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J. Phys. A: Math. Gen. **20** (1987) 5029-5031. Printed in the UK

COMMENT

Critical properties of the three-dimensional self-avoiding walk

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Received 25 March 1987

Abstract. Accurate Monte Carlo data are used to determine the critical exponent $\nu (=0.590 \pm 0.001)$ or inverse fractal dimension of the three-dimensional self-avoiding walk. The leading correction to scaling term is non-analytic and is near 0.5.

Recent Monte Carlo work (Rapaport 1985a, b, Hunter *et al* 1986) on the two-dimensional self-avoiding walk (SAW) concluded that the leading correction-to-scaling term Δ_1 is analytic, i.e.

$$R_N^2 \sim AN^{2\nu}(1 + BN^{-\Delta_1} + CN^{-\Delta_2} + \ldots) \qquad (1)$$

where R_N is the root-mean-square end-to-end distance of a SAW of N steps, ν is the leading exponent and Δ_1 the leading correction term. This result was at variance with some analyses of the series data and other Monte Carlo work (see e.g. Hunter *et al* (1986) for a discussion and the relevant references). MacDonald *et al* (1987) extended the exact enumeration data for the square lattice (28 terms) and the honeycomb lattice (42 terms) and the additional terms confirmed the Monte Carlo conclusion mentioned above, i.e. $\Delta_1 = 1$!

Rapaport (1985b) extended the series and analysed the data for the three-dimensional SAW and from the extended series together with Monte Carlo results concluded that the leading correction to scaling term Δ_1 is analytic, i.e. $\Delta_1 = 1$ while $\nu = 0.592 \pm 0.002$. This value is in conflict with previous series analysis (Majid *et al* 1983) and the generally accepted highly accurate ε-expansion of the $n \to 0$ limit of the n-vector model (Le Guillou and Zinn-Justin 1985) where the primary conclusions are $\Delta_1 \simeq 0.5$, i.e. the leading correction term is non-analytic and $\nu = 0.589$. Guttmann (1986a, b) recently extended the series for the three-dimensional cubic lattice (20 terms) and reported a value of ν of 0.592 in agreement with Rapaport and slightly higher than the ε-expansion results. This value is closer to Flory's prediction of 0.6 and thus Guttmann's result suggests the possibility that additional terms may push the series results towards 0.6. The second factor to be resolved is whether the correction term is analytic or not. Our comment aims to clarify these two points on the simple cubic lattice.

The 'wiggle' method (MacDonald *et al* 1985) is used to simulate conformations of the SAW from length $N = 10$ to 800. The average RMS end-to-end distance agrees remarkably well (to better than 0.15%) with the exact values and to within 1% for the longer chains reported by Rapaport. At least 200 000 independent conformations were generated for the shorter chains (i.e. $N \leq 120$) and from 150 000 conformations for $N = 150$ to 30 000 conformations for $N = 800$. The 30 000 conformations for $N = 800$ took approximately 450 h on a SUN 3/50 work station.

A simple analysis of the data for long chains ($N \geqslant 150$), i.e. a ln-ln plot of R_N^2 against N, leads to $2\nu = 1.183$ and $A \sim 1.45$ in excellent agreement with Rapaport (1985b) and Guttmann (1986a, b). These values were then used in the analysis of the shorter chains through

$$(R_N^2 - AN^{2\nu}) \text{ against } ABN^{2\nu-\Delta_1}.$$

We were unable to distinguish between $\Delta_1 = 0.5$ and 1 from our data although the correlations were slightly better for $\Delta_1 = 0.5$. A more compelling analysis is made by plotting $2\nu(N-m, N+m)$ against $1/\sqrt{N}$ and $2\nu(N-m, N+m)$ against $1/N$ for segments of length m in N. For the series data $m = 1(N \leqslant 20)$; m varied for the Monte Carlo data from $m = 4$ for $N > 20$ to $m = 200$ for $N = 600$. The results are shown in figure 1(a) and (b). The primary conclusion is that a better fit to a straight line is obtained from $1/\sqrt{N}(N > 16)$ than for $1/N(N > 33)$.

Our main results are (i) we can exclude Flory's value of 0.6 from the investigation of longer chains; (ii) the value of 2ν is 1.180 ± 0.002 and (iii) the correction-to-scaling exponent Δ_1 is ~ 0.5.

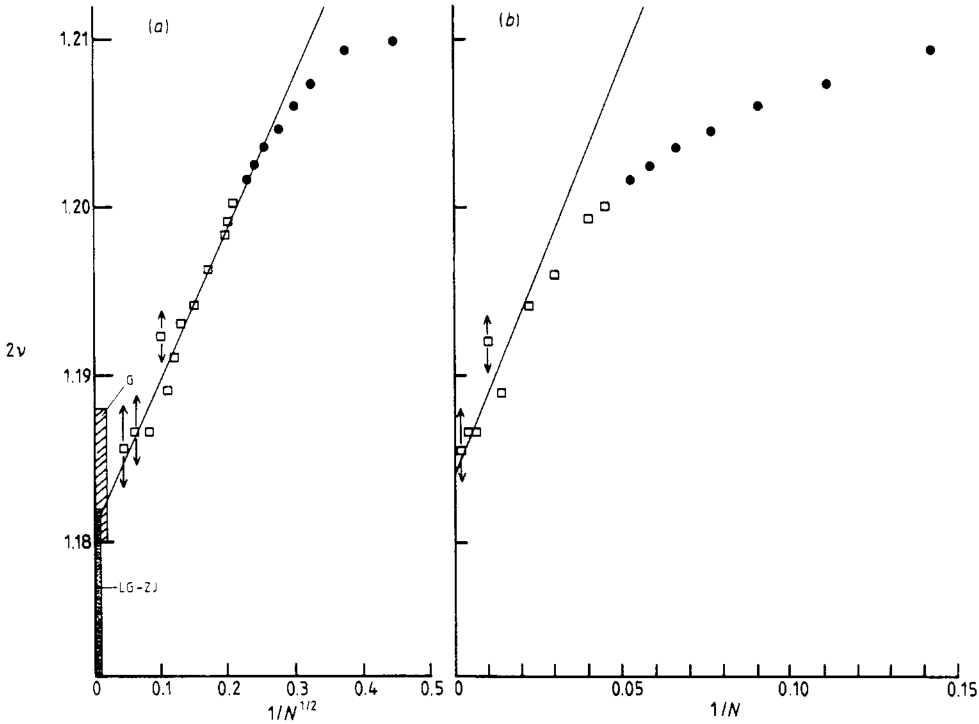

Figure 1. (a) Plot of $2\nu(N-m, N+m)$ against $1/N^{1/2}$ for N varying from 600 to 5. The data are well represented by a straight line for $N > 16$. Results of Guttmann (1986a, b) (G) and Le Guillou and Zinn-Justin (1985) (LG-ZJ) are shown with the corresponding error bars. The series results for ν are indicated by ● and the Monte Carlo results by □. (b) As for (a) except 2ν is plotted against $1/N$. Straight line behaviour is only observed for $N > 33$.

We thank A Guttmann, F Leyvraz and D Stauffer for useful conversations. DLH and NJ are supported by NSERC grants.

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