Stretching helical nano-springs at finite temperature

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Abstract – Using dynamic simulations and analytic methods, we study the elastic response of a helical filament subject to uniaxial tension over a wide range of bend and twist persistence length. A low-pitch helix at low temperatures exhibits a stretching instability and the force-extension curve consists of a sequence of spikes. At elevated temperature (i.e. small persistence lengths) the helix melts and a pronounced force plateau is obtained in the fixed-extension ensemble. The torque boundary condition significantly affects the resulting elastic properties.

The elasticity of flexible filaments has been the subject of intense research efforts, responding to the growing need to understand mechanical and thermodynamic properties of biopolymers such as DNA or filamentous proteins [1]. Various theoretical approaches, ranging from linear elasticity theory [2] to quantum-chemical modelling [3], have been successfully used to describe experimental force-vs.-stretching properties of synthetic and biological polymers. Yet, less is known about mechanical properties of filaments with more complicated ground-state molecular architectures. Helices are ubiquitous motifs in nature [4,5] and provide potential applications in a wide spectrum of engineering and scientific fields [6]. Anorganic nano-springs, like SiC nanowires or single-crystal ZnO nanobelts, are promising key components in nanotechnology [7]. Organic self-assembled helical ribbons are potentially useful for drug delivery system or as biological probes [8].

From the theoretical point of view, the mechanics of elastomeric helices is intriguing due to the coupling of elasticity and geometry. An analysis at zero-temperature (i.e., in the absence of shape fluctuations) revealed a discontinuous multi-step transition of a helical spring with increasing stretching force [9]. Such tension-induced instabilities have been experimentally observed for organic self-assembled helical ribbons using a micromanipulator [8] and for the helical polysaccharide xanthan with the atomic force microscope [10], exhibiting a pronounced force plateau. For experiments on nanoscopic helices at room temperature, shape-fluctuations are expected to modify the resulting elastic response in a crucial way. However, only few theoretical works investigated the interplay of thermal fluctuations and helix elasticity in the presence of external forces [9,11].

In this paper we first present a simple analysis of the force-stretching relation for a helix at zero temperatures, based upon previous theoretical approaches [9,11]. Next, employing dynamic simulations, we systematically study thermal effects on the helix elasticity. For elevated temperatures (low bending persistence length) a force plateau is obtained in the fixed extension ensemble; the characteristic plateau force obeys a simple scaling relation with a numerical prefactor that is determined by simulations. For very high temperatures the helical structure melts and simple worm-like-chain elasticity is recovered. The helix becomes stiffer when terminal rotation is prohibited via an externally applied torque.

To proceed, consider an inextensible filament (or ribbon) with contour length $L$, parameterized by the arclength $s$. A generalized Frenet orthonormal basis $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ is defined along the filament centerline $\mathbf{r}(s)$, where $\hat{e}_3$ points along the tangent and $\hat{e}_1, \hat{e}_2$ correspond to the principal axes of the cross-section. The strain rate vector $\Omega(s) = (\Omega_1, \Omega_2, \Omega_3)$ characterizes the shape of the filament through the kinematic relation $\partial_s \hat{e}_j = \Omega \times \hat{e}_j$, where $\kappa = (\Omega_1^2 + \Omega_2^2)^{1/2}$ is the curvature, $\Omega_3$ the twist density, and $\partial_s$ denotes the partial derivative with respect to $s$. According to linear elasticity theory, the bending and twisting energy of an inextensible filament reads

$$E = \frac{A_1}{2} \int_0^L \! ds(\Omega_1 - \Omega_1^0)^2 + \frac{A_2}{2} \int_0^L \! ds(\Omega_2 - \Omega_2^0)^2$$

