

Unzipping of two random heteropolymers: Ground-state energy and finite-size effects

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We consider a pair of random heteropolymer chains with quenched primary sequences. For this system we have analyzed the dependence of average ground state energy per monomer \mathcal{E} on chain length n in the ensemble of chains with uniform distribution of primary sequences of monomers. Every monomer of the first (second) chain is randomly and independently chosen with the uniform probability distribution $p=1/c$ from a set of c different types $A, B, C, D, \dots (A', B', C', D', \dots)$. Monomers of the first chain could form saturating reversible bonds with monomers of the second chain. The bonds between similar monomer types (such as $A-A', B-B', C-C'$, etc.) have the attraction energy u , while the bonds between different monomer types (such as $A-B', A-D', B-D'$, etc.) have the attraction energy v . The main attention is paid to the computation of the normalized free energy $\mathcal{E}(n)$ for intermediate chain lengths n and different ratios $a=v/u$ at sufficiently low temperatures, when the entropic contribution of the loop formation is negligible compared to direct energetic interactions between chain monomers, and when the partition function of the chains is dominated by the ground state. The performed analysis allows one to derive the force $f(x)$ which is necessary to apply for unzipping of two random heteropolymers of equal lengths whose ends are separated by the distance x , averaged over all equally distributed primary structures at low temperatures for fixed values a and c .

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I. INTRODUCTION

Recent progress in nanotechnology has offered a possibility of single-molecular experiments. The corresponding technique allows one to investigate many physicochemical and biological properties of individual molecules. One of the modern biophysical key experiments deals with the mechanical unzipping of individual double-stranded DNA macromolecule under the action of external force applied to the ends of strands. This system has been analyzed theoretically in a number of important contributions [1–9]. Some of them are devoted to the consideration of unzipping transition in an effective homopolymer chain, the other pay attention to the heterogeneity of primary sequence of complimentary strands constituting the DNA molecule.

In our work we address a problem of unzipping of a complex of two random heteropolymers of finite lengths at sufficiently low temperatures when the partition function is dominated by the ground state. We demonstrate that this problem can be mapped to the alignment of two random sequences with the general “cost function” which takes into account the weights of perfect matches, mismatches, and gaps (all necessary definitions are introduced below). Using this bijection we are able to compute the external work necessary to unzip the complex of two random heteropolymers, averaged over the uniform distribution of all possible primary sequences of heteropolymers. Our consideration allows also to conjecture the scaling corrections to the leading behavior of the force fluctuations due to the finiteness of the lengths of heteropolymer chains.

The paper is organized as follows. In Sec. II we define a model and introduce the basic notations. In Sec. III we con-

sider unzipping of two random heteropolymers from the point of view of the search of longest common subsequence (LCS) of two random sequences. The expectation of the LCS energy is considered in Sec. IV. In the conclusion we give the qualitative explanation of our main results and derive a force, which is necessary to apply to the chain ends to unzip two random heteropolymer chains at low temperatures.

II. THE MODEL

Consider two random heteropolymer chains of lengths $L_1=m\ell$ and $L_2=n\ell$ correspondingly. In what follows we shall measure the lengths of the chains in number of monomers, m and n , supposing that the size of an elementary unit, ℓ , is equal to 1.

Every monomer of the first (second) chain can be randomly and independently chosen with the uniform probability distribution $p=\frac{1}{c}$ from a set of c different types $A, B, C, D, \dots (A', B', C', D', \dots)$. Monomers of the first chain could form saturating reversible bonds with monomers of the second chain. The term “saturating” means that any monomer can form a bond with at most one monomer of the other chain. The bonds between similar types (such as $A-A', B-B', C-C'$, etc.) have the attraction energy u and are called “matches,” while the bonds between different types (such as $A-B', A-D', B-D'$, etc.) have the attraction energy v and are called “mismatches.” Some parts of the chains could form loops, hence contributing to the entropic part of the free energy of the system. It is supposed that the monomers belonging to the same chain do not interact with each other at all. Schematically a particular configuration of the system under consideration for $c=2$ is shown in Fig. 1. Our aim is to compute the free energy of the described model at sufficiently low temperatures when the entropic contribution of the loop formation is negligible compared to the energetic

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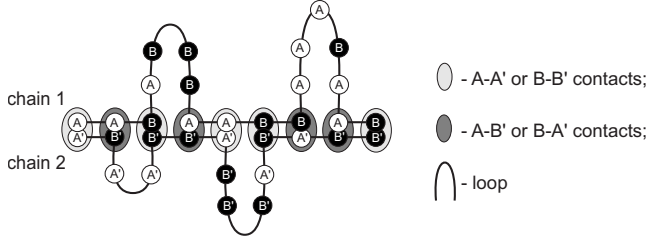


FIG. 1. Schematic picture of a complex of two random heteropolymer chains.

part of the direct interactions between chain monomers.

Consider now the partition function $G_{m,n}$ of such a complex which is the sum over all possible arrangements of bonds. Since we are interested in the low-temperature behavior of $G_{m,n}$, we neglect the entropic contribution of the loop weights which allows us to write $G_{m,n}$ recursively in terms of the partition functions of individual chains g_n :

$$G_{m,n} = g_m g_n + \sum_{i,j=1}^{m,n} \beta_{i,j} G_{i-1,j-1} g_{m-i} g_{n-j}, \quad (1)$$

$$G_{m,0} = g_m; \quad G_{0,n} = g_n; \quad G_{0,0} = 1.$$

The meaning of the Eq. (1) is as follows. Starting from, say, the left ends of the chains shown in Fig. 1, we find the first actually existing contact between the monomers i (of the first chain) and j (of the second chain) and sum over all possible arrangements of this first contact. The term $g_m g_n$ in Eq. (1) contributes to the absence of any contact. The entries $\beta_{i,j}$ ($1 \leq i \leq m$, $1 \leq j \leq n$) are the statistical weights of the bonds which are encoded in a contact map $\{\beta\}$:

$$\beta_{m,n} = \begin{cases} \beta^+ \equiv e^{u/T} & \text{if monomers } i \text{ and } j \text{ match,} \\ \beta^- \equiv e^{v/T} & \text{if monomers } i \text{ and } j \text{ do not match.} \end{cases} \quad (2)$$

For a system of two heteropolymer chains depicted in Fig. 1 the contact map $\{\beta\}$ is shown in Fig. 2.

If one allows for the loop formation within each chain, the partition functions of an individual chain g_n satisfy the recurrent equation [10–12]:

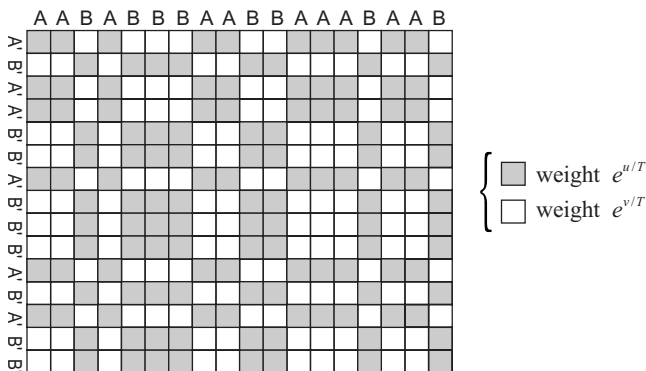


FIG. 2. Contact map $\{\beta\}$ corresponding to the complex of two random heteropolymer chains shown in Fig. 1.

$$g_n = 1 + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \beta'_{i,j} g_{j-i-1} g_{n-j}; \quad g_0 = 1, \quad (3)$$

where $\beta'_{i,j}$ are the self-association constants, which are (similarly to $\beta_{m,n}$) random variables encoded in some contact map. According to the definition of our model, it is assumed the absence of self-association, i.e., $\beta' \equiv 0$, hence

$$g_n \equiv 1. \quad (4)$$

The case of nonzero β' was thoroughly investigated recently [13–15] in a setup when the interactions in the system are predetermined instead of being random and we refer the reader to these papers for more details. Note also that throughout our paper we do not allow for the energetic effects due to the folding of dsDNA into globular structure, since (i) these effects are relatively small as compared to the effects of zipping (i.e., formation of double strand itself) and (ii) the dsDNA is known to be very stiff, therefore the formation of globule is possible only for long enough DNA chains, while the finite size effects which are discussed in this paper manifest themselves on much smaller length scales.

