Mechanical Properties of an Intrinsically Curved Semiflexible Biopolymer in Two Dimensions

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We compare the mechanical properties of two elastic models for a two-dimensional intrinsically curved semiflexible biopolymer. Model 1 allows a signed curvature and the model 2 allows a positive definite curvature only. We show exactly that these two models have different ground states. We discretize both models and use the Monte Carlo method to simulate the models, and find that they have also different mechanical properties at finite temperature. Under the same force and with the same intrinsic curvature and bending rigidity, the extension of model 1 is smaller than that of model 2 at low force, but becomes larger at large force. Moreover, the extension of model 1 undergoes a discontinuous transition when the intrinsic curvature is sufficient large, but the extension of model 2 is always a smooth concave function of the force, so that there is no phase transition. The difference between the two models is due to the fact that under an external force model 2 disfavors looped configurations and favors the configurations with moderate extensions.

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I. INTRODUCTION

Semiflexible biopolymers, such as the double-stranded DNA (dsDNA), actin, microtubule, etc., are fundamentally important in life. The term “semiflexible” means that to bend it subjects one to an energy penalty. Consequently, the response of a semiflexible biopolymer to an external force is a very important issue for the understanding of the structure and function of bio-matrlals [1–18]. A well known example is that the translation and transcription of the genetic codes require the straightening and untwisting of a dsDNA. To have a full understanding of the properties of biopolymers, it requires a comparison between experiment and theory. Recent progresses in experimental techniques have provided powerful tools for manipulating a single biomolecule, so they make it possible to compare directly the theoretical predictions and the experimental observations. In theoretical studies, a semiflexible biopolymer is often modeled as an elastic filament. The simplest model for a semiflexible biopolymer is the wormlike chain (WLC) model, which views a biopolymer as an inextensible chain with a uniform bending rigidity but a negligible cross section. The WLC model has successfully described the entropic elasticity of some dsDNA [1–5]. A WLC is intrinsically straight, i.e., its ground state configuration is

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a straight line or its intrinsic curvature is zero. It follows that at a finite temperature the extension of the model is a smooth concave function of the applied force. However, semiflexible biopolymers are not always intrinsically straight, so that the WLC model fails to account for the properties of these biopolymers [6–10]. Especially, it has been reported that a nonvanishing intrinsic curvature can induce a discontinuous transition in the extension of either three-dimensional (3D) [11–14] or two-dimensional (2D) [15] filaments, so this is completely different from the results of the WLC model. However, we have to point out that there are two elastic models for the 2D intrinsically curved filaments [10, 16, 19, 20]. The difference between the two models is in the bending energies, by using a signed curvature or a positive definite curvature, respectively. These two models are sometimes regarded as the same one [19]. Since many experiments for semiflexible biopolymers are performed in a 2D environment [10, 20–27], and in general different models have different physical properties, and so are appropriate to describe different kinds of materials, whether these two models have really the same mechanical property is therefore an intriguing issue which needs to be clarified. In this work, we study and compare the mechanical property of these two models, and show exactly that their ground state configurations (GSCs) are different. Moreover, using Monte-carlo simulation, we find that at a finite temperature these two models still have very different mechanical properties. Especially, we find that the extension of model 1 can undergo a discontinuous transition when the intrinsic curvature is sufficient large, but the extension of model 2 is always a smooth concave function of the force, so that there is no phase transition.

The paper is organized as follows. In Sect. II, we describe our models. In Sect. III, we compare the GSCs of the two models. In Sect. IV, we present the results at a finite temperature. The main text ends with conclusions and discussions.

II. MODELS

II-1. Continuous models

In the 2D case, the configuration of a filament is determined by its tangent vector, 
\[ \mathbf{t} = \frac{d\mathbf{r}}{ds} = \{\cos \phi, \sin \phi\}, \]
to its contour line, where \( \mathbf{r} = (x, y) \) is the locus of the filament, \( s \) is the arclength and the orientational angle \( \phi(s) \) is the angle between the \( x \)-axis and \( \mathbf{t} \), as shown in Fig. 1. One end of the chain (at \( s = 0 \)) is fixed at \( x = y = 0 \). There are two elastic models for a 2D intrinsically curved filament [10, 16, 19, 20]. Applying a uniaxial force (along the \( x \) axis) \( F_x \) to another end at \( s = L \), the elastic energy of model 1 is [10, 16, 20]