$$+ \frac{C}{2} \int_0^L \! ds(\Omega_3 - \Omega_3^0)^2,$$  \hspace{1cm} (1)
where $A_1$ and $A_2$ are the bending rigidities with respect to the two principal axes of the cross-section, and $C$ is the twist rigidity. The filament shape is alternatively described by the original Frenet formulation of space curves in terms of the unit tangent $\hat{e}_3$, normal $\hat{n} = \partial^2 r / \partial t^2$ and binormal vector $\hat{b} = \hat{e}_3 \times \hat{n}$. They satisfy the Frenet equations, $\partial_t \hat{e}_3 = \kappa \hat{n}$, $\partial_t \hat{n} = -\kappa \hat{e}_3 + \tau \hat{b}$, and $\partial_t \hat{b} = -\tau \hat{n}$, where $\kappa$ is the curvature and $\tau$ is the torsion. Transformation from one description to the other is obtained via the rotation by an angle $\psi$ about the common tangent $\hat{e}_3$, i.e. $\hat{e}_1 + i \hat{e}_3 = \exp[-i \psi(s)](n + i b)$, which gives the relation between the strain $\Omega$ and the curvature $\kappa$ and torsion $\tau$ as $\Omega_1 = \kappa \sin \psi$, $\Omega_2 = \kappa \cos \psi$ and $\Omega_3 = \tau + d \psi / ds$. For an equilibrium (stress-free) state, twist about the local tangent is absent ($\psi = 0$), the torsion $\tau$ thus comes only from the intrinsic twist $\Omega_3$, leading to $\Omega_1 = 0$, $\Omega_2 = \kappa_0$ and $\Omega_3 = \tau_0$. The ground-state shape of a filament is completely specified by the spontaneous curvature $\kappa_0$ and torsion $\tau_0$, related to geometrical parameters; for a regular helix with radius $R$ and pitch $P$, one finds $\kappa_0 = 4\pi^2 R / (P^2 + 4\pi^2 R^2)$ and $\tau_0 = 2\pi P / (P^2 + 4\pi^2 R^2)$, see fig. 3(a).

In the dynamic simulation, the filament is modelled as a chain of $N + 1$ connected spheres of diameter $a$. Each bead is specified by its position $r_j$ and a body-fixed right-handed frame $\Sigma_j \equiv (\hat{e}_1, \hat{e}_2, \hat{e}_3)$ corresponding to the local orthogonal frame $\{ \hat{e}_a \}$ in the continuum limit. A finite-angle Euler transformation matrix transforms $\Sigma_j$ into $\Sigma_{j+1}$, where the three Euler angles $\alpha_j$, $\beta_j$, $\gamma_j$ are related to $\Sigma$ vectors as described previously [13]. The strain rate in the discrete model, $\Omega_j$, is given in terms of the Euler angles, which are in this study chosen as $\Omega_{1,j} = -\beta_j \sin \alpha_j$, $\Omega_{2,j} = \beta_j \cos \alpha_j$, and $\Omega_{3,j} = \alpha_j + \gamma_j$, so that they correctly give the local curvature $\kappa_j = \beta_j$ used in the previous studies of linear polymers with $\Omega^0 = 0$ [13]. In the total energy we include a stretching contribution that ensures connectivity of spheres, $E_s = K / 2 \sum_{j=1}^{N} [ | r_{j+1} - r_j | - a ]^2$, and a truncated Lennard-Jones potential to account for filament self-avoidance. The local elastic translational force, $F_j$, and torque about the local tangent, $T_j$, acting on each sphere are calculated using the variational method described previously [13], leading to the coupled Langevin equations $\partial \mathbf{r}_j / \partial t = \sum_{j=1}^{N} \mathbf{u}_j \cdot \mathbf{F}_j + \mathbf{\xi}_j(t)$ and $\partial \phi_j / \partial t = \mu_i T_j + \Xi_j(t)$, where $\phi_j$ is the spinning angle of the bond connecting spheres $j$ and $j + 1$. Neglecting hydrodynamic effects, we take the mobility matrix to be diagonal and use the Stokes translational and rotational mobilities of a sphere $\mu_j = \delta_{ij} 1 / (3 \pi \eta a) \equiv \delta_{ij} \mu_0 1$ and $\mu_\theta = \pi \eta a^3$, respectively ($\eta$ is the solvent viscosity). The vectorial random forcings $\mathbf{\xi}(t)$ and $\Xi(t)$ model the coupling to a heat bath and obey the fluctuation-dissipation relations $\langle \mathbf{\xi}_j(t) \mathbf{\xi}_j(t') \rangle = 2k_B T \mu_j \delta(t - t')$, $\langle \Xi_j(t) \Xi_j(t') \rangle = 2k_B T \mu_\theta \delta(t - t')$ and $\langle \Xi_j(t) \mathbf{\xi}_j(t') \rangle = 0$.