III. UNZIPPING OF TWO RANDOM HETEROPOLYMERS AND SEARCH OF LCS OF TWO RANDOM SEQUENCES

A. Heteropolymer ground-state energy: Local recursive construction

The straightforward computation shows that the partition function $G_{m,n}$ [with $g_n = 1$ —see Eq. (4)] obeys the following exact local recursion:

$$G_{m,n} = G_{m-1,n} + G_{m,n-1} + (\beta_{m,n} - 1)G_{m-1,n-1}. \quad (5)$$

Note that if $\beta_{i,j} = 2$ for all $1 \leq i \leq m$ and $1 \leq j \leq n$, the recursion relation (5) generates the so-called Delannoy numbers [16].

Represent now the partition function $G_{m,n}$ in the following way:

$$G_{m,n} = e^{F_{m,n}/T}, \quad (6)$$

where $-F_{m,n}$ has the sense of the free energy and T stands for the temperature of the pair of heterogeneous chains of lengths m and n . Considering the $T \rightarrow 0$ limit, we get

$$F_{m,n} = \lim_{T \rightarrow 0} T \ln [e^{F_{m-1,n}/T} + e^{F_{m,n-1}/T} + (\beta_{m,n} - 1)e^{F_{m-1,n-1}/T}] \quad (7)$$

which can be regarded as the equation for the ground state energy of a chain. The expression (7) can be rewritten in a symbolic form

$$F_{m,n} = \max[F_{m-1,n}, F_{m,n-1}, F_{m-1,n-1} + \eta_{m,n}], \quad (8)$$

where

$$\eta_{m,n} = T \ln(\beta_{m,n} - 1)$$

$$= \begin{cases} \eta^+ = T \ln(e^{u/T} - 1) & \text{in the case of match,} \\ \eta^- = T \ln(e^{v/T} - 1) & \text{in the case of mismatch.} \end{cases} \quad (9)$$

Taking η^+ as the unit of the energy, we can rewrite Eq. (8) as follows:

$$\tilde{F}_{m,n} = \max[\tilde{F}_{m-1,n}, \tilde{F}_{m,n-1}, \tilde{F}_{m-1,n-1} + \tilde{\eta}_{m,n}], \quad (10)$$

where

$$\tilde{\eta}_{m,n} = \begin{cases} 1 & \text{in the case of match,} \\ a = \frac{\eta^-}{\eta^+} & \text{in the case of mismatch.} \end{cases} \quad (11)$$

In the low-temperature limit the parameter a has a simple expression in terms of coupling constants u and v :

$$a = \frac{\eta^-}{\eta^+} = \frac{\ln(e^{v/T} - 1)}{\ln(e^{u/T} - 1)} \xrightarrow{T \rightarrow 0} = \frac{v}{u}. \quad (12)$$

The initial conditions for $\tilde{F}_{m,n}$ are transformed due to the second of Eqs. (1) into the following ones:

$$\tilde{F}_{0,n} = \tilde{F}_{n,0} = \tilde{F}_{0,0} = 0. \quad (13)$$

B. Matching with gaps: the cost function

In Eqs. (8)–(13) we can recognize the recursive algorithm [17,18] for the determination of the length $F_{m,n}$ of the longest common subsequence (LCS) of two arbitrary sequences of lengths m and n . It is easy to see that the search of $F_{m,n}$ can be completed in polynomial time $\sim O(mn)$.

Recall that the problem of finding the LCS in a pair of sequences drawn from the alphabet of c letters is formulated as follows. Consider two sequences $\alpha = \{\alpha_1, \alpha_2, \dots, \alpha_m\}$ (of length m) and $\beta = \{\beta_1, \beta_2, \dots, \beta_n\}$ (of length n). For example, let α and β be two random sequences of $c=4$ base pairs A, C, G, T of a DNA molecule, e.g., $\alpha = \{A, C, G, C, T, A, C\}$ with $m=6$ and $\beta = \{C, T, G, A, C\}$ with $n=5$. Any subsequence of α (or β) is an ordered sublist of α (and of β) entries which need not to be consecutive, e.g. it could be $CGTC$, but not TGC . A common subsequence of two sequences α and β is a subsequence of both of them. For example, the subsequence $CGAC$ is a common subsequence of both α and β . There are many possible common subsequences of a pair of initial sequences. The aim of the LCS problem is to find the longest of them. This problem and its variants have been widely studied in biology [19–22], computer science [17,23–25], probability theory [26–31], and more recently in statistical physics [18,32–34]. A particularly important application of the LCS problem is to quantify the closeness between two DNA sequences. In evolutionary biology, the genes responsible for building specific proteins evolve with time and by finding the LCS of similar genes in different species, one can learn what has been conserved in time. Also, when a new DNA molecule is sequenced *in vitro*, it is important to know whether it is really new or it is similar

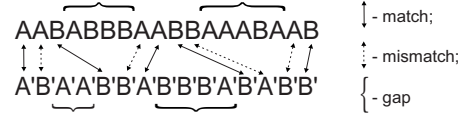


FIG. 3. Matches, mismatches, and gaps in a pair of sequences corresponding to the configuration of two random heteropolymers shown in Fig. 1.

to already existing molecules. This is achieved quantitatively by measuring the LCS of the new molecule with other ones available from database.

In the simplest version of the LCS problem only the number of perfect matches is taken into account, i.e., there is no difference between mismatches and gaps. One can, however, easily construct a generalized model where this difference comes into play. Introduce the general “cost function” \mathcal{S} having a meaning of energy (see, for example, Refs. [35,38] for details)

$$\mathcal{S} = N_{\text{match}} + \mu N_{\text{mis}} + \delta N_{\text{gap}}. \quad (14)$$

In Eq. (14) N_{match} , N_{mis} , and N_{gap} are correspondingly the numbers of matches, mismatches, and gaps in a given pair of sequences—see Fig. 3, and μ and δ are, respectively, the energies of mismatches and gaps. Without the loss of generality, the energy of matches can be always set to 1. In addition to Eq. (14) we have an obvious conservation law

$$n + m = 2N_{\text{match}} + 2N_{\text{mis}} + N_{\text{gap}} \quad (15)$$

which allows one to exclude N_{gap} from Eq. (14) and rewrite this expression as follows:

$$\begin{aligned} \mathcal{S} &= N_{\text{match}} + \mu N_{\text{mis}} + \delta(n + m - 2N_{\text{match}} - 2N_{\text{mis}}) \\ &= (1 - 2\delta)N_{\text{match}} + (\mu - 2\delta)N_{\text{mis}} + \text{const.} \end{aligned} \quad (16)$$

In Eq. (16) the irrelevant constant $\delta(n+m)$ can be dropped out.

Now we can adopt $(1-2\delta)$ as a unit of energy. Finally we arrive at the following expression:

$$\tilde{\mathcal{S}} = N_{\text{match}} + \gamma N_{\text{mis}}, \quad (17)$$

where

$$\gamma = \frac{\mu - 2\delta}{1 - 2\delta} \quad (18)$$

and $\gamma \leq 1$ by definition. The interesting region is $0 \leq \gamma \leq 1$, since otherwise there are no mismatches at all in the ground state (i.e., there is no difference between $\gamma=0$, which corresponds to the simplest version of the LCS problem, and $\gamma < 0$).

It is known [35,38] that the ground-state energy

$$\tilde{\mathcal{S}}^{\max} = \max[N_{\text{match}} + \gamma N_{\text{mis}}] \quad (19)$$

satisfies the recursion relation

$$\tilde{\mathcal{S}}_{m,n}^{\max} = \max[\tilde{\mathcal{S}}_{m-1,n}^{\max}, \tilde{\mathcal{S}}_{m,n-1}^{\max}, \tilde{\mathcal{S}}_{m-1,n-1}^{\max} + \zeta_{m,n}] \quad (20)$$

with

$$\zeta_{m,n} = \begin{cases} 1 & \text{in the case of match} \\ \gamma & \text{in the case of mismatch} \end{cases} \quad (21)$$

Indeed, the ground state may correspond either (i) to the last two monomers connected, then the ground-state energy equals $\tilde{S}_{m-1,n-1}^{\max} + \zeta_{M,N}$ or (ii) to the unconnected end monomer of the first (or second) chain, then the ground-state energy is $\tilde{S}_{m,n-1}^{\max}$ (or $\tilde{S}_{m-1,n}^{\max}$).

