Dynamic Properties of Random Heteropolymer with Correlations in Sequence.

E.Sh.Mamasakhlisov & V.F.Morozov

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Abstract

The some dynamic properties of a random heteropolymer in the condensed state are studied in the mode coupling approximation. In agreement with recent report a dynamic friction increasing is predicted for the random heteropolymer with power-law correlations in comparison with exponential correlations. In the case of strong power-law correlations ($\beta > \beta^*$) the dynamic friction function diverge in the thermodynamic limit. The qualitative explanation is given for the monomer’s dynamics slowing down and diverged energetic barrier between the frozen and random coil states. The possible relations with protein’s function and evolution are discussed.
1 Introduction.

From the molecular point of view the prebiotic evolution is the creation and subsequent change of the set of sequences of proteins and nucleic acids from the primordial soup. The one of important features of biologically functional proteins is the ability of recognizing an a priori given target molecule. One of possible mechanisms of such properties origin was suggested in [1,2]. It is the fast polymerization of monomers in presence the target molecule. It was shown that this procedure produced the slight power-law correlations in sequence of the forming macromolecule due by the interactions between target molecule and monomers. It was shown also that similar type of correlations observed in sequences of real proteins. This result was obtained [1] by averaging over the ensemble of different sequences of the homological proteins. At the last years the some interesting ideas were suggested that try to explain the possible ways to genetic code origin [3,4]. For example, a correspondence between nucleotide and amino acid coding units, may have origin from the sequence-specific interactions between abiotically synthesized polynucleotides and polypeptides [4].This point of view is in interplay with mechanism, proposed by Pande et al.[1].

The role that protein’s and random heteropolymer’s sequence correlation properties play in their structure and function was investigated previously in [5,6]. In particularly, it was shown [6] that in random heteropolymers (RHP) the power-law correlations produced the energetic barrier between folded and random coil states. This result was interpret as an evidence of power-law correlations only in non-coding sequences of DNA, that is corresponded to results of Peng et al. [7,8].

Purely dynamic theories in mode coupling fashion were derived previously in [9-12] for completely random heteropolymers. So, Roan and Shakhnovich [10] derive a mode-mode coupling theory of the RHP and explicitly solved it for a polymer in a good solvent. Thirumalai et al. [11] derived dynamic equations in the framework of dynamic functional integral (DFI) method for a Garel, Leibler and Orland model [13]. The objective of the present study is random heteropolymer’s dynamics treatment in presence of sequence power-law correlations. We have considered here the Langevin dynamics of RHP with correlated sequence in mode-coupling approximation. The main goal of the present article is the investigation of some dynamic properties of the condensed state of RHP.
2 Model and Formalism.

Let us consider the heteropolymer chain with a frozen sequence of different monomers. On the microscopic scale thermal motion in macromolecule produces small deformations of valent bonds and angles and causes rotations around single bonds. It is widely believed [14] that at the low temperatures in the long macromolecules the long-wave fluctuations are dominant. Thus, the global properties of the polymeric chain defined by collisions not merely between monomers, but rather between parts of the chain. It was shown [15] that interactions in the polymeric chain may be qualitatively represented as interactions in the cloud of ”quasimonomers” with the renormalized characteristics of interaction.

Thus, we can assume that the state of the polymer chain described by coarse-grained beads coordinated $\vec{r}(s)$ and their momenta $\vec{p}(s)$ and also by the those coordinates $\vec{r}_\mu$ and $\vec{p}_\mu$ that describe the precise local structure of a polymer.

Specifically, we examine the monomer interaction energy of the form

$$H = E + K + H_{mic}$$

where $K$ is the kinetic energy. The $U_{mic}$ is the potential energy for interactions of microscopic coordinates with other degrees of freedom. $E(r)$ is the coarse-grained ”beads-on the string” Hamiltonian

$$E(r) = \frac{T d}{2a^2} \sum_{s=1}^{N} (r_s - r_{s+1})^2 + \sum_{s<s'} B_{ss'} \delta(r_s - r_{s'}) + V(r)$$

where $B_{ss'} = B\sigma_s\sigma_{s'}$ is second virial coefficient describing two-particle interactions. $\{\sigma_s\}$ are variables, describing species of monomers. $V(r)$ is the excluded volume interactions approximation by effective confinement term

$$V(r) = B^* \sum_s r_s^2$$

where the constant $B^*$ chosen so that the radius of gyration becomes the value, required by the monomers packing density in the globular state [16]. $B_{ss'}$ is the effective second virial coefficient of the interaction between parts of the chain. $B_{ss'}$ represents the collective property of all the monomers of the chain. Taking into account the central limit theorem, we can choose $\{\sigma_s\}$
as random variables, characterized by Gaussian distribution function in the form

\[ P\{\sigma_s\} \propto \exp \left[ -\frac{1}{2} \left( \sigma, \hat{K}^{-1}\sigma \right) \right] \]  

