SELF-SIMILARITY OF MUTUAL AND SELF-INTERSECTIONS OF RANDOM FRACTALS

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The fractal dimensions of various types of intersection sets of random fractals are discussed. This helps a better understanding of issues concerning upper critical dimensionality, Flory approximations or universality of critical behaviour with respect to different excluded volume mechanisms. Diffusion on self-intersecting fractals, and on fractals with local bridges, is also considered in the light of the above discussion, and accurate results for the relative exponents, obtained from analysis of Monte-Carlo generated enumerations, are presented.

1. INTRODUCTION

For many problems of critical behaviour in lattice statistics, like self-avoiding walks (SAW) or related models for linear and branched polymers, mutual or self-intersection properties of random fractals turn out to be relevant in several respects. It is e.g. well known that the upper critical dimension of a problem must be related to the mutual intersection properties of two replicas of the random fractal under consideration. On the other hand, the concept of self-intersections of a fractal enters as a very basic ingredient in the widely applied Flory approximation for the ν -exponent of polymer problems.¹ Indeed, the repulsive energy due to the excluded volume is in this approximation simply estimated as being proportional to the average number of self-contacts of a purely random linear (R.W.) or branched chain.

In the second section of this report, we will review the basic results of the (as far as we know) first systematic investigation of the scaling laws governing the statistical geometry of various kinds of intersections of random fractals on a lattice.² In spite of its relevance, which will be illustrated here, up to now only

scarce attention has been paid to this subject, both in the mathematical and physical literature.³ Besides throwing new light on important issues like the above mentioned connection between intersections and critical dimensionality, or the universality of the ν -exponent with respect to different excluded-volume mechanisms, the study of the laws determining the fractal dimensions of self- and mutual intersections will naturally lead us to a deeper understanding and a nontrivial reinterpretation of the Flory approximation itself, as will be illustrated in the third section.

Random fractals allowing for self-intersections, like k -tolerant walks (i.e. walks that can visit each lattice site at most k times), are not only interesting for the discussion of the above mentioned static properties. An important question is whether such self-intersections are able to allow a nontrivial value ($\neq 1$) for the spectral dimension, which is related to diffusion on the fractal.^{4,5} Such a type of dynamical question, for which new aspects of the geometry of self-intersections are coming into the game, is of particular interest also in con-

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nection with recent debates about the possible mechanisms leading to the noninteger values for the spectral dimension of ferredoxin and hemo-proteins, as measured by spin-lattice relaxation experiments.⁶

2. FRACTAL DIMENSION OF MUTUAL AND SELF-INTERSECTION SETS

The fractal dimension $D(A \cap B)$ of the set of mutual intersection points of two random fractals A and B with fractal dimensions $D(A)$ and $D(B)$ respectively, is expected to be given by the law of codimension additivity:³

$$D(A \cap B) = D(A) + D(B) - d \quad (1)$$

if the r.h.s. is nonnegative, and $D(A \cap B) = 0$ otherwise. In (1), d is the dimension of the embedding Euclidean space. This law can be derived on the basis of simple scaling considerations.²

To be specific, let us consider the case of walks (SAW, R.W. or k -tolerant, etc.) on a d -dimensional lattice. Indicating by W a generic walk, with an extremum at a given origin $\vec{0}$ and with $|W|$ steps, the grandcanonical probability for a walk to visit a site $\vec{r}$ is given by

$$P(\vec{r}) = \sum_W K^{|W|} \chi_{\vec{r}}(W) \cdot \left[\sum_W K^{|W|} \right]^{-1} \quad (2)$$

where K is a step fugacity, and $\chi_{\vec{r}}(W)$ is 1 if W visits site $\vec{r}$, but 0 otherwise. If $\xi(K)$ is the grandcanonical root mean square end-to-end distance of the walks, then the natural scaling assumption for $P(\vec{r})$ is

$$P(\vec{r}) \approx r^{-x} f\left(\frac{r}{\xi}\right) \quad (3)$$

for $r \rightarrow \infty$ and $K \rightarrow K_C^-$, such that $\xi(K) \rightarrow (K_C - K)^{-\nu} \rightarrow \infty$, with ν the end-to-end distance exponent. The function $f(y)$ is expected to approach a constant value for $y \rightarrow 0$. The exponent x can easily be derived in terms of d and ν . Indeed, it is straightforward that $\sum_r P(\vec{r})$ is equal to $\langle \|W\| \rangle$, the average number of *distinct* points

visited by the walk. By definition³ we have that $\langle \|W\| \rangle \sim \xi^{1/\nu} \equiv \xi^D$, where D is the fractal dimension of the walk; thus, on the basis of the above mentioned properties, we may conclude that $\xi^D \sim \xi^{d-x}$, or $x = d - D$.

Consider now two independent walks W_1 and W_2 with the same fractal dimension and origin, for simplicity. In this case one finds

$$\langle \|W_1 \cap W_2\| \rangle = \sum_r P_1(\vec{r}) P_2(\vec{r}) \underset{K \rightarrow K_C^-}{\sim} \xi^{2D-d}, \quad (4)$$

which is consistent with eq. (1).

The law of codimension additivity has been verified directly by Monte-Carlo simulations on k -tolerant walks with k up to 5, in $d=2$ and $d=3$.² In the case of purely random walks, $P(\vec{r})$ can be computed exactly, and turns out to satisfy (3) with $x = d-2$ for $d > 2$ and $x = 0$ for $d \leq 2$, as it should since the fractal dimension is $D=2$ for $d > 2$ and $D=d$ for $d \leq 2$.² According to eq. (4), $d=4$ is the dimensionality below which $\langle \|W \cap W'\| \rangle \rightarrow \infty$, and above which $\langle \|W \cap W'\| \rangle \rightarrow \text{constant}$ for $\xi \rightarrow \infty$, if W and W' are two independent random walks with the same origin. It is remarkable that the quantity $\langle \|W \cap W'\| \rangle$ turns out to be proportional to the integral giving the first order perturbative correction to the 4-point 1-particle irreducible vertex function of a ϕ^4 -theory with ultraviolet cutoff. In this way the appearance of infrared divergences in the ϕ^4 -theory is seen to be directly related to the divergence of $\langle \|W \cap W'\| \rangle$ for two random walks or, equivalently, to their intersection being a fractal with positive Hausdorff dimension.²

The situation is more difficult when we consider the fractal dimension of the self-intersections (if any) of a given fractal. It has been conjectured that the fractal dimension of multiple self-intersection points of m -th order of a fractal (in what follows we will call such points m -ple points) should be determined as if these points would be the mutual intersections of m independent replicas of the fractal.^{3,7}

According to (1), this fractal dimension should then be $mD-(m-1)d$, if D is the dimension of the self-intersecting fractal. This replica idea, however, is contradicted by exact results for random walks and by extensive numerical investigations of k -tolerant walks in $d=2$ and $d=3$.² In the former case, one knows that the average number of m -ple points ($m=2, 3, \dots$) for all random walks with $|W|=N$ grows as a finite fraction of N for $N \rightarrow \infty$.⁸ On the other hand, when $K \rightarrow K_c$, one can exactly calculate the divergence of the correlation length for the probability that two given sites are both visited e.g. twice by a random walk.² This divergence turns out to be proportional to $(K_c - K)^{-1/2}$, which together with the above results implies that the fractal dimension of double points is equal to the fractal dimension of the random walk itself.

k -tolerant walks are an interesting case of nontrivial fractals, in which it is possible to test numerically the self-similarity of m -ple points ($m \leq k$). Such an investigation is a very difficult task, because, already in order to obtain the asymptotic scaling properties of the end-to-end distance of these walks, one must estimate (e.g. by Monte-Carlo sampling) statistical properties of extremely long walks, especially at high k . Such difficulties are becoming much more severe if, like in the present case, one tries to discuss the scaling of the average radius of gyration with respect to the center of mass of e.g. double points. A successful strategy² (a similar strategy was developed independently in ref. 9) consisted in evaluating up to a high degree of accuracy the average radius of gyration of m -ple points for walks of low and intermediate length (typically up to $N \sim 50$) by a Monte-Carlo biased sampling.¹⁰ Such lengths are of course not accessible to exact enumeration, but they still do not require a too large sampling in order to reach a reasonably accuracy. To these approximate numbers

we then applied some standard methods of asymptotic analysis of series expansions. While some techniques (like e.g. the ratio method) are too sensitive to uncertainties in successive data to be of much use in our case, other methods that make use of all the data simultaneously (like Padé approximant methods) are much less sensitive to noise, and they yield rather consistent results. With these methods, very clear evidence could be obtained for the fact that the replica trick does not apply to m -ple points. For each m , like in the random walk case, the average number of m -ple points grows as a finite fraction of N , and their average radius of gyration grows like the end-to-end distance of the walk. This clearly indicates that the fractal dimension of m -ple points is just the same as the one of the whole walk.

