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Static bistable helices in generalized Helfrich elastic theory of a chiral filament

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Abstract

Based on the head-to-tail symmetry only, an elastic theory of a chiral filament is proposed [Langmuir 7 (1991) 567]. Following the same idea, we generalize the theory from the original fourth order to the sixth, such that the coexistence of static bistable helical conformations with opposite handedness is explained.

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1. Introduction

The coexistence of static bistable helical conformations is ubiquitous, from meso- to macroscopic scales. For instance, both the left-handed "Z-DNA" and the right-handed "B-DNA" can coexist [1,2]. Bacterial mobility of flagella filament involves switching between the left- and the right-handed supercoiling states, and they can also coexist [3–7]. Using the same catalyst and under the same temperature, helically coiled carbon tubes can be obtained and they reveal both types of chirality [8–10]. The tendril perversion of climbing plants provides an example of the coexistence of the bistable helices with opposite handedness in macroscopic domain [6,11]. By and large, the distribution of constituents along each filament is continuous and uniform. As a macroscopic theory, it is assumed that the elasticity determines their static conformations [12]. Unfortunately, for a long filament of helical conformation, there has not been an elastic theory so far available to give two energy minima with opposite handedness. This Letter aims at developing such one.

Based on only one assumption of head-to-tail symmetry of a filament, Helfrich has proposed an elastic theory [13], in which the energy density of filaments is expanded to fourth order of torsion τ and/or curvature κ. The theory succeeds in explaining the following facts: the energetic preference of helical conformation over the straight line [13], chirality selection [13], and kink formations from circle DNAs [14], etc. [15]. These facts show that Helfrich theory

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presents the essential part of the static elasticity of uniform and symmetrical filaments. However, the fourth-order elastic theory gives only one energy minimum in helical conformations [13]. In order to account for static helical bistables coexisting in the filaments, a straightforward generalization of the Helfrich's elastic theory from the original fourth- to the higher-order is performed and the sixth-order theory turns out to be necessary and sufficient.

The Letter is organized as what follows. The following Section 2 presents a brief derivation of the sixth-order in energy density expansion of filament elasticity. In Section 3, the bistable helical conformations are demonstrated to coexist with the same elastic moduli and a comparison with experimental data in two cases is made. This Letter is enclosed with a brief summary.

2. The Helfrich theory of a filament and the generalization

A long filament can be viewed as a mathematical line $\mathbf{r} = \mathbf{r}(s)$, where s is arc length. The strains are expressed by vector derivatives $d^n\mathbf{t}/ds^n$ ($n = 1, 2, 3, \ldots$), where $\mathbf{t}$ is unit tangent vector of the line. For the reasons of symmetry, only scalar invariant under simultaneous reversal of both s and $\mathbf{t}$ can occur in the elastic energy associated with the strain [13]. This means that every energy term should be invariant with transforming $(s, \mathbf{t}) \to (-s, -\mathbf{t})$, for it is only a matter of change of symbols without any change of physical contents. In other words, the total number of s and $\mathbf{t}$ in each term must be an even number.

The independent scalars up to the fourth order have been constructed by Helfrich [13],

$$
\begin{aligned}
&\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds},\\
&\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right),\\
&\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right)^2,\\
&\left(\mathbf{t}\times\frac{d^2\mathbf{t}}{ds^2}\right)^2.
\end{aligned}
\tag{1}
$$

The independent fifth and the sixth order are found to be, respectively,

$$
\begin{aligned}
&\left[\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right)\right]\cdot\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right),\\
&\left(\mathbf{t}\times\frac{d^2\mathbf{t}}{ds^2}\right)\cdot\frac{d^3\mathbf{t}}{ds^3},\\
&\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right)^3,\\
&\left[\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right)\right]^2,\\
&\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d^2\mathbf{t}}{ds^2}\right)^2,\\
&\left(\mathbf{t}\cdot\frac{d^3\mathbf{t}}{ds^3}\right)\cdot\left(\frac{d^2\mathbf{t}}{ds^2}\cdot\frac{d\mathbf{t}}{ds}\right),\\
&\left(\frac{d^3\mathbf{t}}{ds^3}\cdot\frac{d^3\mathbf{t}}{ds^3}\right).
\end{aligned}
\tag{2}
$$