For the numerical integrations we discretize the Langevin equations with time step $\Delta$ and rescale all lengths, time and energy and obtain the dimensionless parameter $\tilde{\Delta} = \Delta k_B T \mu_0 / a^2$, which for sufficient numerical accuracy is chosen in the range $\tilde{\Delta} = 10^{-4} - 10^{-5}$. The stretching modulus is set to $K / k_B T a^2 = 10^3 - 10^4$ which keeps bond length fluctuations negligibly small. Observables are calculated every $10^5 - 10^6$ steps, total simulation times are in the order of $10^5 - 10^6$ steps. One filament end is fixed at the origin, and the other end (initially being at its equilibrium position) is moved along the $\hat{z}$-axis (identical to the helix axis). The rescaled displacement speed, $V = V_0 / \mu_0 k_B T$, is set in the range $V = 0.02 - 0.005$. Systematic studies of the rate-dependent elasticity will be published separately [14]. Except at the end of this paper, the two ends of the filament are free to rotate, i.e., no external torque is applied, similar to previous studies [8,9,15]. The number of beads studied is in the range $L / a = N = 40 - 100$. The geometry of a helix may be specified by the two parameters, $\lambda = \tau_0 / K / (2\pi R) = \cot \lambda_0$ with $\alpha_0$ being the equilibrium pitch angle, see fig. 3(a), and $\ell = 2\pi / |\Omega_0| = \sqrt{P^2 + 4\pi^2 R^2}$, the contour length per helical turn. In addition $m = L / \ell$ denotes the number of helical turns and elastic parameters are the bend/twist ratio $\Gamma = C / A$ and the bend persistence length $\ell_p = A / k_B T$. In this study we restrict ourselves to symmetric helices, i.e., $A_1 = A_2 = A$. The helix-stiffness at finite $T$ can be characterized by the two dimensionless numbers $\ell_p / L$ and $\ell_p / \ell$, related to the primary and secondary structure of the filament, respectively. Helix-melting refers to $\ell_p / \ell \sim 1$ in a loose way, keeping in mind that it is strictly not a thermodynamic transition.

We first briefly look at equilibrium properties of fluctuating helices. Using previously established techniques [11], we obtain the bond orientation correlation function for $\Gamma = 1$ as $C(s) = \langle \hat{e}_4(s) \cdot \hat{e}_3(0) \rangle = \cos^2 \alpha_0 e^{-s/\ell_p} + \sin^2 \alpha_0 \cos(2\pi s / \ell_p) e^{-s/\ell_p}$, which agrees well with the numerical data for pitch variable $\lambda = 0.4$ and $\ell_p / \ell = 5$ and 0.8 in fig. 1(a). The end-to-end distance of a helix, $R^2 = \int_0^L ds \int_0^L ds' C(|s - s'|)$, is analytically obtained as $R^2 / R_0^2 = 2L \cos^2 \alpha_0 I (L / \ell_p, 0) + \sin^2 \alpha_0 I (L / \ell_p, 0)$, where $R_0^2 = a^2 N$ is the end-to-end distance of an ideal chain and the function $I(x|Q)$ is defined as $I(x|Q) = x / (x^2 + Q^2) - (x^2 - Q^2) / (x^2 + Q^2)^2 (1 - e^{-x^2} Q^2) + 2xQ / (x^2 + Q^2)^3 e^{-x^2} Q$. Agreement with simulation data in fig. 1(b) is perfect in the low-$T$ limit ($L / \ell_p \rightarrow 0$, where $R_0$ reduces to the end-to-end distance of a perfect helix, $L \cos \alpha_0$). For high $T$, discretization effects lead to deviations between simulation and continuum theory when $\ell_p$ becomes smaller than $2a$ and $R_0 / R_{\ell_p}$ approaches unity.

The zero-temperature response of helices to a stretching force is captured by the following simple analytical argument. Consider a sufficiently long helix with an isotropic bending rigidity $A$, so that end effects are negligible. A homogeneously deformed inextensible helix under external force $f$ is characterized by radius $R$ and pitch $P$, leading to an $s$-independent curvature $\kappa = \sin \alpha / R$ and torsion $\tau = \cos \alpha \sin \alpha / R$, where $\alpha$ is the pitch angle.
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given by \( \tan \alpha = 2\pi R/P = \kappa/\tau \), see fig. 3(a). The elastic energy per unit length is according to eq. (1) given by
\[ e(\psi, R, \alpha) = A/2(\sin \psi \sin^2 \alpha/R)^2 + A/2(\cos \psi \sin^2 \alpha/R - \kappa_0)^2 + C/2(\sin \alpha \cos \alpha/R + \cos \psi/\sin \tau_0 - \tau_0)^2 = f \cos \alpha. \]
Minimization with respect to \( \psi \) yields \( \psi_0 = 0 \) and \( \tilde{e} = e(\psi_0, R, \alpha) \). The force-extension curve (FEC) is obtained by further minimizing \( \tilde{e} \) with respect to \( R \) and \( \alpha \), i.e., \( (\partial e/\partial R)_{\psi_0} = 0 \) and \( (\partial e/\partial \alpha)_{R=0} = 0 \). The former gives the mechanical equilibrium radius, \( \tilde{R}(\alpha) = \sin \alpha (A \sin^2 \alpha + C \cos^2 \alpha)/(\Lambda_0 \sin \alpha + C \tau_0 \cos \alpha) \).

