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LETTER TO THE EDITOR

A new Monte Carlo model for *dense* polymers

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Abstract. We describe a new model for a statistical ensemble of polymers on a cubic lattice with periodic boundary conditions. The system produced describes a network of polymers at intermediate concentrations and, therefore, it obeys des Cloizeaux's law. The great interest of the model is stressed.

A Monte Carlo model to simulate strings on a $d = 3$ spatial dimensional cubic lattice with periodic boundary conditions (3-torus) has recently been developed to show the existence of a new scaling region in the very long string sector [1]. Polymer theory helps in understanding string correlations [2]. In fact, these correlations are given by a screening phenomenon (short range correlations) and by global effects (long range correlations) which are all induced by the topology of the manifold (see also the exact calculations in two dimensions of Duplantier and David [3]). By this suggestion, as we shall see below, this system of strings is exactly a system of self-avoiding walks (SAWs) or polymers [4] in a 'reduced irregular lattice'. Therefore, we shall refer to 'polymers' in the following.

Let us now give a summary description of our Monte Carlo model to generate polymers. It has been developed in great detail in [2] and [5].

In a 3D cubic lattice with periodic boundary conditions we choose at random, on each site of a cell, an element of the discrete Z^3 cyclic group (i.e. [0, 1, 2]). We consider, for any plaquette, the ordered sets 0120, 0112, 0122 and the reversed-ordered sets 0210, 2110, 2210 with all the possible cyclic permutations. A polymer point is identified by any of the above combinations if one of them is realised by the site-values of the given plaquette. The polymer point is then placed at the centre of the plaquette. For any other combination we have no polymer point associated with the corresponding plaquette. Polymer points have a 'sign' which is positive if they are given by one of the former sets of site values or negative if they are given by one of the latter sets. Hence, these polymers (such as polyelectrolytes) are oriented, depending on the sign of the polymer points, looking at the plaquette by the right-hand rule with respect to the positive directions of a conventional reference frame. Starting from any polymer point, we go from cell to cell reading the site values of every plaquette, searching for the next polymer point with the right sign and, then, linking the latter to the former.

We trace the polymer until we gain its end. The algorithm does not stop until every polymer point has been considered.

We remark on three special 'constructive features' of the model.

(*a*) Each polymer point is never passed twice.

(*b*) The possible number of polymer points on the plaquettes constituting the faces of a cell can be 0, 2 or 4. We have the 66% of cells with two polymer points (two-point cells) and the 10% of cells with four polymer points (four-point cells) respectively in the lattice volume *V*.

(*c*) For any polymer point at the centre of a plaquette through which the 'oriented' polymer enters a cell there is at least another polymer point (there are two in the four-point cell, see below), on one of the other faces of the same cell, which does not let the 'oriented' polymer stop.

Elsewhere [2] we have given a physical explanation of these 'intrinsic' properties of the model. However, as we shall also suggest below, they are deeply related to the topological nature of the group structure of the corresponding 'continuum' model. Here, we are only interested in the pure geometrical algorithm which 'naturally implements' the properties listed above.

Two choices have been made on the model.

(i) Periodic boundary conditions have been imposed to force the walk to return into its initial position, so that only closed polymers exist in the system.

(ii) In the four-point cell, when one point has been reached by the polymer, the oriented polymer can continue its walk through two of the other three points left. Two of the three points left have the right sign to let the polymer go ahead. Because of no dynamical input (see below) we make a random choice getween the two polymer points with the right to ensure the complete 'local randomness' into the system.

Before dealing with the main result of the letter, we must emphasise the great generality of this pure geometrical model.

