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LETTER TO THE EDITOR

End-to-end distance of linear polymers in two dimensions: a reassessment

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Abstract. Recent exact enumeration studies of the two-dimensional self-avoiding walk have produced evidence in support of non-analytic scaling corrections. Newly extended series for the triangular and square lattices (to $N = 19$ and 25 respectively) are examined in the light of recent Monte Carlo results suggesting the absence of corrections of this type. Using a modified approach to series analysis, it is concluded that the end-to-end distance can best be understood in terms of analytic corrections alone; in view of the lack of theoretical support there is little reason to introduce additional kinds of correction in attempting to explain the data.

In a recent letter (Rapaport 1985a) we described the results of a Monte Carlo (MC) study of the self-avoiding walk (SAW) on the triangular and square lattices. In addition to providing improved estimates for the dominant asymptotic behaviour of the mean-square end-to-end distance, R_N^2, whose N dependence is given by $R_N^2 \sim AN^{2\nu}$ (N is the number of steps), the results also suggested that the leading-order correction was of the form $N^{2\nu-\Delta}$ with $\Delta = 1$, rather than $\Delta \approx \frac{2}{3}$ as had been reported previously on the basis of series analysis (Djordjevic *et al* 1983, Privman 1984).

In this letter we describe the results obtained by analysing newly extended series for both the triangular (TRI) and square (SQ) lattices; the analysis involves the use of the dominant asymptotic behaviour as predicted by MC, augmented by correction terms that are 'analytic' in nature (i.e., $\Delta = 1, 2, \ldots$). We show that the quality of the fit of the asymptotic expression thus constructed to the exact series data leaves little doubt that, if evidence of correction terms other than of the type included here is to be obtained, it will have to originate from a source other than series analysis. A corresponding absence of non-analytic corrections in the case of the two-dimensional SAW generating function (i.e., the number of walks) was discussed by Guttmann (1984). The situation in three dimensions is also very similar (Rapaport 1985b).

The art and science of numerically extracting the asymptotic behaviour of a function from the early terms of its Taylor expansion has had a comparatively long and fruitful history (Gaunt and Guttmann 1974), and to it are due many of the results that paved the way to the modern theory of critical phenomena (Domb and Green 1972). There is almost certainly a limit, however, to the amount of information that can be gleaned from a series of limited length which, after all, gives only a restricted view of the singularities lying at and beyond the circle of convergence. This is particularly true in view of the highly subjective nature of series analysis; while the various kinds of extrapolation techniques provide sets of numerical estimates for some quantity (e.g., a critical exponent), they are limited in regard to the certainty with which they are able to state that the values are converging to a particular limit, or whether one set of extrapolants is converging faster than another. The three-dimensional SAW provides a good example of this problem (Rapaport 1985b).

Numerical estimation of the exponent ν for walks on the TRI lattice of lengths up to 14 (Martin and Watts 1971) and 16 (Grassberger 1982) led to values 0.744 and 0.746 respectively. With the appearance of a plausible, but non-rigorous, theoretical argument in support of $\nu = \frac{3}{4}$ (Nienhuis 1982), a result difficult to exclude from existing numerical work despite the accuracy claimed, interest turned to the analysis of higher-order corrections to scaling. The fact that a renormalisation-group (RG) treatment (Le Guillou and Zinn-Justin 1980) had produced a non-analytic correction exponent led to a relaxation of the constraint to analytic corrections only, and a recent analysis of the series, by then extended to 18 terms (Djordjevic *et al* 1983), yielded a correction exponent $\Delta \approx \frac{2}{3}$. This value is close to half that predicted by RG namely 1.2, although the latter is of questionable accuracy (Djordjevic *et al* 1983). At the same time, an independent analysis (Privman 1984) using a different approach (see below, however) based on just 16 terms reached essentially the same conclusion.

Though the two calculations are ostensibly dissimilar they are in fact based on a common assumption, and it is this which is responsible for the near identity of their conclusions. Both assume that it suffices to consider the leading-order correction term only and ignore the rest, even though higher-order terms are likely to be significant; the exact R_N^2 are then used to determine the unknowns in the functional form $AN^{2\nu}(1 + b/N^{\Delta})$, either by looking for that value of Δ for which various ratio plots appear most linear on a log-log scale (Djordjevic *et al* 1983), or by requiring that a certain function of the R_N^2 show the least N-dependence (Privman 1984). Both obtain estimates of Δ less than unity, but neither attempts to explore the effect of including the leading-order analytic correction ($N^{2\nu-1}$). In view of the limited length of the series and the extreme unlikelihood of other correction terms not contributing significantly, one is forced to conclude that both calculations are merely searches for that single correction term $N^{-\Delta}$ which best mimics an unknown function of N for N small (the simplest such function is of course an asymptotic expansion in integer powers of N^{-1}), with no assurance that the correct limiting behaviour has been captured.

