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LETTER TO THE EDITOR

The generalised true self-avoiding walk—a model with continuously variable exponent ν

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Abstract. The true self-avoiding walk is generalised by admitting that the self-avoidance parameter depends on the past history of the walk. For the generalised model the end-to-end distance exponent ν is calculated by a method that gives the same result as a Flory-type theory for the usual true self-avoiding walk. The exponent ν is predicted to be continuously variable with one of the parameters of the generalised model. The resulting expression for the exponent ν is confirmed by Monte Carlo simulations.

Recently Amit *et al* (1983) have introduced the true self-avoiding walk (TSAW) which describes the path of a random walker who tries to avoid regions in space visited previously. The properties of this random-walk model are completely different from the properties of the usual self-avoiding walk (SAW), which is a random walk with no self-intersections allowed. For instance, the models differ in their critical exponents and even in their upper critical dimensionalities ($d_c = 2$ for the TSAW while $d_c = 4$ for the SAW (de Gennes 1979)).

In contrast to the SAW, which turned out to provide a fundamental and very accurate model for the configurations of polymers in good solvents (de Gennes 1979), the TSAW seems to be realised in very special physical situations only (Bulgadaev and Obukhov 1983, Family and Daoud 1984). However, great theoretical interest in various generalised random-walk models (Duxbury *et al* 1984, Duxbury and de Queiroz 1984 and references therein) stems from their unusual critical properties.

The TSAW on a d -dimensional lattice is defined as follows. Starting at the origin, the random walker has to move at any step to one of the $2d$ nearest neighbours of the current position i_0 . The probability p_i for moving to the neighbouring site i depends on the number of previous visits n_i of site i through

$$p_i \sim \exp(-gn_i) \quad (1)$$

where the parameter g defines the strength with which the walk avoids itself ($g > 0$).

From a self-consistent approach to the TSAW Pietronero (1983) obtained the universal (independent of g for $0 < g < \infty$) end-to-end distance exponent $\nu = 2/(d+2)$ for $d \leq d_c = 2$ (see also Obukhov 1984, Family and Daoud 1984, Öttinger 1985a). The non-trivial result $\nu = \frac{2}{3}$ in one dimension was confirmed by Monte Carlo simulations (Rammal *et al* 1984, Bernasconi and Pietronero 1984) and by exact enumeration methods (Stella *et al* 1984). The universality of ν has also been supported by renormalisation group studies (de Queiroz *et al* 1984, Obukhov and Peliti 1983, Peliti 1984).

This letter deals with a generalisation of the TSAW which has a very unusual critical property: the exponent ν varies continuously with one parameter of the model. The TSAW is generalised by admitting that the self-avoidance parameter $g(n_0)$ depends on the number of previous visits n_0 of the random walker's current position i_0 . This type of generalisation arises quite naturally if one performs a Monte Carlo renormalisation group study of the TSAW (moreover, one finds an additional tendency to avoid stepping backwards to the site the walker visited immediately before (Öttinger 1985b); in the continuum language, this tendency leads to an enlarged diffusion coefficient which has already been observed by Amit *et al* (1983)). More precisely, we consider the following form of $g(n)$,

$$g(n) = gn^\alpha, \quad (2)$$

involving the parameters g and α only (this generalised TSAW includes the usual TSAW for $\alpha = 0$). We then derive a Flory-type expression for the exponent ν of the generalised TSAW defined by equations (1) and (2) and compare this expression with Monte Carlo results. A brief summary concludes the letter.

For the one-dimensional TSAW in the case of a small self-avoidance parameter Obukhov (1984) obtained a partial differential equation for the dependence of the end-to-end probability distribution $P_N(x)$ on the number of steps N of the walk and the position x ; he found the exponent $\nu = \frac{2}{3}$. Subsequently, Öttinger (1985a) generalised Obukhov's method to arbitrary dimension (in this way, Pietronero's result $\nu = 2/(d+2)$ for $d \leq 2$ was re-derived) and used it to calculate the scaling functions in one dimension. The same method will now be used to derive the exponent ν for the generalised TSAW (1) and (2) for arbitrary dimension d .

