Effect of a force-free end on the mechanical property of a biopolymer — A path integral approach*

Zicong Zhou(周子聪)[1,†] and Béla Joós[2]

[1] Department of Physics, Tamkang University, Taiwan, China
[2] Ottawa Carleton Institute for Physics, University of Ottawa Campus, Ottawa, Ontario, Canada, K1N-6N5

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We study the effect of a force-free end on the mechanical property of a stretched biopolymer. The system can be divided into two parts. The first part consists of the segment counted from the fixed point (i.e., the origin) to the forced point in the biopolymer, with arclength L_f. The second part consists of the segment counted from the forced point to the force-free end with arclength ΔL. We apply the path integral technique to find the relationship between these two parts. At finite temperature and without any constraint at the end, we show exactly that if we focus on the quantities related to the first part, then we can ignore the second part completely. Monte Carlo simulation confirms this conclusion. In contrast, the effect for the quantities related to the second part is dependent on what we want to observe. A force-free end has little effect on the relative extension, but it affects seriously the value of the end-to-end distance if ΔL is comparable to L_f.

Keywords: statistical physics, path integral, biopolymers, mechanical property

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1. Introduction

The conformational and mechanical properties of biopolymers have attracted considerable attentions owing to their importance in understanding the structure and function of biological materials.[1–29] In continuous elastic theory, a biopolymer is often modeled as a filament. The study of a filament has a long history dating back to Euler and Lagrange, and it has an increasing importance because it can be used to described the property of many microscopic objects such as biopolymers.[1–24,28] The simplest model for a biopolymer is the freely jointed chain (FJC) model and it is used to account for the conformational and mechanical properties of a flexible biopolymer. Another example is that the wormlike chain (WLC) model, which views the biopolymer as an inextensible chain with a uniform bending rigidity, has been used successfully to describe the entropic elasticity of a double-stranded DNA (dsDNA) or a semiflexible biopolymer.[1,4,5] Furthermore, the wormlike rod chain (WLRC) model, which is obtained by adding to the WLC model a term related to the intrinsic twist, has been used to explain the supercoiling property of dsDNA.[4,5,8] Owing to the importance of biopolymers, recently there has been a lot of works on the WLC and WLRC models as well as their modifications and extensions.

On the other hand, the path integral provides a powerful technique to study many physical phenomena. The basic idea of this technique can be traced back to Norbert Wiener, who introduced the Wiener integral to solve problems in the theory of diffusion and Brownian motion.[30] The complete method of the path integral was developed in 1948 by Richard Feynman,[31] with the original motivation to obtain a quantum mechanical formulation for the Wheeler–Feynman absorber theory. Since then, the path integral method has been applied widely to different areas in theoretical physics, including quantum field theory, solid state physics, statistical physics, polymer physics, and biophysics.[30–33] It has proved to be especially useful to describe the collective excitations in the theory of critical phenomena. This method often gives a simple way to obtain an exact solution for some physical problems. It also usually provides a solid foundation for the result obtained from other methods, to clarify the limits of their applicability and to indicate the way of finding corrections. For some realistic problems which are not exactly solvable, the path integral technique can help to build up a qualitative picture of the corresponding phenomenon and to develop some approximate methods of calculation.

For a time evolution system, the path integral is an analytic continuation of a method for summing up all possible trajectories of a moving body. It replaces the classical notion of a single, unique trajectory of a system with a sum over infinite possible trajectories to compute an amplitude or propagator. It is straightforward to see that a special configuration of a filament or a chain can be mapped into a trajectory of a moving body, with a replacement of the arclength of the filament by the time of the moving body. Therefore, it is straightforward to generalize the path integral technique to study the conformational and mechanical properties of a filament or a biopolymer.[4,10–12,14,16,21–23,30,32]

*Project supported by the MOST and the NSERC (Canada).
†Corresponding author. E-mail: zzhou@mail.tku.edu.tw
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Traditional studies on the mechanical property of a filament usually assume that the external force or torque is applied exactly at one end of the filament. However, it is not easy to realize such a condition in a microscopic system so in practice the force is applied away from the end leaving a segment with a force-free end. Therefore, to have a complete understanding of the mechanical property of a microscopic filament, it is necessary to clarify the role of such a force-free end. In this paper we apply the path integral technique to answer this question.

