Statistical Mechanics of a Closed Ribbon

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We present a toy model for the statistical mechanics of a closed ribbon with a non-linear coupling between bending and twisting degrees of freedom. Stochastic simulations are in qualitative agreement with previous studies of open ribbons, showing the oscillatory behavior of tangent-tangent correlation function of developable ribbons, and a transition between different types of short-range order from 'railway-track' models. We, however, do not match with the quantitative scaling behavior of previous models on open ribbons.

INTRODUCTION

Real-life polymers are material objects, with one of the most obvious consequence of that fact being that they cannot penetrate themselves. However rough an approximation it might be to the onlooker to neglect this fact, studies of *phantom* polymers has nonetheless been proven to be insightful [1]. Polymer materiality also means that they are endowed with a finite width and internal structure, giving rise for example to stiffness, both in bending [2] and twisting [3]. Moreover, the geometrical structure of the polymer introduces constraint of its own, as in the case of the DNA double-stranded helix: The effect of such a geometry has been studied in the past [4, 5], through different models. The ribbon polymer sees its bending and twisting degrees of freedom coupled through geometrical constraints. The resulting non-linear constraint gives rise to different form of short-range order; Both articles cited here show that the persistence length ℓ_P, characteristic of the stiffness of the polymer is changed from its bare value by the geometry, albeit with different quantitative predictions depending on the underlying model. We here consider an extension of Giomi's and Mahadevan's study [5] of the statistical mechanics of a developable *phantom* ribbon on a ring geