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Julien Fierling, Martin Michael Mueller, Herve Mohrbach, Albert Johner, Igor  
M. Kulic

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# Crunching biofilament rings

JULIEN FIERLING<sup>1</sup>, MARTIN MICHAEL MÜLLER<sup>1,2</sup>, HERVÉ MOHRBACH<sup>1,2</sup>, ALBERT JOHNER<sup>1</sup>  
and IGOR M. KULIĆ<sup>1</sup>

<sup>1</sup> *Institut Charles Sadron, CNRS-UdS - 23 Rue du Loess, BP 84047, 67034 Strasbourg cedex 2, France*

<sup>2</sup> *Equipe BioPhysStat, LCP-A2MC, Université de Lorraine - 1 boulevard Arago, 57070 Metz, France*

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**Abstract** – We discuss a curious example for the collective mechanical behavior of coupled non-linear monomer units entrapped in a circular filament. Within a simple model we elucidate how multistability of monomer units and exponentially large degeneracy of the filament's ground state emerge as a collective feature of the closed filament. Surprisingly, increasing the monomer frustration, *i.e.*, the bending prestrain within the circular filament, leads to a conformational softening of the system. The phenomenon, that we term polymorphic crunching, is discussed and applied to a possible scenario for membrane tube deformation by switchable dynamin or FtsZ filaments. We find an important role of cooperative inter-unit interaction for efficient ring-induced membrane fission.

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**Introduction.** – The classical theme of complex systems centers on the paradigmatic question of how intricate behavior emerges when elementary units assemble and interact with each other. In particular, new phenomena can emerge when the elementary units can switch between several configurational states. Biophysics has developed a keen interest in these kinds of systems as switchable multistable filaments are found everywhere in Living Nature. The list of examples is close to innumerable with the most prominent ones: FtsZ [1,2], Mrb [3], actin [4,5] or bacterial flagella [6,7]. More recently, microtubules were suggested to spontaneously form large-scale superhelices [8,9] and undergo unusual cooperative dynamics [10]. Even whole microorganisms exhibit switchability inherited from their constituent filaments [11,12].

In this letter we study an interesting example for the emergence of an unexpected behavior when non-linear units are entrapped in a circular (bio)filament. More precisely, we pose the following conceptual question: What happens when protein monomers with an intrinsic curvature form a stiff polymer which is forced to close in a ring of different curvature radius? Biofilament rings and shallow helices are a common theme in biological actuation and have been in the focus of numerous experimental studies [1,2,4,5].

As we will see in this letter, the closure constraint can turn the monomers into fluctuating bistable units with rather dramatic effects on the overall shape of the ring.

We find that the ground state is not unique but extremely degenerate. Its number of realizations increases exponentially with the number of monomers  $N$ . As a consequence, increasing the length of the chain  $L$  leads to a conformational softening of the closed filament. We call this phenomenon of extreme shape degeneracy “polymorphic crunching”. In the second part of this letter we investigate the effects of monomer cooperativity and study how a crunching polymorphic ring could constrict a membrane tube and lead to membrane fission. We show that a filament ring can spontaneously crunch even in the absence of cooperativity. However, it can only constrict the membrane in the presence of strong enough inter-monomer cooperativity.

**Emergence of multistability.** – To grasp the flavor of the problem, let us investigate how switchability and multistability of coupled units arise in two simple but generic situations, cf. fig. 1. For this, we consider a collection of identical elastic elements —monomers— each one of them characterized by its curvature  $\kappa_i$ . We assume further that each monomer has a bending energy  $f(\kappa_i)$  where the function  $f$  has a global minimum at  $\kappa = \kappa_m$  corresponding to the monomer's intrinsic curvature, cf. fig. 1(a), right panel.

As a first example let us consider a situation in which  $N$  such monomer units are mechanically coupled in the plane *perpendicular* to their bending axis (see fig. 1(a)).

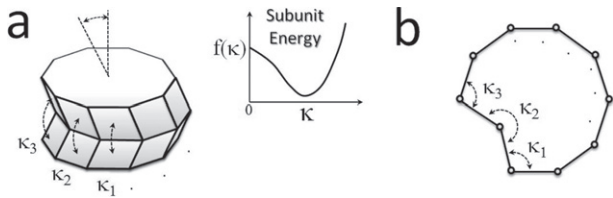


Fig. 1: Two basic types of collective coupling between non-linear units, with curvature  $\kappa_i$  and bending energy  $f(\kappa_i)$ , via a global constraint. (a) Polymorphic buckling as found in bacterial flagella and microtubules. Bendable units are coupled in the plane *perpendicular* to their bending axis [9,10]. (b) Polymorphic crunching, considered in this letter. Non-linear bendable units are coupled *in the plane of bending* by a ring closure constraint.

