

# A simple model of DNA denaturation and mutually avoiding walks statistics

M. Baiesi<sup>1</sup>, E. Carlon<sup>2,a</sup>, E. Orlandini<sup>1</sup>, and A.L. Stella<sup>1</sup>

<sup>1</sup> INFN - Dipartimento di Fisica, Università di Padova, I-35131 Padova, Italy

<sup>2</sup> Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

Received 8 July 2002 / Received in final form 25 July 2002

Published online 17 September 2002 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2002

**Abstract.** Recently Garel, Monthus and Orland [Europhys. Lett. **55**, 132 (2001)] considered a model of DNA denaturation in which excluded volume effects within each strand are neglected, while mutual avoidance is included. Using an approximate scheme they found a first order denaturation. We show that a first order transition for this model follows from exact results for the statistics of two mutually avoiding random walks, whose reunion exponent is  $c > 2$ , both in two and three dimensions. Analytical estimates of  $c$  due to the interactions with other denaturated loops, as well as numerical calculations, indicate that the transition is even sharper than in models where excluded volume effects are fully incorporated. The probability distribution of distances between homologous base pairs decays as a power law at the transition.

**PACS.** 87.14.Gg DNA, RNA – 05.70.Jk Critical point phenomena – 05.70.Fh Phase transitions: general studies – 87.15.Aa Theory and modeling; computer simulation

## 1 Introduction

Simple models of DNA thermal denaturation have attracted a lot of attention for a long time [1–4]. Although it was pointed out rather early that excluded volume effects may be crucial in determining the order of the denaturation transition [2], it was only very recently that such effects were taken into account both at analytical and numerical level [5–8].

Even once accepted excluded volume effects as a key factor in determining the nature of the transition, one can still be interested in understanding how the relaxation of self-avoidance constraints influences the overall behavior of the system. As this can be done in different ways, learning in detail about the effects of various geometrical exclusion constraints can help in conceiving better models or more efficient approximations.

The main general aim of this paper is that of producing a contribution to the debate on these general issues. In particular we analyze the model of DNA denaturation recently introduced and studied by Garel, Monthus and Orland (GMO) [9]. Among other things, we show that this model is a rather ideal context in which a recently proposed representation of DNA in terms of block copolymer networks [8] can be applied.

The Hamiltonian for the GMO model is [9]:

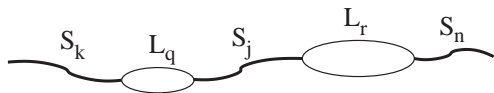
$$H = \frac{1}{2} \sum_{i=1,2} \int_0^N ds \left( \frac{d\mathbf{r}_i(s)}{ds} \right)^2 + \int_0^N ds V(\mathbf{r}_{12}(s)) + g \int_0^N ds \int_0^N ds' \delta(\mathbf{r}_1(s) - \mathbf{r}_2(s')) \quad (1)$$

where  $\mathbf{r}_1(s)$ ,  $\mathbf{r}_2(s)$  describe the conformations of the two strands as functions of the curvilinear coordinate  $s$  and  $V(\mathbf{r}_{12}(s))$  is the attractive interaction between homologous base pairs ( $\mathbf{r}_{12}(s) \equiv \mathbf{r}_1(s) - \mathbf{r}_2(s)$ ). The last term on the r.h.s. of equation (1) is due to excluded volume interactions, which act only between the two chains and not within a single chain. Thus, the self-avoidance constraint is relaxed and each isolated strand obeys a simple random walk (RW) statistics.

The authors of reference [9] simplified further the Hamiltonian (1) by approximating the excluded volume term by a long range interaction between the strands, which allows for an analytical solution of the problem. Within such approximation, the denaturation transition turns out to be of first order type [9], as in models where excluded volume effects are fully incorporated [5–8].

Our purpose here is to clarify further this point. We start from a description *à la* Poland-Scheraga (PS) [1] of the GMO model and use a series of exact results on reunion exponents of mutually avoiding walks, which show

<sup>a</sup> e-mail: carlon@lusi.uni-sb.de



**Fig. 1.** In the Poland-Scheraga model the full partition function of the DNA chain is factorized in terms of products of partition functions  $S_k$  of bound segments of length  $k$  and of partition functions  $L_l$  of denaturated loops of length  $2l$ . Thick lines denote double stranded segments.

indeed that the denaturation transition is first order. More surprisingly, the transition turns out to be even sharper than that occurring in models where excluded volume effects are fully taken into account. This conclusion is corroborated by approximate analytical treatments of excluded volume effects due to loop-loop interactions and by a series of numerical results obtained for polymer lattice models in  $d = 2$  and  $d = 3$ .

