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LETTER TO THE EDITOR

Statistics of the true self-avoiding walk in one dimension

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Abstract. Numerical results of a Monte Carlo study for the true self-avoiding walk in one dimension are presented. For any positive value of the strength parameter ($0<g<\infty$), the root-mean-square displacement R_N and the range S_N of the walk are characterised by two universal exponents $\nu=\frac{2}{3}\pm0.003$ and $s=\frac{2}{3}\pm0.01$ respectively. For negative g (self-attracting walk) both R_N and S_N exhibit a saturation effect: $\lim_{N\to\infty} R_N=R_\infty(g)$ and $\lim_{N\to\infty} S_N=S_\infty(g)$ with $R_\infty(g)\sim(-g)^{-1}$ and $S_\infty(g)\sim(-g)^{-1}$ at $g\leqslant0$. A simple scaling analysis in N and g is proposed and found to be consistent with the Monte Carlo results.

Recently Amit *et al* (1983) have introduced a novel class of non-trivial correlated random walks on a lattice: the true self-avoiding walks (TSAW). They have introduced a self-avoidance parameter g and shown that the upper critical dimensionality for this problem is two ($d_c=2$), whereas it is four for the polymer problem (SAW) (see de Gennes 1979). Logarithmic corrections at $d=2$ have been studied both numerically (Amit *et al* 1983) and by $\varepsilon=2-d$ expansions (Obukhov and Peliti 1983, Peliti 1983). Finally, a self-consistent argument (Pietronero 1983) has been formulated to compute d_c and the exponent ν of a TSAW. The result reproduces correctly $d_c=2$ and suggests a non-trivial value for ν: $\nu=2/(2+d)$ at $d<d_c$. Of particular interest is the prediction of a non-diffusive behaviour, $\nu=\frac{2}{3}$ at $d=1$ for any finite value of the parameter g. The purpose of this letter is to present a brief report of a Monte Carlo study for the TSAW in one dimension, which permits us in particular to check this prediction. Two statistical properties are investigated for positive as well as for negative values of g: the root-mean-square (RMS) displacement R_N and the average number of S_N of distinct visited sites during N-step walks range. Illustrations are limited here to R_N only. More detailed results, in particular for S_N, will be reported elsewhere (Rammal *et al* 1983).

The TSAW problem in one dimension can be formulated as follows: a walker may move at each step to one of the two nearest neighbours of its current position. The (normalised) probability for moving from site i to $i\pm1$ is given by

$$W_i^{\pm}=\{1+\exp[\pm g(n_{i+1}-n_{i-1})]\}^{-1} \tag{1}$$

where n_j denotes the total number of previous visits of site j. Three trivial limits of the TSAW in one dimension are respectively identified: $g=0$, ∞ and $-\infty$. In the first case ($g=0$) we recover the standard random walk problem (RW), where $\nu=\frac{1}{2}$. The second case ($g=\infty$) corresponds to the SAW problem in one dimension, with $\nu=1$. In the last case ($g=-\infty$), the walker oscillates indefinitely between the first two visited sites. For other values of g we have a non-trivial stochastic process with infinitely

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long memory. For $g > 0$ (resp $g < 0$) the walker is discouraged (resp encouraged) from stepping toward previously visited regions. The particular dependence (equation (1)) of $W_i^{\mp}$ on $\{n_i\}$ is at the origin of non-trivial statistical properties of the TSAW.

In figure 1 are shown the Monte Carlo results for R_N at different values of the repulsion parameter g. R_N denotes here the RMS displacement at step N: $R_N^2 = \langle x_N^2 \rangle$. All calculations were performed (in assembly language) on processors M 6502 and M 68000. Each set of points corresponds to an average over $10^4 - 2\times10^4$ runs of N-step walks, up to $N = 2^{18}$. As can be seen, R_N crosses over from a RW behaviour at small g (resp SAW at $g \gg 1$) for small N to a TSAW behaviour for larger N. The asymptotic slope converges towards a well defined value ν, independent of g and very close to $\frac{2}{3}$. From the best fit of data and using a plot enhancing eventual deviations from this value, we have obtained the following estimation for the exponent ν: $\frac{2}{3} \pm 0.003$. This remarkable result, which differs from $\frac{2}{3}$ only by a very small amount, provides strong support for the corresponding value predicted by the self-consistent argument. A similar behaviour was obtained for the range S_N of the TSAW. A power law $S_N \sim N^s$ is reached asymptotically ($N \gg 1$) in the same range of g values. The crossover observed for R_N is also observed for S_N. The estimated value of the exponent s is $s = \frac{2}{3} \pm 0.01$, which supports an intuitive argument (see below) leading to the prediction $s = \nu$.

