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LETTER TO THE EDITOR

Scaling and crossover in the one-dimensional true self-avoiding walk

S L A de Queiroz†, A L Stella‡ and R B Stinchcombe
Department of Theoretical Physics, 1 Keble Road, Oxford OX1 3NP, UK

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Abstract. We apply scaling and crossover arguments to the one-dimensional true self-avoiding walk, which avoids itself with strength g. The problem is formulated in terms of a grand canonical ensemble; a real-space renormalisation-group analysis shows that for large repulsion, $x = e^{-g}$ is a relevant variable causing crossover from the self-repelling chain (SRC) limit, with crossover exponent $\phi = 1$. A physical interpretation of this result is given in terms of competition between the correlation length and the average distance before the walk turns back on itself. The resulting flow suggests the existence of an intermediate attractive fixed point which makes the exponent ν different from SRC and random-walk values for all x between 0 and 1, in agreement with recent Monte Carlo results.

The term 'self-avoiding random walk' (SAW) has long since been used to refer to the statistical problem of a traveller who steps at random, with the constraint that he is *not allowed* to visit any given place more than once. This is a suitable model to describe the configurational properties of polymeric chains in good solvents (see e.g. de Gennes 1979 and references therein). Recently, however, Amit *et al* (1983) have introduced the problem of the traveller who steps at random but *tries to avoid* places he has already visited, and called this the 'true self-avoiding walk' (TSAW); they argue that the model for polymers, described above, which they prefer to call the 'self-repelling chain' (SRC), should be quite different from the TSAW, and indeed find that the upper critical dimensionality is two for the TSAW, whereas it is four for the SRC (de Gennes 1979). They also studied the logarithmic corrections to scaling at $d = 2$, while Obukhov and Peliti (1983) improved the discussion of such corrections. Pietronero (1983) introduced a self-consistent approach to the TSAW from which he obtained $d_c = 2$ as well as an explicit approximate expression for the 'correlation length' exponent ν for $d \leq 2$, namely

$$\nu = 2/(d+2), \qquad d \leq 2. \tag{1}$$

Though at present it is still not clear what kind of physical phenomenon the TSAW could model (diffusion in a medium with cumulative memory effects being perhaps a likely candidate), it displays some rather unique features which make it deserve further attention from the viewpoint of lattice statistics in its own right, as we shall see.

† On leave from Departmento de Fisica, PUC, 22452 Rio de Janeiro, Brazil.
‡ Permanent address: Dipartimento di Fisica e Unità GNSM del CNR dell'Università di Padova, Padova, Italy.

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Even in one dimension ($d = 1$), the TSAW is interesting and far from trivial. There, Pietronero's expression gives $\nu = \frac{2}{3}$, which is different from both the SRC exponent ($\nu = 1$) and the random walk exponent ($\nu = \frac{1}{2}$). Indeed, Monte Carlo simulations give $\nu = 0.67 \pm 0.01$ in this case (Bernasconi and Pietronero 1983).

In this letter we use scaling and crossover arguments to discuss the TSAW for $d = 1$. The special features are more evident near the SRC limit, and this regime is given particular attention.

The problem is defined in the following way (Amit *et al* 1983): on a lattice, the traveller has to move to one of the z nearest neighbours of the site he is at. The probability P_i of moving to a site i depends on the number of times n_i this site has already been visited:

$$P_i = \exp(-gn_i) / \sum_{j=1}^{z} \exp(-gn_j). \tag{2}$$

The parameter g defines the strength with which the walk avoids itself; the differences between the statistics of this problem and that of the SRC are discussed in Amit *et al* (1983) and Pietronero (1983). In particular, the ordinary random walk (RW) is recovered if $g = 0$, for any space dimensionality; however, it is only in one dimension that the problem becomes the same as the SRC as $g \to \infty$ (which we then call the SRC limit). For space dimensionalities greater than one, 'self-trapped' configurations which are dead ends for SRCs (and hence are not taken into account e.g. in Monte Carlo configuration-generating programmes (Rosenbluth and Rosenbluth 1955)) have a way out in the TSAW case even if $g = \infty$, because of normalisation condition (2) above. Accordingly, the discussion of the $g \to \infty$ limit in two dimensions has concentrated on what the corrections to mean-field behaviour must be, rather than on whether or not there should be a crossover to a SRC regime (Obukhov and Peliti 1983).

