Novel relationships between some coordinate systems and their effects on mechanics of an intrinsically curved filament

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Abstract
The fixed frame, Frenet-Serret frame and generalized Frenet-Serret frame are commonly used coordinate systems in the study of a filament or a moving rigid body. In terms of Eulerian angles, we derive some relations in these frames and apply these relations to find some significant results. Especially, we find the angle between the normal of centerline of a filament and the line of nodes which is the crossover between the horizontal plane of fixed frame and normal plane of centerline. We prove that the general solution of a set of nonlinear differential equations represents a circular helix or the corresponding filament has a unique helical ground-state configuration. We show that the effective description of a planar filament depends on the value of its torsional modulus. Finally, we find the expression of energy for a three-dimensional intrinsically curved filament when its cross-section area vanishes, and show that under an applied force the finite intrinsic curvature alone can induce a discontinuous transition in extension.

1. Introduction
Filamentary structure is ubiquitous in the world and it has wide applications in engineering and science so that the study on the conformal and mechanical properties of a filament has a long history dating back to Euler and Lagrange [1, 2]. The interest in filaments has been increasing owing to that recent experiments and theories have revealed its relevance to microscopic objects such as carbon nanotubes [3] and biomaterials [4–29].

The configuration of a filament is determined by the shape of its centerline and the twist of its cross-section around the centerline. The centerline of a filament is a curve passing through the center of cross-section, so that it can be described by the Frenet-Serret equations introduced in differential geometry [30, 31]. The Frenet-Serret equations define a local Cartesian coordinate system and we refer to it as Frenet-Serret frame. The Frenet-Serret frame can also be used to describe the trajectory of a particle or the center-of-mass of a many-body system. However, a curve has vanishing cross-section so that the Frenet-Serret frame cannot describe the twist of cross-section of a filament. Therefore, when the twist is significant, it is commonly to use another local frame called generalized Frenet-Serret frame [4–10] to study a filament. Meanwhile, to study the motion of a rigid body, in classic mechanics it is more convenient to use Eulerian angles [32] so introduces Euler body-frame which can be identified to the generalized Frenet-Serret frame [4–10]. Moreover, to specify the position of a filament completely it also needs a fixed frame. The relationships between these frames are therefore very important. In particular, Eulerian frame introduces a line-of-nodes which is a line perpendicular to the tangent of centerline of the filament and lies on the horizontal plane of the fixed frame. Note that the normal of centerline is also perpendicular to tangent, we can ask an intriguing question, i.e., would the line-of-nodes coincide with the normal of centerline? The answer to this question helps us to find some significant results as we will report in this paper. Moreover, when the cross-section area of filament tends to zero, independent variables are reduced from 3 (Eulerian angles \( \theta, \phi \) and \( \psi \)) to 2 (curvature and torsion, or \( \theta \) and \( \phi \)), what is \( \psi \) in this limit? The answer to this question helps us to set up a three-dimensional (3D) elastic model to study the effect of a finite intrinsic-curvature (IC) on the mechanical property of a filament.
The conformal and mechanical properties of a filament depend on its intrinsic properties and external physical conditions. In elastic theory, the intrinsic properties are usually characterized by some macroscopic parameters [1, 2, 4–10], such as bending rigidity, twisting rigidity and inertia tensor. On the other hand, external conditions are often referred to as applied forces, applied torques and boundary conditions (BCs). Focusing on different physical properties results in different elastic models. The simplest model is the wormlike chain (WLC) model [11–14] which views a filament as an inextensible chain with a certain bending rigidity but a vanishing cross-section area. Owing to its slender shape, a semiflexible biopolymer is usually modeled as a filament so that the WLC model has been used to account for the entropic elasticity of some semiflexible biopolymers successfully [11–14]. Another often used model is the wormlike rod chain (WLRC) model [6, 12–17] which regards a filament as a chain with a nonvanishing intrinsic twist and a circular cross-section. The WLRC model has been applied successfully to explain supercoiling properties of some double stranded DNA (dsDNA). Both WLC and WLRC models are intrinsically straight or both of them have a vanishing IC. In other words, free of external force and torque, their ground-state configurations (GSCs, or spontaneous configurations, i.e., the configurations with the lowest energy) are a straight line and a cylinder with straight centerline, respectively. Moreover, at a finite temperature (T) the extension of both models is a smooth function of applied force.

However, filaments or semiflexible biopolymers are not always intrinsically straight. For instance, for short dsDNA chains, special sequence orders favor a finite IC [33–36]. Meanwhile, with a long-range correlation in sequence, dsDNA develops a macroscopic (intrinsic) curvature so that WLC model fails to account for its property [18]. Moreover, an intrinsically curved filament has complete different mechanical properties from that of WLC and WLRC models [9, 10, 19–24]. In 3D case, both exact theoretical analysis and experimental observation revealed that an intrinsically curved and twisted biopolymer can form a stable helix and under an applied force the extension of helix can subject to a discontinuous transition [9, 10, 19, 20, 23, 24]. On the other hand, in two-dimensional (2D) case it has been shown that a finite IC alone is enough to induce a discontinuous transition in extension for a stretched filament [21, 22]. Since it is uneasy to realize an ideal 2D system, to compare with experiment it should be better to study a 3D system to check whether a nonvanishing IC alone is enough to induce the discontinuous transition. In this paper we answer this question.

On a 2D system, we have to recall that there are two planar elastic models for an intrinsically curved filament, and they have quite different mechanical properties [18, 21, 22, 25–27]. Especially, the extension of model 1 can undergo a discontinuous transition under a stretching force [21, 22]; but the extension of model 2 is always a smooth concave function of applied force [22]. However, there is only one 3D model in this case, as we will show in this paper. How to obtain two different planar models from the 3D model? We clarify this problem in this paper.