In this manner the monomers form a short slice of a tube of circular cross-section. When the tube section bends in a direction orthogonal to the cross-section and assumes a curvature  $\kappa_{tube}$ , the monomers themselves adapt accordingly and become curved with  $\kappa_i \approx \kappa_{tube} \sin \frac{2\pi i}{N}$  as a result of the geometric projection of the tube's curvature on each monomer unit. The total elastic energy of a tube in this geometry is then given by [9]

$$E_{tube}(\kappa_{tube}) = \sum_{i=1}^N f\left(\kappa_{tube} \sin \frac{2\pi i}{N}\right). \quad (1)$$

In the simplest case of  $N = 2$ , *i.e.*, only two monomers “welded” together, the total energy reads  $E_{tube}(\kappa_{tube}) = f(\kappa_{tube}) + f(-\kappa_{tube})$ , where for simplicity we assume a curvature perpendicular to the welding line. Due to the mirror symmetry of the problem, the total energy depends only on even terms of  $f$ . In the most general case, we expect the system to admit at least three equilibrium configurations: two symmetric bent states looking like  $\langle\langle$  and  $\rangle\rangle$  as well as a straight state  $||$ . The straight state  $||$  becomes unstable when  $\left.\frac{\partial^2 f}{\partial \kappa^2}\right|_{\kappa=0} < 0$ , leading to two (in general  $N$ ) equivalent ground states  $\langle\langle$  and  $\rangle\rangle$ . This symmetry breaking and the emergent bi-/multi-stability is the basic motif in switchable tubular systems (see fig. 1(a)) such as microtubules [9,10] and bacterial flagella [13–16].

In a second example, let us consider an even simpler coupling of monomer units: *in the plane* of their bending degree of freedom (see fig. 1(b)). What happens when a chain of such monomers is forced to close into a planar ring? As in the discussion above, let us start with a model-independent general analysis of such a ring. In two dimensions the conformation of such a filament of length  $L$  consisting of  $N = L/a$  identical monomers of size  $a$  is given by its signed curvature  $\frac{d\theta}{ds} = \kappa(s)$ , where  $s \in [0, L]$  is the arc-length variable and  $\theta$  the tangent angle of the filament's centerline. Again, as in the previous example, each unit has an elastic energy  $f(\kappa)$ . In the present case the total ring energy reads

$$E_{ring} = \int_0^L f[\kappa(s)] ds. \quad (2)$$

For a linearly elastic polymer ring with elastic energy  $f(\kappa) \propto \kappa^2$  the ground state would be a perfect circle of curvature  $\kappa_0 = 2\pi/L$ . What happens for strongly non-linear  $f(\kappa)$ ? For small deviations  $\delta\kappa$  from the circle the curvature can be decomposed:  $\kappa(s) = \kappa_0 + \delta\kappa(s)$  and we can expand the elastic energy

$$E_{ring} = E_0 + \sum_{n \geq 2} \frac{1}{n!} \left. \frac{\partial^n f}{\partial \kappa^n} \right|_{\kappa=\kappa_0} \int_0^L \delta\kappa^n ds, \quad (3)$$

where  $E_0$  is the energy of the perfect circle. The sum starts at  $n = 2$  due to the tangent constraint  $\int_0^L \kappa ds = 2\pi$  implying  $\int_0^L \delta\kappa ds = 0$ .

We see that the circle is locally stable if  $\left.\frac{\partial^2 f}{\partial \kappa^2}\right|_{\kappa=\kappa_0} > 0$ . In the opposite case,  $\left.\frac{\partial^2 f}{\partial \kappa^2}\right|_{\kappa=\kappa_0} < 0$ , the circular ring becomes unstable. One of the main goals of this letter is to study the ground state for such a polymorphic ring. For the sake of concreteness let us assume that each monomer has a bending energy per length given by

$$f(\kappa) = A\kappa - \frac{B}{2}\kappa^2 + \frac{C}{2}\kappa^4, \quad (4)$$

where  $A, B > 0$ , and  $C > 0$  are elastic constants whose signs are chosen in such a way that at least one stable preferred curvature state exists. The constant  $A$  represents a structural *asymmetry* of the monomer unit<sup>1</sup>. An open filament, described by eq. (4), behaves like an intrinsically curved ribbon with two distinguishable inner and outer faces. For  $A$  large enough the monomer has only one preferred state given by  $\kappa \approx -\left(\frac{A}{2C}\right)^{1/3}$ .