It can be used for a realisation of Abelian strings on a lattice. Strings are solutions of gauge theories in which the spontaneous symmetry breaking of a Lie group G into a subgroup H of G determines a non-trivial $\pi_1(G/H)$ group [2, 6]. Strings are Abelian if G is Abelian. In the discrete approximation we have used, the G/H group has been represented by the Z^3 group. Again, the same approximation is implied if localisations or topological line defects are produced in a model whose group G (the symmetry of the dynamical model itself instead of G/H) implies a fundamental homotopical group $\pi_1(G)$ different from zero (such as it is in low temperature physics [6] for vortices in superconductors or in superfluids). Finally, when the algorithm introduced above, given on the lattice by the mathematical correspondence between the Z_3 group and the plaquette, is accepted without any topological group theory background, we can consider [2] the walks generated just as polymers. This is the limit in which all these physical objects are only geometrical linear objects without any thickness or intrinsic structure. In fact, once generated the polymer points on the lattice plaquettes, we essentially restrict our consideration to that irregular lattice only made by the set of polymer points themselves. We have a 3D 'reduced irregular lattice' made by $L = 3N^3 \times 0.296$ points. Of course, 0.296 is the probability of a polymer point given, of course, by model building and $3N^3$ the number of plaquettes of the original lattice having imposed periodic boundary conditions. The total length *L* of the system is almost constant [2] because of only Monte Carlo fluctuations of the order of $1/V^{1/2}$.

Turning to the original cubic lattice, we stress that very important implications come from the existence of a cell whose faces have four polymer points (four-point cell).

The four-point cells imply the possibility of polymer–polymer interaction. We must emphasise that the link size is a persistence length into the system. We mean that inside a cell volume the system ignores what 'locally' happens. Then, if it is not defined by any explicit dynamics in the model, one does not know what interaction, if any, is present between polymers. However, in a polymer model for our walks, the excluded volume dynamics would be enough to constrain a 'local' repulsion in the four-point cells between any two polymers. Therefore, polymers would exactly be SAWs.

In a string model for the walks, again, we do not know what happens 'locally' if we have no dynamics. What we know from the general dynamical theory [7] is that strings can *a priori* pass through each other, topologically interchange their branches or be SAWs. Recently, numerical simulations have shown [8] that oriented strings have usually a very low probability to pass through each other. Thus, in the scenario we are considering we exclude that strings can pass through each other.

However, in [2], we have shown that in spite of any dynamics, explicitly imposed by the model, the system has always (implicit) 'configuration' correlations 'on a torus', coming from the topology of the strings naturally induced by the topology of the manifold itself. In fact, very long thin strings show non-local interactions between and inside themselves [2]. For example, any two points on a very long string at some distance from each other can be very close together in space, or a point on a very long string can lie between two other points of the same string which are close together in space. If we consider the average length of the strings which do not wind around the torus and that of those which instead are not topologically contractable into a point, it comes out that the average length shows interesting implications coming from the strings own topology in the infinite volume limit [1]. In this physical limit $(V \to \infty)$ and for strings which do not wind around the torus the system prefers configurations in which strings have no intersection (or the string segments which pass through a four-point cell repel each other). Some kind of string–string interaction of the order of the excluded volume repulsion could be assumed to conclude that for these configurations, where strings have no intersection, strings are all SAWs. Whereas, the average length of strings with increasing total winding number shows exactly the opposite behaviour [1]; many intersections are favoured. The latter strings might no longer be SAWs.

We have simulated for the network of polymers 200 000 configurations on a $V = 20^3$ lattice and the average of the quantities we consider is calculated over them.

Let us define [9] an average linear size $\zeta(l)$ which measures an average distance between polymers with fixed length l. Since this is a typical linear distance into the system we can identify it by the mean distance the centre of gravity (see below) of a polymer with fixed length l would have with respect to the centre of gravity of another polymer with the same length.

Even if a little intriguing, the linear distances on the 3-torus we are dealing with are all intrinsically well defined just if they were taken in a space with free boundary conditions. In fact one of the most interesting results of [1] is that in a lattice volume $V = N^3$ there are no boundary effects on the physical results (such as scaling laws) if the length of polymers is at most $l \leq N^2$. Thus for the aims of the present letter the 3-torus boundary conditions only artificially close the strings because we keep the root mean square of the following fit on lengths of order $5 \times N$ (i.e. figure 1 for $N = 20$).