The paper is organized as follows. In Section 2 we set up the two-dimensional (2D) model. Section 3 presents the results for the ground state. Section 4 makes a brief discussion in the configuration average. In Section 5 we present the results for the effect of the force-free end at finite temperature. Section 6 gives a brief discussion in the three-dimensional (3D) system. Finally, we end the paper with conclusions and discussions.

2. Two-dimensional model

Many observations on semiflexible biopolymers are conducted in a 2D environment so that the property of biopolymers in 2D has attracted growing interest.[3,13,15–17,19,21,23,28] It is also relatively easier to find some exact results in a 2D system.[21,28] Therefore, we begin from a 2D system.

In two dimensions, the configuration of a filament is determined by a vector, $\boldsymbol{t} \equiv \mathrm{d}\boldsymbol{r}/\mathrm{d}s = \{\cos\phi, \sin\phi\}$, which is tangent to the contour line of the filament, where $\boldsymbol{r} = (x, y)$ is the locus of the filament, s is the arclength, and $\phi(s)$ is the angle between the x axis and $\boldsymbol{t}$, as shown in Fig. 1.

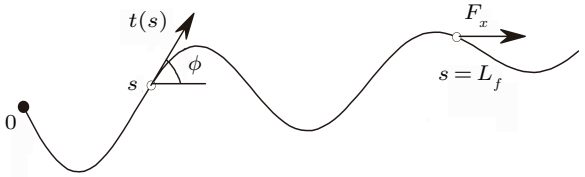


Fig. 1. Schematic diagrams of a curved filament showing the notation used.

Applying a uniaxial force (along the x axis) F_x at $s = L_f$, we can write the reduced elastic energy of a filament as[17,19,21,23,28]

$$\mathscr{E}[\{\phi\}] \equiv \frac{E}{k_{\mathrm{B}}T} = \mathscr{E}_f + \Delta\mathscr{E}, \tag{1}$$

$$\mathscr{E}_f = \frac{1}{2}\int_0^{L_f} k(\dot{\phi} - \tilde{c})^2 \mathrm{d}s - f\int_0^{L_f} \mathrm{d}s\cos\phi, \tag{2}$$

$$\Delta\mathscr{E} = \frac{1}{2}\int_{L_f}^{L} k(\dot{\phi} - \tilde{c})^2 \mathrm{d}s, \tag{3}$$

where E is the energy, T is the temperature, k_{B} is the Boltzmann constant, k is the bending rigidity, L is the total arc length of the filament and is a constant in the model so that the filament is inextensible, and $f \equiv F_x/k_{\mathrm{B}}T$. $\dot{\phi} \equiv \mathrm{d}\phi/\mathrm{d}s$ is the signed curvature and can be either positive or negative, and so does for $\tilde{c}(s)$. $\tilde{c}(s)$ is the intrinsic curvature. $\tilde{c}(s) \neq 0$ means that, when $F_x = 0$, the ground-state configuration (GSC, or the spontaneous configuration, i.e., the configuration with the lowest energy) of the filament is a curve of curvature $\tilde{c}(s)$. When $\tilde{c}(s) = 0$, it reduces to the WLC model. When $k = 0$, it becomes the FJC model.

3. Ground state configuration

Extremizing E, we obtain the shape equation and boundary conditions (BCs) that govern the configuration of a filament in the ground state,

$$k\ddot{\phi} = \begin{cases} F_x \sin\phi, & s \leq L_f, \\ 0, & s > L_f, \end{cases} \tag{4}$$

$$\dot{\phi}_0 = \dot{\phi}_f = \dot{\phi}_L = \tilde{c}, \tag{5}$$

where $\phi_0 = \phi(0)$, $\phi_f = \phi(L_f)$, and $\phi_L = \phi(L)$. Equation (5) gives hinged BC or free BC, i.e., ϕ_0, ϕ_f, and ϕ_L are not fixed. We do not consider other forms of BC since we focus on a filament at finite temperature in this paper.

It is clear that when $s \geq L_f$, $\phi(s) = \phi_f + \tilde{c}s$. Moreover, the equation with $s \leq L_f$ is exactly the same as that of a filament with $L = L_f$. The filament with $L = L_f$ has been studied in detail and it is found exactly that at $T = 0$ and when $\tilde{c} \neq 0$, $x(L)$ undergoes a multiple-step discontinuous transition with increasing force[21,28] for a long filament, i.e., when $L \gg 2\pi/\tilde{c}$, regardless of k.

