Advanced Statistical Physics TD3: The unzipping transition of the DNA

October 2021

The purpose of this exercise, which is largely inspired by the beautiful paper Kafri, Mukamel, and Peliti, Physical Review Letters **85**, 4988 (2000), is to study the unzipping transition of the DNA in a simplified setting.



FIG. 1 – A configuration of the DNA molecule made by a segment of ℓ_1 pairs of bonded monomers and a portion of ℓ_2 unzipped monomers.

We consider a schematic model of the DNA molecule as two filaments composed by a sequence of identical monomers. In order to simplify the treatment of the problem, we will start by assuming that the possible configurations of the DNA molecule are made by two parts, as in figure 1 (Poland-Sheraga model).

- a segment of ℓ_1 pairs of bonded monomers (with $\ell_1 \ge 0$),

- an unzipped portion made by ℓ_2 monomers (with $\ell_2 \ge 0$) on each filament.

The bonding energy associated to each pair of bonded monomers is $-\epsilon_0$ (with $\epsilon_0 > 0$). To simplify the notations we will introduce the Boltzmann factor $\omega = e^{\beta \epsilon_0}$ corresponding to the statistical weight of each bonded pair.

We will assume that the statistical (entropic) weight of the unzipped portion correspond to an entropic gain accounting for all possible configurations of the two filaments of length ℓ_2 (which all have the same energy), which is given by

$$\Omega(\ell_2) = \frac{s^{\ell_2}}{\ell_2^c},\tag{1}$$

with s being a constant (s > 1) and c an exponent which depends on the space dimension.

The analysis of the model is simpler in the grand canonical ensemble. We will then introduce a fugacity $z = e^{\beta\mu}$ associated to the number of pairs of monomer of the DNA (bonded or not).

- 1. Compute the grand partition function Ξ of the molecule in the Poland-Sheraga setting as a function of z, ω and s and show that it is given by the product of the two grand partition functions V_0 (of the bonded segment) and Q (of the unzipped portion) that need to be specified explicitly.
- 2. We now assume, as in Kafri, Mukamel, and Peliti, Physical Review Letters 85, 4988 (2000), that the configurations of the DNA molecule are made by arbitrarily alternating sequences of bonded segments and unzipped portions. Show that the grand partition function Ξ can be expanded as illustrated in figure 2, with U = Q 1 and $V = V_0 1$. Find the expression of Ξ and of the grand potential J.



FIG. 2 – Graphical representation of the expansion of the partition function in powers of $(UV)^n$.

- 3. Write the grand canonical relation which gives the average length of the molecule $\langle L \rangle$ (i.e. the total number of pairs of monomers) from the expression of $\ln \Xi$.
- 4. Henceforth we will focus on the thermodynamic limit, $\langle L \rangle \to \infty$. We define z_{\star} as the smallest value of the fugacity for which $\langle L \rangle$ diverges. Identify the possible values of z_{\star} .
- 5. Show that for c > 1 there is a phase transition between a bonded phase at low temperature and an unzipped phase at high temperature. Find the critical temperature.
- 6. To study the unzipping transition, we will introduce the order parameter $\langle M \rangle$, defined as the average number of bonded pairs of monomers. In the thermodynamic limit the intensive order parameter (i.e. the fraction of bonded pairs) is:

$$m = \lim_{\langle L \rangle \to \infty} \frac{\langle M \rangle}{\langle L \rangle}.$$

Show that m can be written as:

$$m = \frac{\partial \log z_{\star}}{\partial \log \omega}$$

7. We specify now to the case 1 < c < 2 (and $s > \zeta(c) + 1$) and we consider a temperature close to the critical point. We set:

$$\omega = \omega_c + \delta$$
, $z = \frac{1}{s} - \epsilon$.

By expressing ϵ as a function of δ , show that the unzipping transition is second order and compute the critical exponent β such that $m \sim |T - T_c|^{\beta}$.

8. Show that for c > 2 the transition is instead first order.

9. Show that for c < 1 there is no transition and the DNA molecule is in the unzipped phase at all temperature

APPENDIX: Few properties of the polylogarithmic function

The polylogarithmic function is defined as:

$$g_c(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^c} \,.$$

It has the following integral representation:

$$g_c(x) = \frac{1}{\Gamma(c)} \int_0^\infty \frac{t^{c-1} dt}{x^{-1} e^t - 1}$$

- For c > 1 its value in x = 1 is

$$g_c(1) = \zeta(c) \,,$$

where ζ is the Riemann zeta-function.

- For c < 1 the polylogarithmic function diverges for $x \to 1^-$ as:

$$g_c(x) \sim \frac{1}{(1-x)^{1-c}}$$
.

– For c > 1 and $x \to 1^-$ we have that:

$$g_c(1-\epsilon) \approx \zeta(c) - \epsilon^{\gamma},$$

avec $\gamma = \min(1, c - 1)$.