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DNA thermal denaturation by polymer field theory approach: effects of the environment

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We analyse the effects of the environment (solvent quality, presence of extended structures — crowded environment) that may have impact on 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. We find that the effects studied significantly influence the strength of the first order transition. 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 $d = 3$ case, the corresponding diverging $\varepsilon = 4 - d$ expansions are evaluated by restoring their convergence via the resummation technique. For the space dimension $d = 2$, the exponents are deduced from mapping the polymer model onto a two-dimensional random lattice, i.e., in the presence of quantum gravity. We also show that the first order transition is further strengthened by the presence of extended impenetrable regions in a solvent that restrict the number of the macromolecule configurations.

Key words: *DNA denaturation, Poland-Scheraga model, polymer networks, crowded environment*

Nucleic acids together with proteins and carbohydrates belong to macromolecules essential to all known forms of life. Enormous experimental, theoretical, and simulational efforts have been involved to understand and qualitatively describe their physical, chemical and biological properties. In this paper we show how an insight from polymer field theory helps to shed light on properties of a DNA helix-to-coil (also called denaturation, unwinding or unzipping) transition: a phenomenon, that lies at the origin of biological processes involving DNA, as duplication or transcription. The latter phenomena occur in a cell and are complex biological protein-mediated processes. An analogue of DNA unwinding is also observed *in vitro*: when purified DNA solution is heated above the room temperature, the cooperative transition from the hydrogen bound double-stranded helix structure to a single stranded one occurs, see [1] and references therein for review. This phenomenon is known as DNA thermal denaturation and is the subject of our study.

In statistical physics, the DNA thermal denaturation is described in terms of the Poland-Scheraga model [2–4] that allows its treatment in terms of phase transition theory. In a recent paper [5] we have shown that changes in the solvent quality may cause an essential impact on the order of the phase transition between denaturated and bounded DNA states. To quantify this impact, we have calculated $\varepsilon = 4 - d$ expansions for the entropic exponents that govern the denaturated loop distribution in a good solvent and in the θ-solvent regimes and evaluated these (divergent) expansions in $d = 3$. In this paper, we complement such analysis by offering exact results for the exponents at $d = 2$. Moreover, we further analyse possible reasons that may have impact on the order of the transition. In particular, we are interested in the effects caused by the presence of extended structures that restrict the swelling of polymer

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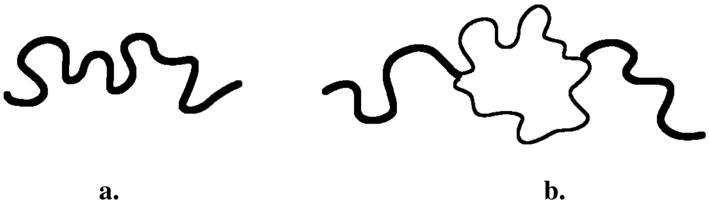


Figure 1. Model of DNA thermal denaturation (unzipping) transition discussed in this paper. At low temperatures T, two DNA strands remain connected by hydrogen bonds and form a single long flexible polymer chain (figure **a**). With an increase of T, the chain unzips and a loop emerges: now the whole structure consists of two different 'species': double stranded side chains, shown by solid lines, and a single stranded loop shown by a thin line in the middle (figure **b**).

chains. By such analysis we make an attempt to consider the situation in a more realistic condition of macromolecules in a crowded environment of a cell [6].

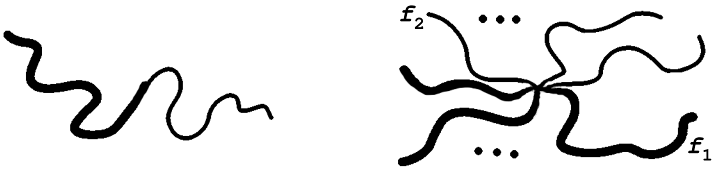
The rest of the paper is organized as follows. In the next section we repeat some of our results for the scaling relations and entropic scaling exponents [5] and give their numerical estimates at $d = 3$. Based on the exact conformal scaling dimensions for two-dimensional copolymers derived from an algebraic structure existing on a random lattice (quantum gravity) [7–9] we derive exact values of the exponents at $d = 2$ and discuss the whole sector $2 \leqslant d \leqslant 4$ in section 2. Crowded environment effects are analysed in section 3, conclusions are summarized in section 4. It is our pleasure and a big honour to contribute by this paper to the Festschrift devoted to Prof. Yu. Kalyuzhnyi on the occasion of his 70th birthday. Doing so we deeply acknowledge his seminal contributions to the soft matter physics in general and to the subject discussed in this paper in particular, see e. g., [10–15]. CvF and YuH also are indebted to the jubilee for a long-lasting friendship, numerous discussions about physics and not only.