Plugging this into the latter condition yields the parametric expression
\[ \frac{z}{L} = \cos \alpha \]
and
\[ \tilde{f} = \frac{f}{A_0^2} = \frac{1}{2}(A \sin^2 \alpha + C \cos^2 \alpha)^2, \]
for the rescaled force \( \tilde{f} \) as a function of the helix linear extension \( z \). Within linear response, the spring constant of a helix follows as \( K_h = \partial f/\partial (L \cos \alpha) \rvert_{\alpha = 0} = (R_0^2 \tau_0^2)/(R_0^2 \tau_0^2 / \Lambda_0 \sin \alpha + C \tau_0 \cos \alpha) \), in agreement with the classical result [16]. The numerically obtained FEC for \( \ell_p/\ell = 5 \), \( \Gamma = 3 \) and \( \lambda = 0.4 \) is compared with eq. (2) in fig. 1(c). The agreement in the high-force-regime is improved by taking the backbone extensibility into account, so that eq. (2) is modified as \( z/L = \cos \alpha + f/K \alpha \), where \( K \) is the stretching modulus.

By virtually closing the open filament (see fig. 3(a) andrefs. [17,18]), we can define the writhe, \( W_r \), which provides a measure of filament spirality and for a regular \( m \)-turn helix is given by \( W_r = m(1 - \cos \alpha) = \sin \alpha(1 - \cos \alpha)/2\pi R \). In the simulations, the writhe from the interior of the chain is obtained by numerically computing the Gaussian integral [17,18]
\[ W_{int} = \frac{1}{4\pi} \int_0^L \int_0^L (r(s) - r(s')) \cdot (\partial_x r \times \partial_y r) \frac{1}{|r(s) - r(s')|^3} ds, \]
The writhe contributions from the virtual extension (to infinity) on both sides (1 and 2 in fig. 3(a)) are evaluated via the expression [17,18]
\[ W_{ext} = \frac{1}{2\pi} \int_0^L \frac{\hat{e}_z \cdot (\hat{u} \times \partial_x \hat{u})}{1 + \hat{u} \cdot \hat{e}_z}, \]
where \( \hat{u} = (r(s) - r(0))/|r(s) - r(0)| \), and \( \hat{e}_z \) is directed parallel to the virtual extension. We then obtain \( W_r = W_{int} + W_{ext,1} + W_{ext,2} \). The twist \( T \) is the integrated rotation along the filament axis, \( T = W_{int} + W_{ext,1} + W_{ext,2} \). When (and only when) rotations of the two ends are prohibited, the linking number \( Lk = T' + W_r = m \) in a stress-free state is a topological invariant during any deformation. For ends that can rotate freely, on the other hand, one has \( d\psi/\sin \alpha = 0 \), i.e., no twisting of the filament about a local tangent occurs during deformation, and the twist \( T \) reads \( T' = \frac{1}{L} \int_0^L \tau(s) ds \), where \( \tau = \frac{1}{L} \int_0^L \tau^2(s) ds \). When \( \tau \) is zero, we still find \( Lk = T' + W_r = m \) but the number of helix turns \( m \) changes as the force is increased. The predictions for \( T \) and \( W_r \) are in nice agreement with the numerical data as shown in the inset of fig. 1(c), demonstrating that the zero-temperature theory captures the elastic properties of a helix as long as \( \ell_p/\ell > 1 \).