Comparing Eqs. (20) and (21) with Eqs. (10) and (11) one sees that they are identical up to the exchange of variables $\gamma \leftrightarrow a$. This establishes the analogy between initial heteropolymer problem formulated in Eqs. (1) and (2) in the low-temperature limit (10) and the standard matching problem with general cost function (14).

For a pair of fixed sequences of lengths m and n , the cost function $\tilde{S}_{m,n}^{\max}$ is just a number. In the stochastic version of the LCS problem one compares two random sequences drawn from alphabet of c letters and hence the cost function $\tilde{S}_{m,n}^{\max}$ is a random variable. We are interested in the computation of the expectation and the variance of $\tilde{S}_{m,n}^{\max}$ for $m=n \gg 1$ and the interpretation of the obtained results for LCS in terms of initial problem of unzipping of two random heteropolymers.

C. Bernoulli model for heteropolymers

We should note that the variables $\tilde{\eta}_{m,n}$ in Eq. (8) are not independent of each other. Actually, consider a simple example of two strings $\alpha=AB$ and $\beta=A'A'$. One has by definition $\tilde{\eta}_{1,1}=\tilde{\eta}_{1,2}=1$ and $\tilde{\eta}_{2,1}=0$. The knowledge of these three variables is sufficient to predict that the last two letters do not match each other, i.e., $\tilde{\eta}_{2,2}=0$. Thus, $\tilde{\eta}_{2,2}$ cannot take its value independently of $\tilde{\eta}_{1,1}$, $\tilde{\eta}_{1,2}$, $\tilde{\eta}_{2,1}$. These residual correlations between the variables $\tilde{\eta}_{i,j}$ make the LCS problem very complicated. However, for two random sequences drawn from the alphabet of c letters, the correlations between $\tilde{\eta}_{m,n}$ vanish for $c \rightarrow \infty$.

In our work we restrict ourselves with the so-called Bernoulli matching (BM) model [18] (which is simpler but yet nontrivial variant of the original LCS problem) where one ignores the correlations between $\tilde{\eta}_{m,n}$ for all c . The cost function $\tilde{F}_{m,n}^{\text{BM}}$ of the BM model satisfies the same recursion relation (8) except that the $\tilde{\eta}_{m,n}$'s are now independent variables, each drawn from the bimodal distribution

$$\tilde{\eta} = \begin{cases} a & \text{with probability } P(\tilde{\eta}) = 1 - \frac{1}{c}, \\ 1 & \text{with probability } P(\tilde{\eta}) = \frac{1}{c}. \end{cases} \quad (22)$$

As has been said already, this approximation is expected to be exact only in the appropriately taken $c \rightarrow \infty$ limit. Nevertheless, for finite c , the results on the BM model can serve as a useful benchmark for original LCS model to decide if indeed the correlations between $\tilde{\eta}_{m,n}$ are important or not.

Note that the problem under discussion can be redefined as follows. Consider a matrix $\tilde{\eta}$ of size $m \times n$ and let the elements of this matrix be independent random variables with bimodal distribution (22). Consider now all directed paths in this matrix, i.e., ordered sequences

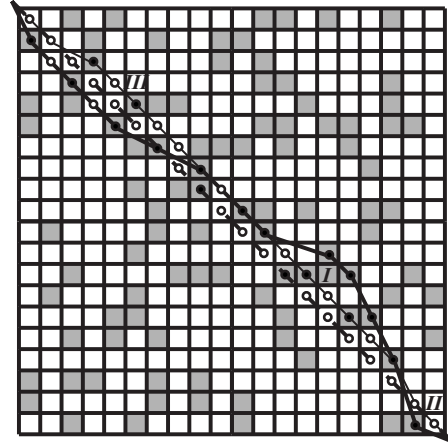


FIG. 4. An example of a random distribution of “1’s” (gray squares) and “a’s” (white squares) on a 20×20 matrix with $c=4$. The optimal path for $a=0$ is shown by the thick line, the diagonal optimal path for $a=1$ by the dashed line, and the evolution of the optimal path with increase of a by the thin line. The 1’s and a’s lying on the optimal paths are marked by filled and open circles, respectively. See the main text for more details.

$\{(m_1, n_1); (m_2, n_2); \dots; (m_k, n_k)\}$ such that $m_i > m_{i-1}$ and $n_i > n_{i-1}$ for $i=2, \dots, k$. Calculating the ground-state energy of the matching problem is obviously equivalent to maximizing the sum of the matrix elements along these directed trajectories:

$$E_{m,n}(a) = \max_{\text{all sequences}} \left[\sum_{i=0}^k \tilde{\eta}_{m_i, n_i} \right]. \quad (23)$$

In Fig. 4 we show an example of the evolution of the optimal path with the increase of a for some particular random distribution of weights “a” and “1” (shown by white and gray squares, respectively) for the alphabet of four letters (i.e., $c=4$).

The optimal path for small a 's is drawn in bold in Fig. 4. With the increase of a , the first change in the optimal path configuration happens at $a = \frac{1}{3}$ when a shortcut I (shown by a thin line) is formed instead of the corresponding section of the bold line. Then, at $a = \frac{1}{2}$ the shortcut marked by II actualizes, then at $a = \frac{2}{3}$ the one marked by III comes into play. So, for $a > \frac{2}{3}$ the optimal path is III-I-II. In what follows we call this path subdiagonal, meaning that it goes only through the diagonal of the matrix ($a_{i,i}$ for $i=1, \dots, n$) and one of its subdiagonals ($a_{i,i+1}$ or $a_{i+1,i}$ for $i=1, \dots, n-1$). Finally, at $a = \frac{5}{6}$ the subdiagonal path III-I-II ceases to be the optimal one, and optimal path sticks to the diagonal (dashed line) where it stays up to $a=1$.

IV. EXPECTATIONS OF LCS ENERGY FOR GENERAL COST FUNCTION \tilde{S}

In this section we consider the dependence of the ground state energy on the parameter a defined in Eqs. (12)–(21). We start with the consideration of the limiting cases: (i) $a \ll 1$ and (ii) $\epsilon = 1 - a \ll 1$ and then, with the physical insight in

hands, proceed to the semiquantitative consideration of the general case.

A. The case $0 < a = \frac{u}{v} \ll 1$

In the limit $a=0$, the problem under consideration corresponds exactly to the simplest version of the longest increasing subsequence (LIS) problem, where the mismatches have no cost at all. The Bernoulli matching model for this problem has been considered in Refs. [18,35] and later, in connection with random matrix theory, in Ref. [36]. An example of the random matrix with the optimal path is outlined by the bold line in Fig. 4 (only filled circles, i.e., points with the weight equal to 1 are relevant in this case). We know that the ground-state energy $E_{m,n}$ as a function of the chain lengths m, n behaves asymptotically for large m and n as

$$E_{m,n}(c, a=0) = \frac{2\sqrt{pmn} - p(m+n)}{q} + \frac{(pmn)^{1/6}}{q} \left[(1+p) - \sqrt{\frac{p}{mn}}(m+n) \right]^{2/3} \chi, \quad (24)$$

where $p=c^{-1}$, $q=1-p$, and χ is a random variable with the Tracy-Widom distribution [37]. The ground-state energy $E_{m,n}(a=0)$ has the meaning of a LIS length of “1” (see Ref. [36]). The mean value $\langle E_{m,n} \rangle$ for $n=m \gg 1$ growth as

$$\langle E_{m,n} \rangle \equiv \langle E_{n,n} \rangle = 2 \frac{\sqrt{p-p}}{q} n = \frac{2}{1+\sqrt{c}} n. \quad (25)$$

Consider now the case $a > 0$ paying special attention to the effects of finite values of m, n on typical fluctuations of E . We assume below $m=n$ for simplicity. If a is a small positive constant $0 < a = \frac{u}{v} \ll 1$ (the meaning of the notation “small” is specified below), then the trajectory of the optimal matching path is not changed with respect to the case of $a=0$. The only difference from the $a=0$ case is that there are mismatches inserted between the matches whenever it is possible (see open circles along the bold line in Fig. 4). It is not difficult to estimate the number of such inserted mismatches. Namely, the typical distance $\langle d \rangle$ between the consequent “1” (i.e., gray squares) along the optimal path in Fig. 4 is dictated by the density of black circles along the optimal path (see Fig. 4). Projecting $\langle d \rangle$ to the horizontal (first chain) and vertical (second chain) axes, we get, correspondingly, $\langle m_{i+1} - m_i \rangle$ and $\langle n_{i+1} - n_i \rangle$. For $m=n \gg 1$ one obviously has

$$\langle d \rangle = \langle m_{i+1} - m_i \rangle = \langle n_{i+1} - n_i \rangle = \frac{n}{\langle E_{n,n} \rangle} = \frac{1+\sqrt{c}}{2}. \quad (26)$$

The average energy gain due to a 's (i.e., white squares in Fig. 4) inserted into the optimal path can be estimated as follows:

$$\langle \Delta E \rangle = \langle E_{n,n} \rangle (\langle \min[m_{i+1} - m_i, n_{i+1} - n_i] \rangle - 1) a. \quad (27)$$

Indeed, we can insert a white square into the optimal path between consequent gray squares if and only if the distance between these consequent gray squares along each axis is

bigger or equal than 2 (we measure the distance in elementary squares). Let us estimate now $\langle \Delta E \rangle$ from above and from below.