1. Poland-Scheraga model: scaling relations and ε-expansion

The model suggested by Poland and Scheraga in middle-sixties [2, 3] describes the DNA thermal denaturation by a proper account of energy-entropy interplay: at low temperatures T, the bound state, figure 1 **a**, is favoured by energy whereas at high T the unbound state, figure 1 **b**, is favoured by entropy as the one having more configurations. Poland and Scheraga's theoretical works lead to a whole family of DNA denaturation models [4, 6, 16–24]. It was shown that the unzipping transition mechanism is governed by the universal loop exponent c which describes scaling of the partition function of a single-stranded DNA loop in double stranded side chains, see figure 1 **b**:

$$\mathcal{Z}_{\text{loop}} \sim \mu^{\ell} \ell^{-c}, \tag{1.1}$$

here, ℓ is loop length (number of unbound segments) and μ is non-universal fugacity. For $c > 1$, the model predicts the denaturation transition whereas for $0 \leqslant c \leqslant 1$ the order parameter (average number of ordered bound pairs in a chain) is a continuous function of T smoothly changing between 1 and 0 when T increases from 0 to ∞. In turn, for larger values of c, the order parameter either continuously vanishes at $T = T_c$ for $1 < c \leqslant 2$ or disappears abruptly at $T = T_c$ for $c > 2$. The last two types of behaviour correspond to the second and first order phase transitions, respectively. However, the value of c is not obvious. First papers on the model suggested $c = d/2$, which lead to the second order transition and $d = 3$ [2, 3]. Later Fisher has considered taking into account the self-avoiding nature of chains that lead to $c = d\nu$ [16], where ν is polymer mean square end-to-end distance scaling exponent. Still, with $\nu(d = 3) \simeq 0.588$ [25], the phase transition remains the second order. This result contradicts experimental observations of the first order nature of the transition [1]. A more general approach to analyze scaling properties of the macromolecule configurations shown in figure 1 was based on polymer network theory, as interaction between the loop and the chain was taken into account [17–21, 26, 27]. Considering both the side chains and the loop as self-avoiding walks (SAWs), it was shown that the phase transition is of



a. **b.**

Figure 2. **a:** block copolymer of two polymer chains of different species, shown by solid and thin lines, linked together. **b:** copolymer star consisting of f_1 chains species 1 and f_2 chains of species 2 tied together at their end points. Its scaling properties are governed by universal copolymer star exponents $\eta_{f_1f_2}$. Note that the block copolymer gives a trivial example of a two-arm copolymer star with an exponent η_{11}.

the first order for $d = 2$ and above. This result was further supported by numerical simulations [26] and it was also suggested that possible heterogeneity in chain structure may strengthen the transition.

Depending on temperature, the asymptotic scaling behaviour of a long flexible polymer macromolecule in a good solvent belongs either to random walk (RW), $T = T_\theta$, or to self-avoiding walk (SAW), $T > T_\theta$ universality classes (T_θ denoting the θ-point) [28, 29]. Therefore, the only difference that may be observed in asymptotic scaling of chains of different species (in our case these are the double- and single-stranded chains) is due to the difference in asymptotic scaling properties of mutually interacting SAWs and RWs. Based on this fact, recently [5] we have applied polymer field theory [9, 25, 32–34] to derive scaling relations that express the loop exponent c (1.1) in terms of the familiar copolymer star exponents $\eta_{f_1f_2}$. The latter govern the scaling of star-like polymer structures that are created by linking together the end points of polymer chains of two different species at a common core, as shown in figure 2. When such a copolymer star is immersed in a good solvent, its asymptotic properties are universal in the limit of long chains. In particular, the partition function (the number of configurations) of a copolymer star made of two sets of f_1 and f_2 mutually avoiding RWs scales with its size R as [9, 32–34]:

