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LETTER TO THE EDITOR

Generalised self-avoiding walk

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Abstract. A generalisation of the self-avoiding walk is introduced in which k or higher multiple points are forbidden ($k = 2$ corresponds to the standard self-avoiding walk). The Flory theory gives the radius of gyration exponent $\nu_k = (k+1)/[(k-1)E+2]$ when $E \leqslant E_c(k) = 2k/(k-1)$. E is the Euclidean dimension of the problem and $E_c(k)$ the upper critical dimension which is also obtained using the fractal set theory.

In the self-avoiding walk (SAW) or excluded volume problem (Barber and Ninham 1970, de Gennes 1979 and references therein) one studies the statistics of a chain without self intersection, equal weights being assigned to the allowed configurations. On a Flory–Huggins lattice (Flory 1953) with mesh size a and Euclidean dimension E, the end-to-end distance for large N is

$$R_N \cong aN^{\nu} \tag{1}$$

where N is the number of steps in the walk. The critical exponent ν is a function of E for $E < E_c = 4$, the upper critical dimension above which the exclusion effect becomes irrelevant. The chain is then Gaussian (random walk with $\nu = \frac{1}{2}$) at large scale.

This problem has been generalised in the Domb–Joyce model (see Domb 1983 for a review) where a weighting factor $1-\omega$ is associated with the self intersections. In the limit $\omega = 0$, a standard random walk is obtained whereas the SAW problem corresponds to $\omega = 1$.

In this letter the SAW is generalised in the following way: the exclusion effect does not take place when a given site is visited less than k times, i.e. allowed configurations have no multiple points of order k (k-multiple points) or more. Such a walk will be called a k-SAW. When $k = 2$ the standard SAW is recovered.

Two different approaches will be used: first the Flory theory (Flory 1953) which is known to give quite accurate values of ν for the standard SAW where the Flory exponent

$$\nu = 3/(E+2) \tag{2}$$

is exact when $E = 1$ or 2 (Nienhuis 1982) but slightly differs from the $\varepsilon = 4-E$ expansion result near E_c (Wilson and Fisher 1972, de Gennes 1972):

$$\nu = \tfrac{1}{2} + \tfrac{1}{16}\varepsilon + O(\varepsilon^2) \quad (\varepsilon \text{ expansion}) \qquad \nu = \tfrac{1}{2} + \tfrac{1}{12}\varepsilon + O(\varepsilon^2) \quad (\text{Flory theory}) \tag{3}$$

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and second the theory of fractal sets (Mandelbrot 1982). For large N values a SAW may be considered as a fractal object with fractal dimension

$$D = 1/\nu \tag{4}$$

so that $D = 2$ for a random walk. Using the fractal properties of the random walk and of its self intersections, Mandelbrot was able to show that $E_c = 4$ in the SAW problem. The same methods will be used here to find out the upper critical dimension $E_c(k)$ of the k-SAW.

The trial Flory free energy for a k-SAW may be written

$$\frac{F_k(R)}{k_B T} = \frac{3R^2}{2a^2N} + \sum_{l=0} v_l \frac{N^{k+l}}{R^{(k+l-1)E}} \tag{5}$$

where the first term is the elastic free energy of a swollen ideal chain† and the second gives the mean field interaction energies between $k, k+1, \ldots, k+l \ldots$ monomers. In a first step, let us ignore the interactions between more than k monomers, an approximation which will be justified below. Through a minimisation of the free energy, we get

$$R_N \cong aN^{(k+1)/[(k-1)E+2]}. \tag{6}$$

The lth term in the interaction energy reads

$$\mathscr{E}_l = k_B T v_l (N^{k+l}/R_N^{(k+l-1)E}) \sim N^{[2(k+l)-E(k+2l-1)]/[(k-1)E+2]}. \tag{7}$$

Higher-order interaction terms $\mathscr{E}_l$ are comparable to $\mathscr{E}_0$ when

$$2(k+l) - E(k+2l-1) = 2k - E(k-1) \tag{8}$$

i.e. when $E = 1$. In higher Euclidean dimensions the interaction terms with $l > 0$ are irrelevant and the approximation leading to (6) is justified. It follows that the fractal dimension of a k-SAW is

$$D_k = 1/\nu_k = [(k-1)E+2]/(k+1). \tag{9}$$

When $E = 1$, we get $D_k = 1\ \forall k$, a result which cannot be modified by higher-order interactions. At the upper critical dimension $\mathscr{E}_0$ (equation (7)) becomes marginal ($\mathscr{E}_0 \sim N^0$) or ν_k takes on the random walk value $\nu = \frac{1}{2}$ so that

$$E_c(k) = 2k/(k-1). \tag{10}$$

With $k = 2$ the standard SAW results are recovered.

