Elasticity of biopolymer filaments

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\textbf{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.

\textbf{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 \textit{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.
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 \( r_1 \) 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:

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

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

\[
u'(s) = \sin \theta, \quad (2)
\]

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

\[
\tau'(s) = k(s) \nu(s), \quad k(s) = \theta'(s), \quad (3)
\]

where \( k \) 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:

\[
\mathbf{p} = t \tau + n \nu, \quad \mathbf{m} = m \tau \times \nu, \quad (4)
\]

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 \( b \), 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]:

\[
t = f \cos \theta - c \sin \theta, \quad n = -f \sin \theta - c \cos \theta, \quad (5)
\]

\[
m' + n = 0, \quad (6)
\]

where the vector relation \( \mathbf{c}(s) = \mathbf{b} \) has been used for convenience, and, without loss of generality, it suffices to take \( \mathbf{c}(s) = c \mathbf{e}_2 \). 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](image-url) 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 \( \tau \) and \( \nu \), respectively, while \( \nu \) makes an angle \( \theta \) with the \( \mathbf{e}_1 \) axis.
Thermal equilibrium over a certain time period would then involve use of an average of $c$ over time.

Instead of including a body force, an essentially equivalent approach would be to consider the filament as initially curved, as in Kabla and Mahadevan [6]. Yet another model based on rod theory, which takes account of different boundary conditions, is that by Purohit et al. [7].

2.3. Constitutive laws

For an inextensible filament the stored elastic energy per unit length is denoted by $U$ and depends only on the curvature $\kappa$. According to Ref. [8], specialized to the case of inextensibility:

$$m = U(\kappa).$$

(7)

A basic simple model for $U$ is the quadratic form:

$$U(\kappa) = \frac{1}{2} B_0 \kappa^2,$$

(8)

where the constant $B_0$ is the bending stiffness (in the notation used in Ref. [1]). By relating this to the statistical physics notation (e.g. [9]) we may write $B_0 = k_B T a_0$, where $k_B = 1.38 \times 10^{-23} \text{Nm}^{-1}$ is the Boltzmann constant, $T$ is the absolute temperature (in K) and $a_0$ is the persistence length (measured in $\mu$m or nm). With Eqs. (7), (8) and (3)2, this gives the linear constitutive equation $m = B_0 \kappa = B_0 \omega$.

2.3.1. Specialization of the equilibrium equations

From Eqs. (6), (5)2 and (7) we obtain the equilibrium equation:

$$U'(\kappa) \theta'(s) - f \sin \theta(s) - c(s) \cos \theta(s) = 0,$$

(9)

where $\kappa = \theta'(s)$ has been used. Once this equation is solved for $\theta(s)$ for a given body force, Eq. (5)1 determines the Lagrange multiplier $\tau$, and Eq. (5)2 determines $n$. For the special model Eq. (8), $U'(\kappa) = B_0$ and if $\theta$ is small, Eq. (9) linearizes to:

$$B_0 \theta'(s) - f \theta(s) - c(s) = 0,$$

(10)

and by using the approximation $\theta \approx u'$ differentiation of Eq. (10) with respect to $s$ gives, by using $c'(s) = b$, the equilibrium equation:

$$B_0 u'' - f u' = b;$$

(11)

see, for example, Ref. [10].

Hereinafter we are assuming small displacements so that a detailed analysis can be carried out. One could, of course, solve the nonlinear equations numerically but this would lead to similar results within the same approximation, and would also allow results to be obtained for large deformations, but only numerically. Nevertheless, the approximation used allows us to obtain an explicit nonlinear relationship between force and extension, which is not possible with a purely numerical approach. This approximation restricts the theory to semi-flexible polymers or to the high force domain of flexible polymers, for which the small lateral displacement approximation is appropriate.

2.3.2. Solution of Eq. (11)

Note that, since $\theta \approx u'$, the left-hand side of Eq. (11) is correct to second order since only terms of third order and higher have been omitted. In the following we set $x_1 = x$. To second order, $x = \cos \theta$ is approximated as $x \approx 1 - \frac{1}{2} u''$ and hence by integrating from $s = 0$ to $l$ we obtain:

$$r^3 - \frac{r}{T} = 1 - \frac{1}{2l} \int_0^l u'' ds,$$

(12)

which defines the scaled end-to-end distance $r^3$.