$$Z^G_{f_1f_2} \sim R^{\eta^G_{f_1f_2}} . \tag{1.2}$$

In turn, the partition function of a copolymer star made of mutually avoiding sets of f_1 SAWs and f_2 RWs scales as:

$$Z^U_{f_1f_2} \sim R^{\eta^U_{f_1f_2} - f_1\eta^U_{20}} . \tag{1.3}$$

The third case which is of interest here is the star of two sets of f_1 and f_2 SAWs. For its partition function, one gets:

$$Z^S_{f_1f_2} \sim R^{\eta^S_{f_1,f_2} - (f_1+f_2)\eta^S_{20}} . \tag{1.4}$$

Indices G, U, S in the above formulae refer to the fixed points (FPs) of the renormalization group transformation that govern the scaling of corresponding mutually avoiding structures: Gaussian FP for RWs, unsymmetric FP for RW and SAW, and symmetric FP for SAWs, see [32–34] for more details. Exponents $\eta^S_{f_1,f_2}$ are related to $\eta^U_{f_1,f_2}$ and to the homogeneous star exponents η_f [30, 31] via: $\eta^S_{f_1,f_2} = \eta^U_{f_1+f_2,0} = \eta_{f_1+f_2}$.

With the above considerations in mind, one is led to four different cases that account for possible inhomogeneities and, therefore, for different scaling exponents of the DNA denaturation model shown in figure 1 **b**:

1. both bound chains and the unbound loop are SAWs (SAW-SAW-SAW);
2. bound chains are SAWs, the loop is RW (SAW-RW-SAW);
3. the chains are RW-like, while the loop is SAW (RW-SAW-RW);
4. both the chains and the loop are RW-like, though they do not intersect each other (RW-RW-RW).

The scaling relations that express the loop exponent c (1.1) in terms of copolymer star exponents $\eta_{f_1 f_2}$ for these four cases read [5]:

$$\begin{aligned}
&\text{1. SAW-SAW-SAW:} &&c_1 = \nu_{\text{SAW}}(3\eta^S_{20} + d - 2\eta^S_{12}), \\
&\text{2. SAW-RW-SAW:} &&c_2 = \nu_{\text{RW}}(\eta^S_{20} + d - 2\eta^U_{12}), \\
&\text{3. RW-SAW-RW:} &&c_3 = \nu_{\text{SAW}}(2\eta^S_{20} + d - 2\eta^U_{21}), \\
&\text{4. RW-RW-RW:} &&c_4 = \nu_{\text{RW}}(d - 2\eta^G_{21}).
\end{aligned} \tag{1.5}$$

Here, $\nu_{\text{RW}} = 1/2$ and ν_{SAW} are the mean square end-to-end distance exponents for the random and self-avoiding walks, correspondingly, and d is space dimension. The exponents $\eta_{f_1 f_2}$ have been calculated within field-theoretical renormalization group approach [9, 32–34] and are currently know in the fourth order of the $\varepsilon = 4 - d$ expansion [35]. Below, we list them together with the ε-expansion for the exponent ν_{SAW} [36] in the corresponding order:

$$\begin{aligned}
\eta^S_{20}(\varepsilon) = &- \varepsilon/4 - 9\varepsilon^2/128 + \varepsilon^3[264\zeta(3) - 49]/2048 \\
&+ \varepsilon^4[704\pi^4 - 297600\zeta(5) + 38160\zeta(3) + 235]/655360,
\end{aligned} \tag{1.6}$$

$$\begin{aligned}
\eta^S_{12}(\varepsilon) = &- 3\varepsilon/4 - 3\varepsilon^2/128 + 3\varepsilon^3[40\zeta(3) + 23]/2048 \\
&+ \varepsilon^4[64\pi^4 - 32640\zeta(5) - 6480\zeta(3) + 3333]/131072,
\end{aligned} \tag{1.7}$$

$$\begin{aligned}
\eta^U_{12}(\varepsilon) = &- 3\varepsilon/4 + \varepsilon^2[42\zeta(3) - 13]/128 + \varepsilon^3[384\zeta(3) - 5]/2048 \\
&+ \varepsilon^4[1024\pi^4 - 528000\zeta(5) + 14880\zeta(3) + 7655]/655360,
\end{aligned} \tag{1.8}$$