3. FLORY APPROXIMATION REVISITED

As mentioned in the introduction, in the Flory approximation for e.g. a linear, self-avoiding chain (polymer) of N steps (monomers), the repulsive energy is estimated as being proportional to the average number of double points of a random walk.¹ This average number is given as $\sim N^2 R^{-d}$, with R the characteristic size of the chain (end-to-end distance). Subtracting from this energy the elastic entropy term $\sim R^2 N^{-1}$, appropriate for a Gaussian chain of elongation R , and extremalizing this free energy with respect to R , leads to $N \sim R^D$ (for $N \rightarrow \infty$) with $D = (2+d)/3$.^{1,11}

A first important remark is that the estimate of the average number of double points as being $\sim N^2 R^{-d}$ is not consistent with what we know about self-intersections. We know that, more correctly, this number should be proportional to N .² On the other hand, the term $N^2 R^{-d}$ can also be read as R^{2D-d} (since $N \sim R^D$). According to the law of codimension additivity, this should be interpreted as the number of mutual

intersections of two *independent* replicas of the chain, which seems to contrast with the intuitive idea at the basis of the approximation.

In order to understand how these two apparently contradictory aspects (mutual vs. self-intersections) can be reconciled, one must arrive at a reinterpretation of the whole approximation, as explained below. The necessity of such a reinterpretation can best be seen when considering the case of the k -tolerant walks, for which a naive application of standard Flory arguments leads to incorrect results. Along the line of the usual derivation for the $k=1$ case, the Flory repulsive energy of a k -tolerant walk, being due to $k+1$ monomer encounters, would seem to be $\sim N^{k+1}R^{-kd}$, leading to a k -dependent fractal dimension $D = (2+kd)/(k+2)$.⁷ This turned out, however, to be a wrong prediction since, for all k , D can be seen to remain equal to its value for $k=1$ (SAW).^{12,13} We clearly need a more reliable criterion for writing the repulsive energy term in a Flory free energy. As we will show, this criterion cannot ignore the correct geometry of both mutual and self-intersections of random fractals.

In order to estimate the free energy of a chain of N monomers, let us first imagine to partition it into N/ℓ segments in such a way that each segment contains a large number ℓ of monomers, and can be considered as a separate fractal. The free energy can then be estimated as the sum over the free energies of N/ℓ segments, plus the free energy due to segment-segment correlations. The first part can simply be written as $\frac{N}{\ell} \cdot F_0(\ell)$, where $F_0(\ell)$ is the free energy of a segment of size ℓ , which is clearly independent of the end-to-end elongation R of the whole chain. In the spirit of the Flory approach, we will treat the various segments as independent random chains (R.W.) of length ℓ . Their mutual repulsive energy is given by segment-segment repulsion effects. In a mean-

field spirit, the number of segment-segment encounters will be proportional to $(N/\ell)^2(R/\ell^{1/2})^{-d}$, taking into account that the elongation of each segment should be $\sim \ell^{1/2}$. Being fractals, two segments will generally have an average number of mutual intersection points proportional to $\ell^{1/2}$ (their elongation) elevated to the power $(2 \cdot 2 - d)$, the fractal dimension of the mutual intersections of two random walks. The entropy of the segments can easily be estimated as the one pertaining to a random chain of N/ℓ ($\gg 1$) segments, with total elongation $R/\ell^{1/2}$. We can finally write for the total free energy:

$$F = \frac{N}{\ell} F_0(\ell) + a \left(\frac{N}{\ell} \right)^2 (R/\ell^{1/2})^{-d} (\ell^{1/2})^{4-d} + b (R/\ell^{1/2})^2 / (N/\ell) \quad (5)$$

with a and b suitable, weakly ℓ -dependent, dimensional factors. A remarkable feature of eq. (5) is that the basic dependence of the free energy on N and R is the same as obtained through the standard Flory derivation of the free energy, in the case of self-avoiding chains. Equation (5), with ℓ playing the role of a rescaling parameter, naturally evokes the inhomogeneous scaling equation for the free energy of a spin model at a fixed point of a renormalization transformation,¹⁴ and shows that there is a form of scaling invariance hidden in the usual expression of the Flory free energy.

The above derivation makes use of the same basic approximations as the standard one,¹ plus the ingredient of a correct description of fractal intersections. An immediate bonus is that we can now understand why the free energy (5), leading to the SAW-exponent, should apply also to k -tolerant walks with $k > 1$. Indeed, the second term should be left invariant, regardless of k , because we may conclude from the considerations of the previous section that $(k+1)$ -ple mutual intersection points of two random walks of ℓ steps should grow, on the

average, like $(\ell^{1/2})^{4-d}$ for all k . These points can indeed be seen as simple intersections of n_1 -ple points of the first walk with n_2 -ple points of the latter, with $n_1+n_2=k+1$. For each n , the n -ple self-intersections of a fractal form themselves a fractal with the same dimension.