Two crossovers must then be expected to exist for a one-dimensional TSAW, as the repulsion parameter is varied from zero to infinity: one from zero to non-zero g (RW $\to$ TSAW) and the other as $g \to \infty$ (TSAW $\to$ SRC). As for the first case, the relevance (the word being taken here in a renormalisation-group sense) of excluded-volume forces is a feature well known to be displayed by models for the θ-transition of polymers in poor solvents (de Gennes 1975, 1979), as well as by a model recently introduced by Stanley *et al* (1983), which is not equivalent to the TSAW, although similar to it. The relevance of anisotropy in random (Derrida and Pomeau 1982) or pure (Napiorkówski 1983) diffusion problems should also be pointed out, for these are further examples of instability of the pure RW relative to perturbations. Thus, it is not all surprising that the one-dimensional TSAW with $g \neq 0$, however small, belongs to a different universality class from the RW, as argued by Pietronero (1983): the existence of a physical mechanism, no matter how weak, which prevents the walk from having equal step probabilities will eventually be dominant on larger scales. This view is consistent with the 'blob' picture of de Gennes (1979).

On the other hand, things are not so clear in the SRC limit, at least as regards the physical mechanism underlying the crossover between TSAWs and SRCs. In what follows, we formulate the problem in terms of a grand canonical ensemble and present a real-space renormalisation-group (RSRG) scheme within which the SRC limit is discussed. A physical picture is presented for the SRC limit, which gives results consistent with those obtained from scaling. It is to be noted also that in this limit Pietronero's effective-medium approach fails, as pointed out by that author (Pietronero 1983); in this sense our approach is complementary to his, whereas we raise some questions of our own as well.

In order to formulate the problem in terms of a grand canonical ensemble, we first associate a fugacitiy K to each step of the walk (Shapiro 1978, de Gennes 1979). We denote a generic walk by α, $|\alpha|$ being the number of steps and r_α its end-to-end (scalar) distance. With $x \equiv e^{-g}$, the probability $P(\alpha, x)$ of a walk α can be deduced from equation (2), with the following normalisation condition:

$$\sum_{\alpha, |\alpha| = N} P(\alpha, x) = 1 \tag{3}$$

for a fixed N. In the grand canonical ensemble, each walk α will be assigned a weight $w(\alpha, x)K^{|\alpha|}$, with $w(\alpha, x)$ proportional to $P(\alpha, x)$. Since for $x = 0$ the only walks with non-zero probability are those with maximal end-to-end distance ($r_\alpha = |\alpha|$) which we denote by $\alpha_{\max}$, a sensible choice is $w(\alpha_{\max}, x) = 1$ for all x, and $w(\alpha, x) = P(\alpha, x)/P(\alpha_{\max}, x)$ for $\alpha \neq \alpha_{\max}$ and $|\alpha| = |\alpha_{\max}|$, and all x. As the number of steps grows large, we expect

$$\sum_{\alpha, |\alpha| = N} w(\alpha, x) \sim N^{\gamma - 1} K_c(x)^{-N} \tag{4}$$

in analogy with the SRC problem (McKenzie 1976, de Gennes 1979). Here, γ is the suceptibility exponent, which equals one in 1D for both $x = 0$ (SRC) and $x = 1$ (RW); the connective constant K_c equals 1 for $x = 0$ and $\frac{1}{2}$ for $x = 1$. Actually, since the weights in our problem are written in terms of probabilities satisfying normalisation condition (3), it follows that $K_c(x) = (1 + x)^{-1}$ and $\gamma = 1$ for all x. In what follows, we shall concentrate on the average end-to-end distance

