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LETTER TO THE EDITOR

Universal distance ratios for 2D SAW: Monte Carlo and exact series results

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Abstract. The mean square distance of a monomer to the origin and the mean square distance of the centre of mass to the origin are studied by Monte Carlo and exact series methods on the square and lattice. The numerical results give strong evidence of a discrepancy with the theoretical prediction of Cardy and Saleur based on conformal invariance theory.

The self-avoiding walks (SAW) model is one of the most successful models of long, flexible chain polymers. It is directly related to the $n \to 0$ limit of the n-vector model [1]. Recently Cardy and Saleur [2] studied one aspect of the metric properties of this model using the c-theorem of Zamolodchikov [3]. Defining

$$\begin{aligned} \nu_N &= \langle R_g^2 \rangle_N / \langle R_e^2 \rangle_N \\ \mu_N &= \langle R_m^2 \rangle_N / \langle R_e^2 \rangle_N \\ F_N(y_t/y_h, \nu_N, \mu_N) &= \left(2 + \frac{y_t}{y_h}\right)\nu_N + \tfrac{1}{8} - \mu_N \end{aligned} \tag{1}$$

they derived a universal relation for SAW on two-dimensional lattices:

$$\lim_{N\to\infty} F_N(y_t/y_h, \nu_N, \mu_N) = 0. \tag{2}$$

Here $\langle R_g^2 \rangle$ and $\langle R_e^2 \rangle$ are the usual mean square radius of gyration and the mean square end-to-end distance respectively, while $\langle R_m^2 \rangle$ is the mean square distance of a monomer to the origin. $\langle \ldots \rangle_N$ denotes the average over the ensemble of N-step SAW. The exponents y_t and y_h are exactly known from Coulomb gas or conformal invariance techniques [4] to be $\frac{4}{3}$ and $\frac{91}{48}$ respectively for 2D SAW.

The most accurately known values of ν_∞ and μ_∞ are those calculated recently by Guttmann and Yang [5] using exact series expansions to 21 terms on the square lattice and 15 terms on the triangular lattice. Their results $\nu_\infty = 0.1396 \pm 0.001$ and $\mu_\infty = 0.4375 \pm 0.002$ yield, when substituted into equation (1), $F_\infty = 0.065 \pm 0.004$. This is in clear disagreement with the theoretical prediction of Cardy and Saleur. However an objection can be raised that this may be caused by a 'short series' effect. In order to check this we perform Monte Carlo calculations here which is a direct extension of the exact series expansion method [6, 7]. This method, called the incomplete enumeration method, had been described before and applied to enumerate configurations of branched and linear polymers [8–12]. It will only be briefly described here.

In the exact enumeration method, the SAW configurations are classified into a tree structure according to their lineage and then enumerated using the backtracking method [13]. In the incomplete enumeration method for a N-step walk, one deletes with probability $(1-p_r)$ where $0<p_r\leqslant 1$ and $r=2,3\ldots N$, all r-step configurations and their descendants from the genealogical tree. The remaining N-step configurations are then systematically enumerated using the backtracking method. Since the set $\{p_i\}$ is pre-chosen, the probability that a particular r-step SAW will be enumerated in a given trial is $p_2, p_3\ldots p_r \equiv P_r$ and is the same for all configurations with the same r. The algorithm thus generates an unbiased sample of configurations. We have chosen here $p_1=1, p_i=\lambda^{-1}$ for $i\geqslant 2$ where $\lambda=2.5$ for the square lattice calculation. The exact enumeration method is recovered by choosing $p_i=1$ for all i.