The paper is organized as follows. In the next section we introduce different frames to describe a filament. In section 3 we set up elastic models. In section 4 we derive some novel relationships for variables in different frames. In section 5 we apply these relations to study mechanical property of an intrinsically curved filament. Finally, the conclusions and discussions conclude the paper.

2. Description of a filament

2.1. Frenet-Serret frame

Using arclength s as variable, the position vector of a curve in a 3D fixed Cartesian coordinate system is written \( \mathbf{r}(s) = (x(s), y(s), z(s)) \). The unit tangent of the curve is defined as \( \mathbf{t}(s) \equiv \frac{d\mathbf{r}}{ds} \), and symbol \( \cdot \) represents the derivative with respect to \( s \). The curvature, \( \kappa(s) \), of the curve is given by

\[
\mathbf{t} = \kappa(s) \mathbf{n},
\]

where \( \mathbf{n} \) is the unit normal. It requires \( \kappa \geq 0 \) in 3D case and \( |\mathbf{t}| = 1 \) results in \( \mathbf{t} \perp \mathbf{n} \). We can define further a binormal unit vector by \( \mathbf{b} = \mathbf{t} \times \mathbf{n} \), so that \( \mathbf{t}, \mathbf{n} \) and \( \mathbf{b} \) form a local right-hand Cartesian coordinate system, i.e., the Frenet-Serret frame, and

\[
\mathbf{n} = -\kappa(s) \mathbf{t} + \tau(s) \mathbf{b}, \quad \mathbf{b} = \frac{d(\mathbf{t} \times \mathbf{n})}{ds} = -\tau(s) \mathbf{n},
\]

where \( \tau \) is the torsion and represents the rotational rate of \( \mathbf{n} \) around \( \mathbf{t} \). The plane perpendicular to \( \mathbf{t} \) is called normal plane. Clearly, both \( \mathbf{n} \) and \( \mathbf{b} \) lie on the normal plane. We can then find \( \kappa \) and \( \tau \) from

\[
\kappa^2 = |\mathbf{t}|^2, \quad \tau = \mathbf{t} \cdot (\mathbf{t} \times \mathbf{t}) / \kappa^3.
\]

Equations (1)–(2) are called Frenet-Serret equations. In differential geometry, it has been shown that once \( \kappa \) and \( \tau \) are known, the shape of a curve is completely determined [30, 31].

The necessary and sufficient condition to have a planar curve is \( \tau = 0 \) at arbitrary \( s \). On the other hand, a general helix is defined as a curve in which \( \mathbf{t} \) makes a constant angle with a fixed direction. This condition is
equivalent to that $\kappa/\tau$ is $s$–independent. When both $\kappa$ and $\tau$ are $s$–independent, the helix is called a circular helix.

2.2. Generalized Frenet-Serret frame

Frenet-Serret equations cannot describe the twist of cross-section of a filament so that we need to generalize them. For a filament with a finite cross-section, we can still represent its centerline by $r$, but it is more convenient to describe its configuration by a triad of unit vectors \( \{ t_i(s) \}_{i=1,2,3} \), where $t_3 \equiv t_1$ and $t_2$ are oriented along the principal axes of cross-section [1, 4–8]. The orientation of the triad is given by the solution of generalized Frenet equations [1, 8, 20, 28],

$$t_i(s) = -\sum_{j,k=1}^{3} \epsilon_{ijk}\omega_j(s)t_k(s),$$

or $t_i = \omega \times t_i$, where $\epsilon_{ijk}$ is the antisymmetric tensor, and $\omega = \omega_1 t_1 + \omega_2 t_2 + \omega_3 t_3$ is a vector in which $\omega_1$ and $\omega_2$ are components of curvature so $\kappa^2 = \omega_1^2 + \omega_2^2$, and $\omega_3$ is the twist rate. $t_1$, $t_2$, and $t_3$ form another local coordinate system and we call it as generalized Frenet-Serret frame.

$t_1$ and $t_2$ are coplanar with $n$ and $b$, so that we can rotate the Frenet-Serret frame counterclockwise an angle $\alpha$ around the common axis $t$ to the generalized Frenet-Serret frame, i.e.,

$$t_1 = \cos \alpha n + \sin \alpha b, \quad t_2 = -\sin \alpha n + \cos \alpha b.$$  \hspace{1cm} (5)

From equations (2)–(5), it is straightforward to show

$$\omega_1 = c \sin \alpha, \quad \omega_2 = c \cos \alpha, \quad \omega_3 = \tau + \chi.$$ \hspace{1cm} (6)

It follows that in general $\omega_3 \equiv \tau$, or $s$–independent $\kappa$ and $\omega_3$ do not result in a helical centerline automatically. Clearly $\alpha$ represents the distortion of cross-section around the centerline.

Note that independent variables in two frames are different. There are two independent variables, $\kappa$ and $\tau$, in Frenet-Serret frame; but there are three independent variables, $\omega_1$, $\omega_2$ and $\omega_3$, in generalized Frenet-Serret frame. Equation (6) provides the relations between these variables.

2.3. In Eulerian angles

In mechanics, it is convenient to use Eulerian angles to describe the motion of a rigid body [32]. The Eulerian angles give relations between a fixed coordinate system and a body-frame rigidly embedded in the rigid body. The same ideas can be readily applied to describe the configuration of a filament by using the generalized Frenet frame as the body-frame and replacing time used in a moving body by $s$ [5–10, 29], since intuitationally the configuration of a filament looks like the trajectory of a flat rigid thin plate. The line common to $x$ – $y$ plane in the fixed frame and $t_1$ – $t_2$ plane is called the line-of-nodes, shown as the green-line in figure 1, where $\xi$ is the unit vector along green-line. The Eulerian angles are generated by three rotations to move the fixed frame into the body-frame [32], as shown in figure 1. The first rotation is through $\phi$, the angle between $x$-axis and line-of-nodes, about $z$-axis so to move $x$-axis into the line of nodes. The second rotation is through an angle $\theta$ about the line-of-nodes, to move $z$-axis to $t$-axis. The final rotation is through an angle $\psi$ about $t$-axis to move $y$-axis into $t_2$-axis.