(1) The upper bound is based on an assumption that the increments of m and n are fully correlated. In this case $\langle \min[m_{i+1} - m_i, n_{i+1} - n_i] \rangle = \langle d \rangle$ with $\langle d \rangle$ computed in Eq. (26). Therefore, for $\langle \Delta E \rangle$ we obtain the following estimate:

$$\langle \Delta E \rangle < \langle E_{n,n} \rangle (\langle d \rangle - 1) a = \left(1 - \frac{2}{1+\sqrt{c}} \right) n a. \quad (28)$$

(2) The construction of the lower bound corresponds to an assumption that the increments of m and n are completely independent. The computations in this case are slightly more involved since we have to compute explicitly the average value of the minimum d_{\min} of two independent increments m and n . The computations presented in Appendix A lead us to the following lower bound of $\langle \Delta E \rangle$:

$$\langle \Delta E \rangle > \langle E_{n,n} \rangle (\langle d_{\min} \rangle - 1) a = \left(\frac{1+\sqrt{c}}{2\sqrt{c}} - \frac{2}{1+\sqrt{c}} \right) n a. \quad (29)$$

Collecting Eqs. (28) and (29) we arrive at the following bilateral estimate of $\langle \Delta E \rangle$ for $0 < a \ll 1$:

$$\left(\frac{1+\sqrt{c}}{2\sqrt{c}} - \frac{2}{1+\sqrt{c}} \right) a < \frac{\langle \Delta E \rangle}{n} < \left(1 - \frac{2}{1+\sqrt{c}} \right) a. \quad (30)$$

It is worthwhile to notice in advance that, according to the numerical simulations, the genuine values of $\langle \Delta E \rangle / n$ are actually very close to the lower bound (29).

B. The case $a=1-\epsilon$ ($0 < \epsilon \ll 1$)

Turn now to the opposite situation $a=1-\epsilon$ ($0 < \epsilon \ll 1$). For $\epsilon=0$ the situation is trivial. Indeed, there is no difference between “1's” and “a's” (i.e., gray and white squares at Fig. 4 are identical) and the optimal path is the diagonal one with the energy

$$E(m, n) \equiv \min[m, n]; \quad E(n, n) \equiv n. \quad (31)$$

Now, for small but finite ϵ and not too long trajectories n (the definition of “not too long” is, once again, to be given below), the longest possible path still sticks to the main diagonal (see Fig. 4). This path is optimal with the ground-state energy given by

$$E_n^{\text{diag}}(a) = n - k\epsilon, \quad (32)$$

where k is the number of a 's on the diagonal, which is a random variable distributed with the binomial law

$$W(k, n) = \frac{n!}{k! (n-k)!} q^k p^{n-k} \quad (33)$$

(recall that $q=1-\frac{1}{c}$ and $p=\frac{1}{c}$). Hence the average energy $\langle E_n^{\text{diag}} \rangle$ per monomer on the diagonal path equals

$$\frac{1}{n}\langle E_n^{\text{diag}} \rangle = 1 - \frac{\langle k \rangle}{n} \epsilon = 1 - (1-p)\epsilon. \quad (34)$$

Let us estimate now the length, n_d , on which the optimal path detaches from the main diagonal. The optimal path of length n is separated from each of the suboptimal ones (i.e., those of length $n-1$) by the energy gap δE :

$$\delta E = (n - k\epsilon) - (n - 1 - k'\epsilon) = 1 - \epsilon\delta k, \quad (35)$$

where $\delta k = k - k'$ is the difference in the number of a 's on the optimal (diagonal) path and on the best of the suboptimal paths of lengths $n-1$ (see Fig. 4). The optimal path detaches from the diagonal when $\delta E < 0$. Since δk cannot exceed $n-1$, the diagonal path is always optimal until

$$1 - \epsilon\delta k < 0 \Rightarrow 1 - (n_d - 1)\epsilon < 0 \Rightarrow n_d > \epsilon^{-1} + 1, \quad (36)$$

where n_d is the length of the optimal path which detaches from the diagonal at energy ϵ . The inequality (36) gives rather crude lower bound for the value of $n = n_d$ for which the detachment of the optimal path from the diagonal actually happens. To acquire better bounds we should take into account the concurrent effects involved. On one hand, the single diagonal path has the advantage of being the longest one. The corresponding value of k has a binomial distribution (33) with the mean $\langle k \rangle = nq$. On the other hand, the suboptimal paths (i.e., those of lengths $n-1$) are disadvantageous because they are shorter, however their intrinsic advantage consists in high degeneracy: one has many such suboptimal trajectories. The number k' of a 's on each particular suboptimal path is a binomial distributed random variable with the probability density $W(k', n-1)$ and the mean $\langle k' \rangle = (n-1)q$. Now we have to find the best (i.e., the minimal) value $\langle k' \rangle$ among \mathcal{N} suboptimal paths. These suboptimal paths (there are $\mathcal{N} \sim n^2/2$ of them) are, however, not independent. It is easy to understand that the number of independent suboptimal paths N_{ind} satisfies the following bilateral inequality:

$$2 \leq N_{\text{ind}} \leq 3n - 2. \quad (37)$$

Indeed, on one hand, there are at least two independent paths coinciding with upper and lower subdiagonals. On the other hand, by definition, the suboptimal paths can visit only these two subdiagonals and the main diagonal itself. The corresponding energetic costs are always linear combinations of the values on the diagonal (n) and two subdiagonals ($n-1$), that is, $n + 2(n-1) = 3n - 2$ accessible matrix elements, which are themselves independent random variables. Evidently one cannot construct more than $3n - 2$ independent linear combinations out of $3n - 2$ independent variables. We are, hence, to compute the average minimum of N_{ind} independent random quantities each distributed with the probability density $W(k', n-1)$. This task is solved in Appendix B. Taking into account the inequality (37) which defines the boundaries of N_{ind} , we can get the upper and lower estimates for $\langle \delta k_{N_{\text{ind}}} \rangle$ ($n \gg 1$), where $\langle \delta k_{N_{\text{ind}}} \rangle$ is defined as follows:

$$\langle \delta k_{N_{\text{ind}}} \rangle = \langle k \rangle - \langle k'_{N_{\text{ind}}} \rangle \equiv npq - \langle k'_{N_{\text{ind}}} \rangle. \quad (38)$$

Substituting into Eq. (38) the expressions derived in Appendix B for $\langle k'_{N_{\text{ind}}} \rangle$, we have

$$q + \frac{1}{\sqrt{\pi}}(npq)^{1/2} < \langle \delta k_{N_{\text{ind}}} \rangle < q + (2npq)^{1/2} \{ \ln[3n^{3/2}(pq)^{1/2}]^{1/2} \}. \quad (39)$$

Remembering now that the optimal path detaches from the diagonal at $\langle \delta k_{N_{\text{ind}}} \rangle \sim \epsilon^{-1}$, and dropping out all constants of order of one, we arrive for $n \gg 1$ at the following approximate bilateral estimate for the detachment length n_d :

$$n_d \leq (\epsilon^2 pq)^{-1}, \quad n_d \ln n_d \geq (\epsilon^2 pq)^{-1} \quad (40)$$

The obtained estimate (40) is compared to our numerical simulations and is discussed at length in the next Section.

C. The general case $a \in [0, 1]$: Detachment, energy cost, and fluctuations

We consider in this section the general case of $a \in [0, 1]$ and define the average ground-state energy $\langle \mathcal{E}_n(c, a) \rangle = \langle E_n(c, a) \rangle / n$ for different values of c and a . The most attention is paid to the finite size effects.