Remarkably, if we now *close* the filament, the asymmetric term  $A \int_0^L \kappa(s) ds = A(\theta(L) - \theta(0)) = 2\pi A$  gives merely a constant in the ring energy, eq. (2), and can thus be discarded. We end up with an *effective* total energy of the ring:

$$E = \int_0^L f_{eff}(\kappa) ds, \quad (5)$$

where

$$f_{eff}(\kappa) = -\frac{B}{2}\kappa^2 + \frac{C}{2}\kappa^4. \quad (6)$$

The closure condition implies an invariance with respect to the choice of the monomer asymmetry  $A$  and has interesting physical implications. In the case in which the *free* monomer has only a single preferred state the constraint induced by chain closure makes the monomer effectively bistable. Indeed, the corresponding effective potential  $f_{eff}(\kappa)$  (an even function) has always two equivalent minima given by  $\kappa = \pm\kappa_1$  with the characteristic curvature

$$\kappa_1 = \sqrt{\frac{B}{2C}} \quad (7)$$

<sup>1</sup>Note that more generally a term  $\propto \kappa^3$  is possible and its presence modifies the emergence of two exactly symmetric minima. In our later exposition, the asymmetry can be incorporated by a biasing “magnetic” field. For simplicity we focus here on the simpler case in which the cubic and higher odd terms are absent or negligible.

and  $f_{eff}(\kappa_1) = -\frac{1}{8}\frac{B^2}{C}$ . Remarkably it is the chain closure, *i.e.*, a global topological property of the system that generates an *emergent bistability* of the local constituent.

If each monomer is close to its ground state,  $\kappa(s) = \pm\kappa_1 + \delta\kappa_{el}(s)$ , with some additional elastic thermal fluctuations  $\delta\kappa_{el}(s)$ , we obtain the total elastic energy up to quadratic order:

$$E_{elastic} = -\frac{L}{8}\frac{B^2}{C} + B \int_0^L \delta\kappa_{el}^2 ds. \quad (8)$$

From this result one could naïvely infer the associated persistence length of the system to be  $l_B = 2B/(k_B T)$ . However, a second contribution of a purely entropic origin due to the degeneracy of the ground state has to be taken into account as we will show in the following.

**The crunching transition.** – The emergence of the two stable monomer states leads to the conclusion that the ground state of the system defined by eq. (5) is highly degenerate. At vanishing temperature, and once the parameter  $\kappa_1/\kappa_0$  surpasses 1, any curvature function of the form  $\kappa(s) = \pm\kappa_1$  gives the same minimum ring energy. In the discrete notation the curvature of the  $n$ -th monomer can be written as  $\kappa_n = \sigma_n \kappa_1$  with the “spins”  $\sigma_n = \pm 1$ ,  $n = 1, \dots, N$ . For  $\kappa_1/\kappa_0 > 1$  exponentially many equivalent ground states with different shapes become possible. The onset of this sudden behavior at  $T = 0$  will be called in the following the crunching transition. Does the sharp onset of the crunching transition persist or does it get “washed out” by the fluctuations at  $T > 0$ ? Let us investigate this question in the following.

For a hypothetically open filament described by eq. (5) —in the absence of the closure condition— the system is formally equivalent to a one-dimensional Ising chain without interactions between the spins. In analogy to the latter, at finite temperature  $T$  we introduce the “average magnetization”

$$M = \left\langle \frac{1}{N} \sum_{n=1}^N \sigma_n \right\rangle, \quad (9)$$

describing the mean of the distribution of positively and negatively curved monomers with the average curvature  $\langle \kappa_n \rangle = \kappa_1 M$ . For a given value of  $M$ , the free energy  $F(M) = E - TS(M)$  decomposes into the elastic energy  $E = -\frac{L}{8}\frac{B^2}{C}$  and the large entropic contribution  $S(M) = k_B \ln W(M)$  due to the high degeneracy of the ground state<sup>2</sup>. Here  $W(M)$  is the number of ring ground states for a given  $M$ . The physical value of  $M$  at any temperature is given by the minimum of  $F(M)$  which is obviously  $M = 0$  for the open filament defined by eq. (5). This implies that the ground states, although degenerate and locally tortuously bent (between  $-\kappa_1$  and  $+\kappa_1$

<sup>2</sup>The elastic thermal fluctuation contributions  $\delta\kappa_{el}$  around the ground states average to  $\langle \delta\kappa_{el} \rangle = 0$ . They only add a constant (entropic) term to the full free energy of the system and can be disregarded from now.