Des Cloizeaux [10] has developed a Lagrangian theory for a system of polymers with no fixed length. The only interaction considered in the model was given by the
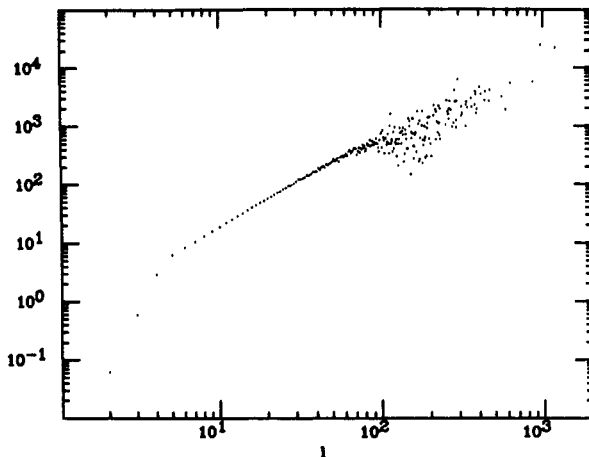
Figure 1. The expectation value of the centre of gravity distances between polymers are plotted against l for the $N = 20$ lattice.

excluded volume repulsion in a two-parameter model. By this approach he deduced a fundamental scaling law in real space R^3 which has been formulated [9] as:

$$\zeta(C) = R_F \left(\frac{C'}{C} \right)^\alpha \tag{1}$$

where ζ is a function of the concentration C. We define [2] C as a function of the length l:

$$C(l) = \frac{n(l)l}{V}.$$

C' is the critical concentration [9] of the system $C'(l) \equiv l/R_F(l)^3$ and $R_F(l) = al^\nu$ is the Flory gyration radius with $\nu = 1/2$ for Brownian polymers and $\nu = 3/5$ for self-avoiding polymers. The α exponent is determined by the critical condition [9] that the exponents of R_F and C' must annihilate.

The important point is that (1) is valid in the approximation $C \gg C'$ (or at intermediate concentrations). We will see that, *a posteriori*, the verification of (1), for the system at hand, implies that the system of polymers we generate is highly concentrated.

The number density of polymers, $n(e)$, with length l can be derived in the following way. We consider, instead of the end-to-end distance R of a closed polymer, its own perimeter size $R = q_1 + q_2 + q_3$. q_i $(i = 1, 2, 3)$ counts the number of cells in the ith direction which bounds the cubic volume occupied by the polymer. For R one can write $n(R)\,dR = R^{-4}\,dR$ by dimensional analysis in three dimensions. Assume a general fractal shape for the string $l = a^{-1}R^D$ with $D = 1/\nu$. Then we easily have

$$n(l)\,dl = \frac{1}{D}\, a^{-3/D} l^{-(3+D)/D}\,dl$$

which for $D = 2$ gives

$$n(l) = \tfrac{1}{2} a^{-3/2} l^{-5/2}. \tag{2}$$

From (1), the definition of $C(l)$ and (2), imposing the critical condition on α, we obtain

$$\zeta(l) = bl^{3/2} \tag{3}$$

where the exponent 3/2 comes from the fundamental assumption that polymers have a Brownian shape; b is determined by a and the fractal dimension D. If (3) is verified by the system then we gain two direct conclusions. First, these polymers are Brownian walks ($D = 2$) and, second, the system is highly concentrated (as we already stated for (1)).

Now we define the mean distance of gravity centres for fixed l in our simulated network of polymers as:

$$\zeta(l) \equiv \frac{1}{2 \times N(l)} \sum_{k=1}^{n(l) \times N_{\text{iter}}} \sum_{i=1}^{n(l) \times N_{\text{iter}}} |G_k(l) - G_i(l)|(1 - \delta_{ik}) \qquad (4)$$

where $G(l)$ is the centre of gravity for the polymers:

$$G_k(l) = \sum_{j=1}^{l(k)} r_k^j \delta_{l(k),l}. \qquad (5)$$

The vector r_k^j denotes the set of coordinates $r_{k,\alpha}^j$ of the k polymer in the 3D cubic lattice. The three spatial dimensions are denoted by j and α is the label of the polymer points. $N(l)$ is for the total number of distances between two polymers with the same length l; $l(k)$ stands for the length of the k polymer and N_{iter} is the number of Monte Carlo iterations for the statistical ensemble. Finally, Kronecker symbols $\delta_{l(k),l}$ and $\delta_{i,k}$ have been introduced to consider, in (5), the sum extended only on a fixed length l and the sums in (4) for $\zeta(l)$, respectively, extended only on different polymers with fixed length.

