Disordered, stretched, and semiflexible biopolymers in two dimensions

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We study the effects of intrinsic sequence-dependent curvature for a two-dimensional semiflexible biopolymer with short-range correlation in intrinsic curvatures. We show exactly that when not subjected to any external force, such a system is equivalent to a system with a well-defined intrinsic curvature and a proper renormalized persistence length. We find the exact expression for the distribution function of the equivalent system. However, we show that such an equivalent system does not always exist for the polymer subjected to an external force. We find that under an external force, the effect of sequence disorder depends upon the averaging order, the degree of disorder, and the experimental conditions, such as the boundary conditions. Furthermore, a short to moderate length biopolymer may be much softer or has a smaller apparent persistent length than what would be expected from the “equivalent system.” Moreover, under a strong stretching force and for a long biopolymer, the sequence disorder is immaterial for elasticity. Finally, the effect of sequence disorder may depend upon the quantity considered.

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I. INTRODUCTION

It is known that sequence-dependent properties of biopolymers play a crucial role in many biological processes. More specifically, sequence disorder has important influences on DNA packaging, transcription, replication, recombination, and repair processes [1–11]. Owing to progress in experimental techniques such as laser or magnetic tweezers and atomic force microscopy, it is now possible to manipulate and observe single biomolecules directly, and thus make a better comparison between theoretical predictions and experimental observations.

In theoretical studies, a semiflexible biopolymer is often modeled as a filament [4–22]. For instance, the wormlike chain (WLC) model, which views the biopolymer as an inextensible chain with a uniform bending rigidity but with a negligible cross section, has been used successfully to describe the entropic elasticity of a long double-stranded DNA (dsDNA) [12–15]. However, the traditional elastic models are usually uniform and ignore the role of sequence disorder. Under what conditions such a simplification is valid is therefore an intriguing question. Based on the elastic models, two effects of sequence disorder need to be considered. First, structural inhomogeneity yields variations of the bending rigidity along the filament, and results in an s-dependent persistence length $l_p(s)$ [8,9], where $s$ is the arc length. It has been reported that for a long biopolymer with short-range correlation (SRC) in $l_p(s)$ and free of external force, this effect can be accounted by a replacement of the $l_p(s)$ by an appropriate average [8,9]. However, for a short biopolymer, inhomogeneity in $l_p(s)$ tends to make physical observables divergent [8,9]. Second, the local structure can be characterized by the intrinsic sequence-dependent curvatures (i.e., the static curvature or the frozen-in curvature) [2–11], and this is also the focus of the present work. For a long biopolymer with zero mean curvature, again it has been demonstrated that the effect of intrinsic sequence-dependent curvatures can also be reduced into a simple correction of the uniform persistence length, either free of external force [8,9,23,24] or under moderate external force [10,11,25]. However, it is argued that sequence disorder is immaterial for the elasticity of a long DNA under strong stretching force [10,15]. In this paper, we prove it exactly for a two-dimensional biopolymer even with a nonvanishing mean intrinsic curvature. Moreover, it is well known that the short- or intermediate-length DNAs play a more important role than the long DNAs in biological processes, from DNA packaging, to transcription, gene regulation, and viral packaging [26–28]. As a consequence, the effect of intrinsic sequence-dependent curvatures for short or intermediate-length biopolymers requires more attention. When the biopolymer is free of external force and with SRC in intrinsic sequence-dependent curvatures, it has been shown exactly that such a three-dimensional (3D) system is equivalent to a system (we will refer it as the “equivalent system” henceforth) with a well-defined (i.e., without randomness) intrinsic mean curvature and a corrected persistence length [8,9], irrespective of its length. In this work, we show that the same conclusion is also valid in the two-dimensional (2D) case and present the general solution of the distribution function of the equivalent 2D system. On the other hand, the effects of intrinsic sequence-dependent curvatures in a short biopolymer under external force are not yet known. In this paper, we demonstrate that under external force, the effect of sequence disorder for a short biopolymer is dependent on the average order and the experimental conditions. Moreover, we find that the results are also dependent on the boundary conditions (BCs), and the short biopolymer looks softer than what is expected from the “equivalent system.” Because theoretically a 2D system is relatively easier...
to study and experiments on the conformations of biopolymers are often conducted in a 2D environment [7,29], this work will focus on the 2D system.

The paper is organized as follows. In Sec. II we set up our model. Section III presents the exact proof of the existence of the “equivalent system” and the general distribution function of the “equivalent system” for a force-free biopolymer. In Sec. IV we focus on the conformation and elasticity of the biopolymer under constant external force. Follows a section discussing the effects of disorder in a segment dependent curvature in the constant-extension ensemble. Finally, we end the paper with conclusions and discussions.

II. MODEL

The configuration of a filament with negligible cross section can be described by the tangent vector, \( \mathbf{t}(s) \), to its contour line, where \( s \) measures the location along the filament. In two dimensions, \( \mathbf{t}(s) = \{ \cos(\phi(s)), \sin(\phi(s)) \} \), where the azimuthal angle \( \phi \) is the angle between the x axis and \( \mathbf{t} \). The locus of the filament can be found by

\[
\mathbf{r}(s) = \{x(s), y(s)\} = \int_0^s \mathbf{t}(u) du.
\]

(1)

The reduced energy of the filament with intrinsic curvature but free of external force can be written as

\[
\mathcal{E}_\alpha[\{\phi(s)\}] = \frac{E}{k_BT} \int_0^L \frac{1}{2} [\phi - \bar{c}]^2 ds,
\]

where \( E \) is the energy, \( \phi = d\phi / ds \), \( T \) is the temperature, \( k_B \) is the Boltzmann constant, \( L \) is the total arc length of the filament and is a constant in the model so that the filament is inextensible, \( k = l_p/2 \) with \( l_p \) the 2D bare persistent length, \( c(s) \) is the intrinsic sequence-dependent curvature. Under a uniaxial applied force \( f_i \) (along x-axis), the reduced energy of the filament becomes

\[
\mathcal{E} = \mathcal{E}_\alpha[\{\phi(s)\}] - \int_0^L \cos \phi ds,
\]

where the reduced force is defined by \( f = f_i / k_BT \). When \( c(s) = 0 \) and \( l_p \) is a constant, it returns to the well-known WLC model [12–15]. Note that with free boundary condition, a negative value of \( f_i \) only extends the polymer in the negative direction rather than the positive direction. So it does for a long polymer since the boundary condition becomes unimportant. Therefore, the sign of the force is meaningless in these cases. However, it is not the case for a short polymer with a fixed initial angle.

If both \( l_p \) and \( c(s) \) are well-defined functions of \( s \), a macroscopic quantity \( B_\phi \) is defined as the average with Boltzmann weights over all possible conformations,

\[
B_\phi = \frac{1}{Z_\alpha} \int \mathcal{D}[\phi(s)] B[\{\phi(s)\}] e^{-\mathcal{E}},
\]

(4)

where \( Z_\alpha = \int \mathcal{D}[\phi] e^{-\mathcal{E}} \). Function \( B[\{\phi(s)\}] \) represents different physical situations. For instance, if \( B[\{\phi(s)\}] = |\mathbf{r}(s_1) - \mathbf{r}(s_2)| \), we find the orientational correlation function (OCF); if \( B[\{\phi(s)\}] = |\mathbf{r}_L - \mathbf{r}_0|^2 \), we obtain the mean end-to-end distance, where \( \mathbf{r}_L = \mathbf{r}(L) \) and \( \mathbf{r}_0 = \mathbf{r}(0) \); if \( B[\{\phi(s)\}] = \delta(\mathbf{R} - \mathbf{r}(s)) \), we get the distribution function of end-to-end vector; if \( B[\{\phi(s)\}] = \delta(\mathbf{r}_L - \mathbf{r}_0) \delta(t(L) - t(0)) \), we find the looping probability. \( B[\{\phi(s)\}] \) is independent of \( k \) and \( c(s) \) but can be a very complex function of \( \phi(s) \) and \( \phi(s) \).