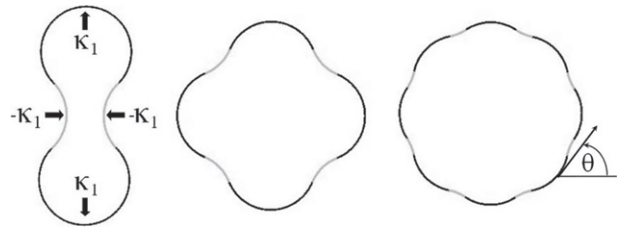


Fig. 2: Crunching of a circularly closed non-linearly elastic filament. A ground state consists of a sequence of positive and negative curvature regions. All depicted states are ground states and have the same elastic energy.

regions) are, however, statistically straight on average. Note that this 2-state model bears some resemblance with other bistable systems like the squeezed helices studied in ref. [17]. It can also be seen as a concrete realization of the block-copolymer model for curvature switchable filaments developed in ref. [18].

Closing the filament imposes three separate constraints. First and second, the closure constraint in the  $(x, y)$ -plane:

$$\int_0^L \cos \theta(s) ds = \int_0^L \sin \theta(s) ds = 0 \quad (10)$$

and third, the condition  $\theta(L) = 2\pi + \theta(0)$ , resulting from the continuity of the tangent angle. In order to adapt to these constraints, the curvature distribution of the monomers along the filament will not be random any more. Indeed the non-linear closure constraints, eq. (10), introduce a weak non-local effective coupling between the individual monomers. Besides, there is now a bias of mean curvature in favor of the curvature  $\kappa_0$ , *i.e.*  $\langle \kappa_n \rangle = \kappa_0$ , necessary for the ring closure.

Nevertheless, similarly to the previous case of the open filament, the ground state shows a high level of degeneracy (see fig. 2). Solving the problem with the non-linear closure constraints, eq. (10), is a rather difficult task, but to illustrate the idea of the ground-state degeneracy we consider a simple case: If the curvature  $\kappa(s)$  displays a fourfold symmetry with respect to the  $x$  and  $y$  axes, then the strict geometric closure is ensured by symmetry. In this case we can restrict ourselves to one of the four quarter copies of the filament with  $N/4$  monomers each.

In contrast to the open chain, once the ring is geometrically closed, it seems that crunching could occur only for  $\kappa_1 > \kappa_0$ . For  $\kappa_1 \leq \kappa_0$  only the perfect circle seems admissible. However, the monomers need not necessarily keep the curvature  $\pm\kappa_1$  but can move slightly away from the minimum of the effective potential (6). Indeed such a shift of the curvature, although energetically costly can be compensated by the entropic contribution. A small additional curvature  $\Delta_\kappa \kappa_1$  (away from the mechanical ground state) added to each monomer  $\kappa_n = (\sigma_n + \Delta_\kappa) \kappa_1$  helps the system to reach macroscopic states with more configurational realizations than in the strict ground state. With this variational ansatz for the constrained ground state(s)



the angular closure constraint implies

$$M = \frac{4}{N} \left\langle \sum_{n=1}^{N/4} \sigma_n \right\rangle = \frac{\kappa_0}{\kappa_1} - \Delta_\kappa, \quad (11)$$

where  $0 < M < 1$ . Note that in the case in which  $\kappa_1 < \kappa_0$ ,  $\Delta_\kappa$  is necessarily non-zero in order to have  $M < 1$ . With this ansatz the statistical average of the curvature is by construction  $\langle \kappa_n \rangle = \kappa_0$ . Again the free energy  $F = E - TS$  of the system contains the elastic energy  $E(\Delta_\kappa)$  and the entropic contribution  $S(\Delta_\kappa) = k_B \ln W(\Delta_\kappa)$  due the high degeneracy of the ground state. Now  $W(\Delta_\kappa)$  is the number of states compatible with the condition (11). For a finite  $N$  and fixed value of the other parameters,  $\Delta_\kappa$  varies with temperature  $T$  and  $N$ . When the energy is dominating over the entropy (small  $T$  or small  $N$ ),  $\Delta_\kappa \approx 0$ .