In order to solve Eq. (11) we set:

$$u = \sum_{n=1}^\infty q_n \sin q_n s,$$

(13)

where $q_n = \pi n / l$, so that $u(0) = u(l) = 0$ (pinned end boundary conditions). This choice of boundary conditions is purely illustrative and other choices lead to similar results.

To match this form of $u$ we set:

$$b = \sum_{n=1}^\infty b_n \sin q_n s,$$

(14)

and substitution into Eq. (11) yields:

$$q_n^2 (B_0 q_n^2 + f) a_n = b_n,$$

(15)

and hence:

$$u = \sum_{n=1}^\infty b_n \sin q_n s, \quad u' = \sum_{n=1}^\infty b_n \cos q_n s.$$

(16)

Substituting the latter expression into Eq. (12) and carrying out the integration, we obtain:

$$r^3 = 1 - \frac{1}{4l} \sum_{n=1}^\infty b_n^2 (B_0 q_n^2 + f),$$

(17)

Since $b = c$, we could also write $c = \sum_{n=1}^\infty c_n \cos q_n s$ so that $b_n = q_n c_n$ and hence:

$$r^3 = 1 - \frac{1}{4l} \sum_{n=1}^\infty c_n^2 (B_0 q_n^2 + f),$$

(18)

which was derived explicitly in Ref. [1] (see Eq. (81) therein) on the basis of simple mechanical arguments. As indicated in Section 2.3.1, and now emphasized here, the analysis leading to Eq. (18) and in the following sections is restricted to situations in which lateral displacements of the filament are small.

2.4. Connection with the work of MacKintosh, and Blundell and Terentjev

To relate the above to the work of MacKintosh [2], which was concerned with semi-flexible filaments, we note that the average value of $a_n^2$ over thermal fluctuations, denoted $< a_n^2 >$, is given by:

$$< a_n^2 > = \frac{2k_B T}{q_n^2} \left( \frac{1}{q_n^2 (B_0 q_n^2 + f)} \right),$$

(19)

which is a result based on statistical mechanics. For details of the derivation of this expression the reader is referred to Ref. [2] (see also Eq. (67) in Ref. [1]). By using Eq. (15) the above expression can be written as:

$$< b_n^2 > = \frac{2k_B T}{q_n^2} q_n^2 (B_0 q_n^2 + f),$$

(20)

and Eq. (17) becomes:

$$r^3 = 1 - \frac{k_B T}{2l} \sum_{n=1}^\infty \frac{1}{B_0 q_n^2 + f}.$$

(21)

Since this formula is based on a two-dimensional calculation, for consistency of comparison we now include a factor 2 to account for the two transverse directions of thermal fluctuations, as in MacKintosh [2]. Therefore, we modify the above as:

$$r^3 = 1 - \frac{k_B T I}{\pi^2 B_0} \sum_{n=1}^\infty \frac{1}{n^2 + f}, \quad f^\circ = \frac{f^0}{\pi^2 B_0},$$

(22)

wherein the notation $f^\circ$ is defined. This is equivalent (in different notation) to the formula (8.10) given in Ref. [2]. Let $f^\circ$ be the value of $r^3$ when $f^\circ = 0$. Then, Eq. (22) reduces to the exact expression $r^3 = 1 - 1/6u_0$, which appears to have been given first by Landau and Lifshitz [11] (see Eq. (148.8) therein), and subsequently in, for example, Refs. [9,12,2,13]. Note that the expression for the
normalized end-to-end distance $r_0^2$ at $F^* = 0$ is accurate only if the contour and persistence lengths are comparable. It is also worth noting that the infinite sum in Eq. (22) can be put in the closed form:

$$\sum_{n=1}^{\infty} \frac{1}{n^2 + r^2} = \frac{\pi}{2}\coth\left(\frac{\pi\sqrt{r^2}}{2}\right) - \frac{1}{2Fr^2},$$

(23)

which was given in Ref. [12] (see Eq. (20) therein).