4. Configurational average

In statistical mechanics, at finite temperature a static macroscopic quantity $\bar{B}$ is defined as the average with Boltzmann weight over all possible conformations. For a continuous system, the average becomes a path integral in the form[4,10–12,14,16,21–23,30–33]

$$\bar{B} = \int \mathscr{D}[\phi(s)] p_L B[\{\phi(s)\}] \mathrm{e}^{-\mathscr{E}} p_0/Z_k, \tag{6}$$

where $Z_k = \int \mathscr{D}[\phi(s)] p_L \mathrm{e}^{-\mathscr{E}} p_0$ is a ϕ-independent normalization constant. $p_0(\phi_0)$ and $p_L(\phi_L)$ are distributions of ϕ_0 and ϕ_L, respectively. p_0 and p_L are specified by the BCs. For instance, if we fix ϕ_0 as ϕ^0 or ϕ_L as ϕ^L, then $p_0 = \delta(\phi_0 - \phi^0)$ or $p_L = \delta(\phi_L - \phi^L)$. If ϕ_0 or ϕ_L is free, then p_0 =constant or p_L =constant. There are some other kinds of BC, such as a hard wall[32] somewhere or forming a loop. In practice, with fixed or free BCs, we can ignore the corresponding p_0 or p_L in Eq. (6), and it is also the most often seen form of the mean in the literature,[4,10–12,14,16,21–23] especially for the time evolution system. In this convention, we should note that fixing ϕ_0 or ϕ_L means that we do not integrate over ϕ_0 or ϕ_L in Eq. (6). In contrast, free ϕ_0 or ϕ_L means that it is necessary to integrate over ϕ_0 or ϕ_L in Eq. (6). Physically, p_0 and p_L represent some constraints, similar to the constraint of a constant volume in the microscopic or macroscopic ensemble in statistical

physics. These constraints are in general ignored in the literature so may result in some confusion.

In the realistic calculations, we can always arrange $B[\{\phi(s)\}]$ properly so that we can write it as $B[\phi,\phi_n,\ldots,\phi_1,\phi_0;s,s_n,\ldots,s_1,s_0]$ with $L\geq s\geq s_n\cdots\geq s_1\geq s_0$, where $\phi\equiv\phi(s)$, $\phi_k=\phi(s_k)$, $k=0,\ldots,n$. For instance, the end-to-end distance can be written as

$$r_L^2=\left(\int_0^L \boldsymbol{t}\,\mathrm{d}s\right)^2=\int_0^L \mathrm{d}s\int_0^L\cos(\phi-\phi_1)\,\mathrm{d}s_1$$
$$=\int_0^L \mathrm{d}s\left[\int_0^s \mathrm{d}s_1\cos(\phi-\phi_1)+\int_s^L \mathrm{d}s_1\cos(\phi-\phi_1)\right],$$

so that inside the square bracket s and s_1 are ordered. Therefore, for convenient in later derivations, we define a distribution function, $P(\phi,s;\phi',s')$ with $s\geq s'$, as

$$P(\phi,s;\phi',s')\equiv C(s,s')\int\mathscr{D}[\phi(u)]\,\mathrm{e}^{-\mathscr{E}'},\tag{7}$$

$$\mathscr{E}'=\begin{cases}\displaystyle\int_{s'}^{s}(\varepsilon_1+\varepsilon_2)\,\mathrm{d}s, & L_f\geq s\geq s',\\ \displaystyle\int_{s'}^{L_f}(\varepsilon_1+\varepsilon_2)\,\mathrm{d}s+\int_{L_f}^{s}\varepsilon_1\,\mathrm{d}s, & s>L_f\geq s',\\ \displaystyle\int_{s'}^{s}\varepsilon_1\,\mathrm{d}s, & s\geq s'>L_f,\end{cases}\tag{8}$$

$$\varepsilon_1=\frac{k}{2}(\dot\phi-\tilde c)^2,\quad \varepsilon_2=-f\cos\phi,\tag{9}$$

where $\phi'=\phi(s')$ and C, which comes from Z_k, is independent of ϕ and ϕ' (but is dependent on BCs), then $\bar B$ can be rewritten as

$$\bar B=\int_{-\infty}^{\infty}\mathrm{d}\phi_L\,\mathrm{d}\phi\,\mathrm{d}\phi_n\cdots\mathrm{d}\phi_2\,\mathrm{d}\phi_1\,\mathrm{d}\phi_0 p_L P(\phi_L,L;\phi,s)P(\phi,s;\phi_n,s_n)\cdots P(\phi_2,s_2;\phi_1,s_1)B[\{\phi(s)\}]P(\phi_1,s_1;\phi_0,0)p_0.\tag{10}$$

Note that if C is dependent on ϕ or ϕ', then equation (10) is invalid.