Equation (4) uses \( \phi \) as the variable of integration. However, the variable of integration can be replaced by \( \phi(s) \), i.e., we have the following identity (see Appendix A for proof)

\[
\frac{\int \mathcal{D}[\phi(s)] B[\{\phi(s)\}] e^{-\mathcal{E}}}{\int \mathcal{D}[\phi(s)] e^{-\mathcal{E}}} = \frac{\int \mathcal{D}[\phi(s)] B[\{\phi(s)\}] e^{-\mathcal{E}}}{\int \mathcal{D}[\phi(s)] e^{-\mathcal{E}}}. 
\]

(5)

For a biopolymer without correlation on \( c(s) \), or with SRC on \( c(s) \) but in the coarse-grained model, the distribution of \( c(s) \), \( W(c(s)) \), can be written as a Gaussian distribution with mean \( \bar{c} \), and root-mean squared deviation \( 1/\sqrt{\alpha} \)

\[
W(c(s)) = \exp \left[ -\frac{1}{2} \alpha (c(s) - \bar{c})^2 \right].
\]

(6)

In this case, we need to average over \( c \) for all biopolymers in the system. Note that averaging can be done in two different orders, either

\[
B = \langle B[\{\phi(s)\}] \rangle = \frac{1}{Z_\alpha} \int \mathcal{D}[c(s)] W(c(s)) B_\phi,
\]

(7)

where \( Z_\alpha = \int \mathcal{D}[c(s)] W(c(s)) \), or

\[
B' = \langle B[\{\phi(s)\}]' \rangle = \frac{1}{Z_k} \int \mathcal{D}[\phi] \left[ \frac{1}{Z_\alpha} \int \mathcal{D}[c] W(c) B[\{\phi\}] e^{-\mathcal{E}} \right] \]

\[
= \frac{1}{Z_k} \int \mathcal{D}[\phi] B[\{\phi\}] \left[ \frac{1}{Z_\alpha} \int \mathcal{D}[c] W(c) e^{-\mathcal{E}} \right].
\]

(8)

Physically, Eq. (7) corresponds to performing a conformational or thermal average over an individual sample first, and then a disorder average over all samples in the system, so we call this a thermal-first system. In contrast, in Eq. (8) a disorder average over an instantaneous conformation of all samples is first performed, followed by a conformational average over all possible conformations, so we refer to the corresponding system as a disorder-first system. To find a macroscopic quantity in the disorder-first system is equivalent to averaging the sequence disorder over all samples first to create an “equivalent” system which is then thermally averaged. So it is always possible to construct an “equivalent system” in that case. However, in experiments and computational simulations thermal-first averages are performed. Therefore, this work will also focus on the thermal-first system and show that in many cases the two systems are not equivalent.

III. DISTRIBUTION FUNCTION FOR THE FORCE-FREE SYSTEM

We first present a brief description of the force-free system. Using the identities Eqs. (5) and
\[
\int \mathcal{D}[c] W\{c\} e^{-\mathcal{E}_0} = \frac{Z_0^b Z_a}{Z_0^a} e^{-\mathcal{H}_0},
\]
and exchanging the order of integration, Eq. (7) becomes
\[
B = \frac{1}{Z_H^a} \int \mathcal{D}[\phi] B\{\phi(s)\} \left\{ \int \mathcal{D}[c]\frac{e^{-\mathcal{E}[c]} W\{c(s)\}}{Z_a} \right\} = \frac{1}{Z_H^a} \int \mathcal{D}[\phi] B\{\phi(s)\} e^{-\mathcal{H}_0},
\] (10)
where
\[
\mathcal{H}_0 = \frac{1}{2} \int_0^L \kappa[\phi(s) - \bar{\phi}]^2 ds,
\] (11)
and the effective persistent length,
\[
l_p^{\text{eff}} = 2\kappa = 2k\alpha/(k + \alpha).
\]
Note that Eq. (10) is valid for any \(L\) and even if \(\bar{\phi}, k \text{ and } \alpha\) are \(s\)-dependent. Comparing Eqs. (4) and (10), we reach the conclusion that a system with SRC in \(c(s)\) is equivalent to a system with a well-defined mean intrinsic curvature \(\bar{\phi}\) and a renormalized persistence length \(l_p^{\text{eff}}\).

The same conclusion has been achieved for 3D biopolymers following similar arguments [8], except that in the 2D case we have to derive Eq. (5) first due to the convention of using \(\phi\) as integral variable. This conclusion also means that the thermal-first system is exactly the same as the disorder-first system in the force-free case.

From the standard connection between the path integral and the Schrödinger equation, we can find that the partition function \(Z_0^b\{\phi(s), s; \phi(0), 0\}\) for the system with effective energy \(\mathcal{H}_0\) satisfies the following partial differential equation [21,22,31],
\[
\frac{\partial Z_0^b}{\partial s} = \left( \frac{1}{2\alpha} \frac{\partial^2}{\partial \phi^2} - \frac{\phi - \bar{\phi}}{\kappa} \right) Z_0^b.
\]
Fixing \(\phi(s)\) at \(s=s_0\), the boundary condition (BC) becomes
\[
Z_0^b(\phi, \phi; 0, \phi) = A[\phi - \varphi],
\]
where \(\varphi = \varphi(s_0)\). In an experiment, one usually takes \(\phi(0) = 0\) when \(f = 0\).

It is straightforward to show that the normalized function (i.e., the distribution function with \(s > s_0\))
\[
P(\phi, \phi; \varphi, \varphi) = \frac{1}{2\pi A(s, s_0)} \exp \left\{ -\int_0^s \frac{\phi - \varphi}{\kappa} ds \right\} \frac{1}{\sqrt{2A(s, s_0)}} \left\{ \int_0^s \frac{\phi - \varphi}{\kappa} ds \right\}
\]
(16)
satisfies Eqs. (14) and (15), where \(A(s, s_0) = \int_0^s ds / \kappa(s)\).

### IV. Conformation and Elasticity of the System under External Force

#### A. On the disorder-first system

When \(f \neq 0\), for the disorder-first system, the derivation leading to Eq. (10) can be generalized easily to obtain an equivalent system with the effective energy
\[
\mathcal{H} = \mathcal{H}_0 - \int_0^L \cos \phi ds,
\]
no matter what the force may be since the force term in \(\mathcal{E}\) is independent of \(c(s)\). The equivalent system has been well studied [22,32,33].

In the three-dimensional case, we can also reach a similar conclusion by a direct generalization of the proof in Ref. [8] to find an equivalent system, and an alternative proof for the three-dimensional filament under weak force can be found in Ref. [10].