(4)

where \( \sigma = \{\sigma_s\} \). \( \hat{K} \) is the matrix describing correlations in the chain sequence

\[ K(\sigma_s, \sigma_{s'}) = \sigma_s \sigma_{s'} \]  

(5)

Following the generalized Rouse theory, derived by Hess [17,18] for the entangled polymeric liquids, consider the dynamic equations, described random heteropolymer behavior.

Let us a complete set of degrees of freedom is \( \{X_i(t)\} \). Then the equation of motion for \( X_i(t) \) is

\[ \frac{d}{dt} X_i(t) = -\hat{L}X_i(t) \]  

(6)

where \( \hat{L} \) is Liouvillian given as

\[ \hat{L} = -\sum_{s=1}^{N} \left[ v(s) \nabla r(s) - \frac{1}{m} \nabla r(s) H \nabla v(s) \right] - \sum_{\mu} (v_{\mu} \nabla_{\mu} - \frac{1}{m_{\mu}} \nabla_{r_{\mu}} H_{\text{mic}} \nabla v_{\mu}) \]  

(7)

\( v(s) \) and \( v_{\mu} \) are velocities of beads (segments) and of microscopic constituents. \( m \) and \( m_{\mu} \) are the corresponding masses. The projection operator formalism shows that Liouville equation can be reduced into the form of generalized Langevin equation [17,18,19]

\[ \frac{d}{dt} r(s,t) = -T \sum_{s',s''} \int_{0}^{t} dt' \mu_{ss'}(t-t') \gamma_{s',s''} r(s'',t') + g(s,t) \]  

(8)

where \( g(s,t) \) satisfied to fluctuation dissipation theorem

\[ \langle g(s,t)g(s',t') \rangle = T \mu_{ss'}(t-t') \]  

(9)

\( \gamma_{s',s''} \) are the elements of the nearest-neighbor matrix for an open ideal chain

\[ \gamma_{s',s''} = -\frac{d}{a^2} \hat{a}_{ss'} \]  

(10)
As it was shown in [18] the dynamic mobility function fulfill the following equation

\[
\mu_{ss'}(t) = \frac{2\delta(t)}{\zeta_0} - \frac{1}{\zeta_0} \int_0^t d\tau \sum_{s''} \mu_{s's''}(t - \tau) \Delta \zeta_{s''s'}(\tau)
\]  

(11)

where \( \Delta \zeta_{s''s'}(\tau) \) is the dynamic friction function produced by force correlations between beads ( coarse-grained coordinates )

\[
\Delta \zeta_{ss'}(t) = \frac{1}{T} \left\langle \bar{f}_p(s) e^{-\hat{Q}\hat{L}t} \bar{f}_p(s') \right\rangle
\]

(12)

\[
\bar{f}_p(s) = -\nabla_{r(s)} H_{int}
\]

where \( H_{int} = \sum_{s<s'} B_{ss'} \delta(r_s - r_s') \)

It was shown that [18]

\[
\Delta \zeta_{ss'}(t) = \beta \left( \bar{f}_p(s) e^{-\hat{Q}\hat{L}t} \bar{f}_p(s') \right) = \beta \left( \bar{f}_p(s) e^{-\hat{L}t} \bar{f}_p(s') \right) + \beta \sum_{s''=1}^N \int_0^t d\tau \left( \bar{f}_p(s) e^{-\hat{L}(t-\tau)} \bar{v}(s'') \right) \Delta \zeta_{s''s'}(\tau)
\]

(13)

The two-particle interaction forces given as

\[
\bar{f}_p(s) = -\nabla_{r(s)} H_{int} = -|\mathbf{b}| T \int_q \hat{i} \mathbf{q} e^{-\mathbf{i} \mathbf{q} \cdot \mathbf{r}(s')} \sigma_s m(\mathbf{q})
\]

(14)

where

\[
m(\mathbf{q}) = \sum_{s'} m_s(\mathbf{q}) = \sum_{s'} \sigma_{s'} \exp \left[ -i \mathbf{q} \cdot \mathbf{r}'(s') \right]
\]

and

\[
\int_q \ldots = \int \frac{d^d q}{(2\pi)^d}
\]

are defined by analogy with the bead’s collective density fluctuations. Thus, the dynamic friction function is equal to

\[
\Delta \zeta_{ss'}(t) = -|\mathbf{b}|^2 T \int_q \int_{\mathbf{p}} \hat{q} \cdot \hat{p} \sum_{s_1 s_2} \left( m_s(\mathbf{q}) m_{s_1}(-\mathbf{q'}) e^{-\hat{L}t} m_{s'}(\mathbf{p}) m_{s_2}(-\mathbf{p'}) \right) -
\]

\[
- |\mathbf{b}| \sum_{s''} \int_q \int_{\mathbf{p}} \hat{q} \cdot \hat{p} \sum_{s_1} \left( m_s(\mathbf{q}) m_{s_1}(-\mathbf{q'}) e^{-\hat{L}(t-\tau)} \hat{v}(s'') \right) \Delta \zeta_{s''s'}(t)
\]
The four-point correlation function at the right side of the last equation cannot be calculated rigorously. Following [18] choose as the simplest approximation for collective density fluctuations

\[ m_s(\vec{q}, t) = \sum_{s'} R_{ss'}(\vec{q}, t) m_s(\vec{q}, 0) \equiv \sum_{s'} R_{ss'}(\vec{q}, t) m_s(\vec{q}) \]  

(16)

The relaxation functions \( R_{ss'}(\vec{q}, t) \) are defined by expression

\[ \langle m_s(\vec{q}, t) m_{s'}(-\vec{q}) \rangle = \sum_{s''} R_{ss''}(\vec{q}, t) \langle m_{s''}(\vec{q}) m_{s'}(-\vec{q}) \rangle \]  

In this approximation

\[ \Delta \zeta_{ss'}(t) = -|b|^2 T \int_q \int_p \frac{\vec{q} \cdot \vec{p}}{\lambda} \sum_{s_1 s_2 s_3} R_{s's''}(\vec{p}, t) R_{s_2 s_3}(-\vec{p}, t) \]  

\[ \langle m_s(\vec{q}) m_{s_1}(-\vec{q}) m_{s''}(\vec{p}) m_{s_3}(-\vec{p}) \rangle - \]  

\[ -|b| \int_q \int_{t'} d\tau (i \vec{q}) \sum_{s_1} \langle m_s(\vec{q}) m_{s_1}(-\vec{q}) e^{-\hat{L}_t v(s'')} \Delta \zeta_{ss'}(\tau) \rangle \]  

It was shown that [18]

\[ \Delta \zeta_{ss'}(t) = -|b|^2 T \int_q \int_p \frac{\vec{q} \cdot \vec{p}}{\lambda} \sum_{s_1 s_2 s_3} R_{s's''}(\vec{p}, t) R_{s_2 s_3}(-\vec{p}, t) \]  

\[ \langle m_s(\vec{q}) m_{s_1}(-\vec{q}) m_{s''}(\vec{p}) m_{s_3}(-\vec{p}) \rangle \]  

(17)

At the integration over \( \vec{q} \) the expression

\[ \langle m_s(\vec{q}) m_{s_1}(-\vec{q}) m_{s''}(\vec{p}) m_{s_3}(-\vec{p}) \rangle \]

gives nonzero contribution only when beads \( s_1 \) and \( s \) are in contact. However, the contact between \( s_1 \) and \( s \) have influence on the contact between the beads \( s_3 \) and \( s'' \), if they belongs to subchain \( (s_1 - s) \) (see fig.1). The loop formation between \( s_1 \) and \( s \) sufficiently reduced the available conformations space as

\[ \frac{\text{Number of subchain}(s_1 - s) \text{ loop conformations}}{\text{Total number of subchain} (s_1 - s) \text{ conformations}} \propto |s_1 - s|^{-4} \]  

(18)

