On three-dimensional self-avoiding walks

1985 J. Phys. A: Math. Gen. 18 113

(http://iopscience.iop.org/0305-4470/18/1/023)

J. Phys. A: Math. Gen. 18 (1985) 113-126. Printed in Great Britain

On three-dimensional self-avoiding walks

D C Rapaport
Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

Received 11 June 1984, in final form 30 July 1984

Abstract. Long self-avoiding walks of up to 2400 steps have been generated on the SC and BCC lattices using an improved Monte Carlo technique. Analysis of the asymptotic length dependence of the end-to-end distance and radius of gyration of the walks leads to values in the range 0.591-0.593 for the critical exponent ν. The simple power-law dependence on length provides an excellent fit to the data over walk lengths between 120 and 2400 with fluctuations around the asymptotic results averaging to a mere 0.13%. Systematic deviations from asymptotic behaviour in short self-avoiding walks have also been examined using Monte Carlo generated walks ranging in length from 12 to 60; the results do not support the existence of the non-analytic correction predicted by the renormalisation group. In the light of this unexpected result, available series expansions for walks on the FCC lattice have been re-examined and previous claims to have observed non-analytic behaviour questioned; equal, if not better convergence of the extrapolated series can be obtained without resorting to non-analytic correction terms. Finally, an analysis has been made of the radius of gyration series to which several new terms have been added.

1. Introduction

The properties of self-avoiding walks (SAWS) on three-dimensional lattices have been studied extensively since it was realised that the SAW might serve as a useful model for the conformational properties of a polymer chain in dilute solution. Prior to the advent of the renormalisation group (RG), numerical results obtained through the use of exact enumeration and Monte Carlo techniques were interpreted as supporting the 'mean-field' result for the asymptotic form of the mean-square end-to-end distance of the SAW, namely

$$R_N^2 \sim AN^{2\nu}, \qquad \nu = \tfrac{3}{5} \tag{1.1}$$

where N denotes the number of steps and A is a constant (the subject is reviewed in McKenzie (1976). A similar result was found to apply to the mean-square radius of gyration as well (Rapaport 1975).

The SAW can also be regarded as the $n=0$ limit of the n-component vector spin model; RG analysis of this model yields the result $\nu = 0.588 \pm 0.001$ and firmly excludes the previously accepted estimate (Baker *et al* 1978, Le Guillou and Zinn-Justin 1980). The same RG analysis also makes a prediction of the leading-order correction term to (1.1)

$$R_N^2 \sim AN^{2\nu}(1 + A_1 N^{-\Delta_1} + A_2 N^{-1} + \mathrm{O}(N^{-1-\Delta_1})) \tag{1.2}$$

with $\Delta_1 = 0.47 \pm 0.03$. The significant feature of this result is that the correction term is non-analytic as $N \to \infty$. The next correction term (N^{-1}) has also been included for later use; prior to the RG result it would have constituted the leading correction to

(1.1). Evidence for the non-analytic correction term has been presented recently based on series and Monte Carlo analyses (Majid *et al* 1983, Havlin and Ben-Avraham 1983).

The asymptotic N-dependence of the number of SAWs of N steps, c_N, has also been extensively studied. Until recently the data were interpreted as having asymptotic behaviour

$$c_N \sim B\mu^N N^{\gamma-1}, \qquad \gamma = \tfrac{7}{6}, \tag{1.3}$$

where μ is the connective constant (or effective coordination number) of the lattice and B a constant (Sykes *et al* 1972). The RG, on the other hand, leads to the prediction

$$c_N \sim B\mu^N N^{\gamma-1}(1+B_1N^{-\Delta_1}+B_2N^{-1}+\mathrm{O}(N^{-1-\Delta_1})) \tag{1.4}$$

with $\gamma = 1.161 \pm 0.003$. Evidence in support of this result has been adduced from series analysis (McKenzie 1979).

The purpose of this paper is threefold. First, a new extensive Monte Carlo study of the three-dimensional SAW problem is described, with particular emphasis on those R_N^2 results which ought to shed light on the nature of the non-analytic corrections. We provide evidence that the exponent ν lies slightly above the RG prediction but distinctly below the old value; an analysis of the deviations from asymptotic behaviour does not support the existence of the RG-predicted non-analytic correction, but indicates an N^{-1} type deviation. Second, we reanalyse existing exact enumeration series for both c_N and R_N^2 on the FCC lattice and show that results of similar quality can be obtained both with and without the inclusion of the non-analytic correction term. A closer look at the behaviour of the correction terms at successive orders—an examination not included in the earlier work—provides a strong hint that the non-analytic corrections are not in fact present. Third, we describe an extension of the series for S_N^2 to $N = 12$ walks, the same length as for R_N^2; analysis yields an exponent estimate consistent with Monte Carlo but with a small discrepancy due to a lack of adequate convergence.

The layout of the paper is as follows. In § 2 we describe the Monte Carlo method and the predicted asymptotic behaviour of the conformational quantities R_N^2 and S_N^2; these results are based on the study of long SAWs. In § 3 attention is focused on shorter walks and the deviations from asymptotic behaviour are examined. Section 4 covers the revised analysis of the R_N^2 series expansion and the new S_N^2 results. The c_N series is reanalysed in § 5. The results are summarised in § 6 and the existence of similar problems in two dimensions discussed.