$$\begin{aligned}
\eta^U_{21}(\varepsilon) = &- \varepsilon + \varepsilon^2[42\zeta(3) + 1]/64 + 17\varepsilon^3/1024 \\
&- \varepsilon^4[1056\zeta(3) - 721]/65536,
\end{aligned} \tag{1.9}$$

$$\eta^G_{21}(\varepsilon) = -\varepsilon, \tag{1.10}$$

$$\begin{aligned}
\nu_{\text{SAW}}(\varepsilon) = &1/2 + \varepsilon/16 + 15\varepsilon^2/512 + \varepsilon^3[135/8192 - (33/1024)\zeta(3)] + \varepsilon^4[3799/524288 \\
&- (873/32768)\zeta(3) - (11/40960)\pi^4 + (465/4096)\zeta(5)],
\end{aligned} \tag{1.11}$$

where $\zeta(x)$ is Riemann zeta-function. Note that the formula for the exponent η^G_{21} contains only linear in ε term and is exact.

Substituting expressions (1.6)-(1.11) into the scaling relations (1.5) one can evaluate loop exponents c_i at any value of d. It is well known, however, that ε-expansions of the field theory are asymptotic at best and proper resummation technique is required to get a reliable numerical information on their basis [37, 38]. Applying resummation technique based on the Borel-Leroy transformation enhanced by conformal mapping of a cut-plane on a disc [39–41], we arrived at the following values of the loop exponents c_i for $d = 3$ [5]:

$$\begin{aligned}
c_1 &= 2.147 \pm 0.009, \quad c_2 = 2.169 \pm 0.004, \\
c_3 &= 2.76 \pm 0.03, \quad c_4 = 2.5.
\end{aligned} \tag{1.12}$$

Clearly, $c > 2$ in all configurations, which confirms the first order transition.

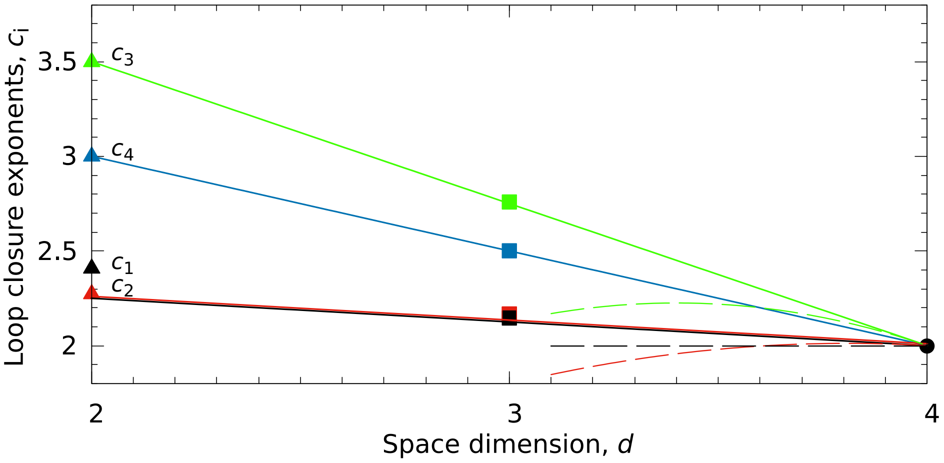


Figure 3. (Colour online) Loop closure exponents c_i at different space dimension d. Triangles show exact results at $d = 2$ (2.3) and squares show most accurate results obtained by resummation at $d = 3$ [5]. The lines show analytic continuation to non-integer d via ε-expansion in the first and second orders, thick solid and thin dashed lines, correspondingly. Note that in the case of mutually avoiding RWs (blue line), loop closure exponents $c_4(\varepsilon)$ are exact and linear in ε.