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**Figure 1.** Rotations defining Eulerian angles. $\xi$ indicates the direction of line-of-nodes.
Replacing $s$ by time, $\omega$ becomes the angular velocity of a rigid body, so we have [32]

$$\omega_1 = \sin \theta \sin \psi \dot{\phi} + \cos \psi \dot{\theta},$$

$$\omega_2 = \sin \theta \cos \psi \dot{\phi} - \sin \psi \dot{\theta},$$

$$\omega_3 = \cos \theta \dot{\phi} + \psi.$$  \tag{7}

In this convention, in fixed frame we can write [32]

$$\mathbf{t} = (\sin \phi \sin \theta, -\cos \phi \sin \theta, \cos \theta),$$

$$t_1 = (\cos \phi \cos \psi - \cos \theta \sin \phi \sin \psi, \sin \phi \cos \psi + \cos \theta \cos \phi \sin \psi, \sin \theta \sin \psi),$$

and $t_2 = t \times t_1$.

Using equations (3) and (10), we can express $\mathbf{t}$, $\mathbf{n}$, $\kappa$ and $\tau$ in Eulerian angles explicitly, as

$$\mathbf{t} = \mathbf{n} = (\cos \theta \sin \phi \dot{\theta} + \cos \phi \sin \theta \dot{\phi},$$

$$- \cos \theta \cos \phi \dot{\theta} + \sin \theta \sin \phi \dot{\phi}, -\sin \theta \dot{\phi}),$$

$$\kappa = \sqrt{\dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2} = \sqrt{\omega_1^2 + \omega_2^2},$$

$$\tau = \cos \theta \dot{\phi} + \frac{\sin \theta (\dot{\theta} \dot{\phi} - \dot{\phi} \dot{\theta}) + \cos \theta \dot{\phi}^2}{\epsilon^2} = \cos \theta \dot{\phi} + d\arctan(\sin \theta \dot{\phi} / \dot{\theta}) / ds.$$ \tag{14}

Equation (14) suggests that for a planar curve, it is always possible to choose $\phi = 0$ so $\tau = 0$ by a proper rotation of the fixed frame.

The advantage of using Eulerian angles to study a filament is that it satisfies $|\mathbf{t}| = 1$ automatically, so we do not need to consider it as a constraint in many calculations and it may simplify calculations greatly.

### 3. Elastic models of a filament

#### 3.1. 3D model

The energy for a 3D filament with a finite IC $\kappa_0$, a finite intrinsic-twist rate $\tau_0$ and under a uniaxial force (along the $z-$axis) is [5–10, 29]

$$E_{3D} = \int_0^L \mathcal{E} ds \equiv \int_0^L (\mathcal{E}_0 - f \cos \theta) ds,$$

$$\mathcal{E}_0 = \frac{k_1}{2}(\omega_1 - \kappa_0)^2 + \frac{k_2}{2}(\omega_2 - \kappa_0)^2 + \frac{k_3}{2}(\omega_3 - \tau_0)^2,$$ \tag{15}

where $k_1$, $k_2$ are bending rigidities and $k_3$ the twisting rigidity or torsional modulus, respectively. $\kappa_0$, $\omega_0$ are components of $\kappa_0$ and $\omega_0$. When $\kappa_0 = \tau_0 = 0$, it reduces into the WLC model.

When $\kappa_0 = \tau_0 = 0$, replacing $s$ by time, $\mathcal{E}$ becomes the Lagrangian of a rigid body with one point fixed and under a constant force, and $k_3$ becomes principal moment of inertia [32]. When $\kappa_0 = 0$ or $\tau_0 = 0$, we can regard $k_1(\omega_1 - \kappa_0) + k_2(\omega_2 - \kappa_0) + k_3(\omega_3 - \tau_0)$ as a special potential energy, though it is difficult to find an analogy in the dynamics of a rigid body, owing to the complex of $\omega_1$.

#### 3.2. 2D models

In 2D case, we can write $\mathbf{t} \equiv \mathbf{r} = (\cos \theta, \sin \theta)$ with $\mathbf{r} = (y, z)$. There are two elastic models for a 2D intrinsically curved filament [18, 25–27]. The energy of the model 1 is [18, 21, 22, 25–27]

$$E_1 \equiv \int_0^L \frac{k}{2}(\dot{\theta} - \kappa_0)^2 ds - f z(L),$$ \tag{16}

where $\dot{\theta} \equiv \dot{y} \dot{z} - \dot{z} \dot{y}$ is the signed curvature, $\kappa_0$ is the intrinsic signed curvature, and $|\dot{\theta}| = |\mathbf{t}|$. In this model, $\dot{\theta}$ and $\kappa_0$ can be either positive or negative. Meanwhile, the energy of the model 2 is [27]

$$E_2 \equiv \int_0^L \frac{k}{2}(|\dot{\theta}| - \kappa_0)^2 ds - f z(L).$$ \tag{17}

In this model, $|\dot{\theta}|$ is curvature.