An extensive use of the two following rules (Mandelbrot 1982) will be made.

(a) *Codimension additivity.* Let S_1 and S_2 be two independent fractal sets in E-dimensional Euclidean space and let $\bar{D}_{1(2)} = E - D_{1(2)}$ be their codimensions; the codimension of their intersection $S_1 \cap S_2$ is

$$\bar{D}_I = E - D_I = \min[E, \bar{D}_1 + \bar{D}_2]. \tag{11}$$

As a consequence two sets of the same dimension D miss one another (have an intersection of dimension zero) when $E \geqslant 2D$. The rule may be extended to more than two sets in an obvious way.

† A logarithmic contribution to the elastic free energy which, at large N, is irrelevant for R_N below E_c has been omitted in (5).

(b) *Replica trick.* For a random set S, with fractal dimension D, the set of its k-multiple points has the same fractal dimension as the intersection of k replicas of S. Applying rule (a), the set of k-multiple points has a fractal dimension

$$D_{\mathrm{I}}(k) = \max[0, E - k(E-D)]. \quad (12)$$

The upper critical dimension E_c of the SAW follows from these two rules (Mandelbrot 1982) by looking at the self intersections of a random walk with $D=2$. Using (12) one gets $D_{\mathrm{I}}(2)=0$ when $E \geqslant 2D$, so that a random walk is self avoiding when $E \geqslant E_c = 4$.

Let us now turn to the k-SAW. Equation (12) tells us that a random walk is k self avoiding, i.e. its set of k-multiple points is of fractal dimension $D_{\mathrm{I}}(k)=0$, when

$$E \geqslant E_c(k) = 2k/(k-1) \quad (13)$$

and the Flory theory result is recovered. It may be also verified that higher-order multiple points play no role at and above E_c since $E_c(k+1) < E_c(k)$.

In the following discussion, first let us mention that upper and lower bounds on $D_k = 1/\nu_k$ below $E_c(k)$ may be deduced from the fractal theory. An upper bound is given by the Euclidean dimension E since a fractal always has (Mandelbrot 1982)

$$D_k \leqslant E. \quad (14)$$

Assuming that rules (a) and (b) still apply for the j-multiple points ($j<k$) below $E_c(k)$†, the fractal dimension $D_{\mathrm{I}}(j)$ of the j-multiple points for k-SAW must be greater than zero below $E_c(k)$, otherwise the upper critical dimension would be $E_c(j)$ or more. Then

$$D_{\mathrm{I}}(j) = \max[0, E - j(E - D_k)] > 0 \quad (15)$$

or

$$D_k > (j-1)E/j. \quad (16)$$

Taking $j=k-1$, below $E_c(k)$ one gets

$$D_k > (k-2)E/(k-1). \quad (17)$$

In the Flory theory, D_k reaches the upper bound when $E=1$ and approaches the lower bound for large k.

For large but finite k values, one may expect two regimes. When $1 \ll N < N^*(k)$ where $N^*(k)$ is a cross-over value below which the k-SAW restrictions play no role, the walk is random ($\nu = \frac{1}{2}$) whereas when $N > N^*(k)$ the asymptotic behaviour is governed by the k-multiple points exclusion and $\nu = 1/D_k$.

The swelling decreases ($E_c(k)$ decreases) when k increases below $E=4$. $E=2$ is an accumulation point for the $E_c(k)$ when $k \to \infty$ and in this limit $D_k = E$ for $1 \leqslant E \leqslant 2$ in the Flory theory‡.

The succession of the upper critical dimensions is the same as for multicritical points of order k (Toulouse and Pfeuty 1975) so that one may expect a thermodynamic analogy with this property, generalising the case $k=2$ (SAW) which is known to be related to the n-vector model (Stanley 1968) in the limit $n=0$ (de Gennes 1972) with an ordinary critical point.

† These rules evidently do not apply for k- or higher-multiple points which are forbidden in k-SAW whereas k replicas may have intersections of this type.

‡ The order of the limits on N and k is important; if the limit $k \to \infty$ is taken first, one gets a random walk with $D=2$ $\forall E$.

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