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LETTER TO THE EDITOR

Two-dimensional polymers: universality and correction to scaling

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Abstract. Improved Monte Carlo methods have been used to study the asymptotic behaviour of self-avoiding walks on two-dimensional lattices. The mean-square end-to-end distance R_N^2 and radius of gyration S_N^2 are both found to scale as $N^{2\nu}$ with exponent values very close to the expected $\nu = \frac{3}{4}$ and an amplitude ratio that is universal. Small- N deviations of R_N^2 from the asymptotic results indicate a correction to scaling exponent $\Delta = 1$, a value that differs from previous estimates.

Although the two-dimensional self-avoiding walk (SAW) remains an unsolved problem a recent analytical argument (Nienhuis 1982) showed that the scaling exponent ν governing the asymptotic length dependence of the mean-square end-to-end distance,

$$R_N^2 \sim AN^{2\nu} \quad (1)$$

(N is the walk length), has a value $\frac{3}{4}$. The argument, though plausible, is not completely rigorous. A variety of numerical techniques—series expansions (Majid *et al* 1983, Djordjevic *et al* 1983), Monte Carlo (MC) (Havlin and Ben-Avraham 1983, Meirovitch 1983), renormalisation group (RG) (Le Guillou and Zinn-Justin 1980), real space renormalisation (Derrida 1981, Redner and Reynolds 1981)—have produced estimates of ν with varying degrees of confidence and precision; though most favour $\nu = \frac{3}{4}$ there are exceptions.

Once the dominant asymptotic behaviour (1) has been determined, the problem of estimating the leading-order correction term becomes somewhat more tractable. Numerical analysis—series (Djordjevic *et al* 1983, Privman 1984), MC (Havlin and Ben-Avraham 1983), RG (Le Guillou and Zinn-Justin 1980)—have so far failed to reach agreement on the value of the correction term exponent.

In this letter we describe the results of a new MC treatment of the $d = 2$ problem. An improved MC technique has allowed the generation of larger samples of long walks than previously possible, with the consequent improvement in the reliability of the results. The key conclusions of the study may be summarised as follows: The numerical ν is extremely close to the 'exact' value, a result which establishes the accuracy of the MC method itself—important because it has also been used for $d = 3$ and 4 (Rapaport 1984a, b). Furthermore, the same value of ν applies to the mean-square radius of gyration S_N^2 as well. The value of ν is lattice independent, as is the $N \rightarrow \infty$ limit of the ratio R_N^2/S_N^2 (or equivalently, the amplitude ratio). Finally, the leading-order correction term for R_N^2 is proportional to $N^{2\nu-1}$, a result not in accord with earlier numerical work. The present treatment of corrections differs from its predecessors in

that the quality of the MC data permits, for the first time, total separation of the correction term calculation from that of the leading-order behaviour.

The MC method used for SAW generation has been described in detail elsewhere (Rapaport 1985a); it is based on the well known enrichment technique (Wall *et al* 1963), but is significantly enhanced by the fact that instead of constructing the walks by adding a single step at a time, as in the original scheme, it operates by combining members of previously generated sets of shorter walks. The method allows the construction of SAWs of sufficient length to be well into the asymptotic region while at the same time not biasing the sample in any way; the efficiency of the algorithm permits the use of large sample sizes to reduce the statistical spread of the data.

The measured values of R_N^2 and S_N^2 for walks of length up to 2400 steps on the triangular (TRI) and square (SQ) lattices are listed in table 1; each value represents the average of $45\text{--}50 \times 10^3$ separate SAW realisations. The confidence limits associated with these values are determined by partitioning the walks into eight groups and computing the spread of the group means; the resulting standard deviations of the mean for each lattice amount to 0.6% (R_N^2) and 0.4% (S_N^2) of the means themselves.

Table 1. Measured values of R_N^2 and S_N^2 .