These two models have very different mechanical properties [21, 22, 27]. Especially, model 1 shows a discontinuous change in $z(L)$ with a varying $f$ [21, 22]; but there is no such a transition in model 2 [27].
4. Some important relations in variables

4.1. A relation between $\alpha$ and Eulerian angles

Equation (6) provides a relation between Frenet-Serret and generalized Frenet-Serret frames. However, using equation (6) to calculate $\alpha$ is uneasy in many cases so that some other ways to calculate $\alpha$ are useful. A related intriguing problem is that after a comparison between equations (6) and (9), we can ask would $\alpha = \psi$? Since $\alpha - \psi$ is the angle between $n$ and $\xi$, the problem is equivalent to finding the relation between $\alpha$ and $\xi$. To find this relation we can combine equations (6), (9) and (14) so obtain

$$\alpha = \psi - \arctan(\sin(\theta \phi / \bar{\theta})) + \beta,$$

where $\beta$ is a $s$–independent constant. From equations (6)–(7), we find further

$$\omega_1 = 0 = \sin \theta \sin \psi \bar{\phi} + \cos \psi \bar{\theta} \text{ or } \tan \psi = -\bar{\theta} / \sin \theta \bar{\phi} \text{ when } \alpha = 0.$$

It follows $\beta = \pi/2$ and

$$\alpha = \psi + \arctan(\bar{\theta} / \sin \theta \bar{\phi}). \tag{19}$$

Equation (19) indicates that $\alpha = \psi$ requires either $\bar{\phi} = 0$ or $\bar{\theta} = 0$, $\bar{\phi} = 0$ gives a planar centerline and $\bar{\theta} = 0$ gives a helical centerline. In more general cases $\alpha \neq \psi$, or $n$ does not coincide with $\xi$.

4.2. Relations in variables when the cross-section area vanishes

Next we consider another unsolved question, i.e., when the cross-section area vanishes, the filament becomes a curve so that we need only two variables, $\theta$ and $\phi$, to describe it, in this case what are the limiting forms of $\psi$? Could we simply take $\psi$ as a $s$–independent constant or even $\psi = 0$ in equations (7)–(9) and (15)? Physically in this case we can ignore the distortion of cross-section and set $\alpha = 0$ so $\omega_3 = \tau$, and then from equation (19) it follows

$$\psi = -\arctan(\bar{\theta} / \sin \theta \bar{\phi}), \sin \psi = -\bar{\theta} / c, \cos \psi = \sin \theta \bar{\phi} / c. \tag{20}$$

Therefore, in general $\psi$ cannot be $s$–independent, $\psi$ is $s$–independent, being $0$ or $-\pi/2$, only when either $\bar{\theta} = 0$ or $\bar{\phi} = 0$, i.e., the filament becomes a helix or a planar curve.

Equations (14), (19) and (20) are very useful and we will apply them to solve some intriguing problems for an intrinsically curved filament.

5. Mechanical property of an intrinsically curved filament

5.1. GSC of the general model when $f = 0$

A very important question on the general 3D model, given by equation (15), is whether it has a unique GSC when $f = 0$. In this case, the GSC of the model is given by $\xi = 0$ so $\omega_1 = \kappa_{01}, \omega_2 = \kappa_{02}$ and $\omega_3 = \tau_0$. Therefore, from equations (7)–(9), we obtain

$$\dot{\theta} = \kappa_{01} \cos \psi - \kappa_{02} \sin \psi, \tag{21}$$

$$\dot{\phi} = (\kappa_{02} \cos \psi + \kappa_{01} \sin \psi) / \sin \theta, \tag{22}$$

$$\dot{\psi} = \tau_0 - (\kappa_{02} \cos \psi + \kappa_{01} \sin \psi) / \tan \theta, \tag{23}$$

$$\kappa^2 = \kappa_0^2 = \kappa_{01}^2 + \kappa_{02}^2. \tag{24}$$

We should stress again that in general $\omega_3 = \tau_0$ is not equivalent to $\tau = \tau_0$. For instance, when $\kappa_0 = 0$, the general solution of equations (21)–(23) is simply a straight twisted cylinder so that $\tau = 0$ but $\alpha = \tau_0$.

When $\kappa_0 \neq 0$, the general solution of equations (21)–(23) is unavailable in literature, and there is not a direct way to find the general solution since these equations are nonlinear. Moreover, even if we could find the general solution, it should have three undetermined parameters and be rather complex, so that it would be difficult to justify the uniqueness of corresponding configuration. Note that it is not necessary to have a unique GSC for every physical model. A typical example is that the model given by equation (17) has uncountable GSCs when $f = 0$ [22]. Fortunately, using equation (19) we can solve this problem readily in an indirect way. Substituting equations (21)–(23) into equation (19), we obtain $\alpha = \psi$. It follows $\omega_3 = \tau = \tau_0$ from equation (6). In other words, when $f = 0$ and $\kappa_0 \neq 0$, the model takes a circular helix as its unique GSC. Note that this conclusion is valid even if $k_0, k_1$ and $k_2$ are $s$–dependent.

We can find a particular solution of equations (22)–(23) by taking $\theta$ as a $s$–independent constant, i.e., let the axis of helix along $z$–axis, so $\tan \psi = \kappa_{01} / \kappa_{02}$, $\tan \theta = \kappa_{02} \sec \psi / \tau_0$ and $\dot{\phi} = \kappa_{02} \csc \theta \sec \psi$. $\psi$ and $\dot{\phi}$ are also $s$–independent in the solution. All other forms of solution can be obtained by a coordinate transformation from this solution. When $\tau_0 = 0$, we get $\theta = \pi/2$ so the GSC becomes a circle. Moreover, $\kappa_{02} = 0$ leads to $\theta = 0$ so gives a straight centerline.
Note that the above conclusions are based on $k_3 > 0$ which leads to equation (23). When $k_3 = 0$, there is not equation (23) so that we have only two equations, equations (21)–(22), but three unknowns, consequently there are infinite numbers of GSCs. In fact, when $k_3 = 0$, the filament can be arbitrarily twisted so that $\psi(s)$ or $\alpha(s)$ can take arbitrary values. Moreover, from equations (21)–(22) we know that $\dot{\theta}$ is coupled to $\phi$ and $\psi$ when $\kappa_0 \neq 0$, so that infinite possibility of $\psi$ results in infinite numbers of GSC.