#### B. General expressions for the thermal-first system under weak force

Note that, mathematically, the conclusion of the existence of an equivalent system in the force-free case results from the fact that both \(Z_0^b\) and \(Z_a\) are Gaussian integrals so are independent of \(c(s)\) or \(\phi\). However, such an argument fails for the thermal-first system with \(f \neq 0\), because \(Z_0\) is no longer a Gaussian integral and is dependent on \(c\), so exchanging the order of integration does not simplify the expression. In other words, there is no simple way to remove the randomness in \(c(s)\) so there is in general no “equivalent system” even under weak force, as we will show exactly below. In this case, to first order in \(f\), as shown in Appendix C,
\[
B = \frac{1}{Z_a} \int \mathcal{D}[\phi] B\{\phi\} e^{-\int_0^L \mathcal{E}[c]} \left\{ \int \mathcal{D}[c] \frac{1}{Z_k} e^{-\mathcal{E}_0} \right\} = B_1 - B_2,
\]
with
\[
B_1 = \langle \mathcal{H}\rangle + \int_0^L ds' \langle B\{\phi(s')\}\cos \gamma(s') \rangle,\]
and
\[
B_2 = \int_0^L ds' \langle B\{\phi(s')\}\cos \gamma(s') + \phi(0) \rangle,\]
(19)
where
\[
A'(s, s_0) = \int_{s_0}^s ds' k'(s), \quad k'(s) = \frac{k(a + k)}{\alpha + 2k},
\]
(20)
\[
\gamma(s) = \int_0^s \dot{\gamma}(s) ds, \quad \dot{\gamma}(s) = \frac{k\dot{\phi} + \alpha \gamma}{\alpha + k},
\]

and \(\phi_0 = \phi(0)\) is the initial azimuthal angle. Note that \(\gamma(s)\) is in general dependent on \(\phi(s)\) making these expressions very complex.

We should remind that when \(f \neq 0\), \(\phi_0\) is not necessarily zero but is dependent on the experimental conditions. In experiments, \(\phi_0\) may be fixed. In this case, the boundary condition at \(s = 0\) is given by Eq. (15). However, experiments on stretching biopolymers usually involve attaching the two ends of the biopolymer to beads, and it does not seem to be easy to completely prohibit the rotation of the beads. As a consequence, it may be difficult to fix \(\phi_0\). In the extreme case, the polymer can rotate freely around the origin. This can be realized by a magnetic tweezer [34]. In the more general case, \(\phi_0\) may have a distribution and therefore finally we need to average over \(\phi_0\). It has been reported that different boundary conditions have considerable effects on the mechanical response of a homopolymer [19,34]. In this work, we come to the same conclusion for a heteropolymer.

On the other hand, for the disorder-first system, we find

\[
B' = \frac{1}{\mathcal{Z}_H} \int \mathcal{D}[\phi] \mathcal{B}[\{\phi]\] \mathrm{e}^{-\mathcal{H}} = B_1 - B_2',
\]

\[
B_2' = f(B[\{\phi(s)\}]) \int_0^L ds \cos(\phi(s)) e^{L f} B_2',
\]

\[
B_2' = \int_0^L \mathrm{e}^{-\lambda s/\sqrt{2}} \cos \left[ \phi_0 + \int_0^s \dot{\gamma}(s) ds \right],
\]

where \(\mathcal{Z}_H = \int \mathcal{D}[\phi] \mathrm{e}^{-\mathcal{H}}\).

It is clear that in general \(B_2 \neq B_2'\) since \(\gamma\) is dependent on \(\phi\). In turn leads to in general \(B \neq B'\). In other words, in general it is impossible to find an equivalent system for the thermal-first system under external force.

C. Elasticity of the thermal-first system under weak force

To figure out how serious the effect of the disorder in \(c(s)\) or how large the discrepancy between \(B\) and \(B'\), we examine the most interesting and also the simplest case with constant \(k, \alpha, \) and \(\varepsilon=0\). It corresponds to the WLC model and is often used to describe the entropic elasticity of biopolymers, such as dsDNA and proteins. Experiments in 3D dsDNA found that \(k=78\) nm and \(\kappa=45\) nm [23,35–37]. It follows that \(k \approx 1.7\kappa\) for DNA. In this case, \(\gamma(s) = \kappa(\phi(s) - \phi_0) / \alpha\), and from Eq. (23), we can obtain

\[
B_2' = 2\kappa f(1 - e^{-L/2\kappa}) \cos \phi_0(B[\{\phi(s)\}]) \varepsilon.
\]

The extension \(X\) in the thermal-first system can be found as (see Appendix D)

\[
X = \left(\langle \chi \rangle - \langle \chi \rangle \right)_{f=0} = 2\kappa f \left[ \frac{1}{L} \frac{k(k+3\alpha)}{k+\alpha} + \frac{k(k+\alpha)}{k-\alpha} e^{-L/k} - \frac{4\kappa^2}{3} \frac{e^{-L/2\kappa}}{k-\alpha} \right]
\]

\[
\kappa^2 \cos(2\phi_0) e^{-2L/k} \frac{X}{3(2k+\alpha)^2}.
\]

\[
X = 6\kappa^2 (e^{L/k} - 1) + 9\kappa^2 (9e^{2L/k} - 16e^{L/k} - 12e^{L/k} + 5) + \alpha^2(3e^{2L/k} - 8e^{L/k} + 6e^{L/k} - 1).
\]

\[
X = \frac{f}{\varepsilon} \left( 1 - e^{-L/2\kappa} ight)^2 + \frac{2\kappa f}{3} \cos(2\phi_0) \times \left( e^{-L/2\kappa} - e^{-L/2\kappa} + 8e^{-L/2\kappa} - 3 \right).
\]

From Eqs. (25) and (26), we can show that \(X \rightarrow X'\) as \(\alpha \rightarrow \infty\), as it should be since in this case the system is free of randomness. Moreover, for a long polymer, we obtain \(X \approx X' \approx 2kL f\), so that the averaging order is irrelevant for a long polymer, and agrees with known results [10,11,25].

However, the discrepancy between the two systems is serious up to moderate length at finite \(\alpha\). From Eqs. (25) and (26), we find that the extensions consist of two terms. The first term is independent of BC or \(\phi_0\), but the second term is dependent on \(\cos 2\phi_0\) so is dependent on the BC. As a consequence, different boundary conditions have strong effects on the elasticity up to moderate length. Without loss in generality, we consider two extreme cases. The first case is to fix \(\phi_0=0\), which gives the most stringent BC effects. The second is to let \(\phi_0\) free so \(\cos 2\phi_0=0\), and only the BC-independent term remains. For a better comparison, we define a ratio of the extensions, \(r_e = X/X'\).

Figures 1 and 2 present some typical results for \(r_e\). From these two figures, we can see that \(r_e\) increases monotonously with increasing \(L\), and in general the disorder in \(c(s)\) makes the biopolymer in the thermal-first system softer, i.e., \(r_e < 1\), than the “equivalent” system, and the effects may be still rather serious up to the length of about \(20\kappa\). Furthermore, we
In contrast, in the disorder-first system, smaller than $L$ is in DISORDERED, STRETCHED, AND SEMIFLEXIBLE $X$ which corresponds to the experimental value of DNA, we can be only about half of $X \cdot t \cdot L = \frac{2}{L} \left(1 - e^{-L/2k}\right) + \frac{4\kappa^2 \cos \phi_0}{9(k - \alpha)^2(2k + \alpha)(3k + \alpha)^2}r''$, with $r'' = 18(k - \alpha)^2(k + \alpha)(2k + \alpha)(3k + \alpha)^2L - 9k(k - \alpha)^2 \times (3k + \alpha)^2(4k^2 + 11\alpha^2 + 22k\alpha) - 16\alpha(2k + \alpha)^3[3(k - \alpha) \times (k + \alpha)(3k + \alpha)L + 4k\alpha(5k + \alpha)(3k + \alpha)]e^{-L/2k} + 18\alpha\alpha(3k + \alpha)^3(k - \alpha)^2e^{-1/(k+2\alpha)} + 18\alpha(3k + \alpha)^2e^{-L/2k} - \alpha(3k + \alpha)^2e^{-2L/2k}$. 