(In the case of ideal Gaussian chain \( d^* = d \).)
By this reason, the loop formation between \( s_1 \) and \( s \) have increased the probability of contact formation for the beads belongs to subchain \((s_1 - s)\). Taking into account this approximation

\[
\Delta \zeta_{ss'}(t) = -|b|^2 T \int_q \sum_{s_1 s_2 s'_3 \in [s, s_1]} q \sum_{s'_2 s'_3 \in [s_2, s_3]} R_{s'_2 s'_3}(\overrightarrow{p'}, t) R_{s_2 s_3}(\overrightarrow{-p'}, t) \times \\
\langle \sigma_s \sigma_{s_1} \sigma_{s'_2} \sigma_{s'_3} e^{-i\overrightarrow{q} \cdot \overrightarrow{L}(ss_1)} e^{-i\overrightarrow{p} \cdot \overrightarrow{L}(s'_2 s'_3)} \rangle
\]

where

\[
\overrightarrow{L}(ss_1) = \overrightarrow{L}(s) - \overrightarrow{L}(s_1)
\]

The last integral can be evaluated as [18]

\[
\langle \int_q q \overrightarrow{p} e^{-i(\overrightarrow{q} + \overrightarrow{p}) \cdot \overrightarrow{L}(ss_1)} \rangle \approx -p^2 \int_Q \langle e^{-iQ \cdot \overrightarrow{L}(ss_1)} \rangle
\]

Thus,

\[
\Delta \zeta_{ss'}(t) \approx |b|^2 T \sum_{p} \sum_{s_1 s_2 s'_3 \in [s, s_1]} \sigma_s \sigma_{s_1} \sigma_{s'_2} \sigma_{s'_3} \int_Q \langle e^{-iQ \cdot \overrightarrow{L}(ss_1)} \rangle \\
\int_p p^2 R_{s'_2 s'_3}(\overrightarrow{p'}, t) R_{s_2 s_3}(\overrightarrow{-p'}, t)
\]

Because of the integral over \( \overrightarrow{p} \) is dominated by the large \( p \) modes only correlations between small numbers of beads have contribution. Then we assume that in the limit of large wave vectors the correlation between different beads vanishes and only single bead propagator survives

\[
\int_p p^2 R_{s'_2 s'_3}(\overrightarrow{p'}, t) R_{s_2 s_3}(\overrightarrow{-p'}, t) \approx \delta_{s'_2 s'_3} \delta_{s_2 s_3} \int_p p^2 G^2(\overrightarrow{p'}, t)
\]

where \( G(\overrightarrow{p'}, t) \) is the single bead propagator.

Consequently, dynamic friction function is

\[
\Delta \zeta_{ss'}(t) = |b|^2 T \Psi_{ss'}(\overrightarrow{\sigma'}) \int_p p^2 G^2(\overrightarrow{p'}, t)
\]
where

$$\Psi_{ss'}(\sigma') = \sum_{s_1 \geq s'} \sum_{s_2 \in [s,s_1]} \sigma_s \sigma_{s_1} \sigma_{s'} \sigma_{s_2} \int_Q \langle e^{-iQ} T^{(ss_1)} \rangle$$

Thus, the generalized Langevin equation for the beads coordinates

$$\frac{d}{dt} r(s,t) = -\frac{T}{a^2} \sum_{s',s''} \int_t^t dt' \mu_{ss'}(t-t') A_{s's''} r(s'',t') + g(s,t) \quad (21)$$

where

$$\langle g(s,t) \rangle = 0$$

$$\langle g(s,t)g(s',t') \rangle = T\hat{\mu}_{ss'}(t-t') \quad (22)$$

$$\mu_{ss'}(t) = \frac{2\delta(t)\delta_{ss'}}{\zeta_0} - \frac{1}{\zeta_0} \int_0^t d\tau \sum_{s''} \mu_{ss''}(t-\tau) \Delta \zeta_{s''s'}(\tau)$$

The dynamic friction functions $\Delta \zeta_{ss'}(t)$ are defined by eqn.(20). In spite of the case investigated in [18], the $A_{ss'}$ are the elements of the nearest-neighbor matrix for the open chain with the confinement interactions (3).