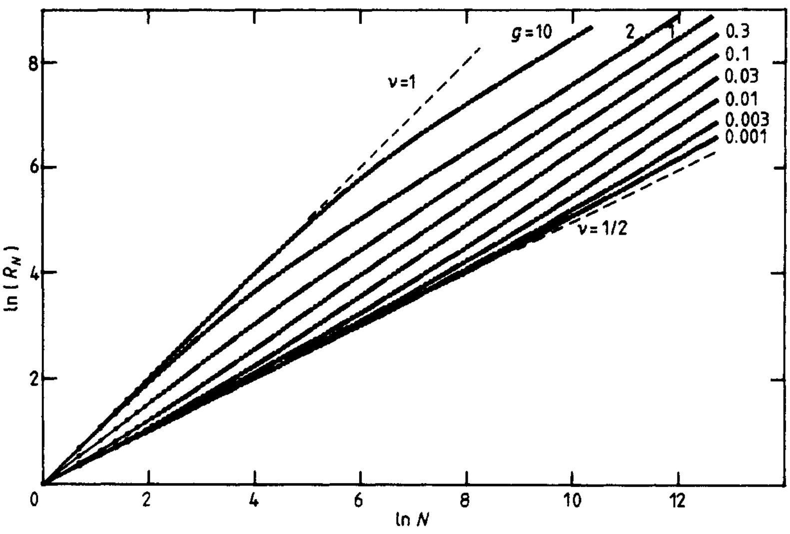

Figure 1. RMS displacement R_N of the TSAW, for different values of the repulsion parameter: $10^{-3} \leq g \leq 10$. For each value of g, an average over $10^4 - 2\times10^4$ runs of up to $N = 2^{18}$ steps was performed. Broken lines correspond to $g = \infty$ (i.e. $\nu = 1$) and $g = 0$ ($\nu = \frac{1}{2}$) respectively. Convergence towards a well defined exponent $\nu \sim \frac{2}{3}$ is clearly shown.

Motivated by the symmetry property $W_i^{\pm}(g) = W_i^{\mp}(-g)$, we have extended the above study to negative values of g. In the extreme limit $g = -\infty$ the TSAW reduces trivially to a simple oscillation between two sites. Such a self-trapping effect was shown to occur also for all other negative values of g. This feature, leading to a saturation of R_N and S_N as functions of N, has been checked by using enumeration methods as well as Monte Carlo calculation. By the former method, we have exactly calculated properties up to a given number of steps ($N \leq 20$) determined by limitations of computer time, for arbitrary values of g. The results behave sufficiently smoothly with N and g that the definition of $R_\infty(g) = \lim_{N\to\infty} R_N(g)$ and $S_\infty(g) = \lim_{N\to\infty} S_N(g)$ is generally possible. To illustrate the results, we have shown, in figure 2, typical variations of R_N as a function of N for different values of negative g, in the vicinity of $g = 0$. As expected $R_\infty(g)$ increases monotonically when g is increased from $g = -\infty$ to $g = 0$. No special behaviour is associated with $g = -\infty$, in contrast with the case $g = \infty$ corresponding to the SAW. Both $R_\infty(g)$ and $S_\infty(g)$ diverge at $g = 0$, following an appropriate power law: $R_\infty(g) \simeq (-g)^{-\nu'}$ and $S_\infty(g) \simeq (-g)^{-s'}$. The best fit of data, close to $g = 0$, leads to the following estimation for exponents: $\nu' = 0.98 + 0.02$ and $s' = 0.99 + 0.02$ respectively. These values are to be compared with the predictions of the scaling analysis: $\nu' = s' = 1$ (see below). It should be noted that errors in ν' and s' estimations reflect the range of plateau levels and extrapolation procedure.