The results for ν_N and μ_N are shown in figures 1 and 2 respectively, plotted against $1/N$. The Monte Carlo data are denoted by dots and the exact results by crosses. The data are obtained using 120 000 trials. The error bars are obtained by dividing the data into ten sets and calculating the standard deviations. From figures 1 and 2 we see that our Monte Carlo data are in excellent agreement with exact series data for both ν_N and μ_N. The extrapolated estimates $\nu_\infty=0.1398\pm0.0005$ and $\mu_\infty=0.4399\pm0.001$ are significant improvements over those of Guttmann and Yang. It should be pointed out that these estimates are very different from those of the second-order ε-expansion [14, 15] $\nu_\infty=0.1428$ and $\mu_\infty=0.4367$. The Monte Carlo data obtained up to $N=100$ steps also exclude the possibility of a 'short series' effect. Using these estimates we find $F_\infty=0.0633\pm0.002$.

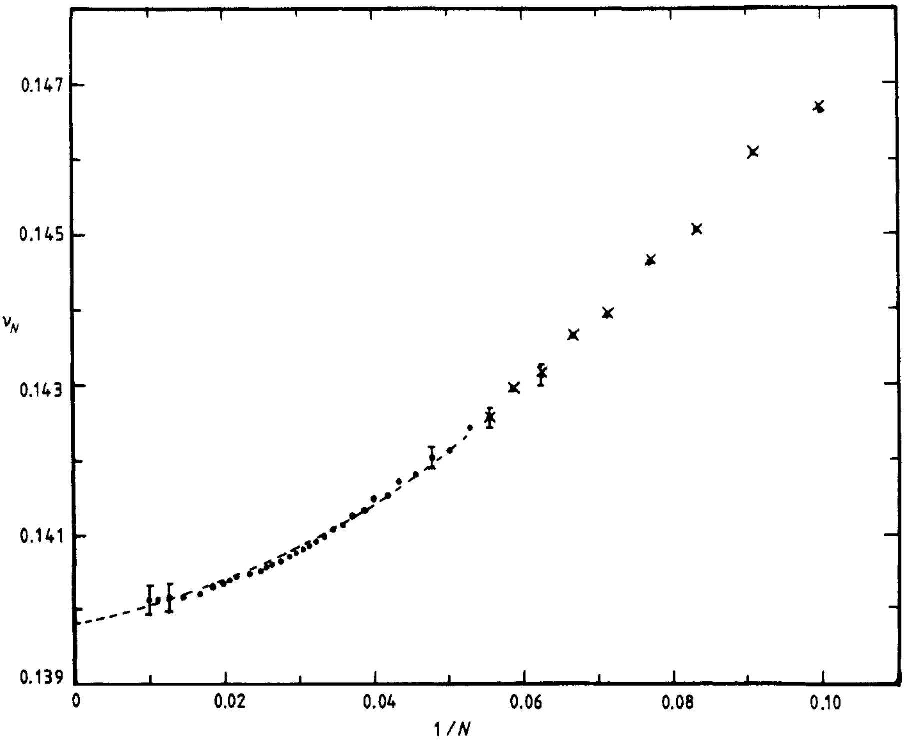

Figure 1. The ratio ν_N against $1/N$. The dots represent Monte Carlo data and the crosses represent the exact series results on the square lattice.

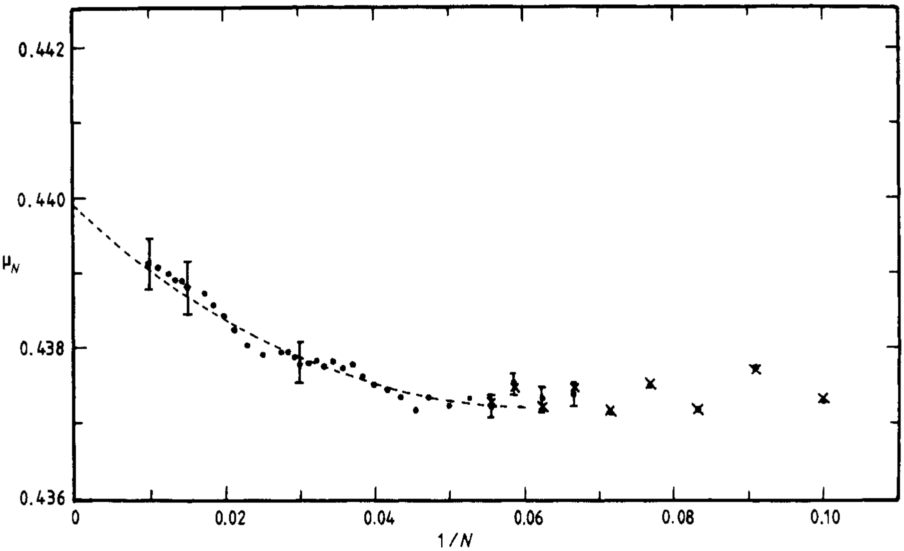

Figure 2. Same as figure 1 but for μ_N.