From Eq. (1) we can see that, when $f\neq 0$, $\mathscr{E}$ is not an invariant with respect to a translation of ϕ, so that P cannot be in the form $P(\phi-\phi',s-s')$. We can also show this conclusion using the series expansion method.[23] It follows that we cannot normalize $P(\phi,s;\phi',s')$ directly since it results in a ϕ'-dependent C. With free ϕ_0 and ϕ_L, $P(\phi,s;\phi',s')$ represents the distribution of ϕ with a fixed ϕ' because all P's in Eq. (10) play the same role. But even in this sense, to normalize P is still meaningless. Moreover, note that BCs can affect the distribution at an arbitrary s, so that if ϕ_0 and ϕ_L are not free, then $P(\phi,s;\phi',s')$ do not have the meaning of a distribution function.

When $f=0$, the exact distribution function, $P(\phi,s;\phi',s')=P_0(\phi,s;\phi',s')$ $(s>s')$, is found to be[23]

$$P_0=\sqrt{\frac{1}{2\pi A}}\exp\left[-\frac{1}{2A}\left(\phi-\phi'-\int_{s'}^{s}\tilde c\,\mathrm{d}s\right)^2\right],\tag{11}$$

$$A(s,s')=\int_{s'}^{s}\frac{\mathrm{d}s}{k(s)}.\tag{12}$$

It is straightforward to show that $(s\geq s_1\geq s')$

$$P_0(\phi,s;\phi',s')=\int\mathrm{d}\phi_1 P_0(\phi,s;\phi_1,s_1)P_0(\phi_1,s_1;\phi',s').\tag{13}$$

In this sense, P_0 is also referred to as a propagator. In quantum mechanics, a propagator always satisfies such a relation. But we should point out that such an expression may be invalid for an arbitrary $P(\phi,s;\phi',s')$ in our system, because C in Eq. (7) must provide $\bar B=1$ when $B[\{\phi(s)\}]=1$, but there is no way to show that it is consistent with Eq. (13) for the arbitrary $P(\phi,s;\phi',s')$ when $f\neq 0$. For instance, a simplest choice of C is to let $C^{n+3}\propto Z_k$, but such a choice is clearly inconsistent with Eq. (13). This should be a very important difference between quantum mechanics description and statistical mechanics description of the path integral method, but the relevant discussion seems unavailable in the literature.

5. Effect of a force-free end at finite temperature

5.1. With free ϕ_L

In experiment, usually ϕ_L is free so that we consider this case first.

5.1.1. When $s\leq L_f$

In this case, using

$$\int\mathrm{d}\phi_L P_0(\phi_L,L;\phi_f,L_f)=1,$$

we find exactly

$$\bar B=\int_{-\infty}^{\infty}\mathrm{d}\phi_f\,\mathrm{d}\phi\,\mathrm{d}\phi_n\cdots\mathrm{d}\phi_2\,\mathrm{d}\phi_1\,\mathrm{d}\phi_0\{P(\phi_f,L_f;\phi,s)P(\phi,s;\phi_n,s_n)\cdots P(\phi_2,s_2;\phi_1,s_1)B[\{\phi(s)\}]P(\phi_1,s_1;\phi_0,0)p_0\}$$
$$=\int\mathscr{D}[\phi(s)]p_0B[\{\phi(s)\}]\,\mathrm{e}^{-\mathscr{E}_f}\Big/\int\mathscr{D}[\phi(s)]p_0\,\mathrm{e}^{-\mathscr{E}_f}.\tag{14}$$

Alternatively, we can use the standard path integral technique to discretize the functional integration in Eq. (6) first, and then integrate it term by term,[21] beginning from ϕ_L, to obtain the same result as in Eq. (14).

Equation (14) is exactly the same as that of the system with $L=L_f$, or it is equivalent to let $\Delta\mathscr{E}=0$. In other words, if we focus on the physical properties related to $s\leq L_f$, then the force-free end does not have any effect. Note that this conclusion is valid even for a filament with s-dependent k and $\tilde c$, including the FJC model with $k=0$.