Let us consider the case of  $N$  large with  $L = Na$  fixed and  $a$  the size of the monomer. With the notation  $\tilde{\kappa}_1 = \kappa_1/\kappa_0$  the energy density can be written as

$$\frac{E}{aBN\kappa_0^2\tilde{\kappa}_1^2} = -\frac{1}{4} + \Delta_\kappa^2 \left( 1 + \frac{\Delta_\kappa}{\tilde{\kappa}_1} - \frac{3}{4}\Delta_\kappa^2 \right) \quad (12)$$

and the entropy per monomer becomes

$$\begin{aligned} \frac{S}{k_B N} &= \ln 2 - \frac{1}{2} \left( 1 - \Delta_\kappa + \frac{1}{\tilde{\kappa}_1} \right) \ln \left( 1 - \Delta_\kappa + \frac{1}{\tilde{\kappa}_1} \right) \\ &\quad - \frac{1}{2} \left( 1 + \Delta_\kappa - \frac{1}{\tilde{\kappa}_1} \right) \ln \left( 1 + \Delta_\kappa - \frac{1}{\tilde{\kappa}_1} \right). \end{aligned} \quad (13)$$

The minimization of  $F$  with respect to  $\Delta_\kappa$  leads to the relation

$$\Delta_\kappa = \frac{1 - \tilde{\kappa}_1 + (1 + \tilde{\kappa}_1) \exp(-\varepsilon)}{\tilde{\kappa}_1 (1 + \exp(-\varepsilon))}, \quad (14)$$

where  $\varepsilon$  is given by

$$\varepsilon = 4al_B\kappa_0^2\tilde{\kappa}_1^2 \left( 2 - 3\Delta_\kappa^2 + 3\frac{\Delta_\kappa}{\tilde{\kappa}_1} \right) \Delta_\kappa. \quad (15)$$

For a very stiff filament whose bending stiffness  $B = l_B kT/2 \gg kT/(a\kappa_0^2)$  dominates over the entropy, the value of  $\Delta_\kappa$  jumps sharply from  $\Delta_\kappa = 1/\tilde{\kappa}_1$  (for  $\tilde{\kappa}_1 < 1$ ) to  $\Delta_\kappa = 0$  (for  $\tilde{\kappa}_1 > 1$ ) close to the ‘‘crunching transition point’’  $\tilde{\kappa}_1 = 1$ . Consequently, the filament forms a ring with  $\kappa = \kappa_0$  below the transition ( $\tilde{\kappa}_1 < 1$ ) and is crunched above it. For more moderate stiffness  $B \lesssim kT/(a\kappa_0^2)$ , the system more gradually interpolates between the uncrunched and crunched state and the transition is smoothed increasingly with decreasing  $B$ .

The lesson from this mean-field analysis is that in general the local curvature  $\kappa_n$  can deviate from its preferred value ( $\pm\kappa_1$ ) by an amount  $\Delta_\kappa\kappa_1$ . Classically, at  $T = 0$ , the crunching occurs only once  $\kappa_1$  surpasses  $\kappa_0$ . However, in the presence of an additional elastic deformation  $\Delta_\kappa$  the filament can ‘‘pre-crunch’’ even for  $\kappa_1 < \kappa_0$ . The exponentially large number of curved-state micro-realizations (reflected in the entropy  $S(\Delta_\kappa) \propto N$  scaling with the system size) competes with the elastic energy  $E(\Delta_\kappa)$  caused by the additional deformation  $\Delta_\kappa$ . This effectively smooths and prevents a strict thermodynamic phase transition at  $\kappa_1 = \kappa_0$  (occurring at  $T = 0$ ) at any finite  $T > 0$ .

**Softening through prestrain.** – How does the presence of exponentially many equivalent states affect the shape fluctuations of a closed ring? From the previous analysis we can now make a coarse-grained approach in the limit of a large number of bistable monomers,  $N \gg 1$ . We further assume that the curvature  $\kappa_1 > \kappa_0$  is supercritical, which gives rise to a negligible  $\Delta_\kappa$  from the previous section. As already mentioned, the closure conditions (10) result in a weak non-local coupling between the individual monomers. This closure coupling, which we previously circumvented by assuming fourfold symmetry, will be treated more elegantly later on by eliminating certain Fourier modes in the coarse-grained filament description. For now, we neglect the strict closure condition and impose the ring conformation on average:  $\langle \kappa_n \rangle = \kappa_0$ . In this way, the spins  $\sigma_n$  can be considered as randomly distributed around an average value  $\langle \sigma_n \rangle = M$  (eq. (11)).