2. Monte Carlo analysis of asymptotic behaviour

There have been a number of attempts in the past to investigate the properties of SAWs using Monte Carlo (MC) methods (e.g., Gans 1965, McCrackin *et al* 1973; further references appear in McKenzie 1976), but, with only one exception (Havlin and Ben-Avraham 1983) which did not involve addressing the asymptotic behaviour directly, there have been no attempts to improve earlier exponent estimates (which leaned towards $\nu = \frac{3}{5}$) in the light of the RG predictions. In this paper we will show that the MC method is capable of producing extremely precise exponent estimates, free both from the need to rely on assumptions regarding the nature of the correction terms and from subjective estimates of error bounds. In this section we briefly describe the MC method and the earlier methods from which it was derived, and the results it produces for walks long enough to be well inside the asymptotic regime.

The goal of the MC method is to generate a sample of SAW conformations which is a representative (and hence unbiased) subset of the ensemble of all possible conformations; an average over the subset of a particular quantity should then be a reliable estimator for the ensemble average of that quantity. In principle, all that must be done is to randomly generate a batch of SAWs of the desired length and compute the necessary averages. The reason why this approach is unfeasible is that there is a serious problem of attrition; essentially all walks attempt to return to a previously visited lattice site after only a few steps, at which stage this simplest of MC approaches discards the entire walk and starts afresh.

In order to overcome the attrition problem the enrichment scheme was proposed (Wall *et al* 1963). With enrichment, when the self-avoidance condition is about to be violated the entire walk is not discarded as before, but only a specified number of the most recently added steps; the remaining portion of the walk is used as the basis for further attempts to complete the construction. The original approach employed step-by-step generation, dividing the walk into sections of s steps and using each newly added section exactly p times in a series of attempts to add sufficient steps to complete a further section. Failure resulted in deletion of the last complete section, and so on. The optimal values of the parameters p and s are functionally related (Wall *et al* 1963); the criteria used to select the values are to maximise the probability of successfully completing each SAW once started, and at the same time to ensure that no single initial section of the walk leads to a disproportionately large number of completed SAWs. The method is clearly unbiased and, if the above precaution observed, also statistically reliable.

The efficiency of the enrichment technique is enhanced if it is combined with the dimerisation technique of SAW generation. Dimerisation was proposed as an alternative method of reducing attrition (Alexandrowicz and Accad 1973) and involves constructing each SAW by randomly combining members of a previously generated selection of shorter SAWs (the term dimerisation reflects the fact that the walk length doubles at each construction stage).

The MC walk generation method used in the present work involves the following three stages. Using exact enumeration techniques a list of all possible short SAW elements of a given length (typically $N=6$) is prepared; this preliminary stage is included to make the second stage more efficient. The next stage is to generate a large batch of SAWs (typically 20 000) of specified intermediate length ($N=60$) by using the principle embodied in enrichment MC to link together randomly selected subsets of the SAW elements; the resulting SAWs are referrred to as segments. The final stage is the generation of SAWs of the desired length (a multiple of the segment length) by again using the enrichment technique, but this time applied to the set of segments. The effective size of the segment set is considerably enlarged by randomly permuting and reflecting the coordinates of each segment before attempting to join it with the previously linked segments. The number of SAWs generated from each segment batch depends on the walk length—the longer the walk the fewer the number of walks in order to maintain adequate sampling; the segment and SAW generation steps are repeated as many times as needed (up to 20) to produce the required number of SAWs. The enrichment parameters are determined empirically; as in the original application of the enrichment technique the two conflicting considerations are the improvement of the SAW completion rate while preventing any given initial element or segment from leading to too many completions.

The generated SAWs ranged in length from $N = 120$ to 2400 for both the SC and BCC lattices; sample sizes lay in the range 40–50 000. In comparison with previous MC work on SAWs, both the maximum walk length and sample size have been enlarged considerably; if the product of these two quantities is taken as a rough measure of the 'extent' of the calculation, then the present analysis is 20–30 times more extensive than its predecessors. The reasons for making the effort to maximise both these quantities are obvious; large N allows deeper probing into the asymptotic region and reduces the dependence of the behaviour on correction terms which are less readily analysed, whereas large sample sizes lead to improved statistics.

The squared end-to-end distance and radius of gyration were measured for each walk generated and the mean-squared averages R_N^2 and S_N^2 computed (each step of the walk is of unit length). The values are shown in table 1. The results were analysed by assuming the asymptotic N-dependence

$$R_N^2 \sim A_R N^{2\nu_R} \tag{2.1}$$

and carrying out a linear regression analysis of log R_N^2 against log N. The exponent ν_R, amplitude A_R and their associated errors are obtained from this computation (e.g., de Groot 1975). The results, as well as those obtained from a similar analysis of S_N^2 (exponent ν_S, amplitude A_s) are summarised in table 2. A preliminary report of the SC results has appeared elsewhere (Rapaport 1984a).

Table 1. Measured values of R_N^2 and S_N^2 and the relative deviations from the leading-order asymptotic predictions.

		R_N^2		S_N^2	
	N	mean	deviation	mean	deviation
	120	328.7	0.0022	52.01	0.0009
	300	968.3	−0.0021	153.99	−0.0010
SC	600	2200.8	−0.0016	351.10	0.0006
	1200	5008.9	0.0003	797.10	−0.0020
	2400	11 390.0	0.0013	1820.84	0.0015
	120	295.2	0.0001	46.89	−0.0010
	300	871.0	−0.0007	138.67	−0.0003
BCC	600	1977.4	−0.0001	315.28	0.0015
	1200	4494.0	0.0018	716.21	0.0024
	2400	10 164.5	−0.0012	1617.43	−0.0026

The degree of reproducibility of the R_N^2 and S_N^2 results of table 1 can be assessed by dividing the walk samples for each N into a number (here 8) of groups and computing the spread of the group means. In each case the spread was close to 1% of the overall mean, with an even smaller uncertainty (0.35%) in the overall mean value (this is in contrast with the broad end-to-end distance and radius of gyration distribution whose standard devitations amount to approximately 60% of the means). Table 1 also shows the relative deviations of the measured values from the predictions of the asymptotic formulae (e.g., (2.1))—the fit is extremely close with deviations in

Table 2. Exponent and amplitude estimates derived from SAWs of lengths 120 to 2400. (The deviations appearing in table 1 are based on estimates with more significant digits than appear here.)

	SC	BCC
ν_R	0.5919 ± 0.0004	0.5909 ± 0.0002
ν_S	0.5933 ± 0.0003	0.5912 ± 0.0004
A_R	1.134 ± 0.005	1.031 ± 0.003
A_S	0.1772 ± 0.0006	0.1633 ± 0.0008

the range 0.03–0.26% (overall average 0.13%); for this reason there is little to be gained by plotting the results.

The error estimates produced by the regresssion analysis (table 2) are of course incapable of including the effects of minute residual corrections which are too small to adversely affect the quality of the fit, but which, nevertheless, could be responsible for a slight shift in the exponent values. There is, however, no way of reliably estimating the contributions of terms of this kind. Table 2 shows that the exponents (ν_R and ν_S) lie between 0.5909 and 0.5933; assuming universality and the equality of ν_R and ν_S the estimate obtained by averaging the four values is

$$\nu = 0.592 \pm 0.002.$$

The value produced by numerical analysis of the appropriate RG perturbation expansion is $\nu = 0.588 \pm 0.001$ (Baker *et al* 1978, Le Guillou and Zinn-Justin 1980); the agreement is satisfactory (see also § 6). The results of series extrapolation will be described in § 4.

3. Monte Carlo analysis of scaling corrections

By considering shorter SAWs than those treated in the preceding section, it should be possible to determine the N-dependence of the deviations from asymptotic behaviour and whether or not the RG predictions are complied with. In this section we describe such a calculation for R_N^2 using the SC lattice.

Walks ranging in length from 12 to 60 (in increments of 6) were generated using a similar MC technique to that described above; because of the small N involved the walks were generated directly from the elements. Since the correction terms were expected to be comparatively small even at low N, much larger sample sizes are required in order to avoid the situation where the statistical uncertainty masked the deviation; for each length 2×10^5 SAWs were generated.

The relative deviations of the measured R_N^2 values from the predictions of the asymptotic result (2.1) are shown in figure 1. The error bars show the spread in values when the walks are divided into twenty groups and each analysed separately; for $N \gtrsim 50$ it is apparent that the deviations drop below the background of statistical 'noise'. The relative deviation is defined as

$$\delta R_N^2 = R_N^2(\text{measured})/R_N^2(\text{asymptotic}) - 1; \tag{3.1}$$

from (1.2) it is clear that the expected N-dependence is given by

$$\delta R_N^2 \sim A_1 N^{-\Delta_1} + A_2 N^{-1} + O(N^{-1-\Delta_1}). \tag{3.2}$$

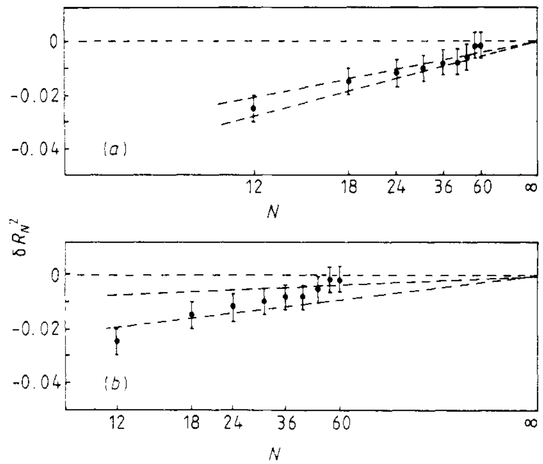

Figure 1. Relative deviations of R_N^2 for short SAWs on the SC lattice from the leading-order asymptotic prediction. The abscissa scales are (*a*) N^{-1}, (*b*) $N^{-0.47}$. The broken lines are visual guides and show the type of behaviour expected if the deviation is due principally to the leading correction terms (*a*) N^{-1} or (*b*) $N^{-0.47}$. The error bars show the average spread of sample means (0.7%).

Thus, if $\Delta_1 < 1$ (the RG prediction is $\Delta_1 = 0.47$, Le Guillou and Zinn-Justin 1980) a plot of δR_N^2 against $N^{-\Delta_1}$ should be approximately linear—although for sufficiently small N the N^{-1} term will also be apparent. If, on the other hand, the leading-order correction is analytic (i.e., proportional to N^{-1}), then linear behaviour ought to be seen when δR_N^2 is plotted against N^{-1}. In both cases $\delta R_N^2 \to 0$ as $N \to \infty$ (N^{-1} or $N^{-\Delta_1} \to 0$). The two possibilities are shown in figure 1; the evidence tends to favour a leading-order correction that is analytic.