\[
E_1 = \frac{k}{2} \int_0^L d\phi (\dot{\phi} - \tilde{c})^2 - F_x x_L \\
= \frac{k}{2} \int_0^L d\phi (\dot{\phi} - \tilde{c})^2 - F_x \int_0^L \cos \phi ds,
\]

where \( k \) is the bending rigidity, \( L \) is the contour length and it is a constant so that the filament is inextensible, \( \dot{\phi} \equiv \dot{x} \dot{y} - \dot{y} \dot{x} \) is the signed curvature, \( \tilde{c} \) is the intrinsic signed
curvature, \( x_L \equiv x(L) \) is the extension. \( \dot{c} \neq 0 \) means that when \( F_x = 0 \), the GSC (or the spontaneous configuration, i.e., the configuration with the lowest energy) of the filament is a curve of curvature \( \dot{c} \). The symbol “\( \cdot \)” represents the derivative with respect to \( s \). \( \dot{c} \) can be \( s \)-dependent, but for simplicity, in this work we consider only a \( s \)-independent or constant \( \dot{c} \). Without loss of generality we also assume \( F_x > 0 \). In this model, both \( \dot{\phi}(s) \) and \( \dot{c}(s) \) can be either positive or negative. It is straightforward to find \( |\dot{\phi}| = |\dot{t}| \). We also define \( |\dot{\phi}| \equiv |d\phi/ds| \) instead of \( d|\phi|/ds \), and similarly for \( |\dot{t}| \). This is a natural choice since \( d|\dot{t}|/ds = 0 \) owing to \( |\dot{t}| = 1 \). When \( \dot{c} = 0 \), it reduces to the WLC model.

\[
\begin{align*}
E_2 &= \frac{k}{2} \int_0^L ds \left[ |\dot{t}(s)| - |\dot{c}(s)| \right]^2 - \int_0^L ds F_x \cdot t(s) \\
&= \frac{k}{2} \int_0^L ds (|\dot{\phi}| - \dot{c})^2 - F_x \int_0^L \cos \phi ds.
\end{align*}
\]

When \( \dot{c} = 0 \), it also reduces into the WLC model. In this model, the curvature, \( |\dot{\phi}| \), is positive definite.

The first term on the right hand side of Eqs. (1)–(2) is referred to as the bending energy, and it also gives the essential difference between these two models. We should also point out that the both models require that \( \phi \) be continuous, i.e., there is no cusp or kink in the filament, to prohibit an infinite \( \dot{\phi} \) and thus an infinite energy. It is required to add extra terms in the energy should we want to consider a cusp or kink.

II-2. Discrete models

It does not seem to be possible to find a closed-from solution for the both models at \( T > 0 \) and under an arbitrary force, so we discretize them and perform Monte Carlo simulation to study them. In the discrete model, the filament consists of \( N \) perfectly straight segments of length \( l_0 \), and joined end by end, as shown in Fig. 2. Label the position vector of the end of \( i \)'s segment as \( r_i \), the direction of the \( i \)'s segment is determined by the unit
vector \( t_i = (r_{i+1} - r_i)/l_0 \). The total length of the chain is \( L = Nl_0 \) and

\[
x_L \equiv x_N = l_0 \sum_{i=1}^{N} t_{ix} = l_0 \sum_{i=1}^{N} \cos \phi_i.
\]

\( (3) \)

![FIG. 2: Schematic diagram of the discrete model.](image)

Replacing \( \dot{\phi} \) by \( (\phi_{i+1} - \phi_i)/l_0 \), we can rewrite \( E_1 \) as

\[
E_1 = k \frac{N-1}{2l_0} \sum_{i=1}^{N-1} (\phi_{i+1} - \phi_i - \bar{c}l_0)^2 - F_x x_N.
\]

\( (4) \)

For convenience, in simulation we introduce the reduced energy of model 1:

\[
\mathcal{E}_1 \equiv \frac{E_1}{k_B T} = \frac{\kappa}{2} \sum_{i=1}^{N-1} (\phi_{i+1} - \phi_i - c)^2 - f x_N / l_0,
\]

\( (5) \)

where \( k_B \) is the Boltzmann constant, \( T \) is the temperature, \( c \equiv \bar{c}l_0 \), \( \kappa \equiv k/l_0k_B T \), and \( f \equiv F_x l_0/k_B T \). Correspondingly, the reduced energy of model 2 becomes

\[
\mathcal{E}_2 \equiv \frac{E_2}{k_B T} = \frac{\kappa}{2} \sum_{i=1}^{N-1} (|\phi_{i+1} - \phi_i| - c)^2 - f x_N / l_0.
\]

\( (6) \)

The relative extension is defined as \( z_N = \langle x_N \rangle / L \), where \( \langle \cdots \rangle \) denotes the configurational or thermal average.

