On the correction-to-scaling exponent of linear polymers in two dimensions

1986 J. Phys. A: Math. Gen. 19 L543

(http://iopscience.iop.org/0305-4470/19/9/015)

J. Phys. A: Math. Gen. 19 (1986) L543-L545. Printed in Great Britain

LETTER TO THE EDITOR

On the correction-to-scaling exponent of linear polymers in two dimensions

D L Hunter, Naeem Jan and Bruce MacDonald

Physics Department, St Francis Xavier University, Antigonish, Nova Scotia B2G 1C0, Canada

Received 17 March 1986

Abstract. We present new results which indicate that the leading correction-to-scaling exponent in the mean squared end-to-end distance in two dimensions is the analytic term. We point out a potential source of the various correction-to-scaling terms reported in the literature.

Considerable attention has been given to the two-dimensional self-avoiding walk (SAW). It is of particular interest as a model for generating polymer conformations in a good solvent (de Gennes 1979). The scaling exponent, ν, for the asymptotic dependence of the mean squared end-to-end distance, R_N^2, upon the length N

$$R_N^2 \approx AN^{2\nu} \tag{1}$$

is more or less agreed to be $\nu = 0.750$ in two dimensions (exact enumeration: Domb 1963, Grassberger 1982, Djordjevic *et al* 1983, Majid *et al* 1983, Adler 1983, Guttman 1984, Privman 1984; Monte Carlo studies: Meirovitch 1983, Havlin and Ben-Avraham 1983, Rapaport 1985, MacDonald *et al* 1985, Lyklema and Kremer 1985; real space renormalisation: Derrida 1981, Redner and Reynolds 1981). Nienhuis (1982, 1984) has shown by reasonable but non-rigorous arguments that the SAW, through its identity with the $n \to 0$ limit of the n-vector model, may be mapped onto the Coulomb gas model, a model onto which many other models (some with exactly known exponents) may be mapped. This common meeting ground is exploited to determine the critical exponents of the SAW. Nienhuis also concluded that the exponent γ defined by

$$C_N \sim \mu^N N^{\gamma-1} \tag{2}$$

is $\frac{43}{32}$ (C_N is the number of distinct walks of N steps and μ the connectivity constant). These exponents are widely believed to be exact and the only numerical evidence which may be inconsistent is the ε-expansion renormalisation group result $\nu = 0.76$ of LeGuillou and Zinn-Justin (1985) for the $d = 2$, $n \to 0$ n-vector model. This discrepancy is perhaps due to the rather large value of the perturbation parameter ($\varepsilon = 2$).

There is a total lack of consensus regarding the leading correction-to-scaling exponent, Δ_1:

$$R_N^2 \sim AN^{2\nu}[1 + BN^{-\Delta_1} + CN^{-\Delta_2} + \ldots]. \tag{3}$$

Whilst Nienhuis' mapping gives $\Delta_1 = \frac{3}{2}$ in qualitative agreement with the RG ε-expansion result $\Delta_1 = 1.29$ (LeGuillou and Zinn-Justin 1985) the exact enumeration studies (refer-

0305-4470/86/090546+03\$02.50

ences given above) suggest a range of values from ~ 0.66 to ~ 0.95 although Guttmann argues that there is no evidence for a value less than 1. The Monte Carlo studies have also been inconclusive. Lyklema and Kremer (1985) find $\Delta_1 = 0.84$, Havlin and Ben-Avraham (1983) report 1.2 whilst Rapaport (1985) finds $\Delta_1 = 1$, i.e. the analytic term is more important than the strongest non-analytic correction. The presence of a non-analytic term less than one would cast doubt on the validity of Nienhuis' mapping.

In this letter we report the results of a Monte Carlo investigation of SAW on the quadratic lattice. We use the 'wiggle' method (MacDonald *et al* 1985, Stellman and Gans 1972a, b, Moti Lal 1969) to generate the end-to-end distance for chains ranging from 10–500 links. Our subsequent analysis depends on the accurate determination of the leading amplitude, A. We assume that corrections to scaling are negligible (or at least small enough not to have any significant statistical effect on the data) for chains of length N in the range 140–500. A least squares fit of our data gives an exponent 2ν of 1.5005 and amplitude A of 0.774 which is in agreement with the extrapolated plot of $R_N^2/N^{3/2}$ against $1/N$ (see also figure 1). We note that the amplitude is extremely sensitive to fluctuations in the data whilst the leading exponent is relatively stable. We now look at the quantity

$$C(N) \triangleq R_N^2 - AN^{2\nu} \sim ABN^{2\nu-\Delta_1(N)} \tag{4}$$

for values of $N \leqslant 22$. We draw upon the exact enumeration data for R_N^2 from Domb (1963) and Grassberger (1983). Examination of $\ln C(N)$ against $\ln N$ for even (and odd) successive values of N indicate that $\Delta_1(N)$ is a monotonically increasing function of alternate integers of N and our extrapolated projection of $\Delta_1(N)$ against $1/N$ leads to $\Delta_1 \approx 1.0$ for $A = 0.774$. If we use, for example the criterion that chains of length $N \geqslant 16$ are influenced *only* by the leading correction-to-scaling term, then we find $\Delta_1(N)$ independent of N and equal to 0.64 (cf the results of Privman (1984) and Djordjevic *et al* (1983)) and A equal to 0.762. However for A equal to 0.782 we find that the above extrapolation leads to Δ_1 equal to 1.50. A change in A of the order of about 2.6% leads to a change in Δ_1 of 100%.