In the Poland-Scheraga (PS) model [1] the DNA chain is treated approximately as a sequence of non-interacting bound double segments and denaturated loops. Within this scheme the full partition function  $Z_N$  for a chain whose constituent strands have lengths  $N$ , is factorized in terms of elementary partition functions for loops and segments (see Fig. 1). In the grand canonical ensemble, where a fugacity  $z$  per lattice step is assigned, the total partition function reads [3]:

$$Z(z) = \sum_N z^N Z_N = \frac{V_0(z)}{1 - L(z)S(z)}, \quad (2)$$

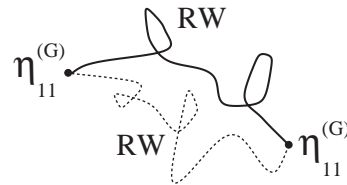
where  $L(z)$  and  $S(z)$  are the grand canonical partition functions for loops and double segments, respectively. The form of the numerator  $V_0(z)$  depends on boundary conditions and is not interesting for our purposes. The partition functions are [3]:

$$S(z) = \sum_k (\mu z e^{\beta\varepsilon})^k k^{\gamma-1} \quad (3)$$

$$L(z) = \sum_l \frac{(\mu^2 z)^l}{(2l)^c}, \quad (4)$$

where  $\beta$  is the inverse temperature and we assigned a contact energy  $\varepsilon$  to each bounded base pair;  $\mu$  is the (non-universal) effective connectivity constant, while  $\gamma$  and  $c$  are universal exponents. The order of the transition is related to the value of  $c$  [3]: At the transition temperature (which in the PS model corresponds to  $\mu^2 z \rightarrow 1$ ) loops are power-law distributed in size with probability  $P(l) \sim l^{-c}$ , thus their average size  $\langle l \rangle = \sum_l l P(l)$  is finite for  $c > 2$ , implying a first order denaturation, while it diverges for  $1 < c \leq 2$  and the transition becomes continuous.

For self- and mutually avoiding strands  $c$  was estimated analytically in an extended PS scheme [6], where excluded volume effects between a self-avoiding loop and the rest of the chain are approximately taken into account. This exponent was also obtained directly by Monte Carlo simulations [7,8] for polymer lattice models. The agreement between the analytical estimates and simulation results for  $c$  is very good both in  $d = 2$  and  $d = 3$  [6–8].



**Fig. 2.** Example of loop in the GMO model. The two strands indicated as dashed and solid lines are allowed to overlap themselves, but are mutually avoiding. Equation (5) gives the associated reunion exponent.

In the next sections we will present analytical and numerical estimates of the exponent  $c$  for the GMO model. The former are based on the theory of copolymer networks, which is briefly reviewed in the Appendix.

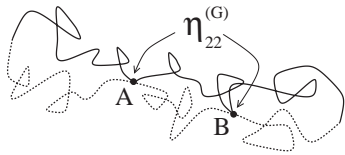
## 2 Mutually avoiding walks

A denaturated loop in the GMO model is formed by two mutually avoiding random walks of equal length  $l$ , with common origin and endpoint (see example of Fig. 2). The probability that two random walks, with common origin, meet for the first time after  $l$  steps decays asymptotically as  $P(l) \sim l^{-c}$  with [10,11]:

$$c = d\nu - 2\nu\eta_{11}^{(G)}. \quad (5)$$

Here  $d$  is the dimensionality of the embedding space,  $\nu = 1/2$  for RWs and  $\eta_{11}^{(G)}$  denotes the contribution of a vertex from which the two walks originate (see Fig. 2). We follow the notation of reference [12] and indicate with  $\eta_{f_1 f_2}^{(G)}$  the exponent associated to a vertex from which  $f_1$  solid and  $f_2$  dashed lines depart, at the Gaussian fixed point, which is the relevant one for our purposes. At this fixed point solid and dashed lines do not interact with themselves, but they avoid the lines of the other group.

