-C and Zinn-Justin J 1976 *Phase Transitions and Critical Phenomena* vol 6, ed C Domb and M S Green (New York: Academic)
- Djordjevic Z V, Majid I, Stanley H E and dos Santos R J 1983 *J. Phys. A: Math. Gen.* **16** L519
- Grassberger P 1982 *Z. Phys. B* **48** 255
- Guttmann A J 1984 *J. Phys. A: Math. Gen.* **17** 455
- 1986a in preparation
- 1986b *Phase Transitions and Critical Phenomena* ed C Domb and J L Lebowitz (New York: Academic) to appear
- Guttmann A J, Ninham B W and Thompson C J 1968 *Phys. Rev.* **172** 554
- Guttmann A J and Sykes M F 1973 *Aust. J. Phys.* **26** 207
- Havlin S and Ben-Avraham D 1983 *Phys. Rev. A* **27** 2759
- Knuth D E 1981 *The Art of Computer Programming* vol 2, 2nd edn (Reading, MA: Addison-Wesley)
- Kremer K and Lyklema J W 1985 *Preprint*
- Le Guillou J-C and Zinn-Justin J 1980 *Phys. Rev. B* **21** 3976
- Majid I, Djordjevic Z V and Stanley H E 1983 *Phys. Rev. Lett.* **51** 143
- Nickel B G 1982 *Phase Transitions (1980 Cargèse lectures)* ed M Lévy, J-C Le Guillou and J Zinn-Justin (New York: Plenum)
- Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
- 1984 *J. Stat. Phys.* **34** 731
- Priestley M B 1981 *Spectral Analysis and Time Series* 2 vols (New York: Academic)
- Privman V 1984 *Physica* **123A** 428
- Rapaport D C 1985a *J. Phys. A: Math. Gen.* **18** L39
- 1985b *J. Phys. A: Math. Gen.* **18** L201
- Rehr J J, Joyce G J and Guttmann A J 1980 *J. Phys. A: Math. Gen.* **13** 1587
- Savit R 1980 *Rev. Mod. Phys.* **52** 453
- Silvey S D 1975 *Statistical Inference* (London: Chapman and Hall)
- Sykes M F and Essam J W 1964 *J. Math. Phys.* **5** 1117
- Syozi I 1972 *Phase Transitions and Critical Phenomna* vol 1, ed C Domb and M S Green (New York: Academic) p 270
- Watson P G 1974 *Physica* **75** 627
- Watts M G 1975 *J. Phys. A: Math. Gen.* **8** 61
- Wegner F J 1972 *Phys. Rev. B* **5** 4529
- Wierman J C 1981 *Adv. Appl. Prob.* **13** 298