For a large number of monomers the piecewise function  $\kappa_n = \pm\kappa_1$  satisfies the central limit theorem so that the probability to find a certain curvature  $\langle \kappa_n \rangle_l$  appropriately coarse-grained on a larger lengthscale  $l \ll Na$  (between the monomer size and the total ring size) is a Gaussian variable. Using this coarse-grained approach, valid on scales  $l \gg a$  beyond the monomer size, we treat the curvature as a continuous Gaussian-distributed function  $\kappa(s)$ . We now introduce a new random Gaussian variable  $\tilde{\kappa}(s) = \kappa(s) - \langle \kappa(s) \rangle = \kappa(s) - \kappa_0$  with zero mean and a standard deviation given by  $\langle \tilde{\kappa}(s)^2 \rangle = \kappa_1^2 - \kappa_0^2 \stackrel{(11)}{=} \kappa_1^2(1 - M^2)$ . Since the curvature is uncorrelated on larger scales,  $\langle \tilde{\kappa}(s)\tilde{\kappa}(s') \rangle \approx \delta(s - s') \langle \tilde{\kappa}(s)^2 \rangle$  for  $|s - s'| \gg l$ . Recast in this form, the polymorphic chain can now be seen in a new light: The coarse-grained curvature  $\tilde{\kappa}(s)$  behaves on larger scales as the curvature of a classical semiflexible chain. The latter is described by the Worm-Like Chain (WLC) model with an effective configurational energy:

$$E_{WLC} = \frac{l_e k_B T}{2} \int_0^L \tilde{\kappa}(s)^2 ds \quad (16)$$

and an effective persistence length given by

$$l_e = \frac{1}{a(\kappa_1^2 - \kappa_0^2)}. \quad (17)$$

Despite this useful analogy with the WLC a note of caution is appropriate. Unlike for the WLC, the persistence length  $l_e$  depends here on the length  $L$  of the filament through  $\kappa_0 = 2\pi/L$  and is moreover temperature independent since it is associated to the conformational entropy of the ground state. From eq. (17) we see that  $l_e$  is a decreasing function of  $L$ . The chain softens for increasing length until  $l_e$  reaches its minimum value  $l_e = 1/(a\kappa_1^2)$ .

Until now we implemented only the mean condition  $\langle \kappa_n \rangle = \kappa_0$ . To enforce the closure conditions (10), let us consider the Fourier decomposition of the tangent angle  $\theta$  around a circular state, *i.e.*,  $\theta(s) = \kappa_0 s + \delta\theta(s)$ , where  $\delta\theta(s)$  is small:  $\delta\theta(s) = \sum_{n=1}^N (a_n^\theta \sin(\kappa_0 ns) + b_n^\theta \cos(\kappa_0 ns))$ . Expanding

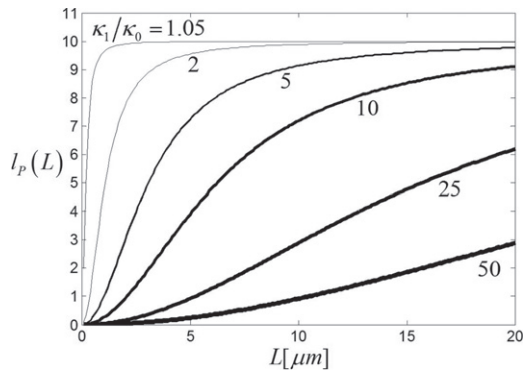


Fig. 3: The persistence length  $l_p$  of crunched filament rings depends on their length (eq. (18)). Parameters:  $a = 1$  nm,  $l_B = 10$   $\mu$ m,  $\kappa_0 = 2\pi/L$  and an increasing polymorphic curvature  $\kappa_1$ .

the  $X$ - $Y$  constraints (10) to lowest order in modes  $a_n^\theta$  and  $b_n^\theta$ , one immediately sees that  $a_1^\theta$  and  $b_1^\theta$  both have to vanish. The higher modes are unaffected and according to the equipartition theorem satisfy  $\langle (a_n^\theta)^2 \rangle = \langle (b_n^\theta)^2 \rangle = (L/2\pi^2 l_e) n^{-2}$ ,  $n \geq 2$ , which are temperature independent due to purely entropic effects.

Including the elastic thermal fluctuations around the ground state(s), it is easy to see that the total persistence length reads

$$l_p(L) = \frac{l_B l_e(L)}{l_B + l_e(L)} \quad (18)$$

which is always smaller than the persistence length  $l_B$  (see fig. 3). We thus observe an effective conformational softening of the filament due to the prestrain induced by the closure. In particular, when the temperature goes to zero or when  $l_B$  is very large (such that  $l_B \gg l_e$ ),  $l_p$  does not diverge as it would for a standard semiflexible filament but stays finite, *i.e.*  $l_p = l_e(L)$ .