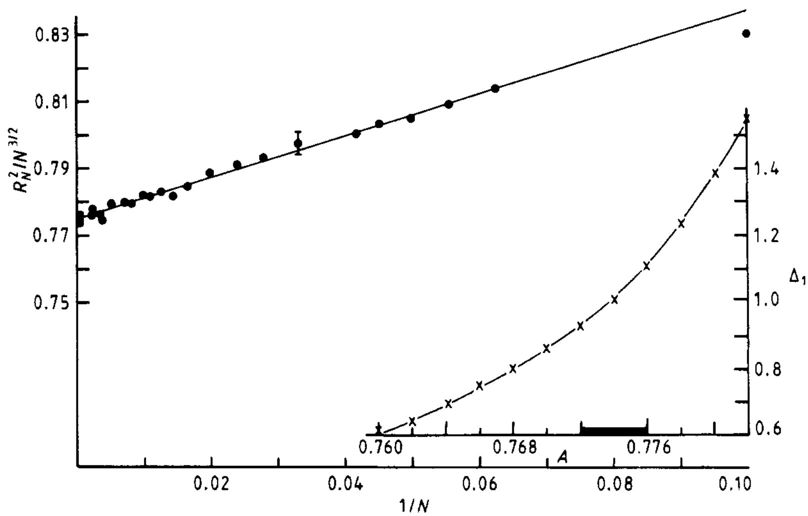

Figure 1. Plot of $R_N^2/N^{3/2} \sim A(1+BN^{-\Delta_1}+\ldots)$ against $1/N$. This should have intercept A if $2\nu = \frac{3}{2}$ and $\Delta_1 = 1$. Inset: dependence of estimates of leading correction exponent Δ_1 on choice of amplitude A.

We continue our analysis; assuming that the dominant correction-to-scaling term is the analytic correction we treat its amplitude B as an adjustable parameter to ensure a leading exponent of $2\nu = 1.50$ for N in the range 50–125. This occurs at B equal to 0.79 and A equal to 0.775, in very good agreement with our previous analysis and the earlier work of Rapaport (1985).

Our main conclusions are: (i) the leading correction-to-scaling term is analytic, i.e. $\Delta_1 = 1.0 \pm 0.1$; (ii) the values obtained for Δ_1 are crucially dependent on the value of the leading amplitude (figure 1) and this therefore may be responsible for the widely varying estimates for Δ_1 reported in the literature; (iii) the Nienhuis value of the leading non-analytic correction exponent $\Delta_2 = \frac{3}{2}$ is not incompatible with this result, and it is plausible that RG analysis which is primarily concerned with the non-analytic part of the free energy is unable to detect the presence of analytic correction terms.

We would like to thank Stu Whittington and Alan Sokal for informing us of previous work on the 'wiggle' method; Kurt Kremer and Dick Lyklema for their unpublished data; B V Liengme, Marty Corsten and Vince Connors for help in developing various algorithms, and Francois Leyvraz for advice on analysing the Monte Carlo data. This research is supported in part by grants from NSERC of Canada and UCR of St Francis Xavier University.

References

Adler J 1983 *J. Phys. A: Math. Gen.* **16** L515
de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
Derrida B 1981 *J. Phys. A: Math. Gen.* **14** L5
Djordjevic Z V, Majid I, Stanley H E and dos Santos R J 1983 *J. Phys. A: Math. Gen.* **16** L519
Domb C 1963 *J. Chem. Phys.* **38** 2957
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
LeGuillou J C and Zinn-Justin J 1985 *J. Physique Lett.* **46** L137
Lyklema J W and Kremer K 1985 *Phys. Rev.* B **31** 3182
MacDonald B, Jan N, Hunter D L and Steinitz M O 1985 *J. Phys. A: Math. Gen.* **18** 2627
Majid I, Djordjevic Z V and Stanley H E 1983 *Phys. Rev. Lett.* **51** 143
Meirovitch H 1983 *J. Chem. Phys.* **79** 502
Moti Lal 1969 *Mol. Phys.* **17** 57
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
—— 1984 *J. Stat. Phys.* **34** 731
Privman V 1984 *Physica* **123A** 428
Rapaport D C 1985 *J. Phys. A: Math. Gen.* **18** L39
Redner S and Reynolds P J 1981 *J. Phys. A: Math. Gen.* **14** 2679
Stellmann S O and Gans P J 1972a *Macromol.* **5** 516
—— 1972b *Macromol.* **5** 720