When $\alpha \rightarrow \infty$, i.e., a system without randomness, we obtain $R^2 = R''^2$ as it should be. Moreover, $L \rightarrow \infty$ also leads to $R^2 \rightarrow R''^2$, again supporting the conclusion that the order in averaging is irrelevant for a long polymer [10,11,25].

Moreover, from Eqs. (29) and (30), we find that the end-to-end distance can also be divided into two terms. The first term is the force-free term and is independent of BC, but the second term is dependent on both BC and force. Especially, for free BC ($\langle \cos 2\phi_0 \rangle = 0$), the force has not effect at all, this is quite different from the force-extension relation. Furthermore, with finite $\langle \cos 2\phi_0 \rangle$, $R^2$ is also smaller than $R''^2$, similar to the force-extension relation. However, the ratio $r_R = R^2/R''^2$ is no longer a monotonic function of $L$, but has a minimum at $L \approx 6\kappa$. Moreover, the discrepancy between $R$ and $R''$ increases with increasing $f$ [see Eqs. (29) and (30)]. Note that our results are valid only for weak force, and for DNA it means that we require $k_BT f < f_s = k_BT f_s$. Taking the generally accepted value $\kappa = 50$ nN, we have $f_s = 0.08$ pN. Figure 3 shows some typical results at $f = 0.5/\kappa$, which correspond to an external force of about 0.04 pN. From Fig. 3, we can see that the discrepancy between $R^2$ and $R''^2$ is much smaller than that for extensions. This is because the force-free term dominates the value of $r_R$. The fact that the disorder in $c(s)$ has quite different effects on the extension and the end-to-end distance may be important in experiments.

In contrast, in the disorder-first system, 

$$S' = 6e^{-r/2\kappa} - 8e^{-(r-S')/2\kappa} + 2e^{(3\kappa - 4\alpha)/2\kappa} - 3e^{-(L+3(r-S'))/2\kappa} - 3e^{-(L+r-S')/2\kappa}. \quad (28)$$

The end-to-end distance can be found as 

$$R^2 \approx 4\kappa L \left[ 1 - \frac{2\kappa}{L} \left(1 - e^{-L/2k}\right) \right] + \frac{4\kappa^2 \cos \phi_0}{9(k - \alpha)^2(2k + \alpha)(3k + \alpha)^2}r'',$$

with $r'' = 18L - 99\kappa + 16(3L + 4\kappa)e^{-L/2k} + 36\kappa e^{-L/2k}$. 

E. Elasticity of the long biopolymer under large force

Again we assume constant $k$, $\alpha$ in this part, but allow a nonvanishing $c(s)$. In the large force limit the filament is nearly straight, thus $t(s)$ is nearly pointing along the direc-

FIG. 2. The ratio $r = \langle t \rangle / L$ for the free BC ($\langle \cos 2\phi_0 \rangle = 0$). From top to bottom, the parameters are: $k = 1.2\kappa$, $\alpha = 6.0\kappa$ (dash); $k = 1.4\kappa$, $\alpha = 3.5\kappa$ (dot); $k = 1.6\kappa$, $\alpha = 2.6\kappa$ (dash dot); $k = 1.8\kappa$, $\alpha = 2.2\kappa$ (solid); $k = 2.0\kappa$, $\alpha = 2.0\kappa$ (short dash). The unit of $L$ is in $\kappa$.

also find that the results are sensitive to BC and randomness of $c(s)$. At first, the effect is much more serious (maybe about twice) in the free BC (Fig. 2) than in fixing BC (Fig. 1). Second, the effect is getting stronger with increasing randomness, i.e., with decreasing $\alpha$. Especially, at $k = 1.7\kappa$ which corresponds to the experimental value of DNA, we find that $X$ can be only about half of $X' \cdot L \approx 10k$ and about 1500 bp. That means DNA is more likely to be in coil state or appears softer and has a smaller apparent persistence length than that in the “equivalent” system up to a rather long length. Finally, these results are independent of the external force, so that a small force may produce a considerable effect. This fact may be important in a stretching experiment for a short polymer since it suggests that the interaction between experimental apparatus and polymer may affect the results seriously.

D. Orientational correlation function and end-to-end distance for the thermal-first system under weak force

Let $B(t(s) \cdot t'(s')) = \cos \phi(s) - \phi(s')$, from Eqs. (18)–(22), we obtain the orientational correlation function (OCF) ($s' > s$) for the thermal-first system and under weak external force (see Appendix E)

$$\langle t(s) \cdot t'(s') \rangle = e^{-(s'-s)/2\kappa} + \frac{\kappa \cos \phi_0 f}{3(3k + \alpha)(k - \alpha)} S,'$$

$$S' = - 6k(k - \alpha)e^{-2[(\alpha + 2k\kappa + (\alpha + 3k\kappa)]2\alpha} + 3k(2k + \alpha)e^{-s'/2\kappa}$$

$$- 6k(3k + \alpha)e^{-2[2\alpha + (k - \alpha)]2\alpha} + (k - \alpha)(3k + \alpha)$$

$$\times[3e^{-(\alpha + 2k\kappa + (\alpha + 3k\kappa)]2\alpha} - 3e^{-(L + 3(s - s'))/2\kappa} + 2e^{-(4s - 3s')/2\kappa} + 3e^{-(\alpha + 2k\kappa + (\alpha - k](s - s'))/2\alpha}].$$

(27)

In contrast, in the disorder-first system,

$$\langle t(s) \cdot t'(s') \rangle = e^{-(s'-s)/2\kappa} + \frac{1}{3} rf \cos \phi_0 S'.$$
The ratio $r_\theta=R^2/R_1^2$ vs $L$. $f=0.5/\kappa$ and $\phi_0=0$ (the fixed BC) for all curves. From bottom to top, the parameters are: $k=1.2\kappa$, $\alpha=6.0\kappa$ (dash); $k=1.4\kappa$, $\alpha=3.5\kappa$ (dot); $k=1.6\kappa$, $\alpha=2.67\kappa$ (dash dot); $k=1.8\kappa$, $\alpha=2.25\kappa$ (solid); $k=2.0\kappa$, $\alpha=2.0\kappa$ (short dash).

The unit of $L$ is in $\kappa$.