**III. ON THE GROUND STATES**

The ground state is the state with the lowest energy, it is also the stable state of the system at zero temperature.

**III-1. Shape equations**

When \( \tilde{c} < 0 \), we have \( |\dot{\mathbf{t}}(s)| - \tilde{c} = |\dot{\mathbf{t}}(s)| + |\tilde{c}| > 0 \), and it reaches the minimum value when \( \dot{\mathbf{t}}(s) = 0 \) or \( \phi(s) \) is a \( s \)-independent constant. Meanwhile, when \( F_x > 0 \), \( -F_x \cos(\phi) \) reaches the minimum value when \( \phi = 0 \). Therefore, from Eq. (2), we find that when \( \tilde{c} < 0 \)
and $F_x > 0$, the GSC of model 2 is always a straight line with $\phi(s) = 0$ and a minimum energy $1/2kL\tilde{c}^2 - F_xL$, instead of a curve with a curvature $\tilde{c}$. Therefore, in model 2, exactly $\tilde{c}$ is no longer an intrinsic curvature when $\tilde{c} < 0$ since it does not affect the GSC. Meanwhile, in model 1, rotating a given configuration with locus $(x(s), y(s))$ $180^\circ$ around the $x$-axis, we obtain a new configuration with $x'(s) = x(s)$, $y'(s) = -y(s)$ and $\dot{\phi}'(s) = -\dot{\phi}(s)$. But this new configuration will have the same energy as the original one if we replace $\tilde{c}$ in $E_1$ by $-\tilde{c}$. Consequently, we do not need to study the case with $\tilde{c} < 0$ in model 1. Therefore, the case with $\tilde{c} < 0$ is less interesting for both models, so we do not consider this case henceforth.

Extremizing $E_1$, we obtain the shape equation, i.e., the equation that governs the configuration of the filament, for model 1

$$k\ddot{\phi} - F_x \sin \phi = 0. \quad (7)$$

The extremum in the energy also yields the free boundary condition (BC) or the hinged BC at $s = 0$ and $s = L$:

$$\dot{\phi}_0 - \tilde{c} = \dot{\phi}_L - \tilde{c} = 0, \quad (8)$$

where $\phi_0 = \phi(0)$ and $\phi_L = \phi(L)$. We do not consider other forms of BC in this work since we focus on a long filament so that the form of the BC is irrelevant. From Eqs. (7)–(8) we find [16]

$$\dot{\phi} = \sqrt{\tilde{c}^2 + F(\cos \phi_L - \cos \phi)}, \quad (9)$$

where $F = 2F_x/\kappa$.

From Eq. (9), we know that $\phi$ in model 1 is a monotonic function of $s$, but $x$ and $y$ can be periodic functions of $s$ [15, 16].

Replacing $\dot{\phi}$ by $|\dot{\phi}|$ in Eqs. (7)–(8), we find the shape equation for model 2, and the solution is in the form

$$|\dot{\phi}| = \sqrt{\tilde{c}^2 \pm F(\cos \phi_L - \cos \phi)}, \quad (10)$$

|\dot{\phi}_0| = |\dot{\phi}_L| = \tilde{c}. \quad (11)$$

We should take “+”(“−”) in Eq. (10) if $\dot{\phi} < 0$ ($\dot{\phi} > 0$). It follows that

$$s(\phi) = \mp \int_{\phi_0}^{\phi} \frac{dx}{\sqrt{\tilde{c}^2 \pm F(\cos \phi_L - \cos x)}}, \quad (12)$$

$$L = \mp \int_{\phi_0}^{\phi_L} \frac{dx}{\sqrt{\tilde{c}^2 \pm F(\cos \phi_L - \cos x)}}. \quad (13)$$