A different approach was adopted by Blundell and Terentjev [3], also in considering semi-flexible filaments and using pinned-end boundary conditions. They introduced a free-energy $F$ as a function of $r/l$. Here we write this in dimensionless form $F^* = F/l^3B_0$. The specific form they chose is (in our notation):

$$F^* = \frac{1}{2}(1 - r^2) + \frac{2\pi\alpha}{1 - r},$$

(24)

where $\alpha = l/(\pi^2l_p^2) = k_B T l / \pi^2 B_0$, the coefficient in front of the sum in Eq. (22) (which differs slightly from the corresponding expression in Ref. [3], namely $k_B T l / \pi^2 B_0$). They employed an approximation for $r^*$ close to 1 (their Eq. (11)) in the form:

$$F^* = 1 - r^* + \frac{2\pi\alpha}{1 - r^*},$$

(25)

The dimensionless force $F^* = dF^*/dr^*$ associated with this approximation is given by:

$$f^* = -1 + \frac{\pi\alpha^2}{(1 - r^*)^2},$$

(26)

which can be inverted to give:

$$r^* = 1 - \sqrt{\frac{\pi^2\alpha}{(1 + f^*)}}.$$  

(27)

This represents the two-term truncation of an infinite series in powers of $(1 + f^*)^{-1/2}$ and should be compared with the two-term truncation of the expression (22), i.e.

$$r^* = 1 - \frac{\alpha}{1 + f^*}.$$  

(28)

The latter can be obtained by considering a free energy:

$$F^* = 1 - r^* - \alpha \log(1 - r^*)$$  

(29)

so that $F^* = -1 + \alpha(1 - r^*)$, which is inverted to give Eq. (28). The free-energy functions (25) and (29) both become infinite as $r^* \rightarrow 1$ and the corresponding forces asymptote to $\infty$ in this limit.

In fact, for many purposes it suffices just to consider the first two terms in Eq. (22) since the subsequent terms in the sum decay very rapidly with $n$. With this in mind another possible choice for $F^*$ is:

$$F^* = 1 - r^* + \frac{1}{\beta} \frac{\alpha^\beta}{1 + f^*}$$  

(30)

for $\beta > 0$, where the constant $\alpha_\beta$ depends on the choice of $\beta$. This yields:

$$f^* = -1 + \frac{\alpha_\beta}{1 + f^*}$$  

(31)

and hence:

$$r^* = 1 - \frac{\alpha_\beta}{(1 + f^*)^\beta/(\beta + 1)}.$$  

(32)

Note that Eq. (27) is recovered for $\beta = 1 (x_3 = \pi^{1/2} \alpha)$ and Eq. (28) for $\beta = 0 (x_3 = \alpha)$. The first two terms in Eq. (18) can also be obtained in a similar way, which requires $\beta = -1/2$, but this yields a finite $F^*$ when $r^* \rightarrow 1$. For the models (27) and (28) we have:

$$r_0^* = 1 - x_3 = 1 - \frac{k_B T l}{\pi^2 B_0} = 1 - \frac{l}{\pi^2 B_0} r_p^0, \quad r_0^* = 1 - \frac{1}{\pi^2 B_0} r_p^0,$$

(33)

respectively, compared with the Landau–Lifshitz formula $1 - l/6l_p$. Thus, both the models of MacKintosh [2] and Blundell and Terentjev [3] include an end-to-end distance $r_0$, even if only implicitly. Palmer and Boyce [13] make explicit use of an $r_0$ partly based on the MacKintosh theory. Thus, for the simple models considered above, $r_0^*$ is given in terms of other filament parameters. This is not the case for more general models. For example, from Eq. (18), by putting $f = 0$, we obtain:

$$r_0^* = 1 - \frac{1}{4B_0^2} \sum_{n=1}^{\infty} \frac{c_n^2}{n^3}$$  

which allows $r_0^*$ to be treated as a free parameter. Finally, we note that the inversions performed for the models (27), (28) and (32) are not in general possible in the statistical physics context. This is because the force–extension curves obtained from isometric experiments (end-to-end distance is held fixed and the force fluctuates) and isentensional experiments (force is held fixed and the end-to-end distance fluctuates) are in general not identical; hence the average extension at fixed force is not the inverse of the average force at fixed extension so that, for example, the two formulas (31) and (32) would be governed by different free energies. For detailed discussion of this issue, see Ref. [12].

We recall from Section 2.1 that $r_0$ is the corresponding value of $r$, so that $r_0 = r_0^* l$. The more general version of the model of Blundell and Terentjev [3] (their Eq. (10)) yields a value of $r_0^*$ given by

$$r_0^* = 1 - 2\pi^2 l_p^2 \alpha$$

and $r_0^* = 0$. The theory of Kabl and Mahadevan [6] also includes an end-to-end distance for $f = 0$, and approximate expressions for the mean square end-to-end distance in the absence of applied force can be found in the book by Flory [14], p. 403, for both flexible and semi-flexible chains.