**Cooperativity.** – Many biofilaments, including dy-namin, FtsZ, tubulin and others, are known to switch cooperatively. To incorporate this effect, in addition to the elastic energy, eq. (5), we assume a cooperative inter-monomer coupling term favoring uniform curvature,

$$E_{couple} = \frac{K}{2} \int_0^L \left( \frac{d\kappa}{ds} \right)^2 ds \quad (19)$$

with an *inter-monomer coupling* constant  $K$ . With cooperativity, domains switch between  $\pm\kappa_1$  on a scale  $\lambda \sim \sqrt{K/B}$  and have transition energy penalty  $J \sim \sqrt{KB}\kappa_1^2$ . The effective block size  $\xi \sim ae^{J/kT}$  of  $\pm\kappa_1$  blocks can now be considered as the effective monomer size  $a_{eff} \sim \xi$ . For short transition lengths  $\lambda \ll \xi$  and intermediate cooperativity,  $a < a_{eff} \sim \xi \ll L$ , all the results from the previous sections stay applicable, however with a *renormalized monomer size*  $a_{eff}$ . In particular the system behaves again like a WLC on larger scales but with smaller persistence length  $l_e \propto 1/a_{eff}$ . For very large  $\xi \gg L$  (in practice  $J \gtrsim 5-10kT$ ) the domain walls become too costly and

$a_{eff} > L$ , with only a minimal number of walls being energetically admissible. In this highly cooperative limit the ring cannot be reduced to a fluctuating WLC, but has a single well-defined ground state, assuming a definite shape with 4 domains as in fig. 2, left panel. This shape will be preferred over the simple circle if the energy of the four transition regions becomes less than the penalty for having a uniform curvature  $\kappa_0$ , *i.e.*  $4J \lesssim \frac{LB^2}{8C} = BL\kappa_1^2/4$ .

**Filament crunching a membrane tube.** – In order to illustrate the model, we apply it to a possible scenario for membrane tube crushing by a polymorphic filament. In Nature one finds many examples of biological polymers interacting with tubular membranes. For instance, the dynamin filament wraps around a neuron's membrane during endocytosis [19,20] to form a helix whose pitch is small. FtsZ filament rings constrict the membranes of tubular bacteria during cell division [1,2]. We do not pretend to specifically model dynamin or FtsZ in this paper but rather set the framework to better understand such interactions in the near future.

We consider a tubular fluid membrane of infinite length, radius  $r$  and bending rigidity  $B_t$ . In terms of the azimuthal angle  $\phi$ , the longitudinal coordinate  $z$ , and the radial displacement field  $u(\phi, z)$  with respect to the cylindrical state the elastic energy reads [21]  $F_t = \int_0^{2\pi} \int_0^L e(\phi, z) d\phi dz$  with  $e(\phi, z) = B_t[(\partial_\phi^2 u)^2 + 3u^2 + 2r^2(\partial_z^2 u)(\partial_\phi^2 u) - 2r^2(\partial_z u)^2 + r^4(\partial_z^2 u)^2 + 4u(\partial_\phi^2 u)]/2r^3$ . The Fourier decomposition of  $u(\phi, z)$  reads

$$u(\phi, z) = \sum_n' \int \frac{dk}{2\pi} A_n(k) e^{i(n\phi + kz)}, \quad (20)$$

where in the sum  $\sum_n'$  the modes  $n = \pm 1$  (for all  $k$ ) are excluded. They would correspond to a net external force, which is absent in our problem. The associated quadratic energy reads [21]

$$F_t = \frac{\pi B_t}{r^3} \sum_n' \int \frac{dk}{2\pi} \mathcal{M}_n(k) A_n(k) A_n(k)^* \quad (21)$$

with  $\mathcal{M}_n(k) = (r^2 k^2 + n^2 - 1)^2 - 2(n^2 - 1)$ .

When the polymorphic filament wraps around the tube, it induces a deformation at position  $z = 0$  of the form  $u(\phi, 0) = \sum_{n=-\infty}^{\infty} a_n e^{in\phi}$ . Expressing the membrane modes  $A_n(k)$  in terms of the filament modes  $a_n$  we obtain the energy of the constrained membrane:

$$F_t = \frac{\pi B_t}{r^2} \sum_n' \frac{|a_n|^2}{I_n}, \quad (22)$$

where  $I_n = r \int \frac{dk}{2\pi} \frac{1}{\mathcal{M}_n(k)}$ . The shape of the membrane can also be easily deduced from filament modes<sup>3</sup>.