Clearly a solution of Eq. (9) is also a solution of Eq. (10). Therefore, one would expect that the two models had the same GSC. But this is not true. From Eq. (10), we see that $\phi$ in model 2 is not necessarily a monotonic function of $s$, but can shift between two branches with different signs. This is an essential difference between the two models and makes it be rather difficult to find an exact GSC for model 2, as we can see in the next two subsections.
For model 2, we should note that for an arbitrary solution of Eqs. (10)–(13), it is easy to find an infinite number of configurations which have different shapes but the same bending energy as the original one. These configurations can be obtained by rotating a part (with $s \geq s_T$ or $s \leq s_T$) of the given configuration $180^\circ$ around $t(s_T)$ at an arbitrary turning point with $s = s_T$. It is not difficult to show that such a rotation results in $\phi'(s) = 2\phi_T - \phi(s)$ so $\phi'(s) = -\phi(s)$, where $\phi'(s)$ is the orientational angle for the new configuration and $\phi_T = \phi(s_T)$. However, we should note that in general the new configurations are not solutions of Eqs. (10)–(13), except for $\phi_T = m\pi/2$ with $m$ being an integer. We will present some examples for such a rotation in the next subsections.

III-2. Free of external force

When $F_x = 0$ and with a fixed $\phi_0$, it is straightforward to find that the GSC of model 1 is unique and is a circle of radius $1/\tilde{c}$. In contrast, in this case a circle of radius $1/\tilde{c}$ is only one of GSCs of model 2, and we can find an infinite number of GSCs with different shapes by performing rotations mentioned in the last paragraph. An example is shown in Fig. 3, with $L = 2.7\pi$ and $\tilde{c} = 0.5$. Fig. 3 (a) is obtained from

$$x(s) = 2\sin(0.5s), \quad y(s) = 2[1 - \cos(0.5s)], \quad \dot{\phi} = 0.5.$$  

\[ \text{(14)} \]

![FIG. 3: Schematic pictures of some possible configurations of a force-free filament with $\dot{\phi}(s) = \pm 0.5$. $\dot{\phi}(s)$ changes sign at the turning points $P_1$, $P_2$, and $P_3$ in (b)–(d).}](image-url)

Rotating the segment with $s > 2L/3$ in Fig. 3 (a) $180^\circ$ around $t(2L/3)$ [dashed line...
in Fig. 3 (b) at point $P_1$, we obtain Fig. 3 (b), with

$$x = \begin{cases} 
2 \sin(0.5s), & s \leq 2L/3 \\
2\sin(0.5s - 2L/3) + 4\sin(L/3), & s > 2L/3
\end{cases} \tag{15}$$

$$y = \begin{cases} 
2[1 - \cos(0.5s)], & s \leq 2L/3 \\
2 + 2\cos(0.5s - 2L/3) - 4\cos(L/3), & s > 2L/3
\end{cases} \tag{16}$$

$$\dot{\phi} = \begin{cases} 
0.5, & s \leq 2L/3 \\
-0.5, & s > 2L/3.
\end{cases} \tag{17}$$

Furthermore, rotating the segment with $s > L/3$ in Fig. 3 (a) 180° around $t(L/3)$ [dashed line in Fig. 3 (c)] at point $P_2$, we obtain Fig. 3 (c), with

$$x = \begin{cases} 
2 \sin(0.5s), & s \leq L/3 \\
2\sin(0.5s - L/3) + 4\sin(L/6), & s > L/3
\end{cases} \tag{18}$$

$$y = \begin{cases} 
2[1 - \cos(0.5s)], & s \leq L/3 \\
2 + 2\cos(0.5s - L/3) - 4\cos(L/6), & s > L/3
\end{cases} \tag{19}$$

$$\dot{\phi} = \begin{cases} 
0.5, & s \leq L/3 \\
-0.5, & s > L/3.
\end{cases} \tag{20}$$

Finally, rotating the segment with $s > L/3$ in Fig. 3 (c) 180° around $t(2L/3)$ [dashed line in Fig. 3 (d)] at point $P_3$, we obtain Fig. 3 (d), with

$$x = \begin{cases} 
2 \sin(0.5s), & s \leq L/3 \\
2\sin(0.5s - L/3) + 4\sin(L/6), & s > L/3
\end{cases} \tag{21}$$

$$y = \begin{cases} 
2[1 - \cos(0.5s)], & s \leq L/3 \\
6 - 2\cos(0.5s - L/3) - 4\cos(L/6), & 2L/3 \geq s > L/3
\end{cases} \tag{22}$$

$$\dot{\phi} = \begin{cases} 
0.5, & s \leq L/3 \\
-0.5, & 2L/3 \geq s > L/3 \\
0.5, & s > 2L/3.
\end{cases} \tag{23}$$

All four configurations in the Fig. 3 are GSCs of model 2 because they all have continuous $\phi$ and $|\dot{\phi}| = 0.5$ and so have the same $E_2(= 0)$. But they have different $\dot{\phi}$ and so have different $E_1$, only the configuration in Fig. 3 (a) gives the GSC of model 1. Therefore, the GSCs of these two models are clearly very different when $F = 0$.