It could be argued that since the correction coefficient A_1 is not predicted by the RG, the non-analytic correction may still be present but with small amplitude. The counter to this argument is contained in figure 1: the analytic N^{-1} correction fits the data to within 0.5% down to as low as $N = 12$ leaving little room for any meaningful contribution from the non-analytic term, and higher order (e.g., N^{-2}) corrections are available to account for any additional discrepancy as $N \to 0$. Quantitatively, the coefficient A_2 is estimated to be -0.32; if the $N^{-\Delta_1}$ term is introduced to help resolve the remaining discrepancy the value of the coefficient A_1 is restricted to $|A_1| < 0.01$. The alternative is to assume that the non-analytic term is able to account for the bulk of the deviation from the asymptotic result. In this case the value $A_1 \sim -0.06$ is obtained from the figure. This correction must also be applied to the results for the longer walks; for $N = 120$ it produces a shift of 0.6%, a value that is three times the deviation (in the wrong direction) of the measured value from the prediction of the leading-order asymptotic formula (2.1). In view of the apparent accuracy of the MC measurements (see below) and the known uncertainties, there is no way to account for the shift demanded by the non-analytic correction.

The accuracy of the MC method can be demonstrated by directly comparing the predictions with exact enumeration results for the SC lattice. For $N = 15$ the exact value of R_N^2 is 27.3931 ... (Martin and Watts 1971) which corresponds to the relative deviation $\delta R_N^2 = -0.021$. When the correction $A_2 N^{-1}$ is allowed for the deviation drops to a mere −0.003, a value easily attributable to a combination of higher-order corrections and statistical uncertainty.

These results should be contrasted with recent series expansion treatment of R_N^2 on the FCC lattice (Majid *et al* 1983). There it was argued that the inclusion of the non-analytic correction is essential to obtain agreement with the RG exponent result. In the following section we will show that by analysing the same data in various ways, both with and without the non-analytic correction, it is reasonable to conclude that the non-analytic term is not essential to achieve reasonable exponent estimates. At this stage it is also appropriate to comment on a recent MC study of the three-dimensional SAW that claimed to observe the $N^{-\Delta_1}$ correction term (Havlin and Ben-Avraham 1983). The quantity measured in that study was not R_N^2 itself, but the set of mean internal separations within the walk; the assumption of a length-invariant self-similarity (motivated by the concept of fractals—Mandelbrot 1982) was then used to derive a measure for ν. The analysis required the simultaneous determination of both exponent and correction term using data from relatively short SAWs ($N \leq 320$) and sites along each walk not more than $N/3$ steps apart, with the final choice being based on a visual goodness-of-fit criterion. Furthermore, it is apparent from the data that the self-similarity assumption is only an approximation, at least for the walk lengths considered. Thus, the evidence in support of the non-analytic correction term obtained by that analysis is judged inconclusive.

4. Series expansions for conformational data

Extrapolation of exact series expansion data provides an alternative means of probing SAW asymptotic behaviour (Domb 1969, McKenzie 1976). Prior to the appearance of the question of non-analytic corrections it was regarded as sufficient to use simple extrapolation techniques; these produced results not inconsistent with the then-accepted value $\nu = 0.600$, both for R_N^2 (Martin and Watts 1971) and S_N^2 (Rapaport 1975). With the appearance of the RG estimate for ν and the prediction of non-analytic corrections it became necessary to handle the extrapolation with greater care to reduce the possibility of ambiguity. The most recent result involves the computation of R_N^2 as far as $N = 12$ on the FCC lattice and an accompanying analysis which claimed to obtain complete agreement with the RG results, both in regard to the exponent value and the leading-order non-analytic correction (Majid *et al* 1983, hereinafter MDS).

In this section we present a detailed comparison of the results obtained when the FCC R_N^2 series data is analysed both with and without the non-analytic correction. As will become apparent from the results below, there is no compelling evidence in support of the presence of the non-analytic terms, hence the results are fully consistent with the MC analysis. We also describe a calculation extending the S_N^2 series to the same order as R_N^2 and the results of analysing this series.

The conformational data (R_N^2 and S_N^2) were generated by an improved version of a counting algorithm used in earlier work (Rapaport 1975). The results are shown in table 3. Comparison of the values of $c_N R_N^2$ (these are the actual quantities computed) for $N = 11$ and 12 with those of MDS reveals a discrepancy of a factor of two, although this is not reflected in their analysis. The values of S_N^2 for $N = 10$–12 are new. The amount of computation required for the evaluation of S_N^2 is double that for R_N^2; the total computer time used was, however, approximately equal to that of MDS (using a similar computer).

Table 3. Exact enumeration data for the FCC lattice (the step length is unity).