Let us estimate the magnitude of the dynamic friction function in dependence of correlations in $\sigma' = \{\sigma_1,...,\sigma_N\}$. Value of the $\Psi_{ss'}(\sigma')$ is defined by the summation over large number of beads and formally similar to the energy with corresponding interaction potential. Thus, $\Psi_{ss'}(\sigma')$ is the extensive quantity. It’s reasonable to suppose that $\Psi_{ss'}(\sigma')$ is the self-averaging quantity. In this case

$$\Psi_{ss'}(\sigma') = \Psi_{ss'}(\sigma) = \sum_{s_1 \geq s'} \sum_{s_2 \in [s,s_1]} \sigma_s \sigma_{s_1} \sigma_{s'} \sigma_{s_2} \int_Q \langle e^{-iQ} T^{(ss_1)} \rangle \quad (23)$$

The main object of our interests is the condensed state of random heteropolymer. It is well known that in this state any subchain behaves as ideal and one-time (equilibrium) correlations described by Gaussian statistics. The deviation from the Gaussian statistics produced a great entropy lost by order $\approx N$. Consequently,

$$\langle e^{-iQ} T^{(ss_1)} \rangle = e^{-Q^2b^2 |s-s_1|}$$

where $b$ is the length of the effective statistical segment. Thus,

$$\Psi_{ss'}(\sigma') = \int_Q \Phi_{ss'}(Q)$$
where
\[
\Phi_{ss'}(\overrightarrow{Q}) = \sum_{s_1 \geq s'} \sum_{s_2 \in [s, s_1]} \sigma_s \sigma_{s_1} \sigma_{s'} \sigma_{s_2} e^{-Q^2 b^2 |s-s_1|} \approx (24)
\]

Because of variables \(s\) are Gaussian distributed and \(\sigma_s = 0\), then
\[
\sigma_s \sigma_{s_1} \sigma_{s'} \sigma_{s_2} = \sigma_s \sigma_{s_1} \cdot \sigma_{s'} \sigma_{s_2} + \sigma_s \sigma_{s_1} \cdot \sigma_{s_1} \sigma_{s_2} + \sigma_s \sigma_{s_2} \cdot \sigma_s \sigma_{s'}
\]

\(Q\) mode of the \(\Psi_{ss'}(\sigma)\) may be estimated as
\[
\Phi_{ss'}(\overrightarrow{Q}) = \sum_{s_1 \geq s'} \sum_{s_2 \in [s, s_1]} \sigma_s \sigma_{s_1} e^{-Q^2 b^2 |s-s_1|} \sum_{s_2 \in [s, s_1]} \sigma_{s'} \sigma_{s_2} + (25)
\]

It is obvious that in dependence of rate of correlation function decay the magnitude of \(\Phi_{ss'}(\overrightarrow{Q})\) may be quite different.

First of all, let us consider the exponential decay of inter monomer’s correlations. In this case
\[
K(s, s') \propto \exp \left( -\frac{|s-s'|}{\xi} \right) \quad (26)
\]

For simplicity, we have restricted our consideration by the case \(s \approx s'\). Then the main term, contributed to \(\Phi_{ss'}(\overrightarrow{Q})\) is
\[
\sum_{s_1 \geq s'} \sum_{s_2 \in [s, s_1]} \sigma_s^2 e^{-Q^2 b^2 |s-s_1|} \approx K \sum_{s_1 \geq s'} e^{-Q^2 b^2 |s-s_1|} \sum_{s_2 \in [s, s_1]} \sigma_{s_1} \sigma_{s_2}
\]

It is obvious that for the exponential correlations
\[
\sum_{s_2 \in [s, s_1]} \sigma_{s_1} \sigma_{s_2} = a_{ss_1} < \infty
\]
is finite for any range of summation. Consequently,

$$\lim_{N \to \infty} \Phi_{ss'}(Q) < \infty$$

for any value of \(Q\). Moreover,

$$\int_Q \sum_{s_1 \geq s'} e^{-Q^2b^2|s-s_1|} \sum_{s_2 \in [s,s_1]} \sigma_{s_1} \sigma_{s_2} \simeq b^{-d}a \sum_{s_1 \geq s} |s-s_1|^{d/2}$$

is finite in the thermodynamic limit (\(N \gg 1\)). In spite of exponential correlations, the power-law decay leads to the following picture. Suppose that

$$K(s, s') \propto |s-s'|^{\beta-1}$$

Then,

$$\Phi_{ss'}(Q) = K \sum_{s_1 \geq s} e^{-Q^2b^2|s-s_1|} \sum_{s_2 \in [s,s_1]} \sigma_{s_1} \sigma_{s_2} \simeq K \sum_{M=0}^{N} e^{-Q^2b^2M} \sum_{S=0}^{M} |M-S|^{\beta-1}$$