The new terms that have been added to the series are listed in table 1. The $N = 19$ values for the TRI lattice are one beyond those given by Djordjevic *et al* (1983); the $N = 23$–25 terms for the SQ lattice are an extension of the series most recently extended by Grassberger (1982). Calculation of the final terms for the two lattices required 216 and 29 hours respectively on the IBM 3081 computer; it appears likely that the limits

Table 1. Extended exact enumeration data for self-avoiding walks on triangular and square lattices (c_N denotes the walk counts).

	N	c_N	$c_N R_N^2$
TRI			
	19	1851 231 376 374	113 279 031 925 422
SQ			
	23	17 266 613 812	1526 445 330 900
	24	46 146 397 316	4347 038 392 480
	25	123 481 354 908	12 341 626 847 324

of the majority of present day computers are about to be reached (especially for the TRI lattice), although the development of a special-purpose processor may merit consideration given the simplicity of the underlying calculations.

The R_N^2 series were subjected to standard extrapolation tests along the lines of the analysis carried out for the three-dimensional problem (Rapaport 1985b) and a similar conclusion reached, namely that merely on the basis of this kind of numerical analysis it is impossible to establish whether or not non-analytic corrections are present. In the case of the SQ lattice there is the additional complication of odd–even oscillations (Watts 1974). These results will not be described here in further detail; suffice it to state that the ν estimates obtained (assuming analytic corrections) were 0.748 (TRI) and 0.749 (SQ), values entirely consistent with the exact $\nu = \frac{3}{4}$, and in disagreement with Grassberger (1982) who excludes this value for both lattices.

The alternative approach to analysing these particular series takes as its starting point the dominant asymptotic behaviour deduced from MC simulations of very long SAWS (Rapaport 1985a). The walks generated ranged in length up to 2400 steps; a simple least-squares fit to the data yielded $\nu = 0.7488$ (TRI) and 0.7479 (SQ), while a biased fit assuming $\nu = \frac{3}{4}$ results in amplitude estimates $A = 0.7145 \pm 0.0036$ (TRI) and 0.7739 ± 0.0048 (SQ). These amplitudes are used as inputs to the present series analysis to allow attention to focus on the correction terms.

The form of the correction is restricted to a second-degree polynomial in $1/N$, so that the full asymptotic expression is

$$R_N^2 \sim AN^{2\nu}[1 + a_1/N + a_2/N^2 + O(N^{-3})]. \tag{1}$$

This form (A and ν are assumed known) can be fitted to any set of R_N^2 values by means of standard least-squares methods. Given the total absence of any *a priori* knowledge concerning the form of the correction terms, it is the quality of the fit which must establish whether (1) is justified. If, as will turn out to be the case, a close fit is obtained, then there is little reason to accept an alternative expression that is capable only of a lower quality fit, unless it is accompanied by convincing theoretical support. Note that (1) applies to the TRI lattice; the oscillatory component of R_N^2 for the SQ lattice requires that odd and even terms be fitted separately.

The fits were carried out for sequences of K values of R_N^2, consecutive for the TRI lattice and alternate for the SQ, with $K \geq 3$ (the actual quantity involved in the fit is $N^2(R_N^2/AR^{2\nu} - 1)$). The fit quality is based on the relative deviation of (1) from the known R_N^2, including smaller N values not used for the fit. Typical results appear in tables 2 and 3 from which it is clear that the deviations can be made extremely small. By way of contrast the corresponding deviations of Djordjevic *et al* (1983), in which the amplitude A is also an adjustable parameter, are some three orders of magnitude greater.

Figure 1 shows the variation of the fitted correction amplitudes, a_1 and a_2, for the TRI lattice (the SQ is similar). Each curve corresponds to a different maximum N, the individual points to different numbers of data values (K) involved in the fit. The estimates of a_1 and a_2, the latter in particular, have yet to settle down, although a hint of imminent convergence is contained in the fact that the spacing of successive points drops as N increases or K decreases. The comparatively slow convergence also reflects a danger inherent in any biased analysis, namely that an error in the assumed A must be compensated for by the correction terms; in view of the fact that a_1 and a_2 are weighted by factors of N^{-1} and N^{-2}, a given relative error in A (the MC value is close to 0.5%) will produce errors in the correction amplitudes that are typically amplified

Table 2. Relative differences between the exact TRI lattice R_N^2 and the asymptotic form (1), where a_1 and a_2 are derived from a fit to the final K values. (Some of the deviations are so small that additional significant digits beyond those given for a_1 and a_2 are required to reproduce the results.)

N \ K	3	5	7
13	3.2×10^{-4}	2.1×10^{-4}	7.6×10^{-5}
14	1.6×10^{-4}	8.1×10^{-5}	-5.3×10^{-6}
15	7.0×10^{-5}	1.8×10^{-5}	-3.6×10^{-5}
16	2.3×10^{-5}	-8.8×10^{-6}	-3.7×10^{-5}
17	1.7×10^{-6}	-1.3×10^{-5}	-2.1×10^{-5}
18	-3.1×10^{-6}	-4.9×10^{-6}	2.8×10^{-6}
19	1.4×10^{-6}	1.0×10^{-5}	3.0×10^{-5}
a_1	0.761 34	0.757 62	0.752 76
a_2	−2.1613	−2.0937	−2.0089

Table 3. Relative differences (as in table 2) for SQ lattice. The odd and even terms of the series are fitted separately.

