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Elasticity of biopolymer filaments

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ABSTRACT

Within the general one-dimensional theory of nonlinear elasticity we analyze the elasticity of biopolymer filaments. The approach adopted is purely mechanical but is reconciled with statistical physics approaches and allows for a proper formulation of boundary-value problems. By specializing the general framework we obtain force–extension relations for inextensible filaments and show how previous work on the biophysics of filaments fits within the framework. On the other hand, within the same framework, the theory of extensible filaments, which is appropriate for semi-flexible filaments such as F-actin, enables us to fit representative F-actin data. The specific formulas derived are relatively simple and the parameters involved have direct mechanical interpretations and are immediately related to the filament properties, including the initial end-to-end length, contour length and persistence length.

1. Introduction

In a recent paper [1] we developed a general two-dimensional framework based on the nonlinear elasticity of one-dimensional continua, incorporating both bending and stretching, for analyzing the elastic behaviour of biopolymer filaments under tension. The general approach adopted embraces the treatment of *both* flexible and semi-flexible filaments and is able to accommodate different degrees of approximation. A key ingredient in the theory is inclusion of a body force term in the equilibrium equation, which in the mechanical setting plays the role of the thermal fluctuations used in the statistical physics approach and enables an inconsistency in the biophysics literature to be reconciled within the context of a mechanical boundary-value problem. Indeed, the body force term was found to be essential for obtaining non-trivial solutions of the governing equations and boundary conditions for filaments *under tension*. Without a body force term mechanical equilibrium cannot be satisfied nontrivially, and therefore the effect of thermal fluctuations on mechanical equilibrium cannot be captured. This general nonlinear one-dimensional theory therefore provides a consistent alternative approach for describing the elasticity of biopolymer filaments.

In the present paper, for simplicity, the theory is illustrated simply for the case of small lateral displacements, for which the equation governing the lateral displacement can be linearized. This approach allows us to obtain explicit formulas in the form of extension–force relationships that include dependence on filament parameters, in particular on the initial end-to-end distance of the filament, and its contour and persistence lengths. These formulas are nonlinear even though the governing equations are linear. By considering inextensible (entropic) versions of the model, we show also how the theory relates to specific models obtained in the biophysics literature. Then, for the extensible (enthalpic) version of the theory we are able to fit force–extension data for semi-flexible filaments, specifically for F-actin.

The general (two-dimensional) theory, however, is applicable to the fully nonlinear case, but then explicit formulas are not in general obtainable. This is why we restrict attention to situations in which the lateral displacement of the filament is small so that the mechanical equilibrium equations can be linearized, which is appropriate for semi-flexible biopolymers or for flexible polymers in the high force domain. To capture the force–extension behaviour of flexible biopolymers in general (e.g., DNA), however, requires adoption of the nonlinear theory, and consequently can only be done numerically, which is not our present interest.

A brief outline of the content of the paper is as follows. In Section 2 we provide a summary of the equations and the constitutive law for an inextensible elastic filament and obtain the general solution of the linearized equilibrium equation for a given general form of the body force (written as a Fourier expansion), and we show, from a purely mechanical standpoint, how the theories of MacKintosh [2] and Blundell and Terentjev [3], which were derived for semi-flexible filaments, relate to our general framework.

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In Section 3 we discuss briefly the case of an extensible filament and we use a particular model within our general framework to fit a set of data on F-actin provided by Liu and Pollack [4]. It then becomes clear that no inextensible model, such as that of MacKintosh [2] or Blundell and Terentjev [3], can fit these data. However, the paper of Blundell and Terentjev [3] also includes an extensible model, but we found that an important formula in their paper is incorrect and could not be used to fit the data.

We emphasize that the approach adopted here is purely mechanical with the aim of establishing formulas relating force to extension in biopolymer filaments. Within a fairly general theory the elastic behaviour of a range of biopolymer filaments can be captured in terms of their contour length, persistence length and the ambient temperature. A formula for the end-to-end distance in the absence of applied tension is also obtained in terms of the contour length and persistence length when the linearized equilibrium equation is adopted.

The choice of F-actin to illustrate the approach is partly because of the availability of suitable data, and because the theory when specialized to the case of small lateral displacements can be used to obtain exact formulas. The nonlinear form of the theory can also be used to model the elastic behaviour of other biopolymer filaments, including the effects of domain unfolding or overstretching.

In a short Appendix we discuss the use of the Gibbs free-energy function as a means of deriving extension–force relations.

2. Elasticity of an inextensible biopolymer filament

Here we treat a single filament as a one-dimensional nonlinear continuum. In particular, we incorporate both bending *and* stretching elasticity. By introducing the relevant kinematics and postulating constitutive laws we derive the equilibrium equation for a single filament explicitly.

2.1. Kinematics

Consider a single inextensible biopolymer filament of length l which is curved due to the effect of thermal fluctuations in the absence of any applied load. We denote by r_0 the end-to-end distance of the filament.