N	c_N	$c_N R_N^2$	$(N+1)^2 c_N S_N^2$
1	12	12	12
2	132	288	552
3	1404	4908	15 360
4	14 700	72 144	335 160
5	152 532	975 780	6312 084
6	1573 716	12 510 768	107 605 728
7	16 172 148	154 540 404	1706 716 656
8	165 697 044	1857 329 520	25 627 095 984
9	1693 773 924	21 857 390 724	368 595 744 612
10	17 281 929 564	252 974 192 304	5120 677 389 624
11	176 064 704 412	2888 610 412 956	69 133 013 891 808
12	1791 455 071 068	32 617 398 861 792	911 241 070 490 664

In order to decide the form of the correction terms and estimate their sizes the data was analysed by computing

$$t_N = \tfrac{1}{2}N(R_N^2/R_{N-1}^2 - 1) \tag{4.1}$$

and then using sets of consecutive t_N values to fit various versions of the general asymptotic expression which follows from (1.2), namely

$$t_N \sim \nu(1 + e_1 N^{-\Delta_1} + f_1 N^{-1} + e_2 N^{-1-\Delta_1} + f_2 N^{-1} + O(N^{-2-\Delta_1})). \tag{4.2}$$

(S_N^2 will be discussed later.) If only integer powers of N^{-1} are present (i.e., no non-analytic terms) then truncation of (4.2) at N^{-k} produces exponent results identical to the kth order Neville table (Gaunt and Guttmann 1974), which itself is equivalent to kth-order polynomial extrapolation in the variable N^{-1}. The number of t_N values required for each calculation of the unkowns in (4.2) depends on the number of correction terms included (Δ_1, if present, is assumed known to avoid the need to solve a nonlinear problem). Due to the limited amount of data available and the observed lack of smooth behaviour if too many terms are included in (4.2), the coefficient e_2 is set to zero and the comparison is between the results obtained with and without the $N^{-\Delta_1}$ term. The value $\Delta_1 = 0.465$ is used when required (this is based on the estimate $\Delta_1 = 0.465 \pm 0.010$ given by Le Guillou and Zinn-Justin 1977 and is used for consistency with the analysis in the next section, the latest value is $\Delta_1 = 0.470 \pm 0.025$—Le Guillou and Zinn-Justin 1980; this minor adjustment has little effect on the analysis).

The coefficients of (4.2) obtained from each of the fits are listed in table 4. Case (a) involves the $N^{-\Delta_1}$ correction only; the convergence is poor but is improved considerably if, as in case (b), the N^{-1} term is included as well. In (b), the value of e_1 is an order of magnitude smaller than f_1 and still falling rapidly at the last available estimate. This behaviour suggests that an attempt is being made to suppress the $N^{-\Delta_1}$ term and that the coefficient e_1 eventually tends to zero. Support for this assertion comes from considering cases (c) and (d) where only analytic corrections to orders N^{-1} and N^{-2} are included; here the estimates of ν are further along the path to convergence than in case (b). These results clearly show that there is no need to include non-analytic corrections in order to obtain a ν estimate in reasonable agreement with that of the MC analysis (or RG); however, in order to examine the quantitative

Table 4. Coefficients of R_N^2 fit using equation (4.2); coefficients not listed are set to zero.

	n	ν	e_1	f_1	f_2
(a)	6	0.381 97	2.084 72		
	7	0.424 73	1.643 21		
	8	0.456 32	1.358 36		
	9	0.478 00	1.177 52		
	10	0.493 60	1.052 47		
	11	0.505 42	0.959 68		
	12	0.514 65	0.887 74		
(b)	7	0.658 09	−0.521 04	1.997 22	
	8	0.660 50	−0.535 39	2.010 46	
	9	0.639 85	−0.398 83	1.865 49	
	10	0.625 81	−0.294 38	1.741 87	
	11	0.617 34	−0.225 38	1.652 64	
	12	0.611 39	−0.173 31	1.580 03	
(c)	6	0.574 98		1.597 86	
	7	0.581 21		1.516 39	
	8	0.586 33		1.442 07	
	9	0.589 36		1.393 50	
	10	0.591 20		1.361 15	
	11	0.592 39		1.338 33	
	12	0.593 18		1.321 94	
(d)	7	0.596 79		1.137 41	1.096 50
	8	0.601 68		1.022 62	1.428 60
	9	0.599 97		1.068 18	1.273 43
	10	0.598 56		1.110 80	1.106 63
	11	0.597 75		1.138 20	0.985 47
	12	0.597 12		1.161 51	0.870 73

behaviour more closely it is necessary to consider extrapolations of higher order than those of table 4.

A concise summary of the exponent estimates for various orders of extrapolation is available directly from the Neville table. Following the recommendations of MDS, several different functions of R_N^2, all of which extrapolate to ν as $N \to \infty$, were used to imbue the results with greater confidence. The functions used were those chosen by MDS, with ρ_N denoting R_N^2:

$$\begin{aligned} u_N^{(a)} &= \tfrac{1}{2}N(\rho_{N+1}/\rho_N - 1) \\ u_N^{(b)} &= \tfrac{1}{2}\ln(\rho_N/\rho_{N-1})/\ln(N/N-1) \\ u_N^{(c)} &= \tfrac{1}{2}(\rho_{N+1}-\rho_N)(\rho_N-\rho_{N-1})/(\rho_N^2-\rho_{N+1}\rho_{N-1}). \end{aligned} \tag{4.3}$$

Note that $u_N^{(a)}$ differs from t_N (4.1) by a shift of index; while this shift affects the lower-order extrapolations, it has negligible effect at higher order.

The Neville table results appear in table 5; the $k=0$ column gives the actual function values. The functions $u_N^{(a)}$ and $u_N^{(b)}$ show small amounts of curvature at all orders of extrapolation, whereas $u_N^{(c)}$ does not vary smoothly at higher order. If allowance is made for the residual drift then the exponent estimates are again seen to be fully consistent with those of the MC calculation.

Table 5. Neville tables for the three formulae (4.3) for estimating the exponent ν from R_N^2; k is the order of extrapolation.