We should address that the method used here should also be instructive in solving other nonlinear differential equations. This is because $\kappa$ and $\tau$ determine the shape of a curve completely [30, 31], and to find $\kappa$ and $\tau$ so identify the solution curve in many cases may be much easier than to find a solution directly.

5.2. $\kappa_{01}$ and $\kappa_{02}$ when the cross-section area vanishes

Another intriguing question is that when the cross-section area vanishes, how to assign $\kappa_{01}$ and $\kappa_{02}$ in $E_3$? To answer this question we can substitute equation (20) into equations (7)–(8) so obtain $\omega_1 = 0$ and $\omega_2 = \kappa$, as well as $\kappa_{01} = 0$ and $\kappa_{02} = \kappa_0$ since at $f = 0$ its GSC has $\kappa^2 = \kappa_{01} + \kappa_{02}$. Note that since $\omega_1$ and $\omega_2$ is either positive or negative, there is not special reason to limit the signs of $\kappa_{01}$ and $\kappa_{02}$ or $\kappa_{02} = \pm \kappa_0$ in this case.

Together with $\omega_3 = \tau$, the energy density in equation (15) is reduced into

$$E_{3D} = \frac{k}{2} (\kappa \pm \kappa_0)^2 + \frac{k_3}{2} (\tau - \tau_0)^2 - f \cos \theta.$$  (25)

This is a natural result for a rigid curve since $\kappa$ and $\tau$ are two independent variables for its shape. In 3D case, we only need to take sign ‘+’ in the first term of $E_{3D}$ since it requires $\kappa > 0$ and $\kappa_0 > 0$. However, to be consistence with 2D models, retaining the sign ‘+’ in equation (25) is still necessary, as we will explain later.

From equations (14) and (25), we know that when $k_3 > 0$ the model requires continuous $\dot{\theta} and \dot{\phi}$ implicitly to prohibit $\dot{\theta} \rightarrow 0$ or $\dot{\phi} \rightarrow 0$ since otherwise it results in infinite $\tau$ and $E_{3D}$ at discontinuous points. The same rule should be also applied to the more general model given by equation (15) to avoid undefined $\tau, \alpha$ and $E_{3D}$.

5.3. From 3D model to 2D models

Next we consider another unsolved question: what is the limit form of equation (25) in 2D case? A planar curve requires $\tau = 0$ at arbitrary $s$ and from equation (14) it is equivalent to $\dot{\phi}(s) = 0$. Consequently, from equations (13) and (25), at first glance the model 2 would be correct. But we have to be careful for the conclusion since these two models have quite different mechanical properties. The key point is that the model 2 allows to change sign of $\dot{\theta}(s)$ at some points [27] or $\dot{\phi}(s)$ without a discontinuous $\dot{\theta}(s)$. However, from the arguments in the last paragraph of section 5.2, we know that $k_3 > 0$ prohibits a discontinuous $\dot{\phi}(s)$. We can confirm this conclusion by looking at a simple case when $\kappa_0$ is independent of $s$. In this case, it is straightforward to find that when $f = 0$ the model 1 has a unique circular GSC but the model 2 has infinite numbers of GSCs [21, 22, 27].

Note that in section 5.1 we have shown that the corresponding 3D model has a unique circular GSC when $f = 0$ and $k_3 > 0$, agreeing with that obtained from the model 1. Therefore, when $k_3 > 0$ the 3D model must be reduced into the model 1.

It is also clear that when $\kappa_0$ keeps the same sign for all $s$, we only need to take sign ‘+’ in the first term of $E_{3D}$.

However, note that in 2D case $\kappa_0$ can be either positive or negative, to maintain a reasonable GSC and be consistent with the 2D model, we need to take the sign ‘+’ in the first term of $E_{3D}$ when $\kappa_0 < 0$. It is also equivalent to adopt the model 1.

In contrast, if $k_3 = 0$ or the effect of $\omega_3$ is negligible, the 3D model should be reduced into the model 2. Ignoring the effect of torsion completely is impractical for a macroscopic filament, but may be a good approximation for some biopolymers. The model 2 is analogous to a free rotating chain model for biopolymers.

In conclusion, exactly two planar elastic models of a filament come from a same 3D model. The model 1 corresponds to taking $k_3 > 0$ in $E_{3D}$ but the model 2 corresponds to taking $k_3 = 0$. Therefore, $k_3$ or the torsional term in energy disappears in 2D models, the effective description of a planar filament still strongly depends on the value of $k_3$.

5.4. Shape equations and boundary conditions for a 3D system with vanishing cross-section

Equation (25) can help clarify the role of a finite $\kappa_0$ to the transition in $z(L)$ for a 3D filament. Using standard variational technique to extremize $E_{3D}$, we obtain the shape equations:

$$\frac{d^2}{ds^2} \left( \frac{\partial E_{3D}}{\partial \theta} \right) - \frac{d}{ds} \left( \frac{\partial E_{3D}}{\partial \dot{\theta}} \right) + \frac{\partial E_{3D}}{\partial \theta} = 0,$$

(26)

$$\frac{d}{ds} \left( \frac{\partial E_{3D}}{\partial \phi} \right) - \frac{\partial E_{3D}}{\partial \dot{\phi}} = 0,$$

(27)
and six BCs
\[ \frac{\partial E_{3D}}{\partial \theta} \bigg|_{\theta=0} = 0, \quad \frac{\partial E_{3D}}{\partial \phi} \bigg|_{\phi=0} = 0, \]
\[ \frac{d}{ds} \left( \frac{\partial E_{3D}}{\partial \theta} \right) - \frac{\partial E_{3D}}{\partial \theta} \bigg|_{\theta=0} = 0. \]  

Equation (26) is a 4th-order nonlinear differential equation in \( \theta \) and equation (27) is a 2nd-order nonlinear differential equation in \( \phi \). Full expressions of both equations are lengthy so we do not present them here. To derived these expressions are rather easy by using some softwares, such as Mathematica.