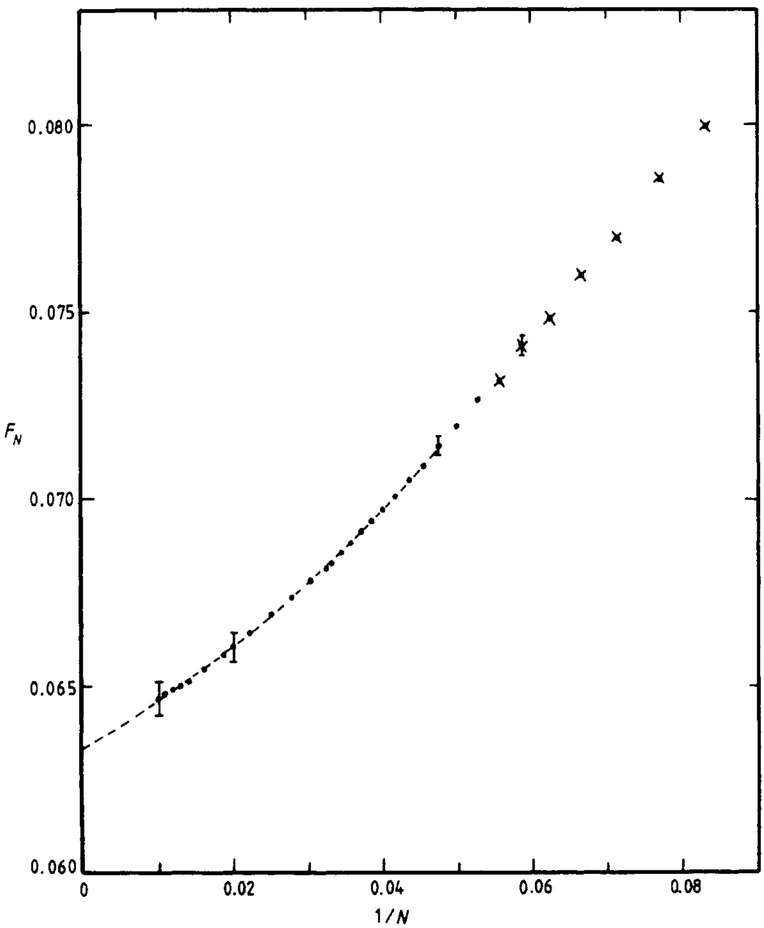

Figure 3. Same as figures 1 and 2 but for F_N.

Rather than extrapolating ν_N and μ_N separately to ν_∞ and μ_∞, it may be more accurate to extrapolate directly F_N to F_∞. This is shown in figure 3 where the F_N values are plotted against $1/N$. We find in this case $F_\infty = 0.0633 \pm 0.001$, in excellent agreement with the previous estimate. We take this to be our best estimate for F_∞.

Both the exact series and Monte Carlo data indicate clear discrepancy with the theoretical predictions of Cardy and Saleur. In view of the present strong numerical evidence, we suggest that the theory of Cardy and Saleur should be carefully re-examined. Our best estimate for F_∞, however suggests that $\tilde{F}_\infty$ with $\tilde{F}_N(y_t/y_h, \nu_N, \mu_N) \equiv (2 + y_t/y_h)\nu_N + \frac{1}{16} - \mu_N$ is very close to zero ($\tilde{F}_\infty = 0.0008 \pm 0.001$).

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