From Eq. (31) it is straightforward to show that when $F^* = 0$ we have $dF^*/dr^* = (\beta + 1)/x_3$. This expression is then the effective extensional modulus of the filament for zero tension and therefore provides a mechanical interpretation for $\beta$. In a recent study [15] a more detailed mechanical interpretation of $\beta$ is provided. In particular, relations between the force $F^*$ and the scaled end-to-end distance $r^*$ are plotted (on a logarithmic scale) for different values of $1/(\beta + 1)$; see Fig. 3a in Ref. [15].

Several of the above formulas express $r^*$ explicitly as a function of $f^*$, whereas use of the free-energy function gives $f^*$ as a function of $r^*$. To obtain $r^*$ as a function of $f^*$ requires use of a Gibbs free-energy function. We discuss this approach in the Appendix.

### 3. Extensible biopolymers

For biopolymers such as F-actin under sufficiently large tension inextensible models are inadequate, and in order to fit the data an extensible model is needed. A class of extensible models has been developed and derived in some detail by Holzapfel and Ogden [11]. Within the same general framework, a modification of their extensible model analogous to Eq. (32) has been adopted by Unterberger et al. [15] and this can be written in the form (Eq. (7) in Ref. [15]):

$$r^* = 1 + \varepsilon f^* - \frac{(1 + 2\varepsilon f^*)}{(1 + f^* + \varepsilon f^*)^2} - \frac{1}{(1 + f^* + \varepsilon f^*)^2}(1 - r_0^*),$$

(34)

where $\varepsilon = \pi^2 B_0 / (\mu_0 l_p^2)$, $l$ is the unstretched filament length, $\mu_0$ is the stretch modulus, $B_0 = k_B T l$, and $\gamma = 1/(\beta + 1)$. The parameter $\beta$ has a similar interpretation to that discussed in the penultimate paragraph of the last section. For $\gamma = 1$ we recover the formula (101) in [11], while in the limit $\mu_0 \rightarrow \infty$ the inextensible model (32) is...
recovered. In this case $r_0^m$ is not given in terms of other parameters and can be considered as an additional free parameter.

Eq. (34) is used to fit the F-actin data given in Fig. 10b of Liu and Pollack [4]. The fit is shown in Fig. 2, for which the parameter values obtained are $l_p = 16 \, \mu$m, $l = 11.264 \, \mu$m, $r_0 = 10.17 \, \mu$m, $\mu_0 = 38.6 \, nN$, $\gamma = 0.438 \, (\beta = 1.283)$. A typical temperature of $T = 294 \, K$ was assumed. Also shown is the corresponding prediction for the inextensible model (32), dashed curve.

The latter cannot be given explicitly in terms of other parameters and cannot be considered as an additional free parameter.

Eq. (34) is used to fit the F-actin data given in Fig. 10b of Liu and Pollack [4]. The fit is shown in Fig. 2, for which the parameter values obtained are $l_p = 16 \, \mu$m, $l = 11.264 \, \mu$m, $r_0 = 10.17 \, \mu$m, $\mu_0 = 38.6 \, nN$, $\gamma = 0.438 \, (\beta = 1.283)$. A typical temperature of $T = 294 \, K$ was assumed. Also shown is the corresponding prediction for the inextensible model (32), dashed curve.

From Fig. 10b of Liu and Pollack [4] using the model (34), the force $F$ is assumed. Also shown is the corresponding prediction for the inextensible model (32). Blundell and Terentjev [3] also considered an extensible model by modifying their Eq. (12), which is equivalent to our Eq. (26), by replacing $l$ by $l(1 + f/\mu_0)$, the extended filament length. However, the result they give, namely Eq. (13) in their paper, is not obtainable by following the procedure they indicate. The essence of their error is that they have rearranged their Eq. (12) as (in our notation):

$$r^c_0 = \sqrt{1 - \frac{(k_BT)^2}{\pi B_0 (f + f_c)}}$$

which is both algebraically and dimensionally incorrect, instead of:

$$r^c_0 = 1 - \frac{k_BT}{\pi B_0 (f + f_c)}$$

where $f_c = \pi B_0 (f + f_c)$. The correct version of their Eq. (13) is, in our notation:

$$r^c_0 = (1 + f) \left( 1 - \frac{k_BT}{\pi B_0} \frac{1 + f}{(1 + f)^2 + f_c} \right),$$