Figure 2, as well as Figures 3–5 below, are examples of so called *copolymer networks*, *i.e.* networks whose constituents are polymers of different species. The relevance of these block copolymer networks for a description of denaturing DNA has been already stressed in the context of models with full excluded volume effects [8]. A general network of this type may be made, for instance, by an arbitrary mixture of random and self-avoiding walks (SAWs). Any pair of these walks may either avoid, or be allowed to cross each other. As for the homopolymer case, the general entropic exponent for a network with arbitrary topology follows from those of the constituents vertex exponents (see Refs. [10,13] for details). The general rule to calculate the entropic exponent of a network is simple and it is reviewed in the Appendix. Restricting to the case in which all constituent polymers have the same  $\nu$  exponent, one associates to each independent loop a factor  $d\nu$  and to each vertex a factor  $-\nu\eta$ , with  $\eta$  the appropriate exponent which depends on the number of outgoing legs, and on their type. The generalization to an arbitrary mixture of polymer segments with distinct  $\nu$ 's, as for instance RWs and SAWs, is also possible.



**Fig. 3.** A small loop (between points A and B) embedded between two much larger loops is characterized by an exponent given by equation (7).

Coming back to equation (5), the vertex exponent for one solid and one dashed line is known exactly in  $d = 2$  [17]. Its value is  $\eta_{11}^{(G)} = -5/4$ , which leads to  $c = 2 + 1/4 > 2$ . In higher dimensions one has to resort to  $\varepsilon$  expansion renormalization group results. In  $d = 3$  resummation techniques yield  $\eta_{11}^{(G)} \approx 0.57$  [12], which implies  $c \approx 2.07$ . Thus, both in  $d = 2$  and 3 the reunion exponent is larger than the threshold value ( $c > 2$ ), which immediately implies a first order denaturation for the GMO model, within the PS picture of non-interacting loops and bound segments.

As a comparison we recall that for an isolated loop made by two self- and mutually avoiding strands the entropic exponent is [15]:

$$c = d\nu. \quad (6)$$

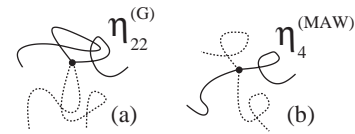
For a SAW one has  $\nu = 3/4$  in  $d = 2$ , which implies  $c = 3/2$ , while  $\nu \approx 0.588$  in  $d = 3$ , implying  $c \approx 1.76$ . Thus, within the PS picture, denaturation is a continuous transition ( $c < 2$ ) when full self-avoidance within a single loop is included [2,3,14].

It is also possible to go beyond the PS approximation in the GMO model, but it is already quite clear at this point that excluded volume effects between a single loop and the rest of the chain “localize” even more the loops and  $c$  can only increase. This can be shown explicitly for some simple geometries in which the loop is embedded. The calculations follow closely those of reference [6] for the model in which self-avoidance is fully included and are also briefly reviewed in the Appendix. We give here only the final results.

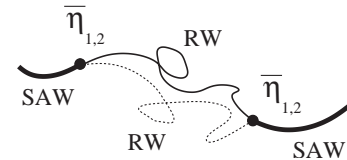
We consider the geometry shown in Figure 3 in which a loop of length  $2l$  is connected to two loops of length  $N - l$  each. In the limit  $l \ll N$  the partition functions of the inner loop is still of the type of equation (4) and factorizes with the partition function of the rest of the chain [6]. As explained in Appendix, the exponent  $c$  is however modified:

$$c = d\nu - \nu\eta_{22}^{(G)}. \quad (7)$$

In  $d = 2$  some care has to be taken in considering vertices, as the order of walks does matter. This is illustrated in Figure 4 where the two possible distinct types of vertices with four outgoing lines, two solid and two dashed, are shown. For a vertex of type (a) more configurations are possible as neighboring lines of the same type are allowed to overlap. In (b), instead, the distinction between solid and dashed lines becomes irrelevant as neighboring



**Fig. 4.** In  $d = 2$  there are two distinct vertices formed by two dashed and two solid lines (see text).



**Fig. 5.** A loop embedded between two long double stranded segments. The latter follow the self-avoiding walks statistics.