	$n\backslash k$	0	1	2	3	4
(a)	6	0.606 10	0.602 85	0.596 87		
	7	0.605 52	0.602 01	0.599 92	0.603 99	
	8	0.604 99	0.601 30	0.599 14	0.597 85	0.591 71
	9	0.604 50	0.600 63	0.598 29	0.596 57	0.594 98
	10	0.604 06	0.600 04	0.597 71	0.596 38	0.596 08
	11	0.603 65	0.599 53	0.597 22	0.595 90	0.595 07
(b)	7	0.596 87	0.602 74	0.594 89		
	8	0.597 50	0.601 89	0.599 35	0.606 78	
	9	0.597 90	0.601 16	0.598 59	0.597 07	0.584 93
	10	0.598 17	0.600 54	0.598 04	0.596 76	0.596 30
	11	0.598 33	0.599 95	0.597 31	0.595 38	0.592 96
	12	0.598 42	0.599 40	0.596 63	0.594 57	0.592 94
(c)	7	0.602 04	0.597 04	0.619 55		
	8	0.601 32	0.596 32	0.594 16	0.551 84	
	9	0.600 65	0.595 32	0.591 85	0.587 23	0.631 46
	10	0.600 07	0.594 85	0.592 93	0.595 44	0.607 77
	11	0.599 56	0.594 44	0.592 61	0.591 75	0.595 28

The earlier analysis of MDS followed a somewhat different approach in which low-order extrapolants are themselves extrapolated; however the final estimate of ν was obtained by passing an arbitrarily chosen curve through the second set of extrapolants (see MDS, figure 1(c)). The final estimate was given as $\nu = 0.5875 \pm 0.0015$, although it is clear from the analysis that a considerable degree of subjectivity was involved in arriving at both the exponent value and the error bound. (Note also that although MDS claimed at one stage to have analysed the radius of gyration, their data is for end-to-end distances only.)

The MC data for S_N^2 was analysed in a similar manner. The results of the Neville table analysis based on the functions (4.3) appear in table 6. The exponent values here are slightly higher than those for R_N^2 (table 5), but it is clear that the incomplete convergence leaves room for a further drop in ν at larger values of N, thereby bringing the results into agreement with the MC exponents. The reduced rate of convergence of S_N^2 relative to R_N^2 is due to the fact that S_N^2 includes contributions from all possible distances between pairs of sites visited by the walk whereas R_N^2 is based only on the endpoint separation; the MC results for larger N show a similar degree of convergence for both quantities.

5. Analysis of SAW counts

The results described in the preceding sections have provided no convincing evidence in favour of the existence of non-analytic corrections to scaling and, in fact, suggest that the contrary may be true. As pointed out in the introduction the same kind of non-analytic correction is also predicted to occur in the asymptotic behaviour of the number of N-step SAWs (1.4). The values of c_N are available as far as $N = 14$ for the FCC lattice and their analysis has been used to establish the existence of the non-analytic

Table 6. Neville tables (see table 5) for S_N^2.

	$n \backslash k$	0	1	2	3
(a)	7	0.552 79	0.599 23	0.607 78	
	8	0.558 85	0.601 28	0.607 41	0.606 79
	9	0.563 69	0.602 45	0.606 56	0.604 87
	10	0.567 64	0.603 12	0.605 78	0.603 95
	11	0.570 89	0.603 47	0.605 05	0.603 12
(b)	8	0.549 09	0.602 37	0.609 23	
	9	0.555 16	0.603 65	0.608 10	0.605 85
	10	0.560 07	0.604 33	0.607 08	0.604 71
	11	0.564 12	0.604 61	0.605 88	0.602 65
	12	0.567 50	0.604 64	0.604 79	0.601 54
(c)	8	0.605 31	0.612 51	0.599 75	
	9	0.605 70	0.608 85	0.596 04	0.588 64
	10	0.605 77	0.606 35	0.596 34	0.597 01
	11	0.605 65	0.604 51	0.596 23	0.595 96

term (McKenzie 1979). In this section we repeat the analysis and show that results of equal, or even better quality can be obtained if the non-analytic correction is omitted.

The correction terms appearing in (1.4) are studied by forming the ratios

$$r_N = c_N / c_{N-1} \tag{5.1}$$

and fitting various versions of the general asymptotic expression based on (1.4), namely

$$r_N \sim \mu(1 + a_1 N^{-1} + b_1 N^{-1-\Delta_1} + a_2 N^{-2} + b_2 N^{-2-\Delta_1} + a_3 N^{-3} + \mathrm{O}(N^{-3-\Delta_1})), \tag{5.2}$$

to sets of consecutive r_N. Here $a_1 = \gamma - 1$. This is the same technique used in the original analysis (McKenzie 1979); but by looking at the results from a different perspective we will show that the original conclusions are not the only ones possible.

Table 7 summarises the results of the fit calculation. The value $\Delta_1 = 0.465$ is used and, because of the impossibility of handling too many unknowns, $b_2 = 0$. Case (a) shows the results obtained when only the N^{-1} and $N^{-1-\Delta_1}$ terms are included. When, as shown in case (b) the N^{-2} term is introduced as well, the value of b_1 drops by a factor of 30, and the last few estimates strongly suggest that $b_1 \to 0$. This phenomenon was also observed for R_N^2 (§ 4) and was interpreted as a sign that the data is attempting to suppress the non-analytic term; a similar conclusion is warranted for the SAW count series data as well. Cases (c) and (d) show the corresponding results when only analytic corrections to orders N^{-2} and N^{-3} are included; here an increase in the order of the fit functions leads to only a minor adjustment in coefficient values, quite unlike cases (a) and (b).

Estimates of μ and $\gamma(=a_1+1)$ obtained from cases (c) and (d) are 10.0364 and 1.163 respectively. The uncertainty inherent in these values can be gauged only by examining the trends in the tabulated results and the amount of additional variation possible before full convergence is achieved. Estimates of this kind are highly subjective and amount to little more than educated guesses; a reasonable error estimate in the present case is ± 1 in the last digit of both μ and γ. The RG estimates for γ are 1.161 ± 0.003 (Baker *et al* 1978) and 1.1615 ± 0.0020 (Le Guillou and Zinn-Justin 1980).

Table 7. Coefficients of c_N fit using equation (5.2); unlisted coefficients are zero.

	n	μ	a_1	b_1	a_2	a_3
(a)	7	10.063 68	0.104 47	0.107 51		
	8	10.034 38	0.164 50	0.010 71		
	9	10.035 51	0.161 82	0.015 34		
	10	10.036 89	0.158 12	0.022 12		
	11	10.037 08	0.157 56	0.023 20		
	12	10.037 16	0.157 31	0.023 70		
	13	10.037 07	0.157 64	0.023 00		
	14	10.036 98	0.157 97	0.022 29		
(b)	8	9.954 59	0.518 46	−1.097 27	1.062 60	
	9	10.039 17	0.143 45	0.076 60	−0.063 20	
	10	10.042 04	0.129 02	0.124 73	−0.112 84	
	11	10.037 87	0.152 58	0.041 67	−0.021 50	
	12	10.037 51	0.154 88	0.033 13	−0.011 55	
	13	10.036 59	0.161 24	0.008 48	0.018 60	
	14	10.036 51	0.161 81	0.006 16	0.021 63	
(c)	7	10.053 85	0.141 41		0.094 82	
	8	10.033 61	0.167 93		0.010 27	
	9	10.034 60	0.166 42		0.015 82	
	10	10.035 79	0.164 39		0.024 33	
	11	10.036 09	0.163 82		0.027 02	
	12	10.036 27	0.163 43		0.029 05	
	13	10.036 31	0.163 34		0.029 55	
	14	10.036 33	0.163 28		0.029 90	
(d)	8	9.999 86	0.239 35		0.482 32	1.133 71
	9	10.036 59	0.161 63		0.053 70	−0.099 95
	10	10.038 55	0.156 91		0.091 00	−0.198 40
	11	10.036 89	0.161 42		0.050 85	−0.078 92
	12	10.036 83	0.161 59		0.049 17	−0.073 37
	13	10.036 44	0.162 88		0.034 99	−0.021 65
	14	10.036 41	0.162 96		0.034 05	−0.017 91

The present estimate is in full agreement with these values, while at the same time apparently excluding the pre-RG value of $\gamma = \frac{7}{6}$ (Sykes *et al* 1972).

Whereas the values of μ and γ just obtained are unbiased, in the sense that both were deduced from the SAW data without assuming anything beyond the presence of analytical correction terms, the results of McKenzie (1979) are biased and were derived by selecting a value of γ and then computing μ. The task of picking the 'best' value of γ involves the subjective comparison of the degree of convergence of the μ-estimates for different γ. The value of γ deemed best was chosen because it produced three final estimates of μ which are practically equal. That this is not a particularly reliable criterion can be seen by repeating the biased analysis but with non-analytic terms to order $N^{-2-\Delta_1}$ included rather than the $N^{-1-\Delta_1}$ term alone; in this instance stationarity is observed for $\gamma = 1.1667$ (the previously accepted value). Clearly the safest form of analysis relies on unbiased estimates only.

Another lesson to be learned from this analysis is that it is not sufficient to monitor μ by itself; both the variation of the coefficients of the correction terms with N and the effect of changing the order of the fit are important indicators as to what is really occurring. The numerical results that reveal the suppression of the leading-order non-analytic term for both c_N and R_N^2 provide a good example of what can be learned from the behaviour of the correction terms.

6. Conclusions

Monte Carlo simulations of three-dimensional self-avoiding walks have shown that the results are represented extremely closely (to within 2-3 parts per 1000) by the simple power law expressions

$$R_N^2 \sim A_R N^{2\nu_R}, \qquad S_N^2 \sim A_S N^{2\nu_S}$$

with $\nu_R = \nu_S = 0.592 \pm 0.002$. These results were obtained by considering walks ranging in length from $N = 120$ to 2400 on both the SC and BCC lattices. When the analysis of R_N^2 on the SC lattice was extended down as far as $N = 12$ it was found that the relative deviation from the simple power law could be closely represented by a term linear in N^{-1}. The exponent estimate is consistent with the value derived from the RG treatment, but the linear deviation at small N is not—the RG predicts a leading order $N^{-0.47}$ deviation.

This discrepancy motivated a reanalysis of previous estimates of asymptotic SAW behaviour based on series extrapolations which claimed to observe the non-analytic corrections required by the RG. The revised extrapolations, both for the SAW counts and for R_N^2, produced exponent estimates which are, respectively, in close agreement with the RG value of γ and consistent with the MC value of ν. These results were obtained without resorting to non-analytic corrections. The overall conclusion regarding the series extrapolation method is that it is unable to make a definitive statement either for or against the existence of non-analytic terms; a stricter criterion, namely the requirement that the data behave in a regular fashion under successive orders of approximation, favours the absence of non-analytic correction terms.