Note that to use a sine series for $\phi(s)$, we can also use the full Fourier series for $c(s)$ and $\bar{c}(s)$ as Fourier series

$$\phi(s) = \sum_{n=1}^{\infty} a_n \sin(q_n s), \quad \bar{c}(s) = \sum_{n=1}^{\infty} \bar{c}_n \cos(q_n s), \quad c(s) = \sum_{n=1}^{\infty} c_n \cos(q_n s).$$

Note that to use a sine series for $\phi(s)$ is reasonable since $\phi_0=\phi(L)=0$. But in general $c(L) \neq 0$ so we cannot use sine series for it. We can also use the full Fourier series for $c(s)$ and $\bar{c}(s)$, but it is straightforward to show that the sine part in the full Fourier series make no contribution at all so we disregard it. Using the orthogonality property of Fourier modes, we can re-express the energy and extension as

$$\mathcal{E} \approx \frac{k_c^2 L}{2} \int_0^L \left[ \phi - c(s) \right]^2 ds + f \int_0^L \frac{1}{2} \phi^2 ds,$$

where we have dropped a constant term $-fL$. For a very long filament, we can use periodic boundary conditions with negligible error, so take $q_n = 2\pi n/L$ with integer $n$, and expand $\phi$, $c(s)$ and $\bar{c}(s)$ as Fourier series

$$\phi(s) = \sum_{n=1}^{\infty} a_n \sin(q_n s), \quad \bar{c}(s) = \sum_{n=1}^{\infty} \bar{c}_n \cos(q_n s), \quad c(s) = \sum_{n=1}^{\infty} c_n \cos(q_n s).$$

Note that to use a sine series for $\phi(s)$ is reasonable since $\phi_0=\phi(L)=0$. But in general $c(L) \neq 0$ so we cannot use sine series for it. We can also use the full Fourier series for $c(s)$ and $\bar{c}(s)$, but it is straightforward to show that the sine part in the full Fourier series make no contribution at all so we disregard it. Using the orthogonality property of Fourier modes, we can re-express the energy and extension as

$$\mathcal{E} \approx \frac{k_c^2 L}{2} + \frac{k_L}{4} \sum_{n=1}^{\infty} (a_n^2 + q_n^2 \bar{c}_n^2) + \frac{fL}{4} \sum_{n=1}^{\infty} a_n^2,$$

with

$$d_n = a_n - \frac{k_n q_n c_n}{k_n^2 q_n + f}, \quad \bar{c}_n = \bar{c}_n - \frac{k_n q_n c_n}{k_n^2 q_n + f}.$$

and

$$\mathcal{E} \approx \int_0^L \cos \phi ds \approx L \left[ 1 - \frac{1}{2} \sum_{n=1}^{\infty} d_n^2 \right] + \frac{fL}{4} \sum_{n=1}^{\infty} a_n^2,$$

where

$$\begin{align*}
\langle x_1 \rangle &= L \left( 1 - \frac{1}{2} \sum_{n=1}^{\infty} d_n^2 \right), \\
\langle x_2 \rangle &= L \left( 1 - \frac{1}{2} \sum_{n=1}^{\infty} d_n^2 \right) - \frac{fL}{4} \sum_{n=1}^{\infty} a_n^2.
\end{align*}$$

From Eqs. (4) and (34)–(38), we see that in the thermal-first system $\langle x \rangle = \langle x_1 \rangle + \langle x_2 \rangle$. $\langle x_1 \rangle$ is independent of $c(s)$, and we recover the well-known result for the WLC model [22,32,38],

$$\frac{\langle x_1 \rangle}{L} = 1 - \frac{1}{2\sqrt{fL}}.$$

In contrast, $x_2$ is independent of $\phi(s)$ and is determined by $c(s)$. Rewriting $W(c(s))$ as

$$W(c(s)) = e^{-\alpha L \left[ c_0 - c_0^2 + 1/2 \sum_{n=1}^{\infty} (c_n - \bar{c}_n)^2 \right]},$$

we obtain

$$\langle x_2 \rangle = \frac{L}{4} \sum_{n=1}^{\infty} \frac{(kq_n)^2}{(kq_n^2 + f)^2} \left( \bar{c}_n^2 + \frac{2}{\alpha L} \right),$$

On the other hand, replacing $k$ and $c_n$ by $\kappa$ and $\bar{c}_n$, respectively, in Eqs. (34)–(38), we find that in the disorder-first system the extension becomes

$$\langle x \rangle' = \langle x \rangle + \frac{x_2}{L} = 1 - \frac{1}{2\sqrt{f_{\text{eff}} L}} + \frac{x_2}{L}.$$
find an “equivalent system” with the effective energy $\mathcal{H}_0$.

On the other hand, the thermal-first average for the constant-extension ensemble can be written

$$B = \frac{1}{Z_e} \int \mathcal{D}[\{\phi\}] W(\{\phi\}) B_e,$$

$$B_e = \frac{1}{Z_e} \int \mathcal{D}[\{\phi\}] B[\{\phi\}] \delta(r_L - \mathbf{b}) e^{-\mathcal{H}_0}.$$  

From Eq. (44), we find that due to the existence of the $\delta(r_L - \mathbf{b})$ term, $Z_e$ is in general dependent on $c(s)$, so that an exchange in the order of integration cannot simplify the expression for $B$. In other words, the existence of an “equivalent system” for the thermal-first system in the constant-extension ensemble is still an open question. From our experience in the constant-force ensemble, such an “equivalent system” does not exist.

Our discussions in this section can be directly generalized to the three-dimensional system, so it completes and reassess the results of our previous work [8].

VI. CONCLUSIONS AND DISCUSSIONS

In summary, we present a rigorous proof that when free of external force, a 2D semiflexible biopolymer without correlation or with SRC in intrinsic curvatures $c(s)$ is equivalent to a system with a well-defined intrinsic curvature and a renormalized persistence length. We obtain exact expressions for the distribution function of the equivalent system. These conclusions can simplify theoretical studies of semiflexible biopolymers, since the disorder in $c(s)$ is completely removed in the equivalent system. For the system under external force, we find that the effect of sequence disorder is dependent on the order in which the averaging is done or the experimental conditions. In the disorder-first system, it is always possible to find an “equivalent system,” no matter the external force, the length of the polymer, the statistical ensemble or the dimension of the system. However, in the thermal-first system, there is in general no “equivalent system” for a biopolymer up to moderate length. Physically, this is because in the thermal-first system the intrinsic curvatures favor defects such as kinks, buckles and loops. To straighten these defects costs extra energy and therefore requires a larger force. In contrast, the disorder-first system erases these extra defects before the application of the force. We find the closed-form expression for the force-extension relationship for the elasticity of a long biopolymer under a strong stretching force. In the thermal-first system, we show exactly that in this case sequence disorder is immaterial even if the biopolymer has a nonvanishing mean intrinsic curvature. Moreover, we find that in the thermal-first system, the results are also dependent on the boundary conditions, and the sequence-dependent effects are much more serious in the case of free BCs than for fixed BCs. Meanwhile, the results are dependent on the degree of randomness and the larger the randomness, the more serious the effect. Our results suggest that the short biopolymer may be much softer so has a smaller apparent persistent length than what the “equivalent system” in
a mechanical experiment would predict. This fact implies that in experiments the interaction between experimental apparatus and polymer, though may be weak, may affect the results seriously for a short polymer. Furthermore, our results suggest that the effects of sequence disorder is dependent upon the quantity measured and how it is measured. We should note that due to the existence of an “equivalent system,” the disorder-first system is much simpler in theoretical studies. However, it is difficult to realize the disorder-first system in experiment.

On the other hand, we considered weak forces and large forces but not intermediate size forces in this work, but we can expect that in this case there will also not be an “equivalent system” even for a long polymer since this is the case for the system under a large force. How the elasticity of a system goes from an “equivalent system” when free of force to a disorder-free system under a large force would be an important question to address. We also do not consider the system with LRC in $c(s)$, which deserves further investigation.