Considerations similar to those presented in the present section can also be formulated for Flory approximations for other problems, like e.g. branched polymers.²

4. SPECTRAL DIMENSION OF k -TOLERANT AND RANDOM WALKS

As mentioned in the introduction, self-intersecting fractals (like e.g. k -tolerant walks) are of interest also from a dynamical point of view. Well known experimental results on the low-frequency behaviour of the density of vibrational states in ferredoxin and some hemo-proteins⁶ were a very important stimulus for the general study of dynamics on fractals.^{4,5} A specific problem connected with the interpretation of such experiments consists in understanding up to which extent the presence of crosslinks (e.g. H-bonds) between different segments of a protein backbone can alter its essentially one-dimensional character as far as dynamics is concerned, leading to a spectral dimension greater than 1.¹⁵

At the level of lattice models for diffusion on random fractals, one can ask the equivalent question whether the exponent characterizing e.g. a random walk on a self-avoiding chain is altered or not, when we allow for extra hoppings between non-adjacent sites of the chain. Extra hopping is generally considered only across short-range bridges, i.e. between neighbouring sites that are both visited by the chain with a certain number of steps in between. An alternative way of realizing a deviation from the law of diffusion on a self-avoiding chain, is to perform a random walk on e.g. a 2-tolerant

walk. The fractal dimension of this 2-tolerant walk is known to be the same as if it would be self-avoiding;^{12,13} the diffusion on it, however, can profit from the many extra hoppings available at the double points.

The problem of diffusion on self-avoiding walks with short-range bridges has very recently been investigated by several authors.^{16,2} A sufficiently accurate determination of the exponent governing such diffusion in two dimensions could be obtained by sampling about 10^7 random walks (for each length from 1 to 50 steps), starting in the middle of self-avoiding walks of 200 steps (to avoid boundary effects).² A different self-avoiding walk configuration was used for every group of 50 random walks. When we apply the series analysis methods mentioned in the previous section to the obtained data, we obtain $D_W = 2.65 \pm 0.03$. This fractal dimension D_W for the diffusion is defined such that the average displacement R , after a large number t of diffusion steps, grows like t^{1/D_W} . The value obtained for this exponent is the same as one would find for simple diffusion on a self-avoiding chain; this implies a spectral dimension equal to 1.

A similar study has been performed for the diffusion on 2-tolerant walks in two dimensions. Also in this case we obtain a rather clear, even if less sharp, evidence for the absence of deviation from the self-avoiding walk case: $D_W = 2.65 \pm 0.15$.

A typical picture of a 2-tolerant walk consistent with this result and with those of the previous section, is that of a configuration in which most of the loops formed by the walk between two visits of its double points are of small scale. After some coarse graining of these small scale loops, the walk looks like a proper self-avoiding structure. Big loops are prevented by a kind of screening effect, due to the presence of a thick and uniform sequence of small loops along the structure. According to

such a picture, the fractal dimension of the double points is clearly identical to the one of the whole walk, as it should be, and diffusion must asymptotically behave like on a simple self-avoiding walk.

We must expect a different situation for diffusion on a pure random walk. In this case, there is no k -tolerance to provide screening, and we can expect loops to be important at all length scales, thus affecting substantially the dynamical exponent. Indeed, extensive enumerations in $d=2$ for this case produced $D_W = 2.99 \pm 0.04$. This result clearly supports the value $D_W=3$ for this case, as indirectly, and less sharply suggested by random chain resistance calculations,¹⁷ and in contrast with the results of reference 18. The spectral dimension^{4,5} of a random walk in two dimensions is thus equal to $2D/D_W = 4/3$, where $D=2$ is the fractal dimension of the random walk.

5. CONCLUDING REMARKS

The above results show that short-range bridges or self-contacts of a basically self-avoiding structure do not affect the diffusion properties on this structure, as was hoped by some authors, in order to give a simple explanation of experimental facts concerning proteins.¹⁵ In order to obtain a spectral dimension greater than one, we must remove completely the self-avoiding, or k -tolerant constraint.

An alternative possibility, while preserving the self-avoiding structure, consists in allowing for long-range hopping rates among different sites of the chain. This was shown on the basis of exact renormalization group calculations for a model of diffusion on a deterministic fractal in two dimensions, which yielded non-universal spectral dimensionalities in the whole range between 1 and $4/3$.¹⁹ Long-range hopping bridges

in this model essentially play the role of the loops at all length scales, affecting diffusion on a purely random unconstrained chain.

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