1. Detachment

In Fig. 5 we show the results of our computer simulation of the average energy of the optimal path as a function of the sequence length for different values of a and p . Here and below all the computer simulation results are the averages of 10^4 independent realizations of disorder. One notes the crossover (for fixed a and p) from the path sticking to the diagonal at low n and the high- n regime, where the optimal path is detached. For $n \gg 1$ the average energy of the path eventually saturates at some value E_∞ , which is a and p dependent. Moreover, though the detachment point is not exactly well defined, the rescaling according to the inequality (40) shows that it gives rather decent estimate of the detachment point. Note also that the plateau region persists up to quite large values of ϵ . Indeed, it is easy to see from Eq. (36) that the detachment happens at $n_d > 2$ (and thus a plateau of at least two points exists) for any $a > a_d = 1/2$. It is less obvious and more important, however, that the more accurate estimate (40) is still relevant in the whole range of $a \in (1/2, 1)$.

2. Energy cost

In Fig. 6 we present the estimates of $\langle \mathcal{E}_n(c, a) \rangle$. These estimates we obtain by the finite size scaling extrapolating $\langle \mathcal{E}_n(c, a) \rangle$ from large, but finite, n to $n \rightarrow \infty$. In our construction we use the following conjecture. One sees from Eq. (24) that at $a=0$ and for $m = n \gg 1$ the average ground-state energy $\langle \mathcal{E}_n(c, a=0) \rangle$ converges to its value at infinity $\langle \mathcal{E}_\infty(c, a=0) \rangle = \frac{2}{1+\nu_c}$ with the scaling exponent $\alpha = \theta_0 - 1 = -2/3$, where $\theta_0 = 1/3$ is the well-known Kardar-Parisi-Zhang (KPZ) exponent [38,39]

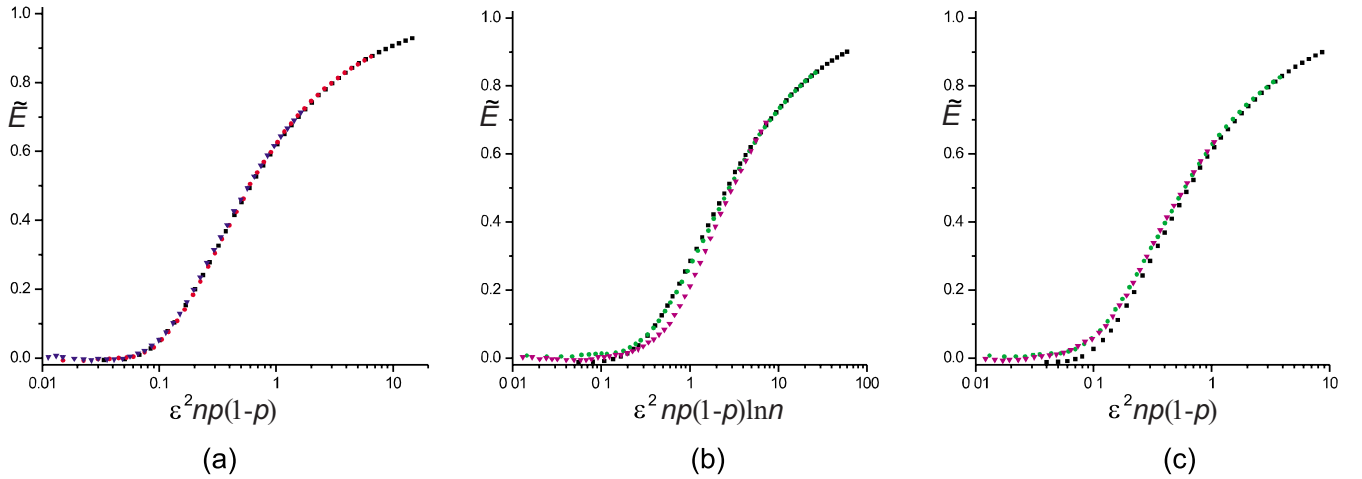


FIG. 5. (Color online) The dependence of the reduced mean energy $\tilde{E} = (\langle \mathcal{E}_n \rangle - \langle \mathcal{E}_0 \rangle) / (\langle \mathcal{E}_\infty \rangle - \langle \mathcal{E}_0 \rangle)$ of the optimal path on the reduced size n of the system: (a) for $c=4$ and $\epsilon=0.3$ (squares), $\epsilon=0.2$ (circles), and $\epsilon=0.1$ (triangles); (b) and (c) for $\epsilon=0.2$ and $c=2$ (squares), $c=8$ (circles), and $c=32$ (triangles). Note that curves for $c=2, 8$ almost collapse after rescaling prescribed by the right-hand side of Eq. (40), while those for $c=8, 32$ collapse with rescaling prescribed by the left-hand side of Eq. (40).

$$\langle \mathcal{E}_n(c, a=0) \rangle = \frac{1}{n} \langle E_{n,n}(c, a=0) \rangle = \frac{2}{1 + \sqrt{c}} + f(c) \langle \chi \rangle n^\alpha, \quad (41)$$

where $f(c) = \frac{c^{1/6}(\sqrt{c}-1)}{\sqrt{c+1}}$ and $\langle \chi \rangle = -1.7711 \dots$ (see Ref. [37]). Recall, that the appearance of the KPZ exponent in Eq. (41) deals with very deep mathematical relation between the Bernoulli matching problem and statistics of largest eigenvalues of ensembles of Gaussian random matrices (see, for example, Ref. [36]).

We assume that the exponent α is a independent and the finite size scaling of $\langle \mathcal{E}_n(c, a) \rangle$ for $a > 0$ and $n \gg 1$ (see also Ref. [38]) is

$$\langle \mathcal{E}_n(c, a) \rangle = \langle \mathcal{E}_\infty(c, a) \rangle + g(c, a) \langle \chi \rangle n^\alpha, \quad (42)$$

where $g(c, a)$ is some function of c and a , but not of n . Extrapolating the data of $\langle \mathcal{E}_n(c, a) \rangle$ computed numerically for large finite n to $\langle \mathcal{E}_\infty(c, a) \rangle$ on the basis of finite size scaling (42), we arrive at the family of curves $\langle \mathcal{E}_\infty(c, a) \rangle$ for $c = 2, 4, 8, 16, 32, 64$ shown in Figs. 6(a) and 6(b). The results presented in Fig. 6(c), as well as those of Ref. [38] demonstrate that the conjecture (42) is actually plausible. Apart from the points obtained by numerical simulation, in Fig. 6(b) we depict (a) the estimates for $\langle \mathcal{E}_\infty(c, a) \rangle$ at small a given by the inequality (30) and (b) the estimates of $\langle \mathcal{E}_\infty(c, a) \rangle$ on the plateau for $a \rightarrow 1$ [Eq. (34)].

One should note that the numerical results for $a \ll 1$ are very close to the lower bound of Eq. (30). We use this fact to