Collecting the terms (1) to (2) and multiplying them with elastic moduli k_i (or k_{ij}), we obtain the elastic energy density up to the sixth-order terms,

$$
\begin{aligned}
f = {}&\frac{1}{2}k_2\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right) + k_3\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right)\\
&+\frac{1}{4}k_{22}\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right)^2 + \frac{1}{2}k_4\left(\mathbf{t}\times\frac{d^2\mathbf{t}}{ds^2}\right)^2\\
&+k_5\left[\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right)\right]\cdot\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right)\\
&+k_{51}\left(\mathbf{t}\times\frac{d^2\mathbf{t}}{ds^2}\right)\cdot\frac{d^3\mathbf{t}}{ds^3} + k_{61}\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d\mathbf{t}}{ds}\right)^3\\
&+k_{62}\left[\mathbf{t}\cdot\left(\frac{d\mathbf{t}}{ds}\times\frac{d^2\mathbf{t}}{ds^2}\right)\right]^2 + k_{63}\left(\frac{d\mathbf{t}}{ds}\cdot\frac{d^2\mathbf{t}}{ds^2}\right)^2\\
&+k_{64}\left(\mathbf{t}\cdot\frac{d^3\mathbf{t}}{ds^3}\right)\cdot\left(\frac{d^2\mathbf{t}}{ds^2}\cdot\frac{d\mathbf{t}}{ds}\right)\\
&+k_{65}\left(\frac{d^3\mathbf{t}}{ds^3}\cdot\frac{d^3\mathbf{t}}{ds^3}\right).
\end{aligned}
\tag{3}
$$

Using the Frenet formulas [16]

$$
\begin{aligned}
&\frac{d\mathbf{t}}{ds} = \kappa\mathbf{n},\\
&\frac{d\mathbf{n}}{ds} = -\kappa\mathbf{t} + \tau\mathbf{b},\\
&\frac{d\mathbf{b}}{ds} = -\tau\mathbf{n},
\end{aligned}
\tag{4}
$$

where **n** and **b** are the normal and binormal unit vector respectively, we have

$$\frac{d^2\mathbf{t}}{ds^2} = \kappa_s \mathbf{n} - \kappa^2 \mathbf{t} + \kappa\tau\mathbf{b}, \tag{5}$$

$$\frac{d^3\mathbf{t}}{ds^3} = (\kappa_{ss} - \kappa^3 - \kappa\tau^2)\mathbf{n} - 3\kappa\kappa_s\mathbf{t} + (2\kappa_s\tau + \kappa\tau_s)\mathbf{b}, \tag{6}$$

where $\kappa_s = d\kappa/ds$, $\tau_s = d\tau/ds$, and so forth. Inserting relations (4)–(6) into Eq. (3), we can rewrite the sixth-order elastic energy density ignoring the boundary terms,

$$\begin{aligned} f = {} & \frac{1}{2}k_2\kappa^2 + k_3\kappa^2\tau + \frac{1}{4}k_{22}\kappa^4 + \frac{1}{2}k_4(\kappa_s^2 + \kappa^2\tau^2) \\ & + k_5\kappa^4\tau \\ & + k_{51}(2\kappa_s^2\tau + \kappa\kappa_s\tau_s - \kappa_{ss}\kappa\tau + \kappa^4\tau + \kappa^2\tau^3) \\ & + k_{61}\kappa^6 + k_{62}\kappa^4\tau^2 + k_{63}\kappa^2\kappa_s^2 \\ & + k_{64}(\kappa^6 + \kappa^4\tau^2 - \kappa^3\kappa_{ss}) \\ & + k_{65}(\kappa_{ss}^2 + \kappa^6 + \kappa^2\tau^4 - 2\kappa^3\kappa_{ss} - 2\kappa\kappa_{ss}\tau^2 \\ & \quad + \kappa^4\tau^2 + 10\kappa^2\tau_s^2 + 4\kappa_s^2\tau^2 + 4\kappa\kappa_s\tau\tau_s). \end{aligned} \tag{7}$$

In general, we must perform the variational calculus of the energy functional to obtain an equilibrium equation; then discuss possible conformations based on the equation. However, it is not necessary to do so because we consider only the helical case in which both the curvature κ and torsion τ are constants. It means that the elastic energy density f is a constant along the filament. Our aim is to see under what elastic moduli the bistable helical states with opposite handedness are possible.