N \ K	3	4	5
16	1.1×10^{-4}	7.8×10^{-5}	3.1×10^{-5}
17	7.4×10^{-5}	5.3×10^{-5}	2.1×10^{-5}
18	2.7×10^{-5}	8.1×10^{-6}	-1.7×10^{-5}
19	1.7×10^{-5}	5.0×10^{-6}	-1.2×10^{-5}
20	1.2×10^{-6}	-7.6×10^{-6}	-1.8×10^{-5}
21	5.5×10^{-7}	-4.9×10^{-6}	-1.2×10^{-5}
22	-1.9×10^{-6}	-3.7×10^{-6}	-3.7×10^{-6}
23	-9.2×10^{-7}	-2.1×10^{-6}	-2.1×10^{-6}
24	8.1×10^{-7}	3.8×10^{-6}	1.1×10^{-5}
25	3.9×10^{-7}	2.3×10^{-6}	7.3×10^{-6}
a_∞(even)	0.951 81	0.950 50	0.948 50
a_1(odd)	0.948 89	0.947 98	0.946 43
a_2(even)	−2.5279	−2.4982	−2.4541
a_2(odd)	−2.9846	−2.9631	−2.9276

by the inverses of these factors. There is indeed no way that the correction terms can converge properly if A is incorrect. It should also be remembered that (1) is a truncated asymptotic expansion and there is therefore a lower limit to N for which it produces results of a specified accuracy; for this reason too the values of a_1 and a_2 might be expected to change as additional terms are added to the series.

In view of these considerations, the best correction amplitude estimates are those that are based on the final few series terms. For the TRI lattice $a_1 = 0.761$, $a_2 = -2.16$. In the case of the SQ lattice the odd/even series terms yield $a_1 = 0.949/0.952$ and $a_2 = -2.98/-2.53$; the two a_1 values are very close, while the a_2 estimates can be combined to give $-2.76 + (-1)^N\ 0.23$ (the fit using the combined correction term is, not surprisingly, of lower quality than the separate odd/even fits).

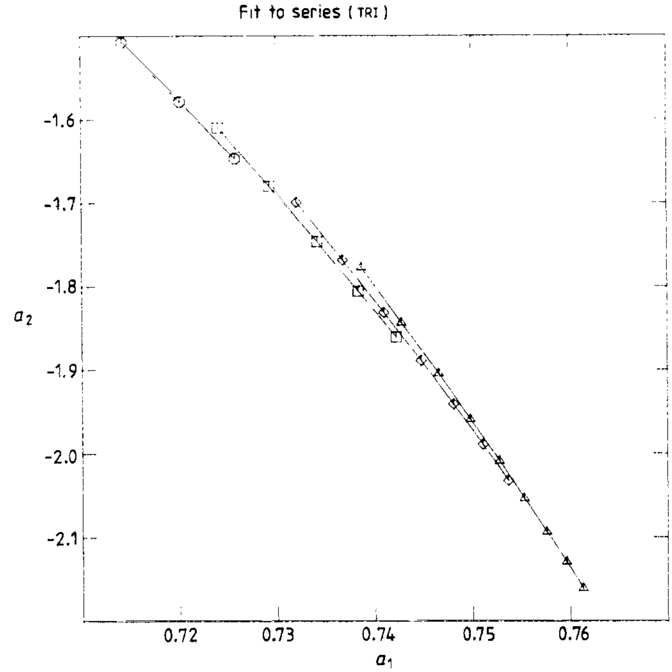

Figure 1. Correction amplitudes a_1 and a_2, obtained by fitting to different sets of R_N^2, for the TRI lattice. Each point corresponds to a distinct set of consecutive values $R_{N-K+1}^2 \ldots R_N^2$. The curves join points with common N; the rightmost point on each curve is for $K=3$, and K increases in unit steps along the curve. ○, $N=13$; □, $N=15$; ◇, $N=17$; △, $N=19$.

Only the $1/N$ correction was discussed in the context of the MC study (Rapaport 1984a) and rough estimates of the correction amplitudes were 0.6 (TRI) and 0.8 (SQ). The present values of a_1 are some 25% higher, but the discrepancy is more than adequately covered by the negative $1/N^2$ correction which leads to the correct curvature of the graphs of R_N^2 against N (Rapaport 1984a, figure 1); the second-order correction is not readily deducible from the MC results alone. The predictions of (1) using the above values of a_1 and a_2 differ from the MC measurements by less than the statistical uncertainty of the data.

In recapitulation, the results confirm the statement made earlier that in view of the very close agreement that can be obtained on the basis of analytic corrections alone, there is no reason to postulate the existence of non-analytic corrections in order to interpret the end-to-end distance series. Only if a well founded theoretical case in support of alternative forms of correction terms is developed will it become necessary to reassess the methods and the results of the numerical analysis.

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