The stretching instability (SI) found in previous works in the limit \( A_1/A_2 \rightarrow \infty \) [9] is exactly reproduced by the stability limit of eq. (3) (although \( A_1/A_3 = 1 \) is assumed in our case). The phase diagram is displayed in fig. 2(a), together with two representative force-extension simulation curves of \( m = 4 \) helices at \( T = 0 \) in the continuous and discontinuous regimes. To see
Fig. 2: (a) Phase diagram in the $(\lambda, \Gamma)$-plane for low-pitch helices under uniaxial tension obtained in zero-temperature simulations for $m = 4$ and $N = 50$ in the fixed-force ensemble, exhibiting continuous (filled squares) and discontinuous (open circles) force-extension curves (FEC); the insets show two typical examples at the specified parameter values. The dashed line is the critical line from the analysis of eq. (3). (b) Typical FECs of flexible helices with varying $\ell_p/\ell = 16.0, 8.0, 4.0$ and 0.20, from top to bottom. The displacement rate $\dot{V}$ is 0.018, 0.009, 0.009 and 0.01, respectively. Black lines are stretching, gray lines are relaxing curves. Throughout (b)-(f), we fix $\lambda = 0.2$ and $\Gamma = 6$, unless stated otherwise. (c) Sequence of snapshots of a helix undergoing stretching for $\ell_p/\ell = 4$. (d) Superposition of scaled FECs of three different contour lengths, $N = 40, 80$ and 100, for $\ell_p/\ell = 5$. The inset shows the un-rescaled FECs. (e) Scaled plateau force $f_{pa}/k_BT$, plotted as a function of $a\ell_p\kappa_0^2$ (we set $\Gamma = 12$ for the data of $\lambda = 0.3$). The broken line is a linear fit with slope 0.66. (f) The FEC of a molten helix, with $N = 100, m = 10$ and $\ell_p/\ell = 0.4$ (with $\dot{V} = 0.16$), compared with the extensible WLC model given in the text. All data are obtained with torque-free boundary conditions.

how the $T=0$ behavior is modified in the presence of thermal fluctuations, we perform a series of simulations for fixed $\lambda = 0.2$ and $\Gamma = 6$ in the discontinuous regime (marked as a star in the diagram in fig. 2(a)), and vary $\ell_p/\ell$ in a wide range. In fig. 2(b), typical FECs for varying $\ell_p/\ell$, are shown. For the largest stiffness $\ell_p/\ell = 16$, the FEC shows a sequence of force spikes at finite stretching speed $\dot{V}$, corresponding to the progressive elimination of helical turns. As $\ell_p/\ell$ decreases, the force response becomes more regular due to the proliferation of thermally assisted escapes from metastable helical configurations. Conversely, for fixed $\ell_p/\ell$, a spiky force response also becomes more regular as the pulling rate $\dot{V}$ decreases. In the limit of a vanishingly small $\dot{V}$, a force plateau is expected to appear for any finite value of $\ell_p/\ell$ [14]. For the rather small pulling rates considered here, hysteresis is already quite weak in general. For the data of $\ell_p/\ell = 0.2$ (i.e. for a molten helix), the entropic elasticity dominates the enthalpic one and the stretching instability is eliminated by thermal fluctuations. In fact, as shown in fig. 2(f), the stretching response of a $N = 100, m = 10$ helix with $\ell_p/\ell = 0.4$ ($\lambda = 0.2$ and
\( \Gamma = 6 \) is well described by the extensible WLC model, \( z/L = 1 - (k_B T/4 \alpha^2) f^1/2 + f/\kappa_0 \), where \( \ell_0/\ell = 0.4 \), \( K = 10^3 k_B T/\alpha^2 \) and \( L = a N \), with no adjustable parameters. Selected snapshots of a helix undergoing stretching and subsequent elimination of helical turns for \( \ell_p/\ell = 4 \) is shown in fig. 2(c).

To gain some insight into the experimentally relevant thermodynamic limit, the stretching responses of helices of different lengths but same persistence length \( \ell_p/\ell = 5 \) are scaled and superimposed in fig. 2(d), resulting in collapse onto a single curve. The extension is normalized by \( L \), and the force is rescaled by \( k_B T \ell_p \kappa_0^2 \), which is the force required to straighten one loop of curvature \( \kappa_0 \) and bending stiffness \( \kappa_0 \). For given helix shape and stiffness, therefore, the helical extension scales linearly with the contour length and the thermodynamic limit is reached already for short filaments. In fig. 2(e) the rescaled force-plateau values, \( f_p/a/k_B T \), obtained in simulations for helices of different geometry, \( \lambda_\ell \) and \( \Lambda_\ell \) stiffness, \( \ell_p \), are plotted against \( a \ell_p \kappa_0^2 \), which demonstrates the relation \( f_p \approx 0.66 k_B T \ell_p \kappa_0^2 \) with a prefactor fitted to simulation data. Incidentally, an almost identical relation follows from the stability limit of eq. (3). In fact, taking the limit \( \Gamma \gg 1 \) (as appropriate for the simulation data considered here), one obtains \( f = \lambda (\cos \alpha - \lambda \sin \alpha)/\cos \alpha \sin \alpha \) with the critical value \( \lambda_c = 4\sqrt{3}/27 \) and \( f_c/\kappa_0^2 = 50\sqrt{10}/243 = 0.65 \) [9], which indicates \( f_p \approx f_c \). An alternative way of estimating the plateau force starts from the total energy \( E_0/\ell \) needed to completely straighten out one helical turn, which turns out to be \( E_0 = A \kappa_0^2 \ell^2/2 \). The average force thus is \( f_a = E_0/((\ell - \ell \cos \alpha_0)) \) which gives a scaling of \( f_a/\kappa_0^2 = 0.62 \) for \( \lambda = 0.2 \) and \( f_a/\kappa_0^2 = 0.70 \) for \( \lambda = 0.3 \), again close to the simulation result for the plateau force.