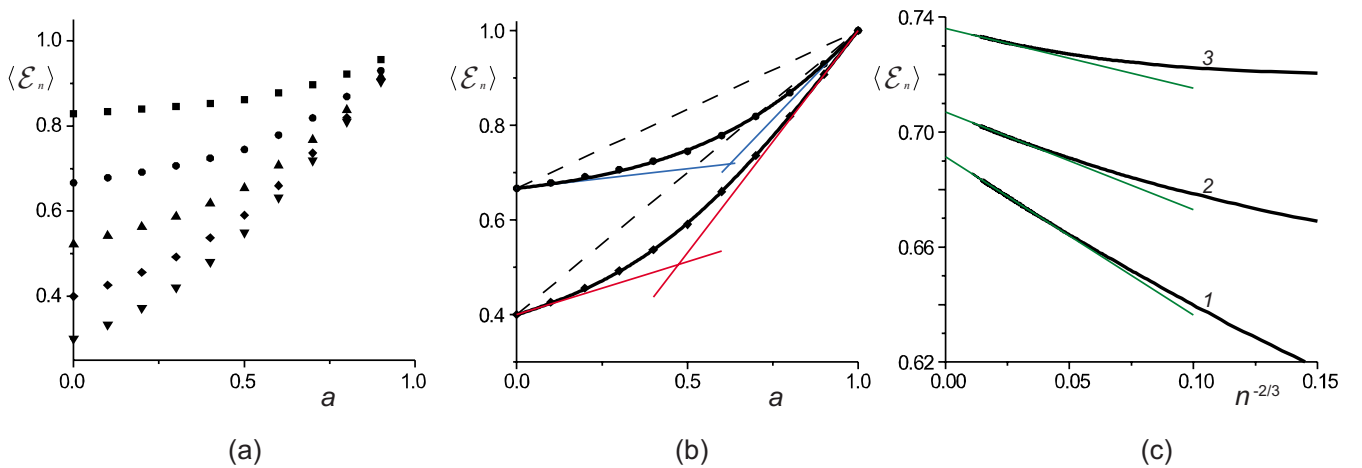


FIG. 6. (Color online) (a) The limiting value of the ground-state energy per cite $\langle \mathcal{E}_n(a) \rangle \equiv \langle E(a) \rangle / n$ as a function of a for different c : $c=2$ (squares), $c=4$ (circles), $c=8$ (up triangles), $c=16$ (diamonds), $c=32$ (down triangles). (b) The upper (dashed line) and lower (thin solid lines) bounds and the hyperbolic fit (thick line) of the $\langle \mathcal{E}_n(a) \equiv \langle E(a) \rangle / n$ dependence for $c=4$ (circles) and $c=16$ (diamonds). (c) The examples of the ground-state energy per cite $\langle \mathcal{E}_n \rangle$ as a function of $n^{-2/3}$ (thick line) and the finite-size scaling fits used to obtain points in (a) (thin lines) for several different values of a and c , line 1: $a=0.2, c=4$, line 2: $a=0.6, c=8$, line 3: $a=0.7, c=16$.

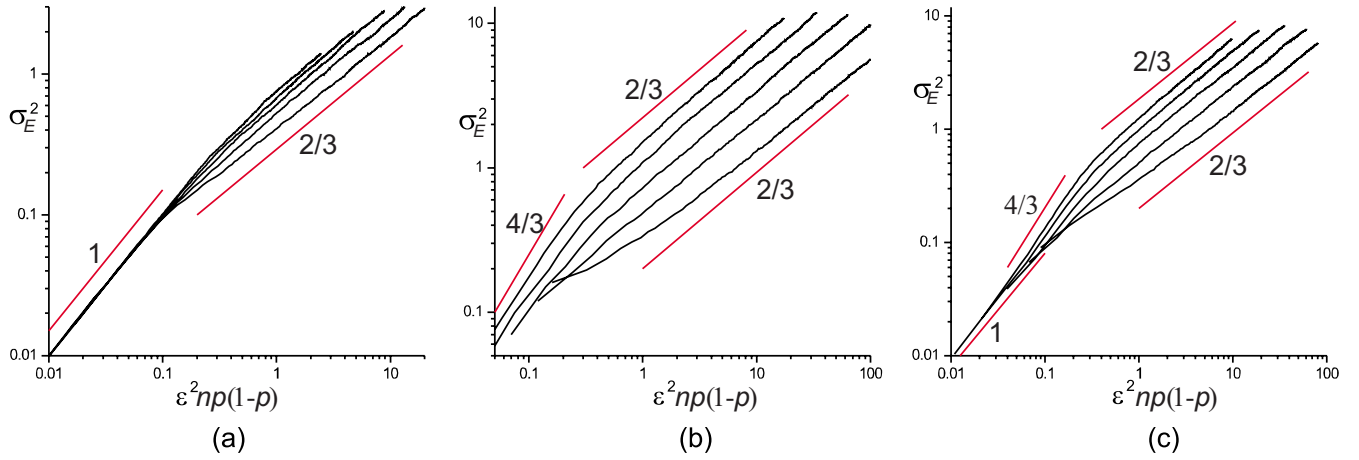


FIG. 7. (Color online) The dispersion σ_E of the ground-state energy as a function of N for different values of a and c . (a) $a=0.7$, (b) $a=0.2$, (c) $a=0.4$. In all figures $c=2, 4, 8, 16, 32$ in ascending order.

produce a fit for the dependence $\langle \mathcal{E}_\infty(c, a) \rangle$ in the whole range of parameter $a \in [0, 1]$ for two values of c ($c=4, 16$). Namely, we fit the data of $\langle \mathcal{E}_\infty(a) \rangle$ by a hyperbola of general form

$$(\langle \mathcal{E}_\infty(a) \rangle + \kappa_1 a + \delta_1)(\langle \mathcal{E}_\infty(a) \rangle + \kappa_2 a + \delta_2) = R, \quad (43)$$

where the constants $\kappa_{1,2}, \delta_{1,2}, R$ are chosen from the constraints that the hyperbola (43) passes through the points $[a, \mathcal{E}_\infty(a)] = [0, 2/(\sqrt{c+1})]$ at $a=0$, and $[a, \mathcal{E}_\infty(a)] = (1, 1)$ at $a=1$ with the slopes given by limiting linear approximations (30) and (34), correspondingly. These four constraints leave us effectively with only one free parameter, which we change to arrive at the best fit of the experimental data. As one sees from Fig. 6(b), the found fits for different values of c are quite good.

3. Fluctuations

Let us now discuss briefly the fluctuations of the average free energy and their dependence on n . One expects for $n \gg 1$ the average fluctuations σ_E^2 to be proportional to $n^{2/3}$, typical for the Kardar-Parisi-Zhang universality class [38]. This conjecture is consistent with the computation of the fluctuations of the averaged length of the LIS in the $a=0$ limit for Bernoulli matching model (see Ref. [36]):

$$\begin{aligned} \sigma_E^2(n) &= \text{var } E_{n,n}(c) = \langle E_{n,n}^2(c) \rangle - \langle E_{n,n}(c) \rangle^2 \\ &\approx (\langle \chi^2 \rangle - \langle \chi \rangle^2) f^2(c) n^{2\theta_0}, \end{aligned} \quad (44)$$

where $\theta_0 = 1/3$ and $\langle \chi^2 \rangle - \langle \chi \rangle^2 = 0.8132, \dots$

The behavior for intermediate values of n is more involved. In particular, for small a and intermediate n one expects for $\sigma_E^2(n)$ the growth with the critical exponent θ_1 :

$$\sigma_E^2(n) \sim n^{2\theta_1}. \quad (45)$$

The exponent θ_1 is known to be typical for the “transitional” regime in the (1+1)D KPZ equation [39,40]. In terms of the work [40] the exponent θ_1 , which governs the short-time behavior of the correlation function of KPZ model, is $\theta_1 = (d+4)/(2z) - 1$, where z is the dynamic exponent [40], and d is the space dimensionality. In $d=1$ the value of z for KPZ

model is known exactly, $z=3/2$, giving the value $\theta_1=2/3$.

For $a=1-\epsilon$ ($\epsilon \ll 1$) the plateau regime for $\mathcal{E}_n(c, a)$ exists at low $n \lesssim n_d$ [where n_d is defined in Eq. (40)]. The arguments of Sec. IV B allow us to expect that, in this case, the variance $\sigma_E^2(n)$ behaves as

$$\sigma_E^2(n) \sim n^{2\theta_2} \quad (46)$$

with the Gaussian exponent $\theta_2=1/2$ since the plateau energy is just the sum of n -independent random variables.

The numerical results presented in Fig. 7 for $\sigma_E^2(n)$ fully confirm the behaviors (44)–(46). In the case of intermediate a shown in Fig. 7(c) the sequence of regimes, at least for large c is more reach: we first note the exponent $2\theta_2=1$ (plateau), then the exponent $2\theta_1=4/3$ (“transitional” KPZ), and finally the exponent $2\theta_0=2/3$ (large-scale KPZ). It looks like the growing plateau region continuously “swallows up” the finite-size KPZ region with the increase of a , and thus at $\epsilon=1-a \ll 1$ one sees only two regimes.

There is a question of how universal the obtained results are with respect to the change of the model settings. Indeed, the exponents $\theta_{0,1,2}$ are obtained in the assumption of Bernoulli matching, i.e., assuming the contact matrix β to have no correlations. Certainly, in reality it is not the case. Though we assume that some of the exponents may be universal, and may even hold in the presence of strong long-ranged correlations in the associating heteropolymer strands, the situation *a priori* is very obscure. A thorough numerical investigation of this question would be, in our opinion, an essential contribution in the field of the KPZ-related studies.

V. CONCLUSION

In this work we have analyzed the average normalized ground-state energy \mathcal{E} of the complex of two random heteropolymers with quenched sequences as a function of chain length n in the ensemble of chains with uniform distribution of primary structures. The main attention is paid to the behavior of the function $\mathcal{E}(n)$ at intermediate chain lengths and low temperatures.