	N	R_N^2	S_N^2
TRI	120	944.4	132.23
	300	3692.7	518.97
	600	10 568.4	1479.15
	1200	29 642.2	4154.40
	2400	83 610.0	11 725.16
SQ	160	1579.3	221.07
	320	4446.6	623.33
	640	12 466.6	1751.32
	1200	31 923.1	4503.13
	2400	90 963.2	12 740.28

The scaling exponent ν appearing in (1) is obtained by linear regression analysis of $\log R_N^2$ against $\log N$, and similarly for S_N^2 . The values of ν thus derived are 0.7488 (R_N^2), 0.7489 (S_N^2) for the TRI lattice, and 0.7479 (R_N^2), 0.7484 (S_N^2) for the SQ; error estimates produced by the regression analysis amount to ± 0.0010 (R_N^2) and ± 0.0006 (S_N^2). In each case the fit of the asymptotic result is so close that the average relative deviation of the data points is only 0.4% (R_N^2) and 0.2% (S_N^2), less than the uncertainties in the data; deviations of this magnitude are barely apparent when the data is graphed. The values obtained for ν all lie approximately 0.2% below $\frac{3}{4}$; the most probable cause of this minor deviation is the residual effect of the leading-order correction terms (see below) which, for $N > 100$, disappear into the statistical noise.

The fit to the asymptotic form can be repeated with the requirement $\nu = \frac{3}{4}$. The quality of the fit is only slightly worse than before, with average deviations of 0.5% (R_N^2) and 0.4% (S_N^2), values that are still no greater than the uncertainty of the data. The resulting estimates of the amplitude A are 0.7145 ± 0.0036 (R_N^2), 0.1002 ± 0.0004 (S_N^2) for the TRI lattice, and 0.7739 ± 0.0048 (R_N^2), 0.1086 ± 0.0004 (S_N^2) for the SQ (the values are quoted to four significant figures to permit reproduction of the results but the last digit is not intended to be taken seriously); the small errors are again an indication

of the closeness of the fit. The $N \rightarrow \infty$ limit of the ratio R_N^2/S_N^2 , i.e., the ratio of the corresponding amplitudes, is equal to 7.131 (TRI) and 7.126 (SQ); the difference is below 0.1% and is strong indication that the amplitude ratio is a universal (lattice independent) quantity (Domb and Hioe 1969).

In order to study the corrections to scaling a series of shorter SAWs were generated by means of the same MC method; the lengths lay in the range $N = 12-60$ (increments of 6) for the TRI lattice and $N = 16-80$ (increment 8) for the SQ. The size of each sample was increased to 2×10^5 walks to further reduce the statistical error. The relative deviations of the measured R_N^2 and S_N^2 from the leading-order asymptotic predictions ((1) with $\nu = \frac{3}{4}$ and appropriate amplitudes) are shown in figure 1 plotted against N^{-1} .

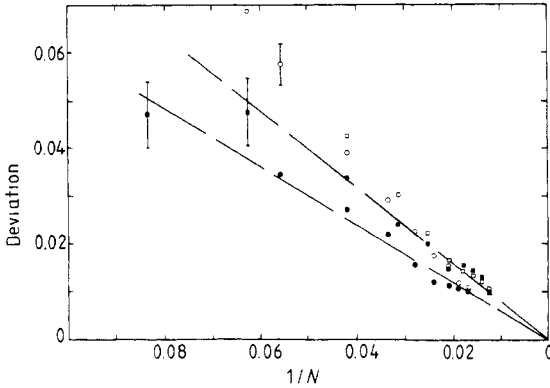


Figure 1. Relative deviations of measured R_N^2 and S_N^2 from the leading order asymptotic predictions with $\nu = \frac{3}{4}$. The symbols \bullet and \circ denote R_N^2 and S_N^2 deviations on the TRI lattice, \blacksquare and \square on the SQ lattice. The straight lines correspond to the N^{-1} correction (2) with coefficients 0.6 (TRI) and 0.8 (SQ). The error bars show the RMS spread of the group means.

It is immediately apparent that the straight lines included in the graph fit the R_N^2 data to well within the error limits. If the generalisation of (1) to include the leading-order scaling correction is

$$R_N^2 \sim AN^{2\nu}(1 + BN^{-1} + O(N^{-2})) \tag{2}$$

then the relative deviation is simply $BN^{-1} + O(N^{-2})$. The results for R_N^2 not only support (2) but also reveal that the N^{-2} correction is negligible down to very small N . The straight lines themselves are drawn to give a good visual fit; they correspond to $B = 0.6$ (TRI) and 0.8 (SQ). The average deviation from (2) is only 0.1%; this is significantly less than the spread of the values themselves (0.7%) when averages based on partitioning the data into 20 groups are computed.