Note that at both \( s = 0 \) and \( s = L \) using
\[ \frac{\partial E_{3D}}{\partial \theta} = \frac{\partial E_{3D}}{\partial \phi} = \frac{d}{ds} \left( \frac{\partial E_{3D}}{\partial \theta} \right) - \frac{\partial E_{3D}}{\partial \theta} = 0, \]

implies that \( \phi(0), \phi(L), \theta(0), \theta(L), \dot{\theta}(0) \) and \( \dot{\theta}(L) \) are free, or adopt the hinged-hinged BCs. The hinged-hinged BCs is also the most commonly used BC in force experiment for a biopolymer. In contrast, one can adopt fully fixed BCs so take \( \phi(0), \phi(L), \theta(0), \theta(L) \) and \( \dot{\theta}(L) \) as constants. We can also choose partial fixed and partial free BCs. Results obtained from different BCs usually require different constraints so are basically different.

Since the model 1 in 2D case corresponds to having a finite \( k_3 \) in 3D case and under an applied force the model 1 shows a discontinuous jump in \( z(L) \), we focus on the case with \( k_3 > 0 \) henceforth.

To find the general solution of shape equations is an arduous task and so does to show exactly that there is a unique solution though physically in most cases the solution should be unique. However, we can examine two simple solutions. The first possible solution is a planar curve and the second is a helix.

Equations (26)–(29) are valid even when \( \kappa_0, \tau_0, k \) and \( k_3 \) are \( s \)-dependent. But in this work we focus on the effect of a finite \( \kappa_0 \) so that for simplicity we assume \( \kappa_0, \tau_0, k \) and \( k_3 \) are all \( s \)-independent henceforth. Moreover, without loss of generality we also assume \( \tau_0 \geq 0 \).

5.5. Planar curve solution
A planar curve requires \( \phi(s) = 0 = \tau \), so that the shape equations are simplified into
\[ k\dot{\theta} = f \sin \theta, \quad k_3 \tau_0 \cos \theta = 0. \]

Therefore, the first important conclusion is that there is not any planar solution when \( \tau_0 = 0 \).

When \( \tau_0 = 0 \), one shape equation and one BC vanish, and the remained shape equation and BC are reduced into
\[ k\dot{\theta} = f \sin \theta, \quad (\theta - \kappa_0) \dot{\theta} \bigg|_{\theta=0} = 0. \]

\( k_3 \) is irrelevant in this case owing to \( \tau = 0 \). Equation (32) recovers the shape equation and BC for model \( 1 \) [21, 22, 26]. The corresponding 2D system has been studied thoroughly [21, 22, 26] and the main conclusions are: in ground state \( z(L) \) can undergo a multiple-step discontinuous transition. The transition is accompanied by unwinding loops, and the critical force reaches a limit quickly with decreasing number of loops [21]. Owing to symmetry, it is natural that free of twist the 3D filament has the same behavior as that of the 2D filament.

5.6. Helix solution
On the other hand, for a helix solution, substitute a \( s \)-independent \( \theta \) into shape equations, we obtain
\[ \phi = \frac{\kappa_0 k \sqrt{1 - z_r^2} + k_3 \tau_0 z_r}{k_3 z_r^2 + k(1 - z_r^2)}, \]
\[ F = \frac{(z_r - \kappa \tau \sqrt{1 - z_r^2})(\kappa_0 k z_r + \sqrt{1 - z_r^2})}{\sqrt{1 - z_r^2}(1 + (k_r - 1)z_r^2)^2}, \]
\[ \mathcal{E}_h = \frac{\kappa_z z_r^4[(k_r - 1)z_r^2 - 1] + \kappa_z^2 [1 + (3k_r - 2)z_r^2 - (k_r - 1)z_r^4]}{2[1 + (k_r - 1)z_r^2]^2} + \frac{\kappa_z z_r^2[1 - z_r^2 - k_r(2 - z_r^2)]}{\sqrt{1 - z_r^2}(1 + (k_r - 1)z_r^2)^2}, \]

where \( F \equiv f / \kappa_0 k_3, \mathcal{E}_h = \mathcal{E}_{3D} / \kappa_0^2 k_3, \kappa_r = \tau_0 / \kappa_0 \) and \( k_3 = k_3/k, z_r \equiv z(L)/L = \cos \theta \) is the relative extension and \( 1 \geq z_r \geq 0 \) for a helix since without loss of generality we can choose \( \tau/2 \geq \theta \geq 0 \). It follows that \( \phi \) is also \( s \)-independent and so does for \( \tau \) since equation (14) gives \( \tau = \cos \theta \dot{\phi} \). Therefore, the filament forms a circular helix. Note that either \( k_3 = 0 \) or \( k = 0 \) leads to \( f = 0 \) or no helix at a finite \( f \).
Four BCs vanish automatically for the helical solution and the remained BCs become

\[
(\dot{\phi} z_r - \tau_0) \delta \thicksim_{l=0}^1 = 0. \tag{36}
\]

If we choose the hinged-hinged BC, from equation (36) we obtain one more equation, i.e., \( \dot{\phi} = \tau_0 / z_r \) at both \( s = 0 \) and \( s = L \). However, substituting \( \dot{\phi} = \tau_0 / z_r \) into equations (33)–(34), we obtain \( z_r = \tau_0 \sqrt{\frac{2}{\tau_0^2 + \kappa_r^2}} \), \( f = 0 \), \( \kappa = \kappa_0 \) and \( \tau = \tau_0 \). Therefore, the hinged-hinged BC results in a free-standing helix, but prohibits any helix at \( f = 0 \).