The behavior of the energy is shown in Figs. 5 and 6. In addition to the formal estimates of the boundaries (30) and

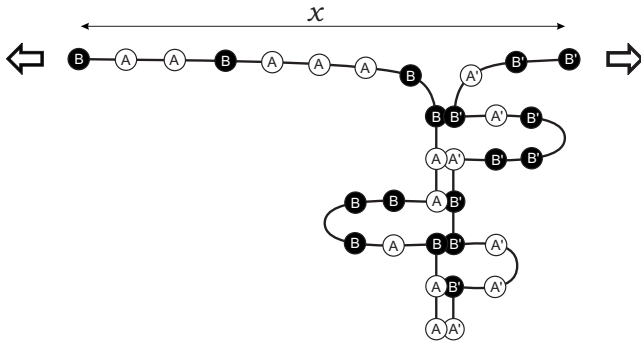


FIG. 8. Unzipping of two random heteropolymers.

(34) and of the crossover length n_d [Eq. (40)], it seems to be desirable to acquire the qualitative understanding of the zipping energy $\langle \mathcal{E}_n \rangle$ for different chain lengths and different values of a .

One sees that the normalized energy $\langle \mathcal{E}_n \rangle$ for relatively long ($n > n_d$) zipped chain configurations, is larger than the corresponding energy in a hairpin state for $n < n_d$. This can be explained in the following way. Longer chains could optimize their energy matching via loops creation, while for short chains the penalty for loop formation is forbiddingly large. Hence, the inequality (40) gives the criterion for the characteristic scale length which separates two kinds of behavior: short chains form the hairpin configuration in which the monomers are forced to bond without any regard of their species, while long chains are capable of adjusting their spatial configurations by loop formation to obtain better matching. The crossover around n_d is, thus, separating the small- n region, where the energy approaches the plateau value (34) exponentially fast with decreasing n , and large- n region, where $\langle \mathcal{E}_n \rangle$ approaches its value at $n \rightarrow \infty$ with the power-law dependence $\langle \mathcal{E}_\infty \rangle - \langle \mathcal{E}_n \rangle \sim n^{-2/3}$. This behavior of $\langle \mathcal{E}_n \rangle$ depends only qualitatively [see Eq. (40)] on the parameter a for suf-

ficiently large $a > a_d \sim 0.5$. (For the definition of a_d see Sec. IV C 1.)

The unzipping process of two random heteropolymer chains is schematically shown in Fig. 8. The results of previous sections allow us to find the dependence of the force $f(x)$ per chain monomer, on an average extension distance x between chain ends. If N is the total length of each heteropolymer chain, and n is the average current length of the heteropolymer complex measured from its common bottom end (see Fig. 8), then by construction, $x = 2(N - n)$. For the sake of simplicity, we neglect here the fluctuations of the unzipped regions of the chain.

The plot of the average force f per chain monomer on the average separation distance x is shown in Fig. 9. To be precise $f(x)$ is the force necessary to unzip two random heteropolymer chains whose ends are separated by the distance x averaged over all equally distributed primary structures at low temperatures for fixed value $a = \frac{v}{u}$ and given number of letters in the alphabet c . The function $f(x)$ can be easily obtained from the dependence $\langle \mathcal{E}_n \rangle$ shown in Fig. 6. Namely, $f(x) = \frac{d}{dn}(n \langle \mathcal{E}_n \rangle)$ at $n = N - x/2$.

Qualitative explanation of this phenomenon repeats the above discussion of the ground-state free energy $\langle \mathcal{E}_n \rangle$. As it has been mentioned already, the main attention in our work is paid to relatively small n , i.e., to large average separation distances x . (For discussions of the peculiarities of the force on the other bound, i.e., at $x \rightarrow 0$, see Ref. [9].) As x tends to the contour length $2N$ the equilibrium unzipping force $f(x)$ gradually decreases as $\text{const} - n^{-2/3} = \text{const} - (N - x/2)^{-2/3}$ until $N - x/2 \sim n_d$ when the force drops further down to reach the limiting plateau value (34) where it saturates independently of further increase of x up to $x_{\text{max}} \equiv 2N$.

Let us stress once more that the obtained result is valid only for values of $f(x)$ averaged over the ensemble of realizations of different heteropolymer sequences: for any given heteropolymer sequence, the equilibrium force would be a

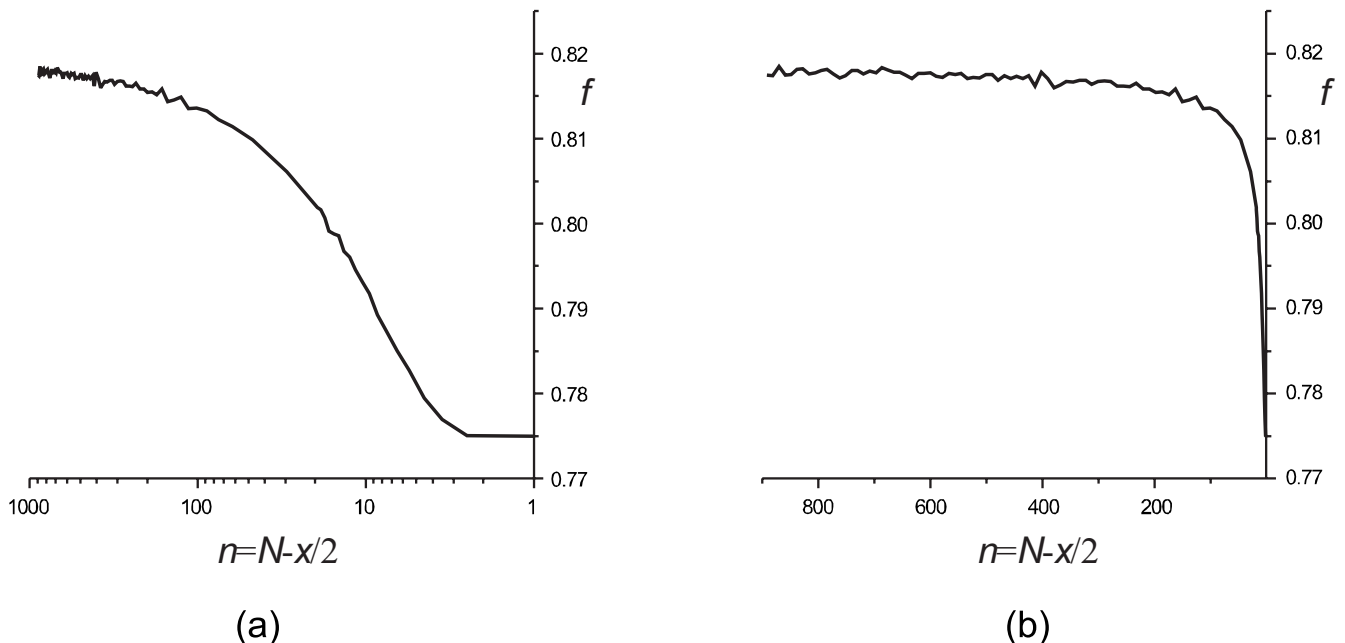


FIG. 9. Dependence of unzipping force f per chain monomer on average separation distance x . (a) Log-linear scale, (b) linear scale.

highly fluctuating function of the distance x . Certainly, the $f(x)$ dependence averaged over the ensemble of quenched heteropolymer sequences does not provide any information about the behavior of the individual pair of zipped heteropolymer chains [41]. However, the investigation of the individual behavior is not a goal of our study. We use the averaged $f(x)$ dependence to extract the information just about the statistics of matchings of two zipped random sequences of finite lengths in the low-temperature limit. From this point of view, the most interesting is the behavior $f(x)$ at large separation distances, when x approaches the total contour lengths $x_{\max}=2N$. Let us emphasize that the results of our study to lesser degree are applied to the DNA molecules, than to a pair of synthetic random heteropolymer chains, since the typical number of mismatches per double DNA strand is very small (of order of few monomers) and it is senseless to talk about any statistics in that situation.

In reality, the unzipping experiments are often set up in a fixed-force ensemble, instead of a fixed distance one (see, for example, Refs. [41–43]), i.e., the constant force is applied to the ends of the chain, and the dynamics of the unzipping under this constant force is studied. In such a setting one can measure the relative occupation times for the different intermediate states, and reconstruct the overall free energy landscape based on this occupation time data. In terms of such a setting, we predict that after the averaging over many realizations with different primary structures, the occupation times for almost unzipped states will be less than those for the almost zipped conformations (the particular difference depending on the applied force). More precisely, these occupation times will gradually decrease with the decrease of x from $2N$ to $2N-2n_d$ and then saturate.