In figure 1 we report the data for the mean distance of gravity centres $\zeta(l)$ as a function of the length l in the system of closed polymers. In figure 1 we see the possibility of a very good linear fit in the bilog scale. We calculate the root mean square fit of the data and find the following scaling law:

$$\zeta(l) = \xi l^\eta \qquad (6)$$

with $\xi = 0.488 \pm 0.005$ and $\eta = 1.556 \pm 0.005$.

As we see, the numerical results for our polymers are in good agreement with the theoretical predictions coming from equation (3) even if small deviations are evident. The reasons for such deviations are deeply related to the 'nature' of the statistical system we have simulated.

On one hand, $\zeta(l)$ is very sensible to the correlations between polymers but much less sensible to correlations between points of the same polymer. In fact, the standard [9] definition of ζ as a function of the concentration of the system (with fixed l) is that it is a certain average mesh size between two polymers. More exactly, this would mean averaging all the point-point distances between two polymers. Since it would be a time consuming numerical calculation to compute the point-point distances, we selected the gravity centre as a special point on the polymer. Thus, a very important approximation which saves computer time but loses some information, consists of restricting ourselves to the gravity centres between different polymers. By doing this we have also excluded contributions to the correlations coming from point-point distances measurable into the same polymer. But, since in most configurations polymers prefer to spread out themselves instead of spatially shrink into balls [2], it is not dangerous, in our opinion [9], to forget about the inner polymer correlations which would almost have a uniform distribution.

On the other hand, a fundamental remark must be made on the l dependence of the concentration $C = C(l)$. Usually, in polymer physics, the system has fixed [9]
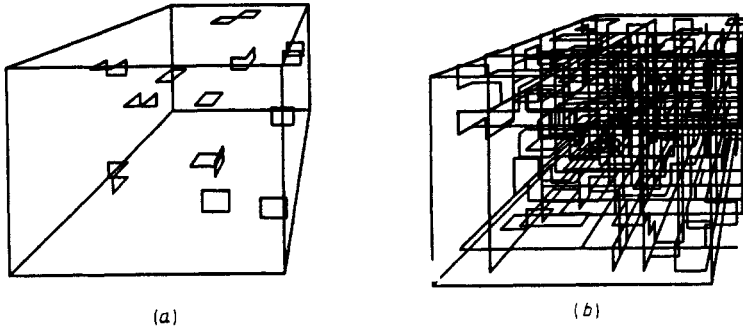
Figure 2. We show typical configurations of strings on a torus: (a) for strings of length $l = 5$ and $l = 6$, (b) for the longest string $l = 694$.

length l. A consequence is that the concentration C of each polymer system has been always l-independent. In our system [10] all possible lengths are living together. When we consider $n(l)$ we suppose to have a system with a 'solute' given by the closed polymers with length l into a 'solvent' given by the plaquette centres which are not polymer points plus the polymer points of the rest of the polymers with every other length different from l. The quantity $\zeta(l)$ has been computed taking a measure on the solute. But, even if we constrain the measure on the solute in this ideal constructive way, the statistical information considered takes into account the complexity due to the simultaneous presence of all polymers with different lengths. In figure 2(a) we report two subsystems of polymers together, each one with fixed but different lengths, $l = 4$ and $l = 6$ respectively, to graphically show how much it increases the complexity of the system. For completeness, we show in figure 2(b) a configuration with just one very long string which fills the whole volume. Furthermore, the increase of concentration (as defined above) can be seen going from figure 2(a) to figure 2(b). Generally, polymers with different lengths are correlated to each other. This means that correlations [2] between polymers with different lengths are present while we are focusing on a 'solute' of all polymers with fixed l. Thus, important influences from outside are contributing on the solute to the behaviour of measurable quantities sensible to any kind of correlations. Any deviation from the theoretical predictions, such as those in (6), must be clearly considered in this picture.

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