That starting point is the Fokker-Planck equation

$$\frac{\partial P_N(x)}{\partial N} = \frac{1}{2} \Delta_x P_N(x) + 2 \frac{\partial}{\partial x} \left(P_N(x) g(n_N(x)) \frac{\partial n_N(x)}{\partial x} \right) \quad (3)$$

where the first term on the right-hand side (involving the Laplace operator) represents a random diffusion and the second term describes a drift which is given by the gradient of the total number of previous visits $n_N(x)$ of point x because the TSAW tries to avoid places already visited (in the limit of large N the variables N and x can be treated as continuous).

Assume that for a fixed value of the parameter α scaling laws of the form (Pietronero 1983, Bernasconi and Pietronero 1984)

$$P_N(x) = (1/R_N^d) f(x/R_N) \quad (4)$$

$$n_N(x) = (N/R_N^d) h(x/R_N) \quad (5)$$

are valid where

$$R_N = \lambda_g N^\nu \quad (6)$$

is the root-mean-square displacement; then by inserting these expressions in equation (3) (with $z = x/R_N$) one obtains

$$-\nu(df(z) + zf'(z)) = \frac{N^{1-2\nu}}{2\lambda_g^2} \Delta_z f(z) + 2g \frac{N^{2+\alpha-\nu[2+(1+\alpha)d]}}{\lambda_g^{2+(1+\alpha)d}} \frac{\partial}{\partial z} \left(f(z) (h/z)^\alpha \frac{\partial}{\partial z} h(z) \right). \quad (7)$$

Provided that the asymptotic behaviour of the generalised TSAW is determined by the self-avoidance, the second term on the right-hand side of equation (7) has to be of the same order of magnitude as the left-hand side (in the limit $N \rightarrow \infty$). Thus, for the exponent ν of the generalised TSAW (independent of the parameter g) one obtains

$$\nu = (2 + \alpha) / [2 + (1 + \alpha)d]. \quad (8)$$

This result is only correct if the influence of the self-avoidance is sufficiently strong for $N \rightarrow \infty$, more precisely if $\alpha > -1$ (independent of d) and below the upper critical dimension $d_c = 2$ (independent of α), because otherwise the pure random-walk term on the right-hand side of equation (7) (with $\nu = \frac{1}{2}$) dominates. Figure 1 shows the dependence of the exponent ν on the parameter α of the generalised TSAW in one dimension. For $\alpha = 0$ equation (8) reproduces Pietronero's (1984) result.

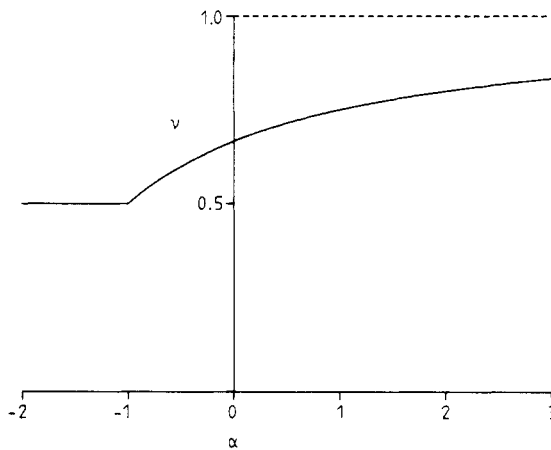


Figure 1. End-to-end distance exponent ν as a function of the parameter α as predicted by equation (8) for the one-dimensional generalised TSAW (the broken line indicates the limiting value of ν for $\alpha \rightarrow \infty$).

Because the scaling functions f and h should be independent of g , one concludes from equation (7) that

$$\lambda_g \sim g^{1/[2+(1+\alpha)d]}. \quad (9)$$

The results (8) and (9) will now be compared with Monte Carlo simulations of the generalised TSAW (1) and (2) in one dimension for several values of g and α .