A similar linear fit for the S_N^2 deviation is not possible, as is clear from the figure. An enlarged N^{-2} correction term could account for the curvature, but the reliable estimation of its coefficient together with that of the N^{-1} term is not possible from the available data. A similar situation is encountered (Rapaport 1985b) when analysing series expansions for R_N^2 and S_N^2 by fitting to (2)— R_N^2 produces better converged estimates than S_N^2 .

The discrepancies between the exact series values of R_N^2 and the MC estimates (or equivalently the asymptotic expressions) are small, and lie well within the limits set

by statistical uncertainty. On the TRI lattice typical differences are 0.1% and 0.2% for $N = 12$ and 19 respectively; these represent a substantial improvement over the 1% and 0.8% differences obtained using a proposed (Djordjevic *et al* 1983) alternative to (2) involving a correction term of form $N^{-\Delta}$ with $\Delta = \frac{2}{3}$. At $N = 20$ on the SQ lattice (Martin and Watts 1971) the difference is only 0.1%, although it increases to 0.4% by $N = 12$ (the MC data are for $N \geq 16$) because of the contribution of higher-order corrections.

The fact that (2) provides a better than adequate fit to the R_N^2 data suggests that attempts (Djordjevic *et al* 1983, Privman 1984) at series analysis assuming an additional $N^{-\Delta}$ correction term with $\Delta < 1$ are not warranted. An analysis (Rapaport 1985b) of the TRI lattice series for R_N^2 , now extended as far as $N = 19$, confirms this conclusion—equal if not better convergence is obtained using the unembellished version of (2). A similar state of affairs exists in three dimensions as well (Rapaport 1985a).

The motivation for introducing correction terms with $\Delta \neq 1$ stems from the RG prediction (Le Guillou and Zinn-Justin 1980) $\Delta = 1.2$; confidence in this particular value is not high because the same RG method predicts that $\nu = 0.77$ —hence the proposal (Djordjevic *et al* 1983) that $\Delta = \frac{2}{3}$. The present analysis cannot of course rule out a value of Δ close to unity (a similar problem arises for the SAW generating function—see Adler (1983) and Guttmann (1984) for conflicting points of view), although there is no evidence that a value $\Delta \neq 1$ is required. If, however, Δ exceeds unity, the N^{-1} term becomes the leading-order correction; this term cannot be seen by the RG since it is associated with the analytic (as opposed to the singular) parts of the SAW generating functions (Rapaport 1985). A recent MC analysis (Havlin and Ben-Avraham 1983) that observed the RG value of Δ neglected the existence of the N^{-1} correction and obtained a negative leading-order correction term, a result clearly incompatible with the present work; the fact that the result was not obtained by direct measurement of R_N^2 but was based on additional assumptions concerning SAW behaviour is the probable explanation of the disagreement.

References

- Adler J 1983 *J. Phys. A: Math. Gen.* **16** L515
 Derrida B 1981 *J. Phys. A: Math. Gen.* **14** L5
 Djordjevic Z V, Majid I, Stanley H E and dos Santos 1983 *J. Phys. A: Math. Gen.* **16** L519
 Domb C and Hioe F T 1969 *J. Chem. Phys.* **51** 1915
 Grassberger P 1982 *Z. Phys.* **B 48** 255
 Guttmann 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 1980 *Phys. Rev. B* **21** 3976
 Majid I, Djordjevic Z V and Stanley H E 1983 *Phys. Rev. Lett.* **51** 143
 Martin J L and Watts M G 1971 *J. Phys. A: Math. Gen.* **4** 456
 Meirovitch H 1983 *J. Chem. Phys.* **79** 502
 Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
 Privman V 1984 *Physica* **123A** 428
 Rapaport D C 1984 *Phys. Rev. B* in press
 — 1985a *J. Phys. A: Math. Gen.* **18** 113
 — 1985b to be published
 Redner S and Reynolds P J 1981 *J. Phys. A: Math. Gen.* **14** 2679
 Wall F T, Windwer S and Gans P J 1963 in *Methods in Computational Physics* vol 1, ed B J Alder *et al* (New York: Academic)