# DNA thermal denaturation by polymer field theory approach Yulian Honchar<sup>1,2,3</sup> Christian von Ferber<sup>2,3</sup> Yurij Holovatch<sup>1,2,3</sup>

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We discuss possible mechanisms that may impact the order of the transition between denaturated and bounded DNA states and lead to changes in the scaling laws that govern conformational properties of DNA strands. To this end, we re-consider the Poland-Scheraga model and apply a polymer field theory to calculate entropic exponents associated with the denaturated loop distribution. For the d = 2 case the latter are deduced from mapping the polymer model onto a two- dimensional random lattice, i.e. in the presence of quantum gravity. For the d = 3 case we get the corresponding (diverging)  $\varepsilon^4$  expansions evaluating them by restoring their convergence via the resummation technique.

## **DNA DENATURATION**

In its native state DNA has a form of a helix that consists of two strands bound together by hydrogen bonds. During biological processes involving DNA (such as duplication or transcription) unbinding occurs, phenomenon known also as denaturation.

The mechanism of such transition may be:

• mechanical (an external pulling force applied to one of DNA strands),



#### **Thermal denaturation of DNA**

One of important experimental observations of the DNA melting curves, where the fraction of the bound pairs  $\theta(T)$  is measured as a function of temperature T is their abrupt behaviour. With an increase of T,  $\theta(T)$  manifests a jump at certain transition temperature clearly signaling that the DNA thermal denaturation is a first order transition. Numerous theoretical approaches to represent the process of DNA thermal denaturation in a two-state Ising-like manner were developed. Here, we concentrate on the Poland-Scheraga type description, where the transition is governed by an interplay of two factors: chain binding energy and configurational entropy [2, 3]. In turn, the entropy of the macromolecule in a good solvent attains a scaling form and this is how the scaling exponents that govern configurational properties of polymer macromolecules of different topology (*Duplantier, Schäfer*) come into play in descriptions of DNA thermal denaturation.





• chemical (changes in the pH of the DNA contained solvent) or

• thermal (heating of the solvent).

The Poland-Scheraga description relies on a representation of the partition function  $\mathcal{Z}$  of a polymer of N segments, each segment being in two possible states (bound and unbound monomers) through the loop closure exponent c for a single loop, defined as

$$\mathcal{Z}_{\text{loop}} \sim \mu^{\ell} \ell^{-c},$$

For c > 1 the order parameter either continuously vanishes at  $T = T_c$ for  $1 < c \le 2$  or disappears abruptly at  $T = T_c$  for c > 2. The two types of behaviour correspond to the second and first order phase transitions respectively.

First attempts to define exponent c analytically let to:

- RW-loop: c = d/2 = 1.5 (*Poland, Scheraga, 1966*)
- SAW-loop:  $c = d\nu_{SAW} = 1.76$  (*Fisher, 1966*)
- MC: c > 2, taking into account the interactions between the loop and the chain (*Causo et al., 2000*)
- SAW system: c(d = 3) = 2.11 (*Kafri et al., 2000; Carlon et al., 2002*)
- Let us find the exponent c. In particular, the partition function (num-

Fig.1. Model of DNA thermal denaturation we consider in this study. A double stranded macromolecule with end points V1 is disattached ('unzipped') at points V3. Resulting heterogeneous polymer network consists of two double strands V1 - V3 (bound nucleobases, bold lines) and a denaturated single-stranded loop V3 - V3 (unbound nucleobases, thin lines). Partition function of the loop attains a power-law scaling [1]

## **MODEL AND POLYMER NETWORK**

$$\eta_{\mathcal{G}} = -d\mathcal{L} + \sum_{f_1 + f_2 \ge 1} n_{f_1, f_2} \eta_{f_1, f_2}, \tag{3}$$

Heterogeneity of the network shown in Fig.1 considering mutual avoidance between all SAWs and RWs leads to four cases: (i) both chains  $V_1 - V_3$  and  $V_3 - V_3$  are SAWs,

$$\eta_{\mathcal{G}} = -d + 2\eta_{12}^S \tag{4}$$

(ii) chains  $V_1 - V_3$  are SAWs, chains  $V_3 - V_3$  are RWs;

$$\eta_{\mathcal{G}} = -d + 2\eta_{12}^U$$

(5)

(6)