III-3. Under a finite force

The ground state of model 1 has been studied in detail [15, 16]. It is found exactly that $x$, $y$, and $E_1$ obtained from Eq. (9) are multiple-valued functions of $F$ when $\dot{c} \neq 0$ and $L > 2\pi/c$. The number of branches, $n$, is less than $cL/2\pi$ and is also the number of loops. The GSC is still unique, but can shift from one branch to another one with varying force resulting in a multiple-step discontinuous transition in $x_L$, regardless of $k$. The transition is accompanied by unwinding loops [15].
Applying an external force removes the degeneracy partly in model 2. For instance, at low force the 4 configurations in Fig. 3 have quite different $E_2$ owing to a different $x_L$, and the configuration in Fig. 3 (d) (by a clockwise rotating) has clearly the lowest $E_2$, since all 4 configurations have the same bending energy, but the configuration in Fig. 3 (d) has the largest $x_N$, and so has the lowest energy, and so is closer to the GSC.

Eqs. (10)–(13) require $\cos \phi_L > 1 - 1/F$. Furthermore, from symmetry, we know that $y(0) = y(L) = 0$. We also only need to consider the case with $0 > \phi_0 \geq -\pi$. This is because the configuration with $\pi > \phi_0 \geq 0$ can be obtained by rotating the filament (with $0 > \phi_0 \geq -\pi$) $180^\circ$ around the $x$–axis. Moreover, we can limit $\pi/2 > \phi(s) > -\pi/2$. This is because $\dot{x} = \cos \phi$, so that $3\pi/2 > \phi(s) > \pi/2$ or $-\pi/2 > \phi(s) > -3\pi/2$ results in a decreasing $x(s)$. But in this case, we can rotate some segments around the tangents passing the points with $\phi = \pm\pi/2$, to make a new configuration with the same bending energy but a larger $x_L$ so a lower energy, and so being closer to the real GSC. A typical example is shown in Fig. 4. In Fig. 4, the black short-dashed line is the GSC of model 1 obtained from Eqs. (8)–(9), and is also a solution of Eqs. (10)–(11). But it is not the GSC of model 2, which we can see as follows. Rotating the segment in the right side of $t(s_1)$ (left vertical line in Fig. 4), with $\phi(s_1) = \pi/2$, around this tangent, we obtain the red short-dotted line, which has the same bending energy as the black short-dashed line. Furthermore, rotating the segment of the red short-dotted line in the right side of $t(s_2)$ (right vertical line), with $\phi(s_2) = -\pi/2$, around this tangent, we obtain the green dash-dotted line, which has also the same bending energy as the black short-dashed line, but has obviously larger $x_L$ so is closer to the GSC of model 2. We should note that all these configurations are solutions of Eqs. (10)–(11), since at the turning points $\phi_T = \pm\pi/2$. Meanwhile, note that $\pi/2 > \phi(s) > -\pi/2$ means that the GSC must be loopless.

![FIG. 4: (Color online) Schematic picture showing why $\pi/2 > \phi(s) > -\pi/2$ in model 2. All three configurations (black short-dashed, red short-dotted, and green dash-dotted) have the same $|\phi(s)|$.](image)