For each combination of g and α displayed in table 1 10 000 walks of up to 100 000 steps have been generated in order to estimate the root-mean-square displacement (these simulations took about 45 h of CPU time on a Sperry 1100/82 computer). Figure 2 shows the results for $\alpha = \frac{1}{2}$ and two different values of g (the error bars on the data are smaller than the size of the symbols). The straight lines indicate the slope $\omega = \frac{3}{5}$ predicted by equation (8) for $d = 1$ and $\alpha = -\frac{1}{2}$. Though it is rather delicate to estimate asymptotic exponents from numerical results for finite N , the data of figure 2 and table 1 provide strong support for the prediction (8).

Equation (9) has been checked for two different values of α . This equation is expected to yield good results for $\alpha < 0$ because in the derivation of the basic equation

Table 1. Monte Carlo results for the exponent ν (column 4) compared with the Flory-type prediction $\nu = (2 + \alpha)/(3 + \alpha)$ (column 3) for several values of the parameters α and g of the one-dimensional generalised TSAW.

α	g	ν	ν_{MC}
$-\frac{3}{4}$	1	$\frac{5}{4}$	0.546 ± 0.009
$-\frac{1}{2}$	1	$\frac{3}{2}$	0.602 ± 0.007
$-\frac{1}{2}$	$\frac{1}{3}$	$\frac{5}{3}$	0.607 ± 0.009
$-\frac{1}{3}$	1	$\frac{5}{3}$	0.631 ± 0.008
$-\frac{1}{3}$	$\frac{1}{3}$	$\frac{7}{6}$	0.636 ± 0.009
$+\frac{1}{3}$	1	$\frac{7}{10}$	0.702 ± 0.006

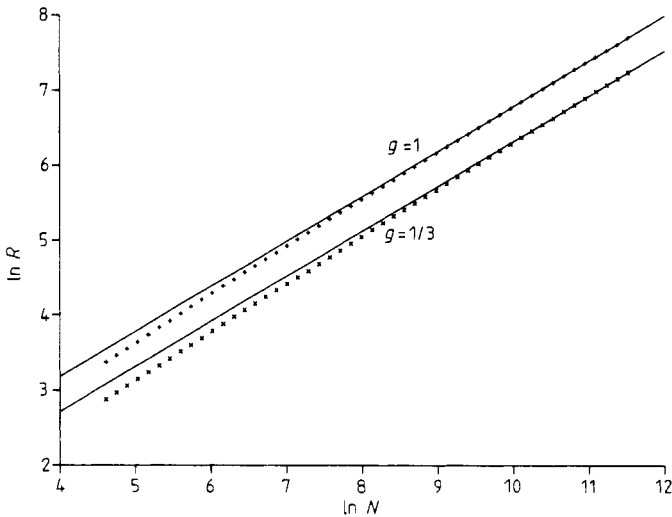


Figure 2. Root-mean-square displacement R_N as a function of number of steps N for the one-dimensional generalised TSAW for $\alpha = -\frac{1}{2}$ and two different values of g .

(3) (Obukhov 1984) $g(n)$ was assumed to be small (for $\alpha < 0$ one has $g(n) \rightarrow 0$ for $n \rightarrow \infty$). The Monte Carlo results for $\alpha = -\frac{1}{2}$, $\lambda_1/\lambda_{1/3} = 1.58 \pm 0.02$, and for $\alpha = -\frac{1}{3}$, $\lambda_1/\lambda_{1/3} = 1.52 \pm 0.02$, are in good agreement with equation (9), which predicts the values 1.55 and 1.51, respectively.

We have generalised the TSAW by admitting that the self-avoidance parameter depends on the number of previous visits of the random walker's current position. This type of generalisation arises quite naturally if one renormalises the usual TSAW. By writing down a partial differential equation for the end-to-end probability distribution one obtains (for arbitrary dimension) an expression for the end-to-end distance exponent ν of the generalised TSAW. For the usual TSAW this method (introduced by Obukhov 1984) gives the same result as a Flory-type theory. The exponent ν obtained in this way (equation (8)) is continuously variable with the parameter α of the generalised TSAW defined by equations (1) and (2). Finally, these theoretical predictions for the exponent ν and the coefficients λ_g in equation (6) have been confirmed by Monte Carlo simulations.

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