It should also be noted that this work focused on 2D systems. However, whether the results apply to 3D systems is an intriguing question. Mathematically we should reach similar conclusions since in the thermal-first system exchanging the order of integration does not simplify the problem. However, physically there exist some fundamental distinctions between the 3D case and the 2D case. At first, the much stronger fluctuations in the 3D system may dominate the intrinsic disorder so the effect may be suppressed. This would explain why the disorder in $c(s)$ has a much smaller effect on the end-to-end distance than on the extension. Moreover, the geometry of a polymer with natural curvature is also very different in the 2D and 3D systems. For example, the looped configuration in the 2D system cannot undergo an out-of-plane buckling that would eliminate loops, but a 3D polymer will exhibit this behavior. Furthermore, in the 2D case it is much easier to form large defects which would be responsible for a larger decrease in extension. Therefore, the difference in the thermal-first or disorder-first ordering may be reduced in a 3D system. But finally let us point out that the studies of the conformations of biopolymers are often performed in a 2D environment (e.g., see [7,29]), so our main findings should be instructive.

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APPENDIX A: PROOF OF EQ. (5)

Using the standard path integral methods [30], for arbitrary function $F(\{\phi(s)\})$, we can write

$$\int D[\phi(s)]F(\{\phi(s)\}) \cong \lim_{N \to \infty} \prod_{j=1}^{N-1} \int d\phi_j F(\{\phi_j\}), \quad (A1)$$

where $\epsilon = L/N$, $\phi_j = \phi((j-1)\epsilon)$ is the discretized $\phi(s)$, $\xi_j = \phi_j - \phi_{j-1}$, and $\phi$ in $B$ and $E$ must be replaced by $(\phi_{j+1} - \phi_j)/\epsilon$. The Jacobian determinant, $J = |\partial \xi/\partial \phi|$, of $\xi_j$'s with respect to $\phi$'s is a constant, therefore

$$\int D[\phi(s)]F(\{\phi(s)\}) \cong \lim_{N \to \infty} \prod_{j=1}^{N-1} \int d\phi_j F(\{\phi_j\}). \quad (A2)$$

Now taking $F = B(\{\phi(s)\})e^{-\epsilon}$ or $e^{-\epsilon}$, from Eq. (A3) we obtain Eq. (5).

$$\int D[\phi(s)]B(\{\phi(s)\})e^{-\epsilon} = \int D[\phi(s)]e^{-\epsilon}. \quad (A3)$$

Intuitively, both sides in the above equation are averages over all possible configurations so they are expected to be equivalent.

APPENDIX B: A DIRECT DERIVATION OF EQ. (16)

In this appendix, we will use the standard path integral method [30] to derive Eq. (16) since it is useful. To account the more general case of $s_0 \neq 0$, we rewrite $H_0$ as

$$H_0 = \frac{1}{2} \int_0^L \kappa^2(\phi(s) - \tilde{c}(s))^2 ds. \quad (B1)$$

For large $N$, the path integral can be approximated as

$$Z_{H_0}^\infty = C \prod_{j=1}^{N-1} \int d\phi_j \exp \left\{-\frac{\epsilon}{2} \sum_{j=0}^{N-1} \kappa_j \left[ \frac{\phi_{j+1} - \phi_j}{\epsilon} - \tilde{c}_j \right]^2 \right\} \quad (B2)$$

$$= C \prod_{j=1}^{N-1} \int d\phi_j \exp \left\{-\frac{1}{2} \sum_{j=0}^{N-1} \kappa_j \left[ \phi_{j+1} - \phi_j - \tilde{c}_j \right]^2 \right\}.$$

where $C$ is a constant, $\epsilon = (L-s_0)/N$, $\phi_j = \phi(s_0 + (j-1)\epsilon)$, $\kappa_j = \kappa(s_0 + (j-1)\epsilon)$ and $\tilde{c}_j = \tilde{c}(s_0 + (j-1)\epsilon)$ are discretized $\phi(s)$, $\kappa(s)$ and $\tilde{c}(s)$, respectively, and $\phi$ in $H_0$ is replaced by $(\phi_{j+1} - \phi_j)/\epsilon$. Now using the identity

$$\int_{-\infty}^{\infty} dx e^{-a(x-x_1)^2 - b(x-x_2)^2} = \sqrt{\frac{\pi}{a+b}} \exp \left\{-\frac{1}{a+b} (x_1-x_2)^2 \right\}. \quad (B3)$$

we obtain

$$Z_{H_0}^\infty \approx \sqrt{\frac{2\pi \epsilon}{\kappa_0 + \kappa_1}} \int d\phi_2 d\phi_3 \cdots d\phi_{N-1} \times \exp \left\{-\frac{1}{2\epsilon} \sum_{j=2}^{N-1} \kappa_j \left[ \phi_{j+1} - \phi_j - \tilde{c}_j \right]^2 \right\} \times \exp \left\{-\frac{1}{2\epsilon} \kappa_0 + \kappa_1 + \frac{\epsilon}{\kappa_0 + \kappa_1} \left[ \phi_2 - \phi_0 - (\tilde{c}_0 + \tilde{c}_1) \right]^2 \right\}.$$
\[ B = \frac{1}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] e^F \left[ \int \mathcal{D}[c] \frac{1}{Z_k} W(c) e^{-E_0} \right] \]

\[ = \frac{1}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] e^F \left[ \int \mathcal{D}[c] W(c) (1 - f) e^{-E_0} \right] \]

\[ = B_1 - B_2, \quad (C2) \]

where

\[ Q = \int_0^L ds \langle \cos \phi(s) \rangle, \quad F = f \int_0^L \cos \phi ds, \quad (C3) \]

\[ B_1 = \frac{1}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] e^F \left[ \int \mathcal{D}[c] W(c) e^{-E_0} \right] \]

\[ = \frac{1}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] e^{E_0} \]

\[ = \langle B \rangle_k + f \int_0^L ds \langle \mathbb{B}[\{\phi(s)\}] \cos \phi(s') \rangle, \quad (C4) \]

\[ B_2 = \frac{f}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] e^F R \]

\[ = \frac{f}{Z_k} \int \mathcal{D}[\phi] \mathbb{B}[\{\phi\}] R, \quad (C5) \]

\[ R = \int \mathcal{D}[c] W(c) Q e^{-E_0}, \quad (C6) \]

and \( \langle \ldots \rangle_k \) denotes the ensemble average with energy \( E_0 \)

\[ \langle \ldots \rangle_k = \frac{1}{Z_k} \int \mathcal{D}[\phi(s)] (\ldots) e^{-E_0}. \quad (C7) \]

Furthermore,

\[ \mathcal{R} = \int_0^L ds' \left[ \int \mathcal{D}[c] W(c) e^{-E_0[\phi(s')]} \right] \frac{1}{Z_k} \int \mathcal{D}[\phi'] \cos[\phi'(s')] e^{-E_0[\phi'(s)']} \]

\[ = \int_0^L ds' \left[ \mathcal{D}[\phi'] \cos[\phi'(s')] \right] \int \mathcal{D}[c] W(c) e^{-E_0[\phi(s')]} \]

\[ = G \int_0^L ds' \left[ \mathcal{D}[\phi'] \cos[\phi'(s')] \right] \int \mathcal{D}[c] W(c) e^{-E_0[\phi(s')]} \]

\[ = \frac{Z_k}{Z_k} e^{-E_0} \int_0^L ds' \left[ \mathcal{D}[\phi'] \cos[\phi'(s')] \right] \int \mathcal{D}[c] W(c) e^{-E_0[\phi(s')]} \]

\[ = \frac{Z_k}{Z_k} e^{-E_0} \int_0^L ds' \left[ e^{-E_0[\phi'(s')]/2} \cos[\phi'(s')] + \phi_0 \right], \quad (C8) \]