Furthermore, the symmetry of the system also requires $x(s) + s(L - s) = 2x(L/2)$ and $y(s) = \pm y(L - s)$; this leads to $\dot{x}(s) = \dot{x}(L - s)$ and $\dot{y}(s) = \pm \dot{y}(L - s)$, i.e., $\cos[\phi(s)] = \cos[\phi(L - s)]$ and $\sin[\phi(s)] = \pm \sin[\phi(L - s)]$, and it follows that $\phi_L = \pm \phi_0$. When $\sin[\phi(s)] = -\sin[\phi(L - s)]$, we find that $\phi(L/2) = 0$ (note that $\pi/2 > \phi(s) > -\pi/2$) and $\phi_L = -\phi_0$. Such a state can be represented as the blue dashed line in Fig. 5 which is also the green dash-dotted line in Fig. 4. However, for such a configuration, we can rotate the part of the filament with $s > L/2$ $180^\circ$ around $t(L/2)$ (straight line in Fig. 5) to obtain a new
configuration with the same $E_2$, shown as the green-dotted line in Fig. 5. Furthermore, rotating the whole green dotted line appropriately (clockwise in this case), we can obtain a new configuration (black-solid line) that has the same bending energy as the original one but has a larger $x_L$ and so a lower energy, and thus is closer to the real GSC of model 2. This means that the original configuration (blue dashed line) cannot be the GSC, though it is a solution of Eqs. (10)–(11). Therefore, the GSC must have $\phi_L = \phi_0$. It follows that $y(s) = -y(L-s)$, $y(0) = y(L/2) = y(L) = 0$, or the GSC has an inverse symmetry with respect to the point $[x(L/2),0]$. We should also note that the blue dashed line and the green dotted line are solutions of Eqs. (10)–(11), since at the turning points $\phi_T = 0$. But we do not know whether the solid black line is a solution of Eqs. (10)–(11), though it has a lower energy and so is closer the GSC. In the similar way, we can find that the GSC of model 2 is at least double degenerated.

In summary, the GSC of model 2 must satisfy $y(L/2) = y(L) = y(0) = 0$, $\phi_L = \phi_0$, and $\pi/2 > \phi(s) > -\pi/2$. In contrast, in the GSC of model 1, at $s = L/2$ $y(s)$ has a local extreme and $\phi_L = 2n\pi - \phi_0$ [15]. Furthermore, there is no loop for the GSC in model 2, and it favors configurations with a larger extension than those of model 1. Note that the discontinuous transition in extension in model 1 is accompanied by unwinding loops, we expect, reasonably, that there is not such a transition in the extension for model 2. Therefore, we can conclude that the GSC of the two models are very different at a finite stretching force.

We have to point out that it is still rather difficult to find the exact GSC in model 2. We do not even know how many degenerated GSCs there are in model 2. The main difficulty comes from the fact that for any solution of Eqs. (10)–(13), we can find an infinite number of configurations with the same bending energy in model 2, but there is not a rule to select a configuration with the largest $x_L$ from so many configurations. For instance, we can rotate further the segments close to the both ends in the black solid line in Fig. 5 to obtain a new configuration with even lower $E_2$.

The above analyses also suggest that at finite temperature model 2 always favors the states with a moderate $x_L$, because in such a state it is easier to rotate some parts of the filament to obtain many new configurations with the same bending energy and nearly the same $x_N$ so that these states may dominate the thermal average. In other words, the
distribution function of $x_N$ in model 2 should have a peak at a moderate $x_N$ regardless of the force. We can then expect that at a finite temperature, up to a moderate force the relative extension of model 2 is larger than that of model 1, but under a large force the relative extension of model 2 is smaller than that of model 1.

IV. RESULTS AT A FINITE TEMPERATURE

At finite temperature the force-extension of model 1 has also been studied in detail \[15, 16\]. In model 1, it was found that a nonvanishing intrinsic curvature can induce a discontinuous change in extension. The critical force increases with increasing $c$. Moreover, the finite temperature represses the sharp transition, so that the discontinuous transition is no longer the multiple-step as at $T = 0$, but becomes one-step, requires large enough $c$ and $\kappa$, and probably occurs only in the thermodynamical limit. These conclusions are valid in both lattice and off-lattice systems. In contrast, the force-extension of model 2 is not yet available.

IV-1. Simulation settings

For the model 1, we perform simulations in both lattice and off-lattice systems to conform the existence of a phase transition. In contrast, in model 2 we consider only the off-lattice system. In our simulation, most of the initial configurations are set randomly. We also set the initial configuration as a circle of curvature $c$ for a few samples but find no difference, except for it requiring a much longer simulation time for model 2 at large force. We equilibrate every sample from $2 \times 10^6$ to $10^7$ Monte Carlo steps (MCS) before performing the average. The thermal average for a sample are taken from $2 \times 10^7$ to $3 \times 10^8$ MCS, and the larger the $N$ or $\kappa$ or $c$, the more MCS. This is because the thermal fluctuations become larger with increasing $N$ or $\kappa$ or $c$. Moreover, we take $N = 20, 50, 100, 150, 200, 250, 300$ to examine the finite size effect. $c = 0.1, 0.2, 0.3, 0.4, 0.5$ and $\kappa = 1, 2, 4, 6, 8$ in most cases. We do not consider larger $c$ because it is impractical. For model 1 when $c = 0.1$, we also take $\kappa = 15, 20, 25$. For model 2 when $c = 0.5$, we also take $\kappa = 10, 15, 20$, and 40. We do not consider larger $\kappa$ in this work because that results in very large fluctuation which should result from the existence of many metastable states, since a larger bending rigidity results in a higher energy barrier, and so the system may be trapped longer in a metastable state.