lines avoid each other. In the latter case the lines form a vertex of four mutually avoiding walks (MAWs) [16]. A vertex with  $L$  outgoing MAWs, has an associated entropic exponent [10,17]:

$$\eta_L^{(\text{MAW})} = -\frac{4L^2 - 1}{12}. \quad (8)$$

Hence, for loops embedded in a geometry as in Figure 3, and formed by vertices of type (b) one finds  $c = d\nu - \nu\eta_4^{(\text{MAW})} = 3 + 5/8 = 3.625$ . Let us consider now vertices of type (a) for which we keep the notation  $\eta_{22}^{(G)}$  to indicate the associated exponent. Using the prescriptions of reference [17] one has  $\eta_{22}^{(G)} = 35/12$  and thus from equation (7)  $c = 2 + 11/24 \approx 2.46$ . Notice that stronger excluded volume effects (as for vertices of type (b)) imply a higher value for  $c$ , with a quite large difference between the two estimated values. We point out that, obviously,  $\eta_{11}^{(G)} = \eta_2^{(\text{MAW})}$  in all dimensions.

In  $d = 3$  the above subtleties do not occur. The vertex exponent  $\eta_{22}^{(G)} \approx -1.81$  was estimated in reference [12] using  $\varepsilon$  expansions and resummation techniques. Thus, from equation (7), one obtains  $c \approx 2.40$ .

We consider now another geometry, where a loop is connected to two long double stranded segments, as illustrated in Figure 5. Using the same method of reference [6] we find (see Appendix):

$$c = d\nu - 2\nu\bar{\eta}_{1,2} \quad (9)$$

where with  $\bar{\eta}_{1,2}$  we indicate the exponent associated to a vertex where one double, and two single stranded segments join. Notice that the double stranded segment is actually a self avoiding walk since, if it would overlap itself in some part, the mutual avoidance condition between the two constituent strands would be violated.

Again in  $d = 2$  one can use the techniques of reference [17] to find  $\bar{\eta}_{1,2} = -2 - 7/16$  which leads to  $c \approx 3.44$ . To our knowledge, there exists no field theoretical analysis for this type of vertices in higher dimensions, thus we are not able to make any predictions for  $c$  in  $d = 3$ , at present.

Table 1 summarizes the exponents found in the GMO model for an isolated loop ( $c^{(\text{IL})}$ ), for a loop interacting

**Table 1.** Summary of the exponents for the GMO model for an isolated loop (IL) and for a loop interacting with neighboring loops (LL) or segments (LS). The results for fully self-avoiding (FSA) strands (from Ref. [6]) are also given. The last column shows the numerical estimates of  $c$  (those for the FSA are taken from Ref. [8]).

	$c^{(\text{IL})}$	$c^{(\text{LL})}$	$c^{(\text{LS})}$	$c$
GMO ( $d = 2$ )	2.25	2.46–3.62	3.44	2.95(5)
FSA ( $d = 2$ )	1.50	2.69	2.41	2.46(9)
GMO ( $d = 3$ )	2.07	2.40	-	2.55(5)
FSA ( $d = 3$ )	1.76	2.22	2.11	2.18(6)

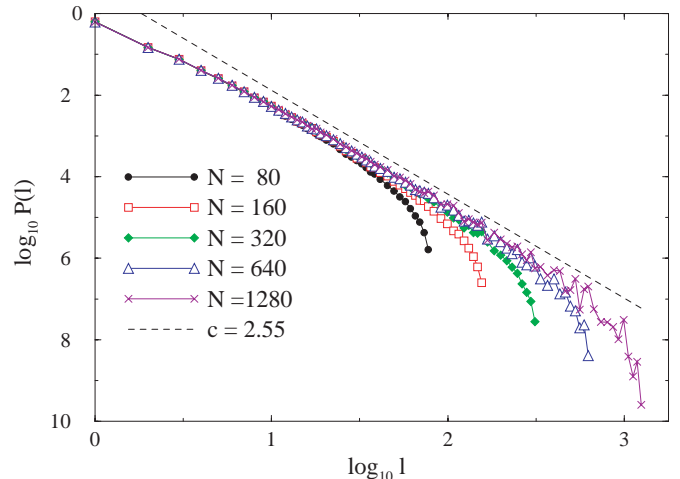
with other loops ( $c^{(\text{LL})}$ ), as in the geometry of Figure 3, and for a loop interacting with double stranded segments ( $c^{(\text{LS})}$ ), as in Figure 5. For the two dimensional case we reported both values of  $c^{(\text{LL})}$  corresponding to the loops formed by the two types of vertices of Figure 4. We notice that, as anticipated above, the interaction with other parts of the chain has the effect of increasing the loop exponent  $c^{(\text{LL})}$ ,  $c^{(\text{LS})} > c^{(\text{IL})}$  as is the case for all other models studied so far [6, 7]. The first order character of the transition in the GMO model is therefore strengthened.