$$\langle \xi(K, x) \rangle = \frac{\sum_N \sum_{\alpha, |\alpha| = N} r_\alpha w(\alpha, x) K^N}{\sum_N \sum_{\alpha, |\alpha| = N} w(\alpha, x) K^N} \tag{5}$$

which is expected to diverge as $(K_c(x) - K)^{-\nu}$ for $K \to K_c(x)^-$, the exponent ν being the same as that discussed by Pietronero (1983).

A RSRG transformation with a scaling factor b should consist of a regular mapping $(K, x) \to (K', x')$, such that $\xi(K', x') = b^{-1}\xi(K, x)$. From the analysis of the fixed points on the critical line $K_c = K_c(x)$ (which should be invariant under the transformation) and their stability, one should obtain the possible values of ν. We have not been able to obtain a set of transformation equations for general (K, x); however we have succeeded in treating the $x \sim 0$ region in a way consistent with what is known for $K_c(x)$. This already allows us to gain considerable physical insight into the crossover between TSAW and SRC in 1D.

First we note that at $x = 0$ no path reversal is allowed, hence $x' = x = 0$. For K' we just apply the standard connectivity ideas used in RSRG to obtain $K' = K^b$ for a b-bond cell, so $(K^*, x^*) = (1,0)$ is a fixed point at which $\nu = \ln b/\ln \lambda = 1$ for all b. These are the exact results for the SRC in 1D (McKenzie 1976).

Near $x = 0$, besides the maximal end-to-end distance walks, one must take into account walks that turn back. A reversal of an $\alpha_{\max}$ path implies a weight reduction from 1 to order x; the simplest modifications of an $\alpha_{\max}$ path are shown in figure 1. For both (a) and (b), up to order x, the weight w is just $x/2$; the factor $\frac{1}{2}$ is necessary because, after the backward step at A, the walk has the same probability of proceeding to the right (a) or to the left (b) when leaving B (see equation (2)).

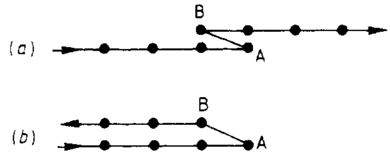

Figure 1. (*a*) and (*b*) Two paths with the same probability to order x (see text).

Of course, other reversals can occur further along the way; however, at $x \sim 0$ we expect that the overall density of backward steps will be low enough so they can be treated independently. For example, one can easily check from figure 1(*b*) that if the walk turns back to the right again, its weight will be $x^2/4$, provided that the second reversal occurs far enough from A.

We thus expect that a 'low density of return steps' approximation correctly applies to the calculation of the transformation in the neighbourhood of $x = 0$. To first order in x, we count in the transformation of K (for rescaling $b = 2$), the three paths in figure 2(*a*), where we make use of the 'centre rule' of Napiorkówski (1983).

This leads to

$$K' = K^2 + xK^4 + O(x^2). \tag{6}$$

This transformation takes into account the fact that, for a $b = 2$ cell, there are only two ways of inserting a modification of the type shown in figure 1(*a*). Under coarse graining these modifications are just smoothed out, and contribute to the effective K'.

In order to determine x' to first order, we must look for the paths which, at the site level, contribute to what would be a reversal as the one shown in figure 1(*b*), at the cell level. We easily realise that these are the configurations shown in figure 2(*b*) for $b = 2$. This means that

$$\tfrac{1}{2}x' = \tfrac{1}{2}x + \tfrac{1}{2}K^2x + O(x^2). \tag{7}$$

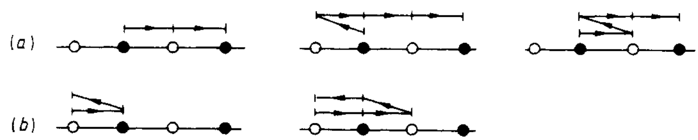

Figure 2. (*a*) Configurations that are counted for the K rescaling. (*b*) Configurations that are counted for the x rescaling. Here $b = 2$. The renormalised lattice is built up by black sites only.