(28)

It is known that [20] the last sum may be asymptotically estimated as

$$\sum_{S=0}^{M} |M-S|^{\beta-1} \leq Const |1-\beta|^{\beta-1} + \frac{M^{\beta}}{\beta} + \frac{1}{2M^{1-\beta}}$$

for \(M \gg 1\). Consequently,

$$\Phi_{ss'}(Q) \simeq K \sum_{M=0}^{N} M^{\beta} e^{-Q^2b^2M}$$

Thus,

$$\Psi_{ss'}(\sigma') = \int_Q \Phi_{ss'}(Q) \simeq b^{-d}K \sum_{M=0}^{N} M^{\beta-d/2}$$

(29)

In the thermodynamic limit \(\Psi_{ss'}(\sigma')\) diverge if

$$\beta > \beta^* = d/2 - 1$$

(30)

In the case of three-dimensional space the "critical value" of \(\beta\) is

$$\beta^* = \frac{1}{2}$$

(31)
Thus, the magnitude of dynamic friction function is strictly dependent from the type of correlations. For the exponential decay the dynamic mobility is more much than in the case of log-range (power-law) correlations. Moreover, for the strong ($\beta > \beta^*$) power-law correlations the long heteropolymer chain ($N \to \infty$) exhibits a zero mobility in the globular state.

This situation is similar to the case of strong entanglements, described in [18], where

$$\int_0^t d\tau \Delta \zeta(\tau) \simeq N$$

3 Discussion

The subject of present article is investigation of relation between the protein’s sequence and its dynamics.

In the case of power-law correlations the dynamic friction behavior is qualitatively distinguished from those in the heteropolymer with short-range correlations. While, for the exponential correlations the $\Delta \zeta_{ss'}(t)$ is finite in the thermodynamic limit, in the case of power-law correlation ($\beta \geq 1/2$)

$$\Delta \zeta_{ss'}(t) \propto N^{\beta-1/2}$$

($N \gg 1$). Consequently, the dynamic mobility of chain segments in the globular state sufficiently decreased with the range of correlations increasing.

This result give us an ability to explain the possible mechanism of large energetic barrier existence between frozen and random coil states that was shown in [6]. The long-range correlations in sequence must be increased the probability of advantageous contacts for the neighbor and especially non-nearest neighbor monomers of chain that effectively slowing down the mutual slip of the chain parts (see fig.2). It may be explain the so strong dependence of dynamic mobility from the range of correlations. The equilibrium properties of the RHP defined by averaging over the all chain conformations. For the long-range correlations in the chain sequence the extended regions of similar monomers are dominated. In the globular state, characterized by monomer’s position fluctuations, the averaging over all conformations included also a very disadvantageous contacts between extended regions of different monomers. This produce a great energetic barrier for the RHP with power-law correlations.
What may be the constructive role of such correlations in sequence?

One of the necessary properties of biologically functional protein is its ground state stability, provided by the energetic barrier existence between native and misfolded states. The long heteropolymer chain have a very low mobility in the state of disordered globule and denaturation/renaturations processes are very difficult in this state. But the real protein’s single chain length in most cases don’t exceed \( \sim 10^2 \) amino acids. It is due not only by the possible errors of replication from the very long segments of RNA. It may be related with necessity to have the stable native state. It is obvious that the random coil may be transferred to the folded (native) state only through the disordered globule state. It’s due by the low entropy of the Gaussian chains in this state in comparison with those in any other state of the polymeric chain [14]. The decreased mobility of disordered globule state should be stabilize the native state of the system.

The results, described above may be relevant to those, obtained by Pande et al. [1,2]. The power-law correlations in sequence can additionally stabilized the frozen state of the heteropolymeric globule.
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Figure 1.
The contact formation between the chain residues $s$ and $s_1$ increased the probability of the internal residues ($s''$ and $s_3$) contact formation.

Figure 2.
Schematic representation of the mutual movement of the chain parts in the presence of the long-range correlations. $z$ are the disadvantageous contacts between different monomers and $x$ are the advantageous contacts between similar monomers.