It is interesting to compare the exponents obtained in this paper with the corresponding ones for the model in which strands are fully self-avoiding (FSA). The latter, taken from reference [6], are given in Table 1. The comparison between the two models indicates that the transition in the GMO model is generally sharper (higher  $c$ ). This is always true with the exception of the exponent  $c^{(\text{LL})}$  in  $d = 2$  for vertices of the type of Figure 4a for which we find  $c^{(\text{LL})} \approx 2.46$ , for the GMO model, while  $c^{(\text{LL})} \approx 2.69$  in the FSA case. This is due to the fact that in the GMO model for the type of vertex considered excluded volume effects are not so pronounced as walks have considerable freedom to overlap.

### 3 Numerical results

We performed a series of numerical calculations for a lattice version of the GMO model both in  $d = 3$  and  $d = 2$  (cubic and square lattices). We considered two random walks of length  $N$ , described by the vectors  $\mathbf{r}_1(i)$  and  $\mathbf{r}_2(i)$  ( $i = 0, 1, 2 \dots N$ ) which identify the positions of the lattice monomers. The walks have common origin ( $\mathbf{r}_1(0) = \mathbf{r}_2(0)$ ), and no specific boundary condition is imposed on the other ends. While each strand can overlap itself, mutual avoidance requires that  $\mathbf{r}_1(i) \neq \mathbf{r}_2(j)$  for  $i \neq j$ . Overlaps at homologous points are however allowed ( $\mathbf{r}_1(i) = \mathbf{r}_2(i)$ ); these correspond to a bound state of complementary base pairs, to which we assign an energy  $\varepsilon = -1$ . At sufficiently low temperature ( $T$ ) the walks are fully bound and form an object obeying self-avoiding walk statistics.

We used the PERM [18] algorithm and computed  $P(l)$  the probability distribution function (pdf) to find a loop of length  $2l$  in the chain. While at low temperatures loops are exponentially distributed in size, at the critical point



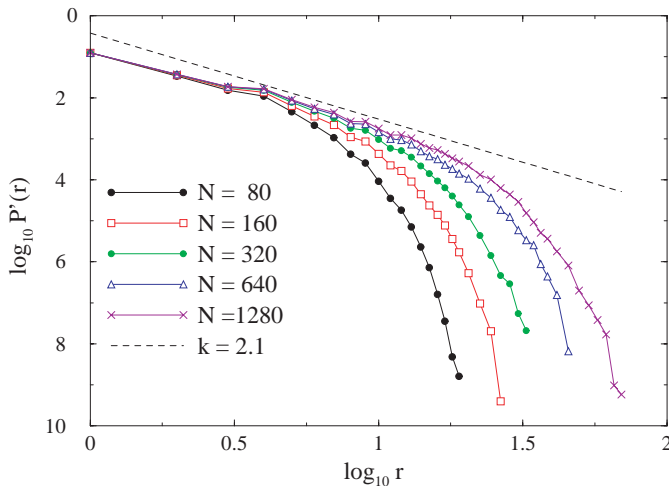
**Fig. 6.** Plot of  $\log_{10} P$  vs.  $\log_{10} l$  at the estimated critical point in  $d = 3$  and up to  $N = 1280$ . A linear fit of the data yields  $c = 2.55(5)$ .

the pdf has an algebraic decay  $P(l) \sim l^{-c}$ , from which we can extract the exponent  $c$  [7, 8]. Figure 6 shows a log-log plot  $P(l)$  vs.  $l$  in  $d = 3$  at the estimated critical point ( $T_c = 0.5181(3)$ ), for chains of lengths up to  $N = 1280$ . A linear fit of the data yields  $c = 2.55(5)$ , not far from the  $c^{(\text{LL})}$  given by equation (7) (see Tab. 1). The result confirms that the transition in the GMO model is sharper than when self-avoidance is fully included. Indeed, in the latter case the most accurate numerical estimate of the loop exponent is  $c = 2.18(6)$  [8].