Last, we address how fixing the linking number modifies the helix elasticity. In the simulations we now block end rotations via an external torque. We study a two-turn helix of \( N = 60 \) and fixed linking number \( Lk = 2 \) in the absence of the stretching instability at zero temperature\(^4\). Figure 3(b) manifests a pronounced change of the stretching response, particularly in the high force regime. The \( Lk \)-conservation results in an increased force compared to the freely rotating case (as found in DNA overstretching experiment [2]). This is due to the twist-stretch coupling: writhe \( Wr \) decreases as the filament is stretched out, while it is simultaneously compensated by the increase of \( T \) (see fig. 3(c)), leading to the twisting of the filament about its local axis, \( d\psi/ds > 0 \). In the freely rotating case in fig. 3(d), on the other hand, twist stemming from the decrease of \( Wr \) can diffuse out from the two ends, at least for slow deformation studied here, resulting in \( d\psi/ds \approx 0 \) and thus \( \Omega_3 \approx \tau \).

In summary, we have studied via simulation and analytical methods the deformation of a fluctuating helix subject to uniaxial tension. The zero-temperature analysis is shown to reproduce well the numerically determined stretching response of stiff high-pitch chains with \( \ell_p/\ell > 1 \). In the fixed extension ensemble, the stretching instability of low-pitch helices yields force spikes for \( \ell_p/L > 1 \) and at finite pulling rate \( V \); a force plateau with a characteristic value of \( f_p \approx 0.66 k_B T \ell_p \kappa_0^2 \) is observed for \( \ell_p/L < 1 \). At even higher temperatures, for \( \ell_p/\ell < 1 \), the elastic response is dominated by entropic effects while the enthalpic stretching instability is eliminated, leading to simple WLC-like elasticity. Fixing the linking number is shown to increase the stiffness of a helical spring, which, for example, may be relevant to nanospring mechanics [6].

The scaling relation for the plateau-force might be observable with helical biopolymers. For example, native xanthan forms a helical secondary structure stabilized by non-covalent bonds in solution (either single or double...)

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\(^4\) Fixing the linking number in the presence of a stretching instability becomes difficult for increasing stretching force since the loop size decreases progressively, pointing to a singularity in the continuum limit.
helices depending on salt conditions) [19], with pitch \( P \sim 4.7 \text{ nm} \) [10]. Assuming a radius \( R \sim 2 \text{ nm} \) large enough to be in the discontinuous regime, one obtains a spontaneous curvature \( \kappa_0 \sim 0.44 \text{ nm}^{-1} \). The reported helix persistence length of native xanthan, \( L_p \), ranges from 30 nm to 150 nm depending on salt concentrations [19]. Using eq. (35) in ref. [11] (and assuming a circular cross-section), the bare bending persistence length \( \ell_p \) is related to \( L_p \) as
\[
\ell_p \approx (1 + \frac{\kappa_0^2}{2 \tau_0^2}) L_p \quad \text{for} \quad \Gamma = C/A \gg 1,
\]
which yields \( \ell_p \sim 730 \text{ nm} \) if we take \( L_p \sim 150 \text{ nm} \). Putting those values together, we obtain a plateau force of \( f_p \approx 0.66 k_B T \ell_p \kappa_0^2 \sim 370 \text{ pN} \), not too different from the plateau-force value \( \sim 400 \text{ pN} \) observed in AFM pulling experiments [10]. The agreement might be coincidence, as interactions beyond the local and linear elasticity level are neglected in our treatment.

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