For a general scaling factor b, equations (6) and (7) can be easily generalised as

$$K' = K^b + O(x), \qquad \frac{x'}{2} = \frac{x}{2} \sum_{l=0}^{b-1} K^{2l} + O(x^2), \tag{8a, b}$$

from which it follows that near the SRC fixed point ($K^* = 1$, $x^* = 0$), $x' = bx$, i.e. x is a relevant parameter. Further, since the Jacobian of the transformation is triangular at the SRC fixed point, the eigenvalues are both equal to b, as can be seen from (8). Hence, the crossover exponent is

$$\phi = (\ln \lambda_k)/(\ln \lambda_x) = 1. \tag{9}$$

This is consistent with a straight critical line near $x=0$, as implied by $K_c(x)=(1+x)^{-1}$, referred to above. In order to gain further physical insight into this result, we recall that at $x\sim 0$ the average number of steps betwen two reversals is of order x^{-1}; this implies the existence of a diverging characteristic length: $N\sim x^{-1}$, for x approaching zero. On the other hand, at the SRC limit $x=0$ the correlation length diverges as

$$\xi_s \propto \delta K^{-\nu_s} \tag{10}$$

with $\delta K = K_c - K$, $K_c=1$, $\nu_s=1$.

We can see then that the physical mechanism underlying the crossover between TSAW and SRC is the competition between these two diverging lengths. From standard scaling arguments it follows that near the SRC limit the correlation length must behave as

$$\xi = \xi_s f(N/\xi_s). \tag{11}$$

Alternatively, the crossover may be viewed in terms of the (relevant) variables x and δK:

$$\xi = \xi_s F(x^{\phi}/\delta K) \tag{12}$$

where ϕ is the crossover exponent.

Comparing (11) and (12),

$$f(N/\xi_s) = F(N^{-\phi}/\xi_s^{-1}) = \tilde{F}(N^{\phi}/\xi_s) \tag{13}$$

so $\phi=1$.

Thus we have a physical explanation of the renormalisation-group result obtained above, which is related to the fact that at $x\sim 0$ the TSAW is similar to a RW with (average) step length N.

The fact that $\phi>0$, that is, x is a relevant variable, has important consequences when combined with standard views about the behaviour near $x=1$: at the $g=0$, RW limit, it is well known that the existence of a physical mechanism that disturbs the isotropic step probability distribution drives one away from the pure RW behaviour (actually a qualitative, effective-medium-like discussion shows that it must happen also for the TSAW case with $x\sim 1$, so nothing surprising is expected in this limit). We are then left with a renormalisation-group flow that is unstable *both* at the RW and the SRC limits: this can only be consistent with a third non-trivial fixed point on the critical frontier in the (K, x) plane, with $x_c \neq 0$, 1 which must be stable along the critical line, as shown schematically in figure 3. This then implies that the exponent for the TSAW in 1D is the same for any finite, non-zero value of the repulsion parameter g, and different from both that of the RW and that of the SRC. This conclusion has been very

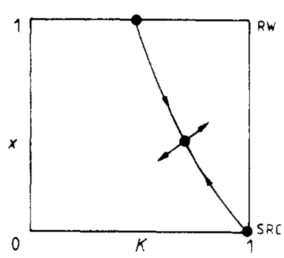

Figure 3. Schematic picture of inferred fixed points and flow.

recently confirmed by the Monte Carlo simulations of Bernasconi and Pietronero (1983).

The precise location of the new intermediate fixed point would be interesting. Further work is in progress along this line.

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