(7)

(iii) chains  $V_1 - V_3$  are RWs, chains  $V_3 - V_3$  are SAWs;

 $\eta_{\mathcal{G}} = -d + 2\eta_{21}^U$ 

(iv) all chains  $V_1 - V_3$  and  $V_3 - V_3$  are RWs.

$$\eta_{\mathcal{G}} = -d + 2\eta_{12}^G$$

When the network is formed by chains of different sizes: R for the

Here f(x) is the scaling function. In the limit  $r/R \to 0$  we apply the short-chain expansion (*Ferber*):  $\mathcal{Z}_{chain} \sim R^{\eta_{chain}}$  with  $\eta_{chain} = \eta_{02}^U = 0$  for RW and  $\eta_{chain} = \eta_{20}^U$  for SAW. This implies the power-law asymptotics for the scaling function:

$$f(x) \sim x^y$$
, with  $y = \eta_{\mathcal{G}} - F_1 \eta_{20}^U - \eta_{\text{chain}}$ . (9)

With (9) the partition function factorizes as

$$\mathcal{Z}_{\mathcal{G}} \sim R^{\eta_{\text{chain}}} \times r^{y} \sim \mathcal{Z}_{\text{chain}} \mathcal{Z}_{\text{loop}}.$$
 (10)

Hence the loop closure exponent c:

$$c = \nu_{\text{loop}} [\eta_{\text{chain}} - \eta_{\mathcal{G}} + F_1 \eta_{20}^U], \qquad (11)$$

and according exponents read:

$$SAW-SAW-SAW: c_{1} = \nu_{SAW}(3\eta_{20}^{S} + d - 2\eta_{12}^{S}), \qquad (12)$$
  

$$SAW-RW-SAW: c_{2} = \nu_{RW}(\eta_{20}^{S} + d - 2\eta_{12}^{U}), \qquad (13)$$
  

$$RW-SAW-RW: c_{3} = \nu_{SAW}(2\eta_{20}^{S} + d - 2\eta_{21}^{U}). \qquad (14)$$
  

$$RW-RW-RW: c_{4} = \nu_{RW}(d - 2\eta_{21}^{G}). \qquad (15)$$

ber of configurations) of a copolymer network  $\mathcal{G}$  (*Ferber*):

 $\mathcal{Z}_{\mathcal{G}} \sim R^{\eta_{\mathcal{G}} - F_1 \eta_{2,0} - F_2 \eta_{0,2}},$ 

S

(1)

Co-polymer star exponents  $\eta_{f_1f_2}$  in scaling relations (12)–(15) have been calculated by means of field-theoretic renormalization group approach and are currently available in  $\varepsilon = 4 - d$ -expansion up to order  $\varepsilon^4$  (*Schulte-Frohlinde*). Perturbative renormalization group expansions have zero radious of convergence and are asymptotic at best. We use the Borel resummation refined by conformal mapping which is known to be a powerful tool in analysis of  $\varepsilon$ -expansions. In general, the method is applied to the function in form of a series expansion:

$$u(x) = \sum_{n=0}^{\infty} c_n x^n, \tag{16}$$

After Borel sum and conformally mapping the cut plane onto a disk of radius 1:

$$=\frac{4}{a}\frac{\omega}{(1-\omega)^2}\,,\tag{17}$$

the procedure is further refined by introducing two additional fit parameters b and  $\alpha$ . The expression for the resummed function reads:

$$\upsilon_R(x) = \sum_n d_n(\alpha, a, b) \int_0^\infty dt \, t^b e^{-t} \frac{\omega^n(xt)}{(1 - \omega(t))^\alpha} \,. \tag{18}$$

ide chains 
$$V1 - V3$$
 and  $r$  for the loop  $V3 - V3$ :  
 $\mathcal{Z}_{\mathcal{G}} \sim R^{\eta_{\mathcal{G}} - F_1 \eta_{20}^U} f(r/R).$ 
(8)