We consider next  $P'(r)$ , the probability that the distance between homologous points in the strands  $|\mathbf{r}_1(k) - \mathbf{r}_2(k)|$  equals  $r$ . This quantity was found to decay as a stretched exponential for  $r \rightarrow \infty$  [9], from an analysis of the Hamiltonian of equation (1).

This conclusion is at odd with the algebraic decay of the loop pdf found here for the GMO model, and also in other similar models with a first order transition [7]. For the numerical calculation of  $P'(r)$  we registered all distances between homologous pairs along the chains  $|\mathbf{r}_1(k) - \mathbf{r}_2(k)|$ , starting from  $k = 1$  and up to the highest  $k$  for which the two strands are in contact ( $\mathbf{r}_1(k) = \mathbf{r}_2(k)$ ). Figure 7 shows a plot of  $\log_{10} P'(r)$  vs.  $\log_{10} r$  at the transition temperature in  $d = 3$ . We cannot fit the data with a stretched exponential decay, but by increasing the system size the data approach a power law decay  $P'(r) \sim r^{-k}$  with  $k = 2.1(1)$ . The fact that  $k > 1$  implies that the probability is normalizable. This is a confirmation that the transition is of first order type (see Ref. [15]). Notice however, that the algebraic nature of  $P'(r)$  implies infinite moments  $\langle r^n \rangle$  starting from  $n = 2$ . We conclude that the exponential decay found in reference [9] is an artifact of the approximation introduced.

We performed a series of calculations also in the two dimensional case. At the estimated critical temperature ( $T_c = 0.5811(7)$ ) we find, from the decay of the probability distributions  $P(l)$  and  $P'(r)$ , the estimates  $c = 2.95(5)$  and  $k = 3.0(1)$ , confirming the first order nature of the



**Fig. 7.** Plot of  $\log_{10} P'$  vs.  $\log_{10} r$ . The sets are the same as in Figure 6. A linear fit yields  $k = 2.1(1)$ .

transition. Again denaturation happens to be sharper than in the case where self-avoidance is fully incorporated, for which  $c \approx 2.46$  [8]. In the PERM algorithm both types of vertices of Figure 4 are generated, thus  $c$  cannot be directly compared with any of the value obtained analytically in the previous section.

## 4 Conclusion

In this paper we studied the model for DNA denaturation recently introduced by Garel *et al.* [9]. Our analysis is complementary to that of reference [9] and it is based on the calculation of the exponent  $c$  describing the algebraic decay of the probability of denaturated loop lengths at the critical point. Using exact results from mutually avoiding walks statistics we find that  $c > 2$  already for isolated loops, implying that the transition is of first order type. This conclusion is in agreement with the results of reference [9], but it is not based on those approximate treatments [19].

For some specific simple geometries in which a loop is embedded in the chain we provide analytical estimates of  $c$ , following ideas from the theory of polymer networks [6, 13]. These calculations show explicitly that  $c$  increases with respect to the isolated loop value, *i.e.* the transition robustly maintains its first order character. More surprising is, at first sight, the fact that the denaturation in the GMO model is sharper than that occurring in models where excluded volume constraints are fully incorporated (higher  $c$ ), as indicated by our analytical and numerical estimates of  $c$  both in  $d = 2$  and 3. This behavior can be explained by taking into account that the self-avoidance of the single strands somehow contrasts the excluded volume effects between each loop and the rest of the molecule. The result is that, when the single strand self-avoidance is relaxed, the loop sizes are further reduced, consistently with an increase of  $c$ .

It is somehow remarkable how results of the theory of block copolymer networks, which are relevant to issues like

that of establishing a link between field theory and multifractal measures (see *e.g.* Ref. [12]), allow to draw reliable predictions on models of the denaturation transition of DNA.

There is another possibility of relaxing the self-avoidance which is somehow complementary to that of the GMO model. One can indeed neglect the mutual avoidance between the strands, while keeping self-avoidance within each stand. This possibility was studied in  $d = 3$  in reference [7] and the denaturation transition turns out to be continuous ( $c < 2$ ). Thus, relaxing the self-avoidance constraint in two different ways within the single loop, results in a softening (as in the latter example) or a sharpening (as in the GMO model) of the transition.