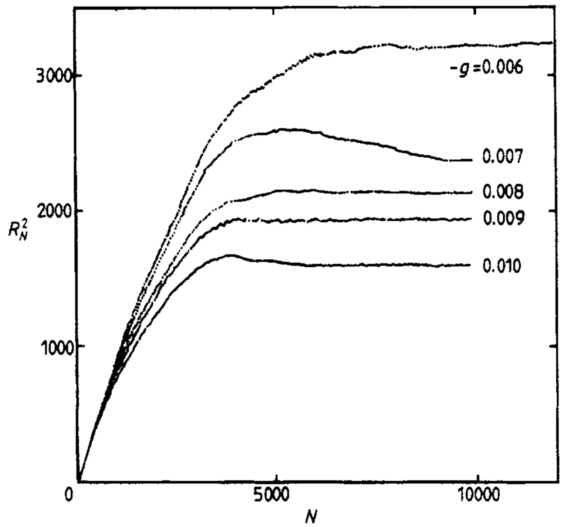

Figure 2. Variation of R_N against N, for different negative values of the strength parameter g in the vicinity of $g = 0$. An average over 4×10^4 runs was performed for each value of g.

The asymptotic properties of the TSAW are therefore very sensitive to the relative sign of the parameter g. In contrast with more simple choices for $W_i^\pm$, the above one (equation (1)) leads to a remarkable phenomenon for $g > 0$ as for $g < 0$. The 'self-attracting' RW has received little study in the past. It is not clear for us to what extent the result obtained here is universal. Other behaviours, corresponding to other choices for $W_i^\pm$, are also possible and cannot be excluded. Our results show the richness of the self-attracting RW and call for further work following similar lines of investigation.

In what follows we will show that the main asymptotical properties of the TSAW can be analysed with the help of a simple scaling argument. From the work of Amit *et al* (1983), it is easy to show that, in a perturbation calculation around $g = 0$, the expansion parameter is $gN^{1-d/2}$ rather than g. For $d = 1$, this leads to a 'virial expansion' in the reduced parameter $z = gN^{1/2}$. The result for R_N can be stated as follows:

$$R_N^2 = N\phi(gN^{1/2}) \tag{2}$$

where $\phi(z) = 1 + a_1 z + a_2 z^2 + \ldots$, and $a_1, a_2 \ldots$ denote numerical factors. The validity of equation (2) was proved by Amit *et al* (1983) up to second order in z. We assume here its validity at all orders in z.

For $g>0$, equation (2) shows that a RW-to-TSAW crossover takes place at $N \simeq N^* \sim g^{-2}$. Assume the following behaviour of R_N in the TSAW regime,

$$R_N \simeq a(g) N^{\nu}, \tag{3}$$

where $a(g)$ is a prefactor which depends on the repulsion parameter g. Matching equation (3) with the RW regime at $N \sim N^*$, one obtains finally

$$a(g) \sim g^{2\nu-1}. \tag{4}$$

From (3), (4) we deduce the scaling law for R_N:

$$\text{TSAW: } gR_N \simeq (gN^{1/2})^{2\nu}, \qquad \text{RW: } gR_N \simeq (gN^{1/2}). \tag{5}$$

Stated otherwise, $\phi(z) \equiv R_N^2/N$ is a universal function of the scaling variable $z \equiv gN^{1/2}$, with the following limits:

$$\begin{aligned} \phi(z) &= 1 + a_1 z + a_2 z + \ldots && \text{at } z \ll 1, \\ &\simeq z^{2(2\nu-1)} && \text{at } z \gg 1. \end{aligned} \tag{6}$$

Perturbation calculation at large g involves the reduced variable Ne^{-g}. The SAW-to-TSAW crossover can be analysed following the same line of argument. This point will not be discussed further here. In figure 3, we have shown the universal plot for R_N, which exhibits clearly the RW-to-TSAW crossover, according to (5).

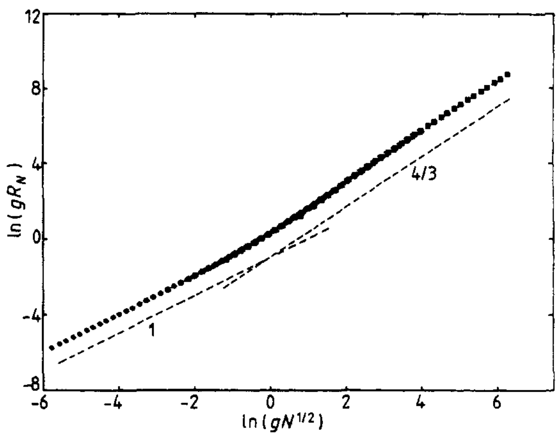

Figure 3. Universal plot of R_N against N, with scaling variables: gR_N against $gN^{1/2}$, showing the RW-to-TSAW crossover. Broken lines, of slopes 1 and $\frac{4}{3}$ respectively, are shown for comparison. □, $g=1$; ▲, $g=3$; ⧖, $g=0.1$; ○, $g=0.03$; ◆, $g=0.01, 0.003, 0.001$.