To check the conclusions obtained from the path integral method, we discretize the model and perform the Monte Carlo simulation method with the Metropolis algorithm to study it in the off-lattice system. For convenience, we only simulate the system with constant k and $\tilde{c}$. In the discrete model, the filament is consisted of N straight segments of length l_0 and joined end by end. The coordinates of two ends of the i-th segment are therefore $\{x_{i-1}, y_{i-1}\}$ and $\{x_i, y_i\}$ with $x_0 = y_0 = 0$. The external force is applied at the N_f-th segment. Replacing $\dot{\phi}$ by $(\phi_{i+1} - \phi_i)/l_0$, the reduced elastic energy becomes

$$\mathscr{E}_N \equiv \frac{E_N}{k_B T} = \frac{\kappa}{2} \sum_{i=2}^{N} (\phi_i - \phi_{i-1} - c)^2 - F \sum_{i=1}^{N_f} \cos\phi_i, \quad (15)$$

where $c \equiv \tilde{c} l_0$, $\kappa \equiv k/l_0 k_B T$, $F \equiv F_x l_0/k_B T$. We also scale length by l_0 so

$$x_N = \sum_{i=1}^{N} \cos\phi_i, \quad x_{N_f} = \sum_{i=1}^{N_f} \cos\phi_i,$$

and the relative extension is given by $z_N = \langle x_{N_f} \rangle / N_f$. Therefore, F and z_N are dimensionless quantities.

We have presented reports on the results with $N = N_f$ (or $L = L_f$) for this model.[28] We found that if $c \neq 0$ and at $T > 0$, z_N undergoes a one-step first-order transition in the thermodynamical limit if the filament has a sufficiently large κ.

In this work we simulate the system with $\Delta N \equiv N - N_f > 0$. We take $c = 0$, 0.1, 0.2, and 0.5 in this work. We set $\kappa = 6$ when $c = 0$ and 0.5; $\kappa = 20$ when $c = 0.1$; $\kappa = 2$ and 6 when $c = 0.2$. $N_f = 50$, 100, 200, and 300. $\Delta N = 2$, 4, 6, 8, 10, 15, 20, 30, 40, and 50. The initial configurations are set randomly in this work. We equilibrate every sample for 10^6 Monte Carlo steps (MCS) before performing the averaging. The thermal average for a sample is taken to be 5×10^6 MCS. The MCS in this work are much less than that used in Ref. [28] since here we need only some qualitative results.

Some typical simulation results for z_N are shown in Fig. 2. From Fig. 2, we can see that z_N's for the system with $\Delta N = 0$ and $\Delta N > 0$ are almost the same, so that these results support the conclusion that a force-free end indeed has no effect on the physical properties of a filament.

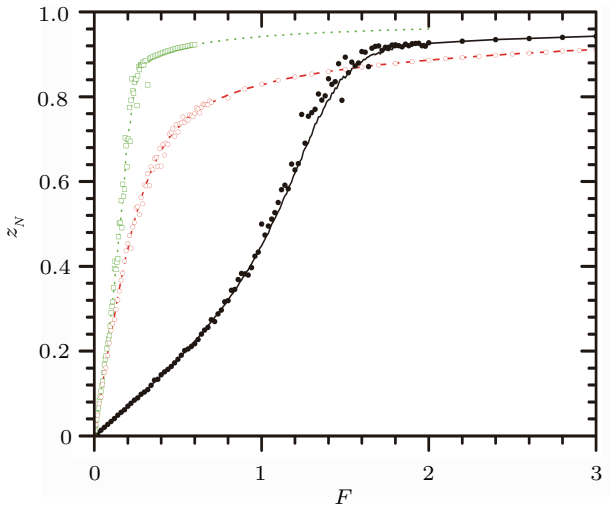


Fig. 2. (color online) z_N versus F when $\kappa = 6$, $c = 0.5$ (black); $\kappa = 2$, $c = 0.2$ (red); and $\kappa = 20$, $c = 0.1$ (green). $N_f = 300$ in all cases. The lines (solid, dashed, dotted) are the systems with $N = N_f$ and MCS $= 3 \times 10^8$.[28] The black solid circle is for a filament with $N = 315$, the red empty-circle is for a filament with $N = 320$, and the green empty-square is for a filament with $N = 310$. MCS $= 5 \times 10^6$ for circles and squares. Reduced units are used.