Finally, we also considered the probability distribution of the distances between homologous monomers of the two strands. We found that this quantity decays as a power law at the transition point, in disagreement with the stretched exponential behavior found in reference [9], which is probably an artifact of the approximation introduced there. The algebraic decay of various quantities at denaturation, even in the case of first order transitions, is a common feature of other similar models. Finding the appropriate treatment of the Hamiltonian (1), which provides power-law decays at the transition point is still an open issue.

We are grateful to David Mukamel for useful discussions. Financial support by MUR through COFIN 2001 and by INFN through PAIS 2001 is gratefully acknowledged.

## Appendix

We review here some known results for entropic exponents of networks of arbitrary topology. We focus mainly on networks whose constituent polymers are all of the same type, and just briefly mention copolymer networks.

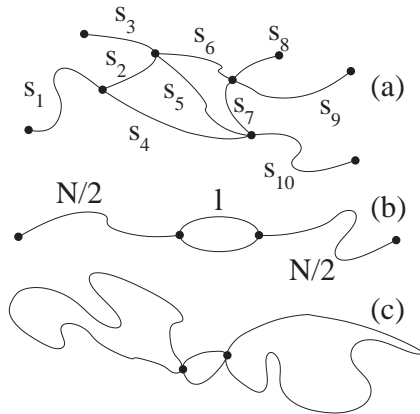
Let us consider a network made of self-avoiding walks, all avoiding each other, as the one shown in Figure 8a. Let  $N = \sum_i s_i$  be the total length of the network, where each segment has length  $s_i$ . In the asymptotic limit  $N \rightarrow \infty$ ,  $s_i \rightarrow \infty$ , the total number of configurations for the network scales as [13]:

$$\Gamma \sim \mu^N N^{\gamma_G - 1} f\left(\frac{s_1}{N}, \frac{s_2}{N}, \dots\right) \quad (10)$$

where the factor  $\mu$  is the effective connectivity constant for the walks (see *e.g.* Ref. [20]) and  $f$  is a scaling function. The universal exponent  $\gamma_G$  depends only on the number of independent loops,  $\mathcal{L}$ , and the number of vertices with  $k$  outgoing segments  $n_k$  as [13]

$$\gamma_G = 1 - \mathcal{L}d\nu + \sum_k \nu \eta_k n_k \quad (11)$$

where  $\eta_k$  are exponents associated to a vertex with  $k$  outgoing legs. Such exponents are known exactly in  $d = 2$  from conformal invariance [13], while they have been obtained from renormalization group and resummation techniques in  $d = 3$  [21]. We notice that it is also customary to use the definition  $\sigma_k \equiv \nu \eta_k$ .



**Fig. 8.** Examples of polymer networks with (a)  $\mathcal{L} = 2$ ,  $n_1 = 5$ ,  $n_3 = 2$  and  $n_4 = 2$ , (b)  $\mathcal{L} = 1$ ,  $n_1 = 2$ ,  $n_3 = 2$  and (c)  $\mathcal{L} = 3$ ,  $n_4 = 2$ .

This theory was recently applied to the denaturation problem [6]. In this case one considers network geometries as that of Figure 8b, in which a loop of total length  $2l$  is connected to two polymers of lengths  $N/2$  each. Following the above notation one has  $\mathcal{L} = 1$ ,  $n_1 = 2$  and  $n_3 = 2$  and thus the total number of configurations scale as:

$$\Gamma \sim \mu^N N^{\tilde{\gamma}-1} f\left(\frac{l}{N}\right) \quad (12)$$

with  $\tilde{\gamma} = 1 - d\nu + 2\nu(\eta_1 + \eta_3)$ . Now in the limit  $l \ll N$  one should recover the partition function for a self-avoiding walk of total length  $N$  which has an entropic exponent  $\gamma = 1 + 2\nu\eta_1$ . This requires that:

$$f(x) \sim x^{2\nu\eta_3 - d\nu} \quad (13)$$

in the limit  $x \rightarrow 0$ . Thus, loops of length  $l$  embedded within a long chain of length  $N$  ( $\gg l$ ) are distributed according to the probability  $P(l) \sim l^{-c}$ , with [6]:

$$c = d\nu - 2\nu\eta_3. \quad (14)$$

As second example we consider a loop of length  $2l$  embedded between two long loops of total length  $2N$ , as depicted in Figure 8b. The total number of configurations is still given by equation (12) with  $\tilde{\gamma} = 1 - 3d\nu + 2\nu\eta_4$ , as the network has now  $\mathcal{L} = 3$  independent loops and two vertices with four outgoing legs, *i.e.*  $n_4 = 2$ . In the limit  $l \ll N$  one should find the partition function of two loops joined at a single vertex. Matching the scaling function in this limit yields