ACKNOWLEDGMENTS

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APPENDIX A: AVERAGE VALUE OF THE MINIMUM OF TWO INDEPENDENT INCREMENTS

First of all we should make a conjecture about the distribution of intervals $d_m=m_{i+1}-m_i$ and $d_n=n_{i+1}-n_i$. It seems to be rather natural to suppose that the intervals $d_{m,n}$ have the exponential distribution, i.e., $p(d_{m,n})\sim e^{-kd_{m,n}}$ (one can easily check that at least the tails of this distribution are indeed exponential). Normalizing $p(d_{m,n})$, we get

$$p(d_{m,n}) = \frac{e^{-kd_{m,n}}}{\sum_{d_{m,n}=1}^{\infty} e^{-kd_{m,n}}} = (e^k - 1)e^{-kd_{m,n}}. \quad (\text{A1})$$

The mean values $\langle d_m \rangle$ and $\langle d_n \rangle$ are

$$\langle d_m \rangle = \langle d_n \rangle = \sum_{d_{m,n}=1}^{\infty} d_{m,n} p(d_{m,n}) = \frac{e^k}{e^k - 1}. \quad (\text{A2})$$

Now we are to find the averaged joined minimum $\langle d_{\min} \rangle$ of two random variables d_m and d_n distributed with Eq. (A1). To do that we proceed as follows. First of all find the discrete integral distribution function $F_1(z)$ for each random distribution $p(d_m)$ and $p(d_n)$:

$$F_1(z) = \sum_{d_{m,n}=1}^z p(d_{m,n}) = 1 - e^{-kz}. \quad (\text{A3})$$

Following the general procedure, define now the joined discrete integral distribution function $F_2(z)$

$$F_2(z) = 1 - [1 - F_1(z)]^2 = 1 - e^{-2kz}. \quad (\text{A4})$$

Taking the discrete derivative, $p_2(z) = F_2(z) - F_2(z-1)$, we find the probability distribution, $p_2(z=d)$ for the minimum $d_{\min} = \min[m_{i+1}-m_i, n_{i+1}-n_i]$. The last step consists in taking average $\langle d_{\min} \rangle$ with respect to the joined distribution function $p_2(d)$:

$$\langle d_{\min} \rangle = \sum_{z=1}^{\infty} z p_2(z) = \frac{e^{2k}}{e^{2k} - 1}. \quad (\text{A5})$$

Collecting Eqs. (26), (A2), and (A5), we get

$$\frac{e^k}{e^k - 1} = \frac{1 + \sqrt{c}}{2}, \quad (\text{A6})$$

$$\frac{e^{2k}}{e^{2k} - 1} = \langle d_{\min} \rangle$$

and thus, resolving Eq. (A6),

$$\langle d_{\min} \rangle = \frac{(1 + \sqrt{c})^2}{4\sqrt{c}}. \quad (\text{A7})$$

Substituting Eq. (A7) into Eq. (27) one finally obtains the estimate of ΔE from below:

$$\Delta E > \langle L_{n,n} \rangle (\langle d_{\min} \rangle - 1) a = \left(\frac{1 + \sqrt{c}}{2\sqrt{c}} - \frac{2}{1 + \sqrt{c}} \right) na. \quad (\text{A8})$$

APPENDIX B: AUXILIARY CONSTRUCTION FOR ESTIMATION OF THE DETACHMENT LENGTH

Assuming $\frac{n}{c} \gg 1$ one can replace the binomial distribution (33) with the Gaussian one and approximate $W(k)$ as follows:

$$\tilde{W}(k, n) = \frac{1}{\sqrt{2\pi npq}} \exp\left(-\frac{(k - \langle k \rangle)^2}{2npq}\right), \quad (\text{B1})$$

where $\langle k \rangle = nq$. The distribution function $W(k', n-1)$ for the variable k' is completely similar up to the replacement $n \rightarrow n-1$.

We are now to compute the mean minimal value $\langle k'_{\text{ind}} \rangle$ of N_{ind} random variables, each distributed with $W(k', n-1)$

$\equiv W(k')$. Repeating the same procedure as in the Appendix A, we proceed as follows. First of all pass to the integral distribution function $\tilde{F}(z)$:

$$\tilde{F}(z) = \int_{-\infty}^z \tilde{W}(k') dk' = \frac{1}{2} \left(1 + \operatorname{erf} \left[\frac{z - (n-1)q}{\sqrt{2(n-1)pq}} \right] \right). \quad (\text{B2})$$

Now construct the new probability distribution function $Q(z)$ for the joint distribution, as follows:

$$Q(z) = \frac{d}{dz} \{1 - [1 - \tilde{F}(z)]^{N_{\text{ind}}}\} = N_{\text{ind}} \tilde{F}'(z) [1 - \tilde{F}(z)]^{N_{\text{ind}}-1}. \quad (\text{B3})$$

The desired mean minimal value $\langle k'_{N_{\text{ind}}} \rangle$ now reads

$$\langle k'_{N_{\text{ind}}} \rangle = \int_{-\infty}^{\infty} z Q(z) dz. \quad (\text{B4})$$

Now, taking the estimate (37) into account one readily arrives at the lower bound for $\langle k'_{N_{\text{ind}}} \rangle$. Indeed, for $N_{\text{ind}}=2$

$$\begin{aligned} \langle k'_{N_{\text{ind}}} \rangle &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} [y \sqrt{2(n-1)pq} + (n-1)q] e^{-y^2} [1 - \operatorname{erf}(y)] dy \\ &= (n-1)q - \frac{1}{\sqrt{\pi}} [(n-1)pq]^{1/2}. \end{aligned} \quad (\text{B5})$$

For $N_{\text{ind}}=3n-2 \gg 1$ [see Eq. (37)] the integral (B4) cannot be computed analytically and therefore one needs to apply some approximate approach. We proceed as follows. The function $\tilde{F}(z)$ has a sense of the area under the curve $\tilde{W}(k)$ in the interval $k' \in (-\infty, z]$. Consider now $N_{\text{ind}} \gg 1$ independent ran-

dom variables each distributed with $\tilde{W}(k')$. For $\frac{z-(n-1)q}{\sqrt{(n-1)pq}} \ll -1$ on average one point of N_{ind} equally distributed random points lies in the area $\tilde{F}(z) \sim N_{\text{ind}}^{-1}$. Since this area is the area under the left tail of the distribution $\tilde{W}(k')$, the point inside this area is the minimal one by construction. So, expanding $\tilde{F}(z)$ for $\frac{z-(n-1)q}{\sqrt{(n-1)pq}} \ll -1$, we get

$$\begin{aligned} \tilde{F}(z) &= \frac{1}{2} \left(1 + \operatorname{erf} \left[\frac{z - (n-1)q}{\sqrt{2(n-1)pq}} \right] \right) \\ &\simeq \frac{\sqrt{(n-1)pq}}{\sqrt{2\pi}[(n-1)q - z]} \exp \left(-\frac{[z - (n-1)q]^2}{2(n-1)pq} \right) \sim \frac{1}{N_{\text{ind}}}. \end{aligned} \quad (\text{B6})$$

Since the term in the exponent in Eq. (B6) varies much faster than the pre-exponential term, we can roughly estimate $z = \langle k'_{N_{\text{ind}}} \rangle$ as follows:

$$\langle k'_{N_{\text{ind}}} \rangle \simeq (n-1)q - [2(n-1)pq]^{1/2} (\ln\{N_{\text{ind}}[(n-1)pq]^{1/2}\})^{1/2}. \quad (\text{B7})$$

Note that Eq. (B7) is obtained from Eq. (B6) under the condition $z < (n-1)q$ which fixes the correct sign of the square root branch of the second term in Eq. (B7).

Substituting $N_{\text{ind}}=3n-2$ into Eq. (B7) and taking into account that $n \gg 1$, we get the following desired estimate for $\langle k'_{N_{\text{ind}}} \rangle$:

$$\langle k'_{N_{\text{ind}}} \rangle \simeq (n-1)q - (2npq)^{1/2} \{\ln[n^{3/2}(pq)^{1/2}]\}^{1/2}. \quad (\text{B8})$$

Now we can use the boundaries Eqs. (B5) and (B8) for getting lower and upper bounds of $\langle \delta k'_{N_{\text{ind}}} \rangle$ and of the detachment length n_d —see Eqs. (39) and (40).

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