5.1.2. When $s > L_f$

In the same way as in the last section, when $s > L_f$, $\bar{B}$ can be found in two steps

$$\bar{B} = \int \mathrm{d}\phi_f \mathrm{d}\phi_- \cdots \mathrm{d}\phi_1 \mathrm{d}\phi_0 g(\phi_f, L_f) P(\phi_f, L_f; \phi_-, s_-) \cdots P(\phi_2, s_2; \phi_1, s_1) P(\phi_1, s_1; \phi_0, 0) p_0, \quad (16)$$

$$g = \int \mathrm{d}\phi \mathrm{d}\phi_n \mathrm{d}\phi' \cdots \mathrm{d}\phi_+ P_0(\phi, s; \phi_n, s_n) P_0(\phi_n, s_n; \phi', s') \cdots P_0(\phi_+, s_+; \phi_f, L_f) B[\{\phi(s)\}], \quad (17)$$

where $s > s_n > s' > s_+ > L_f > s_-$. $g(\phi_f, L_f)$ is dependent on ϕ_f and L_f, and is the same as the mean of the same quantity in a force-free system with an effective length $\Delta L = \Delta N = L - L_f$ and a fixed initial angle $\phi_0 = \phi_f$. Since P_0 is well known, in many cases we can find a closed form for $g(\phi_f, L_f)$. For instance, for $x_L = \int_0^L \mathrm{d}s \cos\phi$ and constant k and $\tilde{c}$, using (this can be shown exactly using the standard path integral technique[21,23])

$$P(\phi, s; \phi_0, 0) = \int_{-\infty}^{\infty} \mathrm{d}\phi_f P_0(\phi, s; \phi_f, L_f) P(\phi_f, L_f; \phi_0, 0),$$

we obtain

$$\Delta x_L \equiv \langle x_L - x_f \rangle = \int_{L_f}^{L} \mathrm{d}s \langle \cos\phi(s) \rangle$$

$$= \int_{L_f}^{L} \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}\phi P(\phi, s; \phi_0, 0) \cos\phi(s) p_0$$

$$= \frac{2kG}{1 + 4\tilde{c}^2 k^2}, \quad (18)$$

$$G = [1 + \mathrm{e}^{-\Delta L/2k}(2\tilde{c}k \sin\gamma_f - \cos\gamma_f)] \langle \cos\phi_f \rangle - [2\tilde{c}k - \mathrm{e}^{-\Delta L/2k}(2\tilde{c}k \cos\gamma_f + \sin\gamma_f)] \langle \sin\phi_f \rangle. \quad (19)$$

where $\gamma_f = \tilde{c}\Delta L$. When $k = 0$, i.e., for the FJC model, we obtain $\Delta x_L = 0$ as it should be. Equation (18) is in fact valid for all x_s with $s > L_f$.

Replacing ΔL by L, $\langle \cos\phi_f \rangle$ by $\cos\phi_0$, and $\langle \sin\phi_f \rangle$ by $\sin\phi_0$, equation (18) recovers the x_L of a force-free filament with a fixed ϕ_0. This seems to be a trivial result, but we should note that exactly the behavior of Eq. (18) is different from that of the x_L of a force-free filament with a fixed ϕ_0. A typical example is that, with a free ϕ_0, exactly $\langle \cos\phi_f \rangle = \langle \sin\phi_f \rangle = 0$ when $f = 0$ so that $\Delta x_L = 0$, regardless of k, L and $\tilde{c}$. But when ϕ_0 is fixed, clearly $\Delta x_L \neq 0$. This is because the two terms in

the right-hand side of Eq. (19) are strongly correlated when ϕ_0 is fixed since

$$\sin\phi_0 = \pm\sqrt{1-\cos\phi_0^2}.$$

In contrast, in general $\langle\cos\phi_f\rangle^2 + \langle\sin\phi_f\rangle^2$ varies with f and is not a constant, as shown in Fig. 3, so that knowing $\langle\cos\phi_f\rangle$ does not mean knowing $\langle\sin\phi_f\rangle$.