$$f(x) \sim x^{\nu\eta_4 - d\nu} \quad (15)$$

for  $x \rightarrow 0$ . One finds thus that loops are distributed according to the probability  $P(l) \sim l^{-c}$ , with [6]:

$$c = d\nu - \nu\eta_4. \quad (16)$$

The theory can be generalized to the case of networks with more than one type of polymer, as for *copolymer* networks. Equation (11) can be generalized easily in the case

that the constituting polymers have all the same metric exponents (for instance in the case of mutually avoiding random walks). The only difference is that now vertex exponents will not depend only on the number of outgoing legs, but also on the type of polymers forming the vertex and, in two dimensions, also on the order. As an example we consider a network with the geometry given in Figure 3. In the limit where the inner loop is much smaller than the two outer ones the exponent  $c$  is given by equation (7), which is the copolymer network counterpart of equation (16). Notice that while for homopolymers  $\eta_2 = 0$ , in general a vertex with two outgoing polymers of different type will have a non-vanishing exponent (as is the case of the  $\eta_{11}^{(G)}$  introduced in Fig. 2).

Finally, if the polymers constituting the inhomogeneous network have a different  $\nu$  exponent, as for networks formed by a mixture of random and self-avoiding walks, equation (10) is still valid, but in a form involving the radii of gyrations  $R_i$  of the constituent polymers, where  $R_i \sim s_i^\nu$ , for a segment of length  $s_i$ .

## References

1. D. Poland, H.A. Scheraga, J. Chem. Phys. **45**, 1456 (1966); **45**, 1464 (1966)
2. M.E. Fisher, J. Chem. Phys. **45**, 1469 (1966)
3. M.E. Fisher, J. Stat. Phys. **34**, 667 (1984)
4. M. Peyrard, A.R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989)
5. M.S. Causo, B. Coluzzi, P. Grassberger, Phys. Rev. E **62**, 3958 (2000)
6. Y. Kafri, D. Mukamel, L. Peliti, Phys. Rev. Lett. **85**, 4988 (2000); Y. Kafri, D. Mukamel, L. Peliti, Eur. Phys. J. B **27**, 135 (2002)
7. E. Carlon, E. Orlandini, A.L. Stella, Phys. Rev. Lett. **88**, 198101 (2002)
8. M. Baiesi, E. Carlon, A.L. Stella, Phys. Rev. E, **66**, 021804 (2002)
9. T. Garel, C. Monthus, H. Orland, Europhys. Lett. **55**, 132 (2001)
10. B. Duplantier, K.-H. Kwon, Phys. Rev. Lett. **61**, 2514 (1988)
11. B. Duplantier, Commun. Math. Phys. **117**, 279 (1988)
12. C. von Ferber, Yu. Holovatch, Europhys. Lett. **39**, 31 (1997); C. von Ferber, Yu. Holovatch, Phys. Rev. E **56**, 6370 (1997)
13. B. Duplantier, Phys. Rev. Lett. **57**, 941 (1986)
14. Notice that denaturation becomes first order for  $d > 4$ , since  $\nu = 1/2$  and thus  $c = d\nu = d/2 > 2$
15. P.G. de Gennes, *Scaling concepts in Polymer Physics* (Cornell University Press, Ithaca, NY, 1979)
16. C. von Ferber, Yu. Holovatch, Phys. Rev. E **65**, 042801 (2002)
17. B. Duplantier, Phys. Rev. Lett. **82**, 880 (1999)
18. P. Grassberger, Phys. Rev. E **56**, 3682 (1997)
19. The approximate treatment of the excluded volume interaction as done in reference [9] has been the subject of recent debate. See: S.M. Bhattacharjee, Europhys. Lett. **57**, 772 (2002); T. Garel, C. Monthus, H. Orland, Europhys. Lett. **57**, 774 (2002)
20. C. Vanderzande, *Lattice Models of Polymers* (Cambridge University Press, Cambridge, United Kingdom, 1998)
21. L. Schäfer, C. von Ferber, U. Lehr, B. Duplantier, Nucl. Phys. B **374**, 473 (1992)