For simplicity we confine attention to two dimensions so that the curved filament lies in the plane defined by the unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$, with corresponding coordinates x_1 and x_2. One end of the filament is located at a fixed origin, $x_1 = 0$, while the other end is located on the x_1 axis, and the arc length measured from the origin is denoted by s. A tensile force f is applied at the right-hand end in the x_1 direction, as a result of which the end-to-end distance r_0 becomes r; see Fig. 1.

With reference to Fig. 1 we have:

$$\boldsymbol{\tau}(s) = \cos\theta(s)\mathbf{e}_1 + \sin\theta(s)\mathbf{e}_2, \quad \boldsymbol{\nu}(s) = -\sin\theta(s)\mathbf{e}_1 + \cos\theta(s)\mathbf{e}_2, \tag{1}$$

where $\boldsymbol{\tau}$ is the unit tangent to the filament, $\boldsymbol{\nu}$ is the unit normal in the sense shown in Fig. 1, θ is the angle between $\boldsymbol{\tau}$ and the $\mathbf{e}_1$ axis, and $u = x_2$ is the lateral displacement from the $\mathbf{e}_1$ axis, with:

$$u'(s) = \sin\theta, \tag{2}$$

where the prime denotes the derivative with respect to the parameter s. Then:

$$\boldsymbol{\tau}'(s) = \kappa(s)\boldsymbol{\nu}(s), \quad \kappa(s) = \theta'(s), \tag{3}$$

where κ is the curvature, which may take different signs for different values of s.

We have chosen the tensile force f along the end-to-end direction, as is usually done in the literature. More generally it is possible to include a transverse force but for equilibrium this must be balanced by a moment, as is also the case if f is not aligned with the end-to-end direction. A three-dimensional setting would also require the consideration of torsional couples; however, accommodation of such details is possible but it makes the analysis significantly more complicated and does not affect the main features of our proposed framework.

2.2. Equilibrium equations

The filament is assumed to be "unshearable" as well as inextensible. On the filament cross-section at location s there act tangential and normal components of the resultant contact force, say $\mathbf{p}$, and a resultant contact couple, say $\mathbf{m}$, such that:

$$\mathbf{p} = t\boldsymbol{\tau} + n\boldsymbol{\nu}, \quad \mathbf{m} = m\boldsymbol{\tau}\times\boldsymbol{\nu}, \tag{4}$$

where t, the tension in the tangential direction, and n, the normal component, are Lagrange multipliers required to prevent extension and through-thickness shearing, respectively, while m is the bending moment in the filament (for detailed background on the mechanics of rods and beams, see Ref. [5]). Note that t, n and m depend, in general, on s. We recall from [1] that if there is no body force, then in the absence of the applied axial tension the filament is necessarily straight, and hence *the effect of thermal fluctuations on the equation that governs mechanical equilibrium* is equivalent to the effect of a transverse body force distribution. Thus, to ensure that the statistical physics approach is consistent with the equations of mechanics, we include a body force term. This is denoted by $\mathbf{b}$, defined per unit length and also dependent on s. Therefore, from the purely mechanical point of view the body force can be thought of as the driving mechanism for the thermal fluctuations.

For the two-dimensional problem the equilibrium of the filament is governed by two translational and one rotational balance equations of the form [1]:

$$t = f\cos\theta - c\sin\theta, \quad n = -f\sin\theta - c\cos\theta, \tag{5}$$

$$m' + n = 0, \tag{6}$$

where the vector relation $\mathbf{c}'(s) = \mathbf{b}$ has been used for convenience, and, without loss of generality, it suffices to take $\mathbf{c}(s) = c(s)\mathbf{e}_2$. Note that here we are referring to mechanical equilibrium at a certain time; hence, the balance equations hold for a snapshot in time.

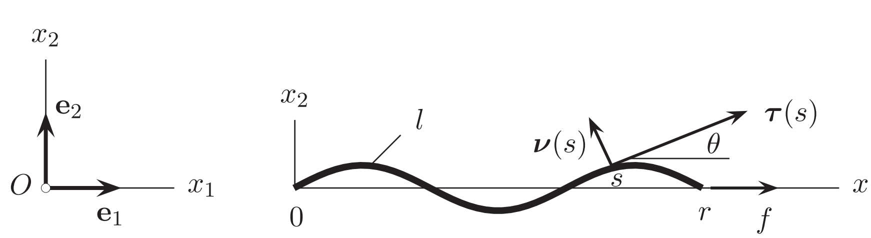

Fig. 1. An inextensible elastic filament with length l and arc length s subject to a tensile force f applied along $\mathbf{e}_1$ at $x_1 = r$, where r is the end-to-end distance. The unit tangent and the normal vector to the filament are $\boldsymbol{\tau}$ and $\boldsymbol{\nu}$, respectively, while $\boldsymbol{\tau}$ makes an angle θ with the $\mathbf{e}_1$ axis.