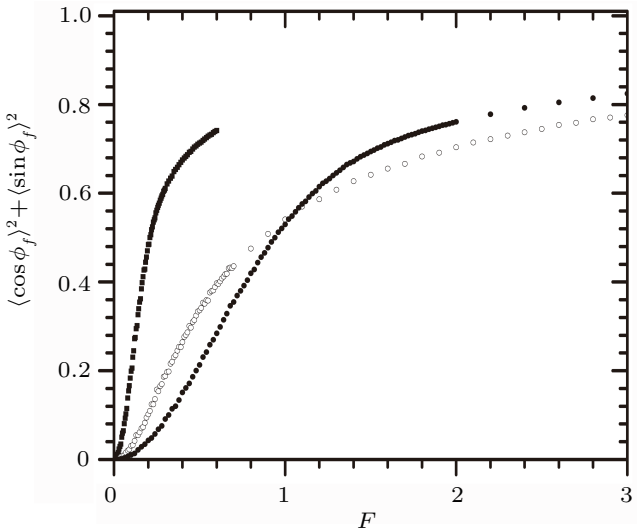


Fig. 3. $\langle\cos\phi_f\rangle^2 + \langle\sin\phi_f\rangle^2$ versus F for a filament when $\kappa = 6$, $c = 0.5$ (solid-circle); $\kappa = 2$, $c = 0.2$ (empty-circle); and $\kappa = 20$, $c = 0.1$ (solid-square). $N_f = 300$ in all cases. Reduced units are used.

From Eq. (18), it is clear that $\Delta x_L/L_f \to 0$ when $L_f \to \infty$. Note further that ΔL appears in the form of $\mathrm{e}^{-\Delta L/2k}$, we conclude that x_L/L and x_f/L_f should be almost indistinguishable in experiment. Therefore, for a long filament, the effect of the force-free end for the relative extension is negligible, regardless of ΔL.

We can find similar results for some other quantities. Especially, replacing ΔL by L, we can show that $\Delta\boldsymbol{r}_L^2 \equiv \langle(\boldsymbol{r}_L - \boldsymbol{r}_f)^2\rangle$ is independent of ϕ_f, and is exactly the same as the $\boldsymbol{r}_L^2$ of a force-free filament, which is basically dependent linearly on L.[21] In this case, if ΔL is comparable to L_f, then $\langle\boldsymbol{r}_L^2\rangle$ and $\langle\boldsymbol{r}_f^2\rangle$ will be quite different, so that one must be very careful to distinguish these two quantities in experiments.

5.2. With a Gaussian distribution on ϕ_L

Intuitively, it is very difficult to apply a constraint on ϕ_L without an associated force, except for binding some parts of a filament to form loops. Evaluating the effect of loops is a rather complex task so we will not discuss it in this work. For simplicity, we only present some expressions for a constraint in the form of a Gaussian distribution in ϕ_L, to demonstrate the complicated nature of the problem. Fixing ϕ_L can be regarded as taking $\alpha \to \infty$, so we do not consider it separately. In this case

$$p_L = \sqrt{\alpha/\pi}\,\mathrm{e}^{-\alpha(\phi_L-\beta)^2}. \tag{20}$$

Define

$$\begin{aligned} p(\phi,s) &\equiv \int_{-\infty}^{\infty} \mathrm{d}\phi_L p_L P_0(\phi_L, L; \phi, s) \\ &= \sqrt{\alpha_s/\pi}\,\mathrm{e}^{-\alpha_s(\phi-\beta_s)^2}, \end{aligned} \tag{21}$$

$$\alpha_s = \frac{\alpha}{2\alpha A(L,s)+1}, \quad \beta_s = \beta - \int_s^L \mathrm{d}s\tilde{c}(s), \tag{22}$$

when $s \le L_f$, we can obtain

$$\bar{B} = \frac{\int \mathscr{D}[\phi(s)] p_0 B[\{\phi(s)\}]\,\mathrm{e}^{-\mathscr{E}_f} p(\phi_f, L_f)}{\int \mathscr{D}[\phi(s)] p_0\,\mathrm{e}^{-\mathscr{E}_f} p(\phi_f, L_f)}. \tag{23}$$

Again equation (23) is the same as that of the system with $L = L_f$, or it is equivalent to let $\Delta\mathscr{E} = 0$ but with an effective Gaussian distribution, $p(\phi_f, L_f)$, for ϕ_f. But in this case we cannot say that the force-free end has no effect since $p(\phi_f, L_f)$ is dependent on both α and β.