On the other hand, from equation (36) we know that the fixed BC requires \( \dot{\theta}(0) = \dot{\theta}(L) = 0 \). For a helix, \( \theta = \theta(0) \) is already a constant so that the BC does not yield any new equation. In other words, with the fixed BC it is possible to form the helical filament when \( f = 0 \) so that we focus on such a system henceforth in this subsection.

We should point out that a stable configuration requires \( g(z_r) \equiv df / dz_r > 0 \) or extension increases with increasing force. Moreover, if \( g(z_r) \) has more than one real zeros within \( 1 \geq z_r \geq 0 \), there will have an abrupt change in \( z_r \).

From equation (34) we know that when \( \tau_0 = 0 \) it has always \( F \geq 0 \) and \( g(z_r) \) has only one zero at \( z_r = z_1 \equiv 1 / \sqrt{3(\kappa_r - 1)} \). Consequently, when \( k_r < 4/3 \), it has always \( g(z_r) > 0 \) so that the helix is stable. Moreover, when \( k_r > 4/3 \), if \( z_r > z_1, g(z_r) < 0 \) so that the helix is unstable; but if \( z_r < z_1, g(z_r) > 0 \) so that the helix is stable. Therefore, \( \tau_0 = 0 \) and a large \( k_r \) favors the helix with a large \( z_r \). In another limit when \( \kappa_0 = 0 \), we find that when \( k_r < 4/3 \), it has always \( g(z_r) < 0 \) so that the helix is unstable. In contrast, when \( k_r > 4/3 \), if \( z_r < z_1, g(z_r) < 0 \) so that the helix is unstable; but if \( z_r > z_1, g(z_r) > 0 \) so that the helix is stable. In other words, \( \kappa_0 = 0 \) and a large \( k_r \) favors the helix with a large \( z_r \). These results suggest that \( \tau_0 \) and \( \kappa_0 \) play an opposite role in stabilizing a helix. There is no discontinuous transition in \( z_r \) when either \( \tau_0 = 0 \) or \( \kappa_0 = 0 \) since \( g(z_r) \) has only one real zero.

A finite \( \kappa_0 \) results in a significant difference. From equation (34) we find \( g(z_r) \sim k\kappa_0 / z_r \) (1 - \( z_r \)) \( ^{3/2} \)/ 2 \( \sqrt{2} > 0 \) when \( z_r \sim 1 \) so that the helix with a large \( z_r \) is always stable when \( \kappa_0 \tau_0 > 0 \). In another limit, we find \( g(0) = \kappa_0 k_r (1 - \kappa_r^2 k_r) \), so that \( g(0) < 0 \) when \( \kappa_r > 1 / \sqrt{3} k_r \), or the helix with a small \( z_r \) is unstable up to a special \( z_r = z_n \). Numerical calculations of equation (34) show that the larger the \( \kappa_r \) or \( \kappa_0 \), the larger the \( z_r \) or a large \( \tau_0 \) or \( k_r \) favors the helix with a small \( z_r \), as shown in figure 2. From figure 2, we can see that when \( \kappa_r \) is small, \( z_r \) increases quickly with increasing \( \kappa_r \); but when \( \kappa_r \) is large, \( z_r \) increases very slowly. We also find that if \( k_r < 4/3 \), \( z_r \rightarrow 1 \) when \( \kappa_r \rightarrow \infty \); but if \( k_r > 4/3 \), \( z_r \rightarrow z_1 \) when \( \kappa_r \rightarrow \infty \).

Moreover, we find that there may exist a discontinuous transition in \( z_r \) even when \( \kappa_0 \) is small. In a special case, i.e., when \( k_r = 0 \) or \( k_r \rightarrow \infty \), we find exactly that when \( \kappa_r < 4/3 \), it has always \( g(z_r) > 0 \) so that \( z_r \) is a single-valued function of \( F \). However, when \( \kappa_r > 4/3 \), \( g(z_r) \) has always two zeros at

\[
z_r^\pm = \sqrt{(3\kappa_r^2 - 2 \pm \kappa_r \sqrt{9\kappa_r^2 - 16}) / (6 + 6\kappa_r^2)} \text{ so that between } z_r^+, \text{ } z_r \text{ becomes a triple-valued function of } F, \text{ as shown in figure 3, and } F < 0 \text{ when } z_r < 1 / (1 + \kappa_r^2). \text{ At } \kappa_r = 4/3, \text{ } z_r^+ \text{ merge. It is easy to show that } z_r^- < z_r^+ < 1 / (1 + \kappa_r^2), \text{ so that under a compressive force (} F < 0 \text{), the helix can collapse or extend suddenly. A typical example with } \kappa_r = 1.5 \text{ is shown in figure 3. From figure 3, we can see that the } E - F \text{ curve is self-crossed, and the crossover point gives the lowest energy under a given } F. \text{ In figure 5, points } P_1 \text{ and } P_4 \text{ have different } z_r \text{ but the same } F = 1.407, \text{ and at this } F \text{ the } E - F \text{ curve has a crossover point. Meanwhile, points } P_2 \text{ and } P_3 \text{ correspond to } z_r^\pm. \text{ Therefore, in a quasi-static process, } z_r \text{ will collapse suddenly at crossover point of } E, \text{ or from } P_2 \text{ to } P_1. \text{ Moreover, tips in both } z_r - F \text{ and } E - F \text{ curves define two metastable regimes, one is from } P_1 \text{ to } P_2 \text{ and the}
The phase diagram for the helix can be divided into four regimes, as shown in Figure 4. In this case, the transition occurs at the hinged-hinged BC. A typical example with \( k_r = 20 \) and \( \kappa_r = 0.28 \) is shown in Figure 4, in which \( g(z_r) \) has always two zeros, so \( z_r \) also shows a discontinuous change in \( z_r \), similar to that presented in Figure 3.

In the model, \( g(z_r) \) can have three real zeros when \( \kappa_r > 1/\sqrt{k_r} \). A typical example with \( k_r = 20 \) and \( \kappa_r = 0.28 \) is shown in Figure 4. In this case, the first zero of \( g(z_r) \) indicates that a helix with \( z_r < z_1 \) is unstable, and the second and third zeros of \( g(z_r) \) gives a critical regime similar to that presented in Figure 3. We should also note that the critical regime of \( F \) becomes much narrower and the change of \( z_r(\Delta z) \) becomes quite large in this case, owing to the larger linear regime at low \( F \). For instance, in Figure 4 the critical regime is \( \Delta F = 0.03298 - 0.03037 = 0.00261 \) and \( \Delta z \approx 0.6 \) which is about twice of \( z_r \) before transition. Such a small \( \Delta F \) and large \( \Delta z \) means that the hysteresis may be negligible so that the filament may work as a sensitive switch or sensor. Moreover, the sharp transition of \( z_r \) occurs at \( F > 0 \) in this sample.

Our above discussions reveal that \( g(z_r) \) can have not any real zero, have one real zero, have two real zeros and have three real zeros results in different mechanical behaviors. Consequently, the phase diagram for the helix can be divided into four regimes, as shown in Figure 5. In regime I, \( g(z_r) \) has no real zero, so \( z \) varies smoothly between \( 0 \) to \( 1 \). In regime II, \( g(z_r) \) has only one real zero and \( g(0) < 0 \), so that the helix with a small \( z \) is unstable, but \( z \) of the stable helix increases smoothly to \( 1 \) with increasing \( F \). In regime III, \( g(z_r) \) has two real zeros and \( g(0) > 0 \), and there exists a critical regime bounded by \( z_r^\pm \) in which \( z_r \) has a first order transition with varying \( F \), similar to that shown in Figure 3. We also note that the regime III has two disconnected parts separated by regime I, as shown in Figure 5. Finally, in regime IV, \( g(z_r) \) has three real zeros and \( g(0) < 0 \), so that the helix with a small \( z \) is unstable, and there is a critical regime, bounded by the remained two real zeros, in
which $z_r$ shows a discontinuous change, similar to that shown in figure 4. From figure 5, we also find that at either $1.35 > k_r > 0.492$ or $3/2 > k_r > \sqrt{32/243}$, there is not discontinuous change in $z_r$.

In conclusion, in this subsection we show exactly that an intrinsically curved 3D filament has a planar GSC only when $\tau_0 = 0$ and it recovers 2D results. It follows that a finite IC alone is indeed enough to induce a discontinuous change in $z(L)$ even in 3D case. Moreover, with hinged-hinged BC, the filament can form a helix only when $f = 0$. In contrast, with fixed BC and proper parameters, the filament can form a helix and $z_r$ of the helix can subject to a first order transition. These results suggest that a finite $\kappa_0$ is crucial for the conformal and mechanical properties of a filament. In contrast, a finite $\tau_0$ is not a necessity for the phase transition.

6. Conclusions and discussions

In summary, in terms of Eulerian angles, we derive some useful relations in variables between some coordinate systems. Especially, we find the angle between the normal of centerline of a filament and the line of nodes defined in Eulerian frame.

We apply these relations to explore some physical problems. We show exactly that free of external force and torque, the ground-state configuration of a three-dimensional filament is unique and is a circular helix when the filament has a finite torsional modulus. A byproduct is that the general solution of a set of nonlinear differential equations represents a circular helix. We derive the expression of energy for a three-dimensional intrinsically curved filament when its cross-section area vanishes. We show that the effective description of a planar filament depends on the way to take the planar limit. More exactly, it depends on whether the torsion becomes zero at a fixed torsional modulus or the torsion and torsional modulus go to zero simultaneously. It also helps explain why the two planar models have very different mechanical properties. We find that when the intrinsic torsion is zero, the three-dimensional filament has the same ground-state configuration as that of the two-dimensional one, so that a finite intrinsic-curvature alone is indeed enough to induce the first order transition in extension.

We show that under a finite external force to form a helix it requires the fixed boundary conditions, and present the phase diagram for such a helix. We reveal that with proper parameters, a helical filament can subject to a first order phase transition in extension. The transition can be sensitive to applied force, so that such a filament may be used as a sensitive switch or sensor. Our results confirm that the finite intrinsic-curvature plays the key role in the phase transition but a finite intrinsic torsion is not so crucial for the transition.

In this work we do not consider the effect of temperature so that our results on filament can be applied only to the systems with negligible thermal effect, such as a macroscopic filament or a very rigid biopolymer. However, ignoring thermal effect may be inappropriate for many biopolymers. Indeed, in two-dimensional systems it has been shown that a finite temperature can suppress transition [21, 22]. Note that in general the temperature results in a much stronger thermal fluctuation in a three-dimensional system than that in a two-dimensional case, we can expect that the temperature may depress the transition further so lead to different results. Therefore, the effect of a finite temperature on a three-dimensional system deserves a further study.

Our results are not only helpful for the understanding of the mechanical property of a semiflexible biopolymer or a filament, but also useful for the study of dynamics of a rigid body. The new relations in variables for different frames may be also significant in differential geometry. Finally, the method to find the helix solution for nonlinear differential equations may be instructive to other mathematical or physical problems.
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