where

\[ 061911-9 \]
\[ k(s) = \frac{k(\alpha + k)}{\alpha + 2k}, \quad \dot{\gamma}(s) = \frac{k\dot{\phi} + \alpha c}{\alpha + k}, \quad \gamma(s) = \int_0^s \dot{\gamma}(s) ds, \]
\[ G = \int [D(c) e^{-1/2d(2k+\alpha)c^2}] ds/k'(s), \quad A'(s,s_0) = \int_{s_0}^s ds/k'(s), \]
\[ \gamma(s) = \int_0^s \dot{\gamma}(s) ds, \]
\[ (C9) \]

and we have used an expression similar to Eq. (16) in the last two lines in Eq. (C8) to transform the path integral into simple integral. \( \gamma(s) \) is in general dependent on \( \phi(s) \) and it makes the expression complex. Now the Eq. (C5) can be reduced into
\[ B_2 = \frac{f}{2\pi \hbar} \int [D(\phi) B\{\{\phi(s)\}\}] e^{-\gamma_0} \]
\[ = \int_0^L ds' e^{-A'(s',0)/2} \cos[\gamma(s') + \phi_0] \]
\[ = \int_0^L ds' e^{-A'(s',0)/2} \{B\{\phi(s)\}\} \cos[\gamma(s') + \phi_0] \}
\[ (C10) \]

where \( \phi_0 = \phi(0) \). Equations (C4) and (C10) are exactly the same as Eqs. (19) and (20).

**APPENDIX D: CALCULATIONS OF THE EXTENSION**

In this case \( B\{\{\phi(s)\}\} \) corresponds to \( \cos \phi(s) \), and so from Eqs. (19) and (20), we obtain
\[ X = \langle x \rangle - \langle x \rangle_{f=0} \]
\[ = \int_0^L ds \langle \cos \phi(s) \rangle - \int_0^L ds \langle \cos \phi(s) \rangle_{f=0} \]
\[ = \int_0^L ds \int_0^L ds' \langle \cos \phi(s) \cos \phi(s') \rangle \]
\[ - e^{-s'/2k} \langle \cos \phi(s) \rangle \cos [\gamma(s') + \phi_0] \} \]
\[ (D1) \]

Note that Eq. (16) is valid only if \( s > s_0 \). Therefore, the integral for \( s' \) in Eq. (D1) should be divided into two parts, one is from 0 to \( s \) and the other is from \( s \) to \( L \). When \( s > s' \), we have
\[ \langle \cos \phi(s) \cos \phi(s') \rangle \}
\[ = \int_{-\infty}^\infty d\phi d\phi' P(\phi,s';\phi',s') \cos \phi \cos \phi' P(\phi',s';\phi_0,0) \]
\[ = e^{(-s'/2k)} \int_{-\infty}^\infty d\phi \cos^2 \phi' \cos \phi' P(\phi',s';\phi_0,0) \]
\[ = \frac{1}{2} e^{(-s'/2k)} \int_{-\infty}^\infty \cos(2\phi_0) \]
\[ (D2) \]

and
\[ \langle \cos \phi(s) \cos [\gamma(s') + \phi_0] \rangle \}
\[ = \int_{-\infty}^\infty d\phi d\phi' P(\phi,s';\phi',s') \cos \phi \cos \phi' P(\phi',s';\phi_0,0) \]
\[ \times \cos [\kappa(\phi' - \phi_0)/\alpha + \phi_0] P(\phi',s';\phi_0,0) \]
\[ = e^{-i(s'/\alpha)k} \int_{-\infty}^\infty d\phi \cos^2 \phi \cos (\kappa(\phi' - \phi_0)/\alpha + \phi_0) \]
\[ \times P(\phi',s';\phi_0,0) \]
\[ = \frac{1}{2} e^{(-s'/\alpha)k} [1 + e^{-2s'/\alpha} \cos(2\phi_0) + e^{2s'/\alpha}] \]
\[ (D3) \]

When \( s < s' \), we obtain
\[ \langle \cos \phi(s) \cos \phi(s') \rangle \}
\[ = \int_{-\infty}^\infty d\phi d\phi' P(\phi',s';\phi,s) \cos \phi \cos \phi' P(\phi,s';\phi_0,0) \]
\[ = e^{-i(s'/\alpha)k} \int_{-\infty}^\infty d\phi \cos^2 \phi \cos \phi' \cos \phi P(\phi,s';\phi_0,0) \]
\[ = \frac{1}{2} e^{i(s'/\alpha)k} [1 + e^{-2s'/\alpha} \cos(2\phi_0) + e^{2s'/\alpha}] \]
\[ (D4) \]

It follows
\[ X = 2k \left[ \frac{k(k + 3\alpha)}{k + \alpha} + \frac{k(k + \alpha)}{\alpha} + \frac{4\kappa\alpha}{k - \alpha} - \frac{\kappa^2 \cos(2\phi_0) e^{-2L/k}}{3(2k + \alpha)(3k + \alpha)} \right] \]
\[ = 6k^2 (e^{L/k} - 1) + k\alpha(9e^{2L/k} - 16e^{3L/k} + 12e^{L/k} - 5) \]
\[ + \alpha^2 (3e^{2L/k} - 8e^{3L/k} + 6e^{L/k} - 1) \]
\[ (D6) \]

In the limit \( \alpha \to k \), \( X \) is still finite and
\[ \langle \cos \phi(s) \cos [\gamma(s') + \phi_0] \rangle \}
\[ = 2k \left[ L - k(k + 3\alpha)/k + k(k + \alpha)/\alpha - \frac{4\kappa\alpha}{k - \alpha} - \frac{\kappa^2 \cos(2\phi_0) e^{-2L/k}}{3(2k + \alpha)(3k + \alpha)} \right] \]
\[ (D6) \]

**On the other hand, in disorder-first system,**
\[ X' = \langle x' \rangle - \langle x' \rangle_{f=0} \]
\[ = \int_{0}^{L} ds \langle \cos \phi(s) \rangle' - \int_{0}^{L} \langle \cos \phi(s) \rangle_{\kappa} \]
\[ = \int_{0}^{L} ds \int_{0}^{L} \langle \cos \phi(s) \rangle_{\kappa} \]
\[ - \left[ \int_{0}^{L} ds \langle \cos \phi(s) \rangle_{\kappa} \right]^{2} \frac{\kappa^{2} f}{3} \left( e^{-2L/\kappa} - 6e^{-L/\kappa} + 8e^{-L/2\kappa} - 3 \cos(2\phi_{0}) \right). \]
\[ = 2\kappa f \left[ L + \kappa - \kappa(e^{-L/2\kappa} - 2)^{2} \right] + \frac{\kappa^{2} f}{3} \left( e^{-2L/\kappa} - 6e^{-L/\kappa} + 8e^{-L/2\kappa} - 3 \cos(2\phi_{0}) \right). \]
\[ \text{(D8)} \]

When \( \alpha \to \infty \), it is clearly that \( X \to X' \).