For $g<0$, the scaling variable $z = gN^{1/2}$ implies, in a saturation regime, the result

$$R_\infty^2(g) \simeq (-g)^{-2\nu'} \tag{7}$$

with $\nu' = 1$. The corresponding plot is shown in figure 4.

The same scaling analysis leads to the prediction $s' = 1$ for the exponent of $S_\infty(g)$, and similar expressions at $g>0$, with $s=\nu$. In one dimension S_N and R_N have the

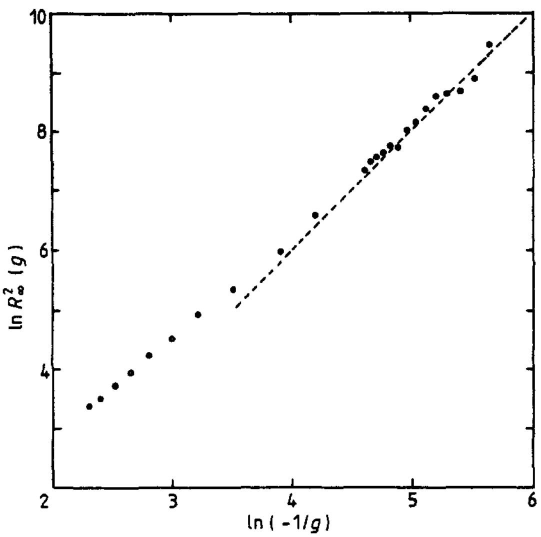

Figure 4. Power law behaviour of the limiting value $R^2_\infty(g) = \lim_{N\to\infty} R^2_N(g)$ as function of g (negative) close to $g = 0$. The broken line has the slope 2, predicted by the scaling analysis.

same exponents. The meaning of this is evident from the consideration that the RMS excursion of the walker is proportional to N^ν, and in *one dimension*, while sites inside this distance will almost always have been visited, sites outside it will not. This argument is known to be exact for $g = 0$. Our results support its validity for all g.

Using the numerical results, we have checked that the expression of $\phi(z)$ in powers of z gives the correct slope of R^2_N/N at $z = 0$; $a_1 = 2\pi^{1/2}/3 = 1.1816\ldots$. The singular behaviour at $g < 0$ leads to the following conclusion. The expansion of R^2_N/N in powers of z has a radius of convergence near $|z| \sim N^{-1/2}$, gives the correct slope a_1 at $z = 0$, but such a function cannot be generally used for finite z. The perturbation series for R^2_N/N is not convergent except at $z = 0$. It is doubtful that the first few terms of this series can provide any insight into the asymptotic behaviour of R_N at finite z. This suggests strongly that the perturbational approach is fruitless.

In summary, we have presented in this letter a brief report on a Monte Carlo study for the TSAW in one dimension. Our results provide strong support for the value $\nu = \frac{2}{3}$ of the RMS displacement exponent $R_N \sim N^\nu$, for all values $(0 < g < \infty)$ of the repulsion parameter. A similar behaviour was found also for the range $S_N \sim N^s$ of the TSAW. For negative g (self-attracting walks), we have shown a saturation effect, corresponding to a self-trapping of the walker, with $R_\infty(g) \sim (-g)^{-1}$ and $S_\infty(g) \sim (-g)^{-1}$ at $g < 0$. A simple scaling analysis of the TSAW statistics was outlined, providing in particular a simple explanation of the singular behaviour at $g \leqslant 0$. In this respect, it is of interest to extend this study $(g \leqslant 0)$ to $d = 2$. Extension to fractal structures is now in progress (Angles d'Auriac and Rammal 1983). Comparison with other models of correlated RW and more detailed results will be reported in a forthcoming paper (Rammal *et al* 1983).

We are grateful to Dr G Toulouse and Professor L Peliti for stimulating discussions. After this work was completed, we learned that J Bernasconi and L Pietronero (1983

preprint) have also performed similar calculations for ν at $g > 0$. Their results are in very good agreement with ours. We thank Professor L Peliti for bringing this work to our attention.

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