2. Exact results at $d = 2$ and quantum gravity

As has been discussed above, the ε-expansions for the c_i may serve as a basis for reliable numerical estimates at $d = 3$ provided appropriate resummation technique is applied. With the perturbative expansions and their numerical estimates at hand, it is instructive to corroborate the results by comparing them with the data for other space dimensions, if available. One obvious result is obtained for $d = 4$: there, as it is easy to check via equations (1.5), all exponents are equal: $c_i(d = 4) = 2$. Besides, there is a tempting opportunity to get exact values for the exponents at $d = 2$. Indeed, to this end one can make use of the exact results for the scaling exponents of $d = 2$ copolymer stars of mutually avoiding bunches of SAW and RW [7, 8]. There, the relations between exponents in fluctuating geometry (quantum gravity) and flat $d = 2$ geometry have been used to extract the exact values of the exponents. In notations of the previous section, the exponents read:[1]

$$\eta^G_{f_1 f_2} = \frac{1}{48}\left\{4 - \left[\sqrt{24 f_1 + 1} + \sqrt{24 f_2 + 1} - 2\right]^2\right\}, \tag{2.1}$$

$$\eta^U_{f_1 f_2} = \frac{1}{48}\left\{4 + 5 f_1 - \left[3 f_1 + \sqrt{24 f_2 + 1} - 1\right]^2\right\}. \tag{2.2}$$

Substituting these formulae into equations (1.5) and taking into account that $\nu_{\text{SAW}}(d = 2) = 3/4$ [25], one gets the following exact values of the exponents c_i at $d = 2$:

$$\begin{aligned} c_1 &= \frac{77}{32} \simeq 2.406, \quad c_2 = \frac{109}{48} \simeq 2.271, \\ c_3 &= \frac{7}{2}, \quad c_4 = 3\,. \end{aligned} \tag{2.3}$$

These values are shown by triangles in figure 3. The obtained result for the exponent c_3 recovers the value predicted at $d = 2$ by the exact formula that follows from equation (1.5) and is also valid for other values of d: $c_3 = 2 + \varepsilon/2$.

Comparing the values of the loop closure exponents c_i at $d = 2$ and at $d = 3$ one can arrive at certain conclusions about an impact of chain heterogeneity on the strength of the DNA thermal denaturation

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[1] Cf. equations (100), (101) of [9].

transition. The first observation is that passing from the homogeneous SAW composition within the Poland-Scheraga model (as described by the exponent c_1) usually leads to strengthening of the first order transition. When the SAW side chains are substituted by RWs, the strength of the transition increases: $c_3 > c_1$, $c_4 > c_2$. In turn, when the side chains remain unchanged, the change of the SAW loop to the RW loop decreases the strength of the first order transition: $c_3 > c_4$ and $c_1 > c_2$. The last effect is more pronounced for the RW side chains and at space dimension $d = 2$. In general, the following rule holds: $c_2 < c_1 < c_4 < c_3$ (with $c_2 \sim c_1$ at $d = 3$).

Another striking feature that follows from the comparison of the exact and perturbative results shown in figure 3 is a rather unusual behaviour of the ε-expansion curves. Indeed, the first order ε-expansion for the exponents c_i (solid lines in the plot) nicely corresponds to the resummed ε^4-data at $d = 3$ and to the exact values at $d = 2$. Such a behaviour is obvious for the exponent c_3, where the first order ε-expansion provides an exact number. However, for the other exponents, an account of the higher orders of the perturbative expansion needs careful application of the resummation technique. Being evaluated naïvely by simple adding higher order contribution, the ε-expansion holds only very close to the upper critical dimension $d = 4$, as shown in the figure by the thin dashed lines for the case of ε^2-data. Therefore, the first order ε-expansion provides the so-called optimal truncation [38] for the $c_i(\varepsilon)$ series.

3. Crowded environment

In two former sections, 1 and 2, we discussed an impact of the solvent quantity on the order of the DNA thermal denaturation transition. Another factor that may modify the scaling exponents of long flexible polymer macromolecules is the presence of impurities — impenetrable regions in a solvent that restrict the number of polymer configurations, see e.g., [42] and references therein. Statistics of polymers in disordered medium is of interest for a number of reasons. In the context of our study it is important to mention its relevance for treating macromolecules in a cell, composed of many different kinds of biochemical species [43–45].