<sup>3</sup>The membrane shape is then given by  $u(\phi, z) = \sum_n' a_n e^{in\phi} J_n(z)/I_n$  with  $J_n(z) = (8\sqrt{2}\sqrt{n^2-1})^{-1} (e^{-\frac{z}{r}\gamma^-}/\gamma^- - e^{-\frac{z}{r}\gamma^+}/\gamma^+)$  and  $\gamma^\pm = (\sqrt{n^2-1}(\sqrt{n^2-1} \pm \sqrt{2}))^{1/2}$ ,  $I_n = J_n(0)$  for  $|n| \neq 1$  and  $I_0 \approx 0.06$ .

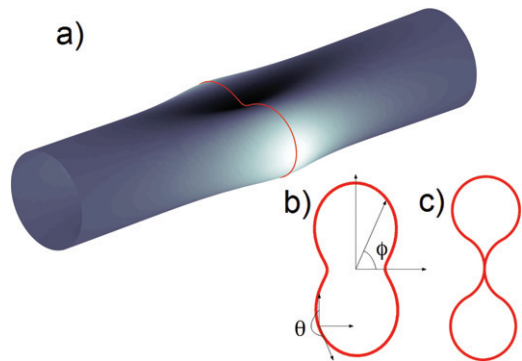


Fig. 4: (Colour on-line) (a) A crunching polymer ring on a fluid membrane, (b) weakly deformed, (c) critically deformed with self-contact for  $\kappa_1/\kappa_0 = 7/3$ .

Can a polymorphic filament deform or even crunch the membrane tube? We consider first the case in which cooperativity is negligible and the filament behaves like a WLC on large scales. In the limit of large  $l_B \gg l_e$  we can neglect the elastic fluctuations and  $l_p \approx l_e$ . The total free energy in this case becomes  $F = F_{WLC} + F_t$ , where  $F_{WLC}$  and  $F_t$  are given by eqs. (16) and (22), respectively. In terms of the Fourier modes  $a_n$  of the radial displacement  $u$ , the ring contribution is  $F_{WLC} = \frac{k_B T l_e \kappa_0^2 L}{r^2} \sum_n n^4 |a_n|^2$ . Applying the equipartition theorem to each mode we obtain  $\langle |a_n|^2 \rangle = 2r^2 / (\frac{\pi l_e}{r} n^4 + \frac{\pi B_t}{l_n k_B T})$  for  $|n| \neq 1$ . We note that the filament always *reduces* the free membrane fluctuations (given by  $l_e/r \rightarrow 0$ ). Therefore, a filament which is lacking structural cooperativity is unable to deform the membrane.

However, the presence of high cooperativity (eq. (19)) changes this picture completely and boosts dramatically the deformation of the membrane. A very stiff filament  $B \gg r B_t$  with high cooperativity  $J \gg kT$  dominates entirely over the membrane. For  $\kappa_1 > 4\sqrt{J/BL}$  the filament establishes a peanut shape, cf. fig. 4. The tube deforms strongly and establishes a self-contact for  $\kappa_1/\kappa_0 = 7/3$  (“kissing condition”, cf. fig. 4). Beyond this critical value the membrane would be forced to tear and rupture due to strong self-interaction and the localized shear induced by the filament slicing through it.

**Conclusions.** – We have shown that the conceptually simple procedure of circular closure transforms a simple mundane object—an anharmonic filament with a unique ground state—into a complex multistable filament with an exponentially large number of degenerate ground states. When the filament thermally explores this multistable energy landscape, it exhibits anomalous fluctuations. We have shown that in the limit of low

cooperativity the filament ring can be modelled as a worm-like chain but with an effective (length-dependent) persistence length which is dominated by configurational fluctuations between the ground states.

Motivated by FtsZ and dynamin filaments we have started to explore the interaction of such a multistable crunching filament with a tubular fluid membrane. We have seen that a crunching ring can deform a membrane tube only in the presence of strong inter-monomer cooperativity. In this cooperative limit the membrane could undergo fission in a novel geometric scenario: The membrane is forced through itself and possibly ruptured by the crunching filament slicing through it. The self-contact of the membrane driven by localized normal pressure along a line (the filament) and the subsequent recombination pathway of the upper and lower membrane leaflets is an interesting problem, worthwhile exploring in future.

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