At finite temperature the fluctuations can suppress sharp transitions, especially for a finite size system. Therefore, to examine the possible phase transition and to identify the nature of the transition, one often has to evaluate the finite size effects. For this purpose, we study the specific heat $C_N$ and stretching strength $\mu_N$. They are expressed as

$$C_N \equiv \frac{\langle E_N^2 \rangle - \langle E_N \rangle^2}{N} \propto \frac{1}{N} \frac{\partial \langle E \rangle}{\partial T},$$

(24)

$$\mu_N \equiv \frac{1}{N} \frac{\partial \langle x_N \rangle}{\partial f} = \frac{\langle x_N^2 \rangle - \langle x_N \rangle^2}{N}.$$

(25)
The thermodynamical limit in this work means that we keep both \( l_0 \) and \( c \) as constants, but let \( N \to \infty \) so that the total length \( L = Nl_0 \to \infty \).

**IV-2. Results**

In the off-lattice system, first of all, under low force we find analytically [16] that in model 1 the relationship between \( z_N \) and \( f \) obeys approximately

\[
\frac{z_N}{f} = \frac{2f\kappa}{1 + 4c^2\kappa^2},
\]

and the larger the \( N \), the better the agreement, as shown in Figs. 6–7. This agreement provides a robust proof on the reliability of the simulation results. But model 2 does not obey such a relation, and the larger the \( \kappa \) or \( c \), the larger the deviation, as shown in Figs. 6 and 7.

![FIG. 6: (Color online) \( z_N \) vs \( f \) for the two models when \( \kappa = 2 \), \( c = 0.2 \). The lengths are \( N = 50 \) (black short-dashed and empty square), 100 (magenta dash-dotted and empty circle), and 300 (black solid and empty triangle). The dash-dot-dotted straight lines are given by Eq. (26). Pure lines represent the data for model 1. Lines and symbols represent the data for model 2. The inset presents the same data but with a larger range in \( f \). Reduced units are used.](image-url)

It is also interesting to know whether it is possible to find a united empirical expression of \( z_N(f) \) for the two models, similar to that for the WLC model [5]. In other words, we would like to know whether it is possible to find a universal curve for \( z_N(f) \) by choosing a proper scale, regardless of \( \kappa \) and \( c \). Using Eq. (26), it is clear that if there is a united expression for model 1, a proper choice for the scaling factor is to replace \( f \) by \( f' = f\kappa/(1 + 4c^2\kappa^2) \). However, though at low \( f \) such a scaling is indeed pretty good, but it fails clearly at moderate force. For model 2, we have the same problem.

From Fig. 6, we can see that when both \( \kappa \) and \( c \) are small, the results for the two models are close to each other, and the extensions in both models are simple concave
functions of $f$, i.e., the larger the $f$, the smaller the $\partial z_N/\partial f$. This is a natural result since a small $c$ means that both models are close to the WLC model, and so should have a similar behavior. Meanwhile, small $\kappa$ means that the filament is rather flexible so that the bending energy is less important. However, large $\kappa$ or $c$ makes a very different picture. As we can expect, under low force the $z_N$ of model 2 is always larger than that of model 1, as shown in Figs. 6 and 7, as a consequence of that, model 2 favors a larger $x_N$ in the GSCs. In contrast, from Figs. 6 and 7, we find that under large force, the $z_N$ of model 2 becomes smaller than that of model 1. Therefore, we can conclude that model 2 always favors the configurations with a moderate extension, agreeing well with the analysis at the end of section III.

However, from Figs. 6 and 7, we find that when $\kappa$ is large, in model 1 $z_N$ is no longer a concave function of $f$. There exists an inflection point at which the curve of $z_N(f)$ changes from being convex to concave. In other words, before the inflection point, the larger the $f$, the larger the $\partial z_N/\partial f$; but after the inflection point, the larger the $f$, the smaller the $\partial z_N/\partial f$. In contrast, there is no such inflection point in model 2, so that its $z_N(f)$ is still a simple concave function.