At this juncture it is appropriate to recall the fact that the RG addresses a continuum model; while it is reasonable to expect that universality applies to the leading-order exponents, there is no guarantee that the discrete lattice in which the SAW is embedded has no effect on the correction terms. The actual numerical exponent estimates derived by RG methods are themselves subject to problems of accuracy and convergence, and caveats have been issued by those responsible for the results (Le Guillou and Zinn-Justin 1980, Nickel 1982). Finally, RG does not predict the amplitudes of the non-analytic corrections; if they turn out to be sufficiently small they will not be observable in the kinds of calculation described here.

A similar situation has arisen for the two-dimensional SAW. The exponent ν has been shown (by a plausible but non-rigorous argument) to have the value $\frac{3}{4}$ (Nienhuis 1982). The RG prediction is $\nu = 0.77$ (no error bounds were given) and a correction term $N^{-\Delta_1}$ with $\Delta_1 = 1.2$ (Le Guillou and Zinn-Justin 1980). Recent MC analysis using the self-similarity idea (as discussed in § 3) yielded $\nu = 0.753 \pm 0.004$ and $\Delta_1 = 1.2 \pm 0.1$ (Havlin and Ben-Avraham 1983). Series extrapolation of R_N^2 on the triangular lattice (Djordjevic *et al* 1983, see also Privman 1984) gave the results $\nu = 0.750$ and $\Delta_1 = 0.66 \pm 0.07$, a correction exponent far removed from the RG result. Analysis of the SAW counts (Guttmann 1984) failed to find any evidence in support of a value of Δ_1 significantly below unity (see, however, Adler (1983) for an alternative point of view).

Finally, an MC study similar to that of the present article yielded $\nu = 0.7488 \pm 0.0009$ for R_N^2 on the triangular lattice, and the same apparent absence of non-analytic correction terms observed in three dimensions (Rapaport 1985). It is difficult to envisage a situation in which the leading-order correction has an exponent $\Delta_1 > 1$; while not completely impossible it is reasonable to expect that, if no non-analytic term with $\Delta_1 < 1$ is present, then the leading-order correction will be the analytic term N^{-1}. A term of this kind may be invisible to the RG since the correction to scaling exponent originates in the singular part of the free energy (Wegner 1972), whereas the N^{-1} correction could arise from the analytic parts of the generating functions whose coefficients are the numbers c_N and $c_N R_N^2$ (namely the susceptibility and second spherical moment series of the SAW). Why no such N^{-1} term was observed in the earlier MC study (Havlin and Ben-Avraham 1983) is not clear.

The close agreement between the exponent estimate obtained when the present MC technique is applied to the two-dimensional problem and the theoretical value $\nu = \frac{3}{4}$ provides additional evidence in support of the accuracy claimed for the MC method. Finally, a similar study in four dimensions (Rapaport 1984) clearly reveals the presence of logarithmic corrections consistent with the RG prediction.

References

Adler J 1983 *J. Phys. A: Math. Gen.* **16** L515
Alexandrowicz Z and Accad Y 1973 *Macromolecules* **6** 251
Baker G A, Nickel B G and Meiron D I 1978 *Phys. Rev.* B **17** 1365
de Groot M H 1975 *Probability and statistics* (Reading: Addison-Wesley)
Djordjevic Z V, Majid I, Stanley H E and dos Santos R J 1983 *J. Phys. A: Math. Gen.* **16** L519
Domb C 1969 *Adv. Chem. Phys.* **15** 229
Gans P J 1965 *J. Chem. Phys.* **42** 4159
Gaunt D S and Guttmann A J 1974 in *Phase transitions and critical phenomena* vol 3, ed C Domb and M S Green (London: Academic)
Gutmann A J 1984 *J. Phys. A: Math. Gen.* **17** 455
Havlin S and Ben-Avraham D 1983 *Phys. Rev.* A **27** 2759
Le Guillou J C and Zinn-Justin J 1977 *Phys. Rev. Lett.* **39** 95
—— 1980 *Phys. Rev.* B **21** 3976
Majid I, Djordjevic Z V and Stanley H E 1983 *Phys. Rev. Lett.* **51** 1282
Mandelbrot B B 1982 *The fractal geometry of nature* (San Francisco: Freeman)
Martin J L and Watts M G 1971 *J. Phys. A: Math. Gen.* **4** 456
McCrackin F L, Mazur J and Guttman C M 1973 *Macromolecules* **6** 859
McKenzie D S 1976 *Phys. Rep.* **27** 35
McKenzie S 1979 *J. Phys. A: Math. Gen.* **12** L267
Nickel B G 1982 in *Phase transitions: Cargèse 1980* ed M Lévy, J C Le Guillou and J Zinn-Justin (New York: Plenum)
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
Privman V 1984 *Physica* **123A** 428
Rapaport D C 1975 *J. Phys. A: Math. Gen.* **8** 1328
—— 1984 *Phys. Rev.* B **30** 2906
—— 1985 *J. Phys. A: Math. Gen.* to be published
Sykes M F, Guttmann A J, Watts M G and Roberts P D 1972 *J. Phys. A: Math. Gen.* **5** 653
Wall F T, Windwer S and Gans P J 1963 in *Methods in Computation Physics* vol 1 (New York: Academic)
Wegner F J 1972 *Phys. Rev.* B **5** 4529