Since both curvature and torsion are constants, we have $\kappa_s = 0$, $\kappa_{ss} = 0$ and $\tau_s = 0$, the energy density (7) is then,

$$\begin{aligned} f = {} & \frac{1}{2}k_2\kappa^2 + k_3\kappa^2\tau + \frac{1}{4}k_{22}\kappa^4 + \frac{1}{2}k_4\kappa^2\tau^2 \\ & + k_5\kappa^4\tau + k_{51}(\kappa^4\tau + \kappa^2\tau^3) + k_{61}\kappa^6 \\ & + k_{62}\kappa^4\tau^2 + k_{64}(\kappa^6 + \kappa^4\tau^2) \\ & + k_{65}(\kappa^6 + \kappa^2\tau^4 + \kappa^4\tau^2), \end{aligned} \tag{8}$$

which, with the following replacements,

$$\begin{aligned} & k_{51} + k_5 \to k_5, \\ & k_{61} + k_{64} \to k_6, \\ & k_{62} + k_{64} + k_{65} \to k_{61}, \\ & k_{65} \to k_{62} \quad \text{and} \quad \kappa^2 \to y, \end{aligned} \tag{9}$$

becomes,

$$\begin{aligned} f = {} & \frac{1}{2}k_2 y + k_3 y\tau + \frac{1}{4}k_{22}y^2 + \frac{1}{2}k_4 y\tau^2 + k_5 y^2\tau \\ & + k_{51}y\tau^3 + k_6 y^3 + k_{61}y^2\tau^2 + k_{62}y\tau^4, \end{aligned} \tag{10}$$

where $k_2 > 0$ [14] and $y = \kappa^2 > 0$. In the next section, we will discuss the coexistence of the bistables based on the above energy density (10).

3. Two energy minima of the filament

For simplicity, all elastic moduli can be scaled relative to k_2, i.e., $k_2 = 1$. The first and the second derivative of f (10) with respect to y and τ are then given by,

$$\begin{aligned} f'_y = {} & \frac{1}{2} + k_3\tau + \frac{1}{2}k_4\tau^2 + k_{51}\tau^3 + k_{62}\tau^4 \\ & + \frac{1}{2}k_{22}y + 2k_5 y\tau + 2k_{61}y\tau^2 + 3k_6 y^2, \end{aligned} \tag{11}$$

$$\begin{aligned} f'_\tau = {} & y(k_3 + k_4\tau + 3k_{51}\tau^2 + 4k_{62}\tau^3 \\ & + k_5 y + 2k_{61}\tau y), \end{aligned} \tag{12}$$

$$f''_{yy} = \frac{1}{2}k_{22} + 2\tau(k_5 + k_{61}\tau) + 6k_{61}y, \tag{13}$$

$$f''_{\tau\tau} = y(k_4 + 6\tau(k_{51} + 2k_{62}\tau) + 2k_{61}y), \tag{14}$$

$$\begin{aligned} f''_{\tau y} = {} & k_3 + 2k_5 y \\ & + \tau(k_4 + 3k_{51}\tau + 4k_{62}\tau^2 + 4k_{61}y). \end{aligned} \tag{15}$$

For our purpose to give solutions representing the bistable helical conformations, we must require that either helix be in energy minimum state. Therefore, these states must satisfy following five equations:

$$\begin{aligned} & f'_y = 0, \\ & f'_\tau = 0, \\ & f''_{yy} > 0, \\ & f''_{\tau\tau} > 0, \\ & f''_{yy}f''_{\tau\tau} - f''^2_{\tau y} > 0. \end{aligned} \tag{16}$$

In addition, an inequality should be added for the helical conformations are energetically preferred only when their energies lower than a straight line whose energy density f is zero [13]; and it is,

$$f < 0. \tag{17}$$

The mathematical way to tackle this problem is firstly to associate two equalities in Eqs. (16) to find the solutions for y and τ, then substituting these solutions into the inequalities in Eqs. (16) and (17) to see under what set of parameters the bistable helices are possible. Lengthy calculation can show that without the sixth-order terms, i.e., $k_6 = k_{61} = k_{62} = 0$, Eqs. (16) and (17) give no satisfactory solution. This is why we resort to the sixth-order theory.

Since the equation determining τ is a sixth-order one, we can always obtain two torsions with plus and minus sign, respectively. For demonstrating that our theory is successful, we match our theory with two experimental results in the following.

Case 1. The occurrence of bistable helices is equally probable. In an experiment, Li et al. used a Ti catalyst at 770 °C and found that two types of carbon tubes with left and right handedness, respectively, have almost the same number [9]. The experimental group measured the pitch p and radius r of the helices and found that pitch $p = 0.23$ µm and radius $r = 0.11$ µm, respectively; i.e., curvature and torsions are $\kappa = 8.1/\mu\text{m}$, $\tau = \pm 2.7/\mu\text{m}$, respectively. Then two equalities in Eqs. (16) give four independent equations. To note that in this case the energies for each type of chirality are equal. So we have five equations whose compatibility determines five parameters. A convenient choose of these parameters is

$$k_3 = k_5 = k_{51} = 0,$$
$$k_{22} = -(1 + 486k_6 + 18k_{61} - 2k_{62})/9,$$
$$k_4 = -2(9k_{61} + 2k_{62}). \tag{18}$$

The vanishing of k_3, k_5 and k_{51} is easily understandable for they stand for chiral dependence of energy density. Now the energy density (10) is $f = \frac{1}{4}\kappa^2(2 + 2k_{61}(-2 + \kappa^2) + 2k_{62}(-2 + \kappa^2) + \kappa^2(-1 - 6k_6 - 4k_6\kappa^2)$ in length unit (1/2.7) µm and in energy unit k_2. There are many sets of parameters (k_6, k_{61}, k_{62}) giving satisfactory solutions to Eqs. (16) and (17). For instance, we find a set of parameters $(k_6, k_{61}, k_{62}) = (1/12304, 1/21, 1/3)$ being theoretically satisfactory for we have $(f, f''_{yy}, f''_{\tau\tau}, f''_{yy}f''_{\tau\tau} - f''^2_{\tau y}) = (-1.2, 0.03, 24, 0.02)$.

Case 2. The occurrence of bistable helices is not equally probable. In another experiment, Volodin et al. used a Si substrate to produce two kinds of helically coiled carbon tubes [10]. For the right-handed helix pitch $p = 0.25$ µm and radius $r = 0.95$ µm, i.e., $\kappa = 8.96/\mu\text{m}$ and $\tau = 3.75/\mu\text{m}$; and for left-handed helix the pitch $p = 0.50$ µm and radius $r = 0.85$ µm, i.e., $\kappa = 6.27/\mu\text{m}$ and $\tau = -5.87/\mu\text{m}$. Then two equalities in Eqs. (16) give four independent equations whose compatibility determines four parameters in length unit (1/3.75) µm and in energy unit k_2,

$$k_{22} = -0.53 + 3.43k_3 + 22.0k_5 + 7.29k_{51} + 0.43k_{62}, \tag{19}$$
$$k_4 = 2.21k_3 + 8.98k_5 + 12.1k_{51} - 15.4k_{62}, \tag{20}$$
$$k_6 = 0.01 - 0.09k_3 - 0.65k_5 - 0.13k_{51} - 0.06k_{62}, \tag{21}$$
$$k_{61} = -0.28k_3 - 1.29k_5 - 1.32k_{51} + 1.00k_{62}. \tag{22}$$

There are also many sets of parameters $(k_3, k_5, k_{51}, k_{62})$ giving satisfactory solutions to all Eqs. (16) and (17). For instance, we find a set of parameters $(k_3, k_5, k_{51}, k_{62}) = (-1, -1/6, 9/8, 25/32)$ being theoretically satisfactory for we have that for right-handed helix, $(f, f''_{yy}, f''_{\tau\tau}, f''_{yy}f''_{\tau\tau} - f''^2_{\tau y}) = (-0.31, 0.18, 66, 0.31)$, whereas for the left-handed, $(f, f''_{yy}, f''_{\tau\tau}, f''_{yy}f''_{\tau\tau} - f''^2_{\tau y}) = (-0.37, 0.17, 25, 2.47)$.

4. Summary

After generalizing Helfrich's theory of elastic filament from the original fourth-order theory to the sixth-, the coexistence of bistable helices with opposite handedness is explained. Two sets of the experimental result on helically coiled carbon tubes are used to demonstrate the validity of our theory. In our approach, we cannot fix all elastic moduli theoretically but impose some limitations on the intervals of their values (17). In fact, in some cases, more elastic moduli can be determined. For example, in the production of helical conformations of carbon tubes under the same environment, more than two sets of pitch and radius can frequently be observed. The degrees of freedom in elastic moduli can then be reduced by examining the simultaneous appearance of other helical formations, which is not the purpose of present Letter and will be done elsewhere.

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