There exist different analytic frameworks to model an impact of disordered medium on the scaling properties of (interacting) SAWs and RWs. To give a few examples, the latter are studied on a percolation cluster [46, 47] or at presence of quenched defects [48–55]. Taking into consideration that the uncorrelated defects do not influence polymer scaling [48, 49], the so-called 'extended' or long-range correlated structural disorder has been shown to be relevant. A model of long-range correlated disorder has been suggested in [50] and further exploited in studies of polymers [52–55]. Within this model, one considers the defects, characterized by the density-density pair correlation function $g(r)$ decaying at a large distance r according to the power law

$$g(r) \sim r^{-a} \, . \tag{3.1}$$

For integer values of a, such defects have a direct interpretation: the case $a = d$ corresponds to point-like defects, while $a = d - 1$ ($a = d - 2$) correspond to straight lines (planes) of defects of random orientation. Sometimes non-integer values of a are interpreted in terms of fractal structures.[2] Detailed analysis of an impact of the long-range correlated disorder (3.1) on possible changes in the exponents (1.5) and hence on the DNA thermal denaturation is beyond the scope of this study. However, we will use some of the previously obtained results in order to understand and qualitatively describe this possible impact.

It is easy to see that the presence of long-range correlated impurities may or may not be relevant and change the polymer scaling exponents depending on the value of a. Indeed, large-distance asymptotics of the pair correlation function (3.1) corresponds to the power-law behaviour of its Fourier-image at small wave vector k in the form k^{a-d}. Therefore, by simple power counting, one arrives at the conclusion that such a term becomes relevant at small k for $a < d$. Applying field-theoretic renormalization group technique, the corresponding polymer model has been analysed and the scaling exponents were calculated in the two-loop approximation at fixed $d = 3$ and different values of the correlation parameter a as well as in a one-loop order by the double expansion in $\varepsilon = 4 - d$ and $\delta = 4 - a$ [52–54]. The derivation given below is based on these double ε, δ expansions. In particular, it has been shown that for certain

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[2] See also [56–58], where the relation of fractal dimension to the analytically continued non-integer dimension is discussed in more details.

region of parameters $\varepsilon/2 < \delta < \varepsilon$, the scaling properties of a single flexible polymer chain in porous environment with a long-range correlated structure are governed by a new, 'long-range' fixed point L. The mean square end-to-end distance exponent ν_{SAW} in the first order of ε, δ expansion reads [52]:

$$\nu^{L}_{\text{SAW}} = 1/2 + \delta/8 + \dots . \tag{3.2}$$

In turn, the $\eta_{f_1 f_2}$ exponents for co-polymer stars in porous environment with long-range correlated structure are given by:[3]

$$\begin{aligned}
\eta^{S_L}_{f_1 f_2} &= \frac{-(f_1+f_2)(f_1+f_2-1)\delta}{4}, && (3.3)\\
\eta^{U_L}_{f_1 f_2} &= \frac{-f_1(f_1+3f_2-1)\delta}{4}, && (3.4)\\
\eta^{G_L}_{f_1 f_2} &= -f_1 f_2 \delta . && (3.5)
\end{aligned}$$

In equations (3.3)–(3.5), the first exponent $\eta^{S_L}_{f_1 f_2}$ corresponds to the star of $f_1 + f_2$ SAWs, the second exponent $\eta^{U_L}_{f_1 f_2}$ describes the star of mutually avoiding sets of f_1 SAWs and f_2 RWs, and the third exponent $\eta^{G_L}_{f_1 f_2}$ describes the star of two mutually avoiding sets of f_1 and f_2 RWs.

Two cautions are at place here. First, the 'long-range' fixed point S_L is accessible in the region where the above mentioned power counting shows that the disorder is irrelevant. Second, the fixed points U_L and G_L can be reached only for specific initial conditions. Similar situation is also encountered when the ε, δ expansion is applied to study models of m-vector magnets with long-range correlated quenched disorder [50]. However, an account of higher order contributions restores the physical region of stability of the 'long-range' fixed point confirming a qualitatively correct result of the first-order analysis, see e.g., [59] and references therein. Therefore, with an aim of getting a qualitative description of an impact of extended long-range correlated impurities on the DNA thermal denaturation transition, we proceed with formulae (3.2)–(3.5) substituting them into the scaling relations (1.5) and arrive at the following first-order values for the c_i exponents:

$$\begin{aligned}
c^{L}_{1} &= c^{L}_{2} = 2 - \varepsilon/2 + 5\delta/4, && (3.6)\\
c^{L}_{3} &= c^{L}_{4} = 2 - \varepsilon/2 + 2\delta. && (3.7)
\end{aligned}$$