(35)

which is obtained by replacing $l$ by $l(1 + f)$ in the definitions of $r^c_0$ and $f_c$, where $f = f/\mu_0 = q^{c_0}$. Blundell and Terentjev did not fit their model to data, and we have found that it is not possible to fit the Liu and Pollack data with the (incorrect) Eq. (13) from [3], and for this reason it is important that the error is identified. However, if we use Eq. (35) the fit to the data shown in Fig. 2 is very good. This is also the case with the Odijk model [16], which is also an extensible worm-like chain model. We have found that the fit is indistinguishable from the plot based on Eq. (35). Note, however, that low force data, for which the Odijk model is known to be unsatisfactory, were not included. For the model (35) we obtain the parameters $l_p = 14.839 \, \mu$m, $l = 11.258 \, \mu$m, $\mu_0 = 36.08 \, nN$, and for the Odijk model $l_p = 11.702 \, \mu$m, $l = 11.258 \, \mu$m, $\mu_0 = 36.12 \, nN$. The latter values are a little different from those obtained in Ref. [4], which are $l_p = 9.9 \, \mu$m, $l = 11.263 \, \mu$m, $\mu_0 = 32.2 \, nN$.

However, models of this kind are rather ad hoc in nature and do not have the benefit of a rational development based on the elasticity of filaments that has been adopted in the present paper. We note that the present work embodies simple formulas, e.g. Eq. (33), for the (scaled) end-to-end distance $r_0^m$ in the absence of an applied tension.

4. Concluding remarks

In the present study we have focused on the description of the purely mechanical behaviour of elastic filaments. This is a starting point for more general considerations related to chemistry of biomolecules and the important effects of solvent, pH and other influences which require a fully thermodynamic setting. Within the general theoretical mechanical framework we have thus far considered very specific example models in order to predict the behaviour of the filament F-actin and then to fit a representative set of data. Other specific examples of the general theory can be adopted as necessary for other biomolecules, including those for which the linear theory is appropriate.

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Appendix. A complementary energy approach

In terms of the (dimensionless) free-energy function $F^c$, we have $F^c = dF^c/dr^c$. In order to invert this relationship we introduce a Gibbs free-energy function (or complementary energy function or chemical potential), also dimensionless, via the Legendre transformation:

$$G^c(r^c) = r^c F^c - F^c(r^c),$$

which assumes implicitly that $r^c$ can be determined uniquely as a function of $F^c$. This yields:

$$r^c = \frac{dG^c}{dF^c}.$$

Since we require $r^c \to 1$ as $F^c \to \infty$, an appropriate form for $dG^c/dF^c$ consistent with the expressions in Section 2.4 is:

$$r^c = 1 - \sum_{n=1}^{\infty} \frac{A_n}{(n^2 + f_0^2)^{\gamma}},$$

where $\gamma > 0$ is a disposable parameter. Apart from an additive constant this corresponds to:

$$G^c = f^c - \sum_{n=1}^{\infty} \frac{A_n}{(n^2 + f_0^2)^{\gamma}},$$

and

$$F^c = \sum_{n=1}^{\infty} \frac{A_n(n^2 + f_0^2)^{\gamma}}{(1 - \gamma)(n^2 + f_0^2)^{\gamma}}.$$

The latter cannot be given explicitly in terms of $r^c$ in general, but must blow up as $F^c \to \infty$, which requires that $\gamma \leq 1$. Thus, $0 < \gamma \leq 1$ and we note that the limiting case $\gamma = 1$ corresponds to
the log function considered in Eq. (29) (in order to take this limit the additive constant must be included in the expression for $F^q$).

If we consider just a single term, then:

$$r^q = 1 - \frac{A_1}{1 + f^q}, \quad f^q = -1 + \left( \frac{A_1}{1 - r^q} \right)^{1/\gamma},$$

and

$$F^q = 1 - r^q + \frac{\gamma}{1 - \gamma} A_1^{1/\gamma} \left[ \frac{1}{(1 - r^q)^{1/\gamma - 1}} \right],$$

again apart from an additive constant. The last term blows up as $r^q \to 1$ if $0 < \gamma \leq 1$, and again we remark that in the limiting case $\gamma \to 1$ the additive constant must be included and the final term becomes $- A_1 \log (1 - r^q)$. Note that the latter expression for $F^q$ is equivalent to Eq. (30), as can be seen by setting $\gamma = 1/(\beta + 1)$ and $A_1 = 2\phi$

References