![Fig. 7](image1.png)

FIG. 7: (Color online) $z_N$ vs $f$ for the two models when $\kappa = 6$ and (a) $c = 0.2$; (b) $c = 0.5$. The symbols are the same as in Fig. 6. Reduced units are used.

![Fig. 8](image2.png)

FIG. 8: (Color online) $\mu_N$ vs $f$ for the model 2 when $\kappa = 6$ and (a) $c = 0.3$; (b) and $c = 0.5$. The lengths are $N = 20$ (black short-dashed), 50 (blue dotted), 100 (magenta dash-dotted), 200 (green dashed), and 300 (black solid). Reduced units are used.
The existence of the inflection point can be seen more clear by examining $\mu_N$. As reported in Ref. [15], when $\kappa$ is large, $\mu_N$ of model 1 has a peak, corresponding to the inflection point in $z_N(f)$ and the height of the peak increases with increasing $N$. It means that there is a discontinuous transition in $z_N$ in the thermodynamical limit. In contrast, from Fig. 8, we can see that the $\mu_N$ of model 2 always decreases monotonically with increasing $f$. Therefore, there is no phase transition in extension for model 2.

In simulations, $\langle y_N \rangle$ is well zeroed for both models, as it should be. To have a complete picture, we also evaluate $\Delta y_N \equiv \langle y_N^2 \rangle / N$ and find that $\Delta y_N$ has also rather different behavior between the two models. In model 1, when $\kappa$ and $c$ are small, $\Delta y_N$ decreases monotonically with increasing $f$. However, when $\kappa$ or $c$ is large, we find that there is a peak in $\Delta y_N$, and the larger the $N$, the sharper the peak, as shown in Fig. 9(a). The existence of the sharp peak in $\Delta y_N$ in model 1 should be due to a very large fluctuation near to the critical point, and gives another evidence on the existence of a phase transition. In contrast, in model 2 $\Delta y_N$ always decreases monotonically with increasing $f$, as shown in Fig. 9(b).

Finally, we find that for model 2, at the same $\kappa$ and $f$, the larger the $c$, the smaller the $z_N$. This is a natural result since with a large $c$, the filament is more likely to stay in a curled state and so has a small $\langle x_N \rangle$. Moreover, at the same $c$ and $f$, when $c$ is small, the larger the $\kappa$, the larger the $z_N$. In contrast, at the same $c$ and $f$, and when $c$ is large, then at small $f$, the larger the $\kappa$, the larger the $z_N$; but at large $f$, the larger the $\kappa$, the smaller the $z_N$, as shown in Fig. 10. Again this is due to the system preferring to stay in the states with a moderate extension.

Therefore, we can conclude that at finite $T$ the mechanical properties of these two models are still very different. The intrinsic curvature plays a very important role in model 1, but has relatively less effect in model 2.
FIG. 10: (Color online) $z_N$ vs $f$ when $c = 0.5$ and $N = 300$ for model 2. The bending rigidities are $\kappa = 2$ (black solid square), $\kappa = 8$ (red empty circle), $\kappa = 20$ (green solid triangle), and $\kappa = 40$ (blue empty diamond). The inset is the blow up of the regime with large $z_N$. Reduced units are used.

V. CONCLUSIONS

In summary, we compared two elastic models for two-dimensional intrinsically curved semiflexible biopolymers. We show exactly that these two models have very different ground states. Using computer simulation we find further that the two models still have different mechanical properties at a finite temperate. Our results show that under the same force, with the same intrinsic curvature and bending rigidity, the extension of model 1 is smaller than that of model 2 at low force, but becomes larger at large force. The difference is due to the fact that model 2 favors the configurations with moderate extensions. More important, the extension of model 1 is subjected to a discontinuous transition when the intrinsic curvature and bending rigidity are sufficiently large, but there is no such phase transition in model 2, so that the extension of model 2 is always a concave function of force. Therefore, we should distinguish these two models carefully. Model 1 should be appropriate for describing a biopolymer with nearly the same bond angle between nearest-neighbor monomers. In contrast, model 2 should be more appropriate for describing a biopolymer which allows different signs in bond angles. Finally, in this work we considered only a constant intrinsic curvature, but it is reasonable to expect that the main conclusions should still be valid for a system with a $s$-dependent intrinsic curvature.

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