#### $\varepsilon$ -EXPANSION RESUMMATION

Explicit form of the coefficients  $d_n(\alpha, a, b)$  is found on the base of known expansion coefficients  $c_n$  in Eq. (16). In practice, procedure (18) is applied to the truncated series (16), which is known up to order L. Let us denote the value of the resummed truncated function at given fixed x by  $v_R^{(L)}$ . Ideally, such value (that usually corresponds to certain physical observable) should not dependent on resummation parameters  $\alpha$  and b. To eliminate such dependence, for each perturbation theory order L one choses optimal values of  $\alpha_{opt}^{(L)}$ ,  $b_{opt}^{(L)}$  which satisfy condition of minimal sensitivity (*Delamotte, Dudka, Mouhanna*):

$$\frac{\partial v_R^{(L)}(b,\alpha)}{\partial b}\Big|_{b_{opt}^{(L)},\alpha_{opt}^{(L)}} = \frac{\partial v_R^{(L)}(b,\alpha)}{\partial \alpha}\Big|_{b_{opt}^{(L)},\alpha_{opt}^{(L)}} = 0.$$
(19)

In this way, a set of optimal values  $(b, \alpha)^L$  is obtained for every perturbation theory order L. Out of these points one has to choose those that ensure the fastest converge by minimizing values:

$$\upsilon_R^{(L+1)}(b^{(L+1)}, \alpha^{(L+1)}) - \upsilon_R^{(L)}(b^{(L)}, \alpha^{(L)}).$$
(20)

### **RESULTS AND CONCLUSIONS**



Fig.2.Loop closure exponent c for DNA of heterogeneous compositions modeled as sequences of random and self-avoiding walks in different orders of  $\varepsilon = 4 - d$  expansion at space dimension d = 3. Solid and dashed lines show resummed (convergent) and non-resummed (divergent) values, correspondingly. Value c = 2 discriminates between the first (at  $c \ge 2$  and the second (at  $1 \le c < 2$ ) order transition.

The above described procedure has been applied to obtain the results discussed below.

	Ι	II	III	IV
$\nu_{SAW}$	0.54(3)	0.56(2)	0.582(8)	0.585(3)
$\eta_{20}^S$	-0.25(6)	-0.292(4)	-0.289 (5)	-0.276(3)
$\eta_{12}^S$	-0.75(4)	-0.77(2)	-0.75(1)	-0.743(5)
$\eta_{12}^{ar{U}}$	-0.75(8)	-0.82(5)	-0.77(3)	-0.795(5)
$\eta_{21}^{U}$	-1.(2)	-0.9(8)	-0.95(8)	-0.98(3)

**Table 1:** Scaling exponents  $\nu$ ,  $\eta_{f_1f_2}$  obtained at d = 3 by resummation of  $\varepsilon$ -expansion in different orders of perturbation theory. [1]

	Ι	II	III	IV
$c_1$ (SAW-SAW-SAW)	2.04 (15)	2.05 (9)	2.12 (4)	2.147 (9)
$c_2$ (SAW-RW-SAW)	2.12 (7)	2.17 (2)	2.16 (1)	2.169 (4)
$c_3$ (RW-SAW-RW)	2.7 (3)	2.8 (1)	2.76 (8)	2.76 (3)
$c_4$ (RW-RW-RW)	2.5	2.5	2.5	2.5

**Table 2:** Loop closure exponents  $c_i$  (12)–(15) in different orders of perturbation theory for different combinations of interacting SAWs and RWs. [1]



Fig.3. Loop closure exponents  $c_i$  of the heterogeneous co-polymer network of interacting SAWs and RWs (as shown in Fig.1) in different orders of the perturbation theory. [1]

Influence of possible heterogeneity in entropic scaling exponents of bound and denaturated DNA strands on the loop closure exponent c is manifest by an interplay of two factors. On the one hand, the number of configurations of a denaturated loop, is influenced by the loop

self-avoidance interactions (the number is larger for the RW loop and smaller of the SAW one). On the other hand, the number of loop configurations is restricted by the side chains. Calculations presented here give a reliable way to judge about the values of exponents  $c_i$  for different heterogeneity conditions and hence to judge about the order of DNA thermal denaturation transition. Our analysis is grounded on the field theory of co-polymer networks (*Ferber*). By scaling relations (12)–(15) we connect loop closure exponents  $c_i$  to scaling exponents  $\eta_{f1f2}$  that govern entropic properties of co-polymer stars made by mutually interacting sets of SAWs and RWs. As one can see, the effects of heterogeneity significantly influence the strength of the first order transition (the exponent c increases in comparison to the usual homogeneous SAW case).

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