As it follows from equation (3.1), the smaller is a, the stronger are the correlations in porous structure that restricts the volume available for the macromolecule. Indeed, the density-density correlation function $g(r)$ decays slower with a decrease of a, attaining the fat-tail features. The positive sign at the linear in δ terms in equations (3.6), (3.7) brings about an increase in the exponents c_i with an increase of $\delta = 4 - a$. This allows to conclude, that an increase in density correlations of the porous structure leads to strengthening of the DNA thermal denaturation transition. Moreover, comparing equations (3.6) and (3.7), one concludes that $c^{L}_{3}, c^{4}_{4} > c^{L}_{1}, c^{L}_{2}$, similar to what was observed for the DNA denaturation in a pure solvent without porous medium. The difference between the exponents increases with an increase of δ: $c^{L}_{3,4} - c^{L}_{1,2} = 3\delta/4$. Of course, with all cautions mentioned above, these results should be considered as qualitative predictions, rather than a quantitative description of DNA denaturation in a crowded environment. The above obtained relations $c^{L}_{1} = c^{L}_{2}$ and $c^{L}_{3} = c^{L}_{4}$ may be (and perhaps indeed are) violated in the second order of the perturbation theory. However, it is worth mentioning that the scaling arguments supported by the renormalization group calculations predict the effect of strengthening the order of the denaturation transition when it occurs in presence of extended structures that restrict the swelling of the polymer coil.

4. Conclusions

The value of the loop closure exponent c (1.1) discriminates between different ways the thermal denaturation of the DNA occurs: for $c > 2$, the denaturated loop emerges abruptly, in the first order

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[3] Cf. equation (39) from [55].

phase transition manner, for $1 < c < 2$, the transition is continuous, and for $c < 1$, no transition happens. Numerous attempts of theoretical description and numerical simulation of this phenomenon finally led to the coherent picture, observed also in the *in vitro* experiments and simulations [1, 17, 27, 60]: the transition is of the first order and $c > 2$. Besides, the factors that may have an impact on the strength, and, eventually, even on the order, of this transition are discussed in the literature [6]. In a recent paper [5], we have derived scaling relations that express the loop closure exponent c of the Poland-Scheraga model in terms of the copolymer star exponents $\eta_{f_1 f_2}$ [32–34]. This enabled us to analyse an impact of inhomogeneities in DNA chain composition and solvent quality on the order of the transition. As it has been shown in [5] and as it is briefly discussed in the above section 1, consideration of the macromolecule as sets of mutually avoiding SAWs and RWs (see figure 1) leads to an increase in value of c and $d = 3$ and, hence, strengthens the first order transition. In the present paper, we support this observation providing exact results at $d = 2$. Moreover, we show that the effect of strengthening is further enhanced by the so-called crowded environment with the long-range correlated inhomogeneities.

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Термічна денатурація ДНК в підході теорії поля для полімерів: вплив середовища

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Ми розглянули вплив середовища (якість розчинника, присутність витягнутих структур (перешкод) — «зайняте» середовище), який може змінити рід переходу між денатурованим та зв’язаним станами ДНК і привести до змін законів скейлінґу для конформаційних властивостей ланцюжків ДНК. Показано, що досліджені ефекти значним чином впливають на інтенсивність переходу першого роду. З цією метою, ми розглянули модель Поланда-Шераги і застосували підхід теорії поля для полімерів, щоби обчислити ентропійні показники, пов’язані з розподілом денатурованих петель на ланцюгу. Для випадку $d = 3$ проаналізовано відповідні розбіжні $\varepsilon = 4-d$ розклади, оцінюючи їх за допомогою відновлення збіжності методами пересумовування степеневих рядів. Для вимірності $d = 2$ їх обчислено завдяки проектуванню полімерної моделі на двовимірну випадкову ґратку, тобто розглянуто систему за присутності квантової ґравітації. Ми також показуємо, що інтенсивність переходу першого роду посилюється за наявності у розчиннику протяжних непроникних областей, що обмежують кількість конфігурацій макромолекули.

Ключові слова: *денатурація ДНК, модель Поланда-Шераги, полімерні мережі, невпорядковане середовище*