Similarly, when $s > L_f$, we can find

$$\bar{B} = \int \mathrm{d}\phi_f \mathrm{d}\phi_- \cdots \mathrm{d}\phi_1 \mathrm{d}\phi_0 g_1(\phi_f, L_f) P(\phi_f, L_f; \phi_-, s_-) \cdots P(\phi_2, s_2; \phi_1, s_1) P(\phi_1, s_1; \phi_0, 0) p_0, \tag{24}$$

$$g_1 = \int \mathrm{d}\phi \mathrm{d}\phi_n \mathrm{d}\phi' \cdots \mathrm{d}\phi_+ p(\phi, s) P_0(\phi, s; \phi_n, s_n) P_0(\phi_n, s_n; \phi', s') \cdots P_0(\phi_+, s_+; \phi_f, L_f) B[\{\phi(s)\}], \tag{25}$$

Again, since P_0 and $p(\phi,s)$ are well known, it is possible to find a closed form for some quantities with complex expressions.

6. On three-dimensional system

In the 3D case, the configuration of a filament can be described by a triad of unit vectors $\{\boldsymbol{t}_i(s)\}_{i=1,2,3}$, where $\boldsymbol{t}_3 \equiv \mathrm{d}\boldsymbol{r}(s)/\mathrm{d}s$ is the tangent to the center line $\boldsymbol{m}(s)$ of the filament, and $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ are oriented along the principal axes of the cross section. The orientation of the triad as one moves along the filament is given by the solution of the generalized Frenet equations that describe the rotation of the triad vectors,[12,14]

$$\mathrm{d}\boldsymbol{t}_i(s)/\mathrm{d}s = -\sum_{j,k} \varepsilon_{ijk}\omega_j(s)\boldsymbol{t}_k(s),$$

where ε_{ijk} is the antisymmetric tensor, and $\{\omega_i(s)\}$ are the curvature and torsion parameters.

Applying a uniaxial force (along the z axis) F_z at $s = L_f$, we can write the reduced elastic energy of a filament with intrinsic curvatures $\zeta_1(s)$, $\zeta_2(s)$, intrinsic twist rates $\zeta_3(s)$ and persistence lengths $a_i(s)$ as[12,14]

$$\mathscr{E} \equiv \frac{E}{k_\mathrm{B}T} = \sum_{i=1}^{3} \int_0^L \frac{a_i}{2}(\omega_i - \zeta_i)^2 \mathrm{d}s - f\int_0^{L_f} \mathrm{d}s\cos\theta, \tag{26}$$

where $\theta(s)$ is the angle between the force and the z axis.

Again, a static macroscopic quantity $\bar{B}$ is defined as a path integral

$$\bar{B} \equiv \frac{\int \mathscr{D}[\omega_i] p_0 B[\{\omega_i(s)\}] \, \mathrm{e}^{-\mathscr{E}} p_L}{\int \mathscr{D}[\omega_i] p_0 \, \mathrm{e}^{-\mathscr{E}} p_L}. \tag{27}$$

Similar to the 2D case, we can show exactly that when $s \leq L_f$ and with a free end at $s = L$,

$$\bar{B} = \frac{\int \mathscr{D}[\omega_i] p_0 B[\{\omega_i(s)\}] \, \mathrm{e}^{-\mathscr{E}_f}}{\int \mathscr{D}[\omega_i] p_0 \, \mathrm{e}^{-\mathscr{E}_f}}, \tag{28}$$

$$\mathscr{E}_f = \sum_{i=1}^{3} \int_0^{L_f} \frac{a_i}{2} (\omega_i - \zeta_i)^2 \, \mathrm{d}s - f \int_0^{L_f} \mathrm{d}s \cos\theta. \tag{29}$$

Therefore, we find exactly the same conclusion as that in the 2D case, i.e., if we focus on the quantities with $s \leq L_f$, then we can ignore the free end. Replacing the force by a torque, we can obtain the same conclusion. Moreover, for the quantities related to $s > L_f$, we can also find some results similar to that in 2D.

7. Conclusions and discussions

In summary, using the path integral technique, at finite temperature, we show exactly that for a filament if we focus on the quantities related to $s \leq L_f$, then we can ignore the force-free end completely. In this paper we consider a uniaxial force only, but it is straightforward to generalize this conclusion to more general cases. In contrast, if we are interested in the quantities related to $s > L_f$, then the importance of a force-free end is quantity-dependence. A force-free end has little effect on the relative extension. But if ΔL is comparable to L_f, then a force-free end affects seriously the value of the end-to-end distance. Our conclusions are valid in both 2D and 3D, regardless of bending rigidity, intrinsic curvatures and intrinsic twist rates.

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