**APPENDIX E: CALCULATIONS OF THE ORIENTATIONAL CORRELATION FUNCTION AND THE END-TO-END DISTANCE**

In this case, \( B_{1}[\phi] = \mathbf{t}(s) \cdot \mathbf{t}(s') = \cos[\phi(s) - \phi(s')] \). From Eqs. (18)–(22), we obtain
\[ \langle \mathbf{t}(s) \cdot \mathbf{t}(s') \rangle = \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \frac{1}{2} \left[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} + \langle \gamma(s') \rangle_{\kappa} \right] \]
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} = \frac{1}{2} e^{-L/\kappa}. \]  
\[ \text{(E1)} \]

The first term in above equation is simple, as
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \int_{-\infty}^{\infty} d\phi d\phi' P(\phi,s'; \phi',s') \cos(\phi - \phi') P(\phi',s'; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma. \]  
\[ \text{(E2)} \]

Again, due to that Eq. (16) is valid only if \( s > s_{0} \), the integral for \( s'' \) in Eq. (E1) should be divided into several parts. If \( s > s' > s'' \), we have
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \int_{-\infty}^{\infty} d\phi d\phi' d\phi'' P(\phi,s'; \phi',s''; \phi'',s') P(\phi',s''; \phi'',s'') \]
\[ \times \cos(\phi - \phi') \cos(\phi' - \phi'') \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \int_{-\infty}^{\infty} d\phi'' \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \cos(\phi_{0}). \]  
\[ \text{(E3)} \]

If \( s > s'' > s' \), we obtain
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \int_{-\infty}^{\infty} d\phi d\phi' d\phi'' P(\phi,s'; \phi'',s'') P(\phi'',s''; \phi',s') \cos(\phi - \phi') \cos(\phi' - \phi'') \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi',s'; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \int_{-\infty}^{\infty} d\phi'' \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \cos(\phi_{0} + \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \cos(2\phi_{0}). \]  
\[ \text{(E4)} \]

If \( s'' > s > s' \), we find
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \int_{-\infty}^{\infty} d\phi d\phi' d\phi'' P(\phi,s'; \phi',s') P(\phi',s'; \phi'') \cos(\phi - \phi') \cos(\phi' - \phi'') \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \int_{-\infty}^{\infty} d\phi'' \cos(\phi'' - \phi_{0}) \alpha + \phi_{0}) P(\phi'',s''; \phi_{0},0) \]
\[ = e^{-L/\kappa} \gamma \cos(\phi_{0}) \cos(\phi_{0}). \]  
\[ \text{(E5)} \]

Similarly, if \( s > s'' > s' \), then
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = e^{-L/\kappa} \gamma \cos(\phi_{0}). \]  
\[ \text{(E6)} \]

If \( s'' > s > s' \), then
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = e^{-L/\kappa} \gamma \cos(\phi_{0}). \]  
\[ \text{(E7)} \]

If \( s'' > s > s' \), then
\[ \langle \cos[\phi(s) - \phi(s')] \rangle_{\kappa} \]
\[ = \frac{1}{2} e^{-L/\kappa} \gamma \cos(\phi_{0}). \]  
\[ \text{(E8)} \]
Combining Eqs. (E1) and (E2), we finally obtain for $s > s'$

$$\langle t(s) \cdot t(s') \rangle = e^{-(s-s')/2k} + \frac{\kappa \cos \phi_0 f}{3(3k + \alpha)(k - \alpha)} S,$$

$$S = -6k(k - \alpha)e^{-(2(\alpha+2k) + (\alpha+3l)')/2\kappa} + 8\alpha(2k + \alpha)e^{-2\kappa/2k} - 6k(3k + \alpha)e^{-2\kappa/2k} + (k - \alpha)(3k + \alpha)
\times [3e^{-(\alpha+3l')/2\kappa} - 3e^{-(L+3(s'-l)/2k}) + 6e^{-(s'/2k)} - 3e^{-(L+s'-l)/2k}]
\times 2e^{-(4s - 3s')/2k} + 3e^{-(\alpha+3l'+(\alpha-k)(s'-l)/2\kappa)}].$$

(E9)

$$\langle t(s) \cdot t(s') \rangle'$$ is also finite when $\alpha \rightarrow k$ because in this case,

$$\langle t(s) \cdot t(s') \rangle = e^{-(s-s')/2k} + \frac{13}{6} e^{-2s'/k} + \frac{1}{2} e^{-2(s+s')/k} + e^{-2L(s-l)/k}
\times \frac{2}{3} e^{-(4s - 3s')/k} + e^{-(L+3(s'-l)/k)} + \frac{s'-s}{k} e^{-s'/k}.$$  

(E10)

In contrast,

$$\langle t(s) \cdot t(s') \rangle' = \langle \cos[\phi(s) - \phi(s')] \rangle_k
+ \int_0^L ds'' \langle \cos[\phi(s) - \phi(s')] \cos[ \phi(s'')] \rangle_k
- \langle \cos[\phi(s) - \phi(s')] \rangle_k \int_0^L ds'' \langle \cos[\phi(s'')] \rangle_k
= e^{-(s-s')/2k} + \int_0^L ds'' \langle \cos[\phi(s) - \phi(s'')] \rangle
\times \cos[\phi(s'')] - 2\kappa f \cos \phi_0 e^{-(s-s')/2k}
\times \left(1 - e^{-L/2\kappa} \right)
= e^{-(s-s')/2k} + \frac{1}{3} \kappa f \cos \phi_0 (6e^{-s'/2k} - 8e^{-s'/2k}).$$

When $\alpha \rightarrow \infty$, we obtain $\langle t(s) \cdot t(s') \rangle \rightarrow \langle t(s) \cdot t(s') \rangle'$. The end-to-end distance can be found by

$$R^2 = \int_0^L ds \int_0^L ds' \langle t(s) \cdot t(s') \rangle'$$

$$= 2 \int_0^L ds \int_0^L ds' \langle \cos[\phi(s) - \phi(s')] \rangle_k$$

$$= 4\kappa L \left[ 1 - \frac{2\kappa}{L} (1 - e^{-L/2\kappa}) \right]$$

$$+ \frac{4\kappa^2 \cos \phi_0 f}{9(k - \alpha)^2(k + \alpha)(2k + \alpha)(3k + \alpha)^2}.$$  

(E12)

$$R^2 = 18(k - \alpha)^2(k + \alpha)(2k + \alpha)(3k + \alpha)^2L - 9(k - \alpha)^2
\times (3k + \alpha)^2(4k^2 + 122k + 16\alpha^2(2k + \alpha)^2[3(k - \alpha)]
\times (k + \alpha)(3k + \alpha) + 4k^2a^2(5k + \alpha)(3k - \alpha)e^{-L/2\kappa} + 18\kappa a
\times (k + \alpha)^3(k - \alpha)^2e^{-(1/2)\kappa} + 18(k + \alpha)^2(2k + \alpha)
\times (3k + \alpha)^2e^{-L/2\kappa} - \kappa(\alpha)(2k + \alpha)(3k + \alpha)^2e^{-2L/2\kappa}.$$  

(E13)

when $\alpha \rightarrow k$,

$$R^2 = 2KL \left[ 1 - \frac{k}{L} (1 - e^{-L/2\kappa}) \right] + \frac{k \cos \phi_0 f}{18} [36KL - 11k^2
+ (18L^2 + 78kL + 109k^2)e^{-L/2k} + 3k^3e^{-3L/2k} - k^2e^{-4L/2k}]$$

(E14)

On the other hand

$$R^2 = 4\kappa L \left[ 1 - \frac{2\kappa}{L} (1 - e^{-L/2k}) \right] + \frac{1}{9} \kappa^2 \cos \phi_0 f [18L - 99k
+ 16(3L + 4\kappa)e^{-L/2k} + 36\kappa e^{-2L/2k} - \kappa e^{-2L/2k}].$$

(E15)

When $\alpha \rightarrow \infty$, we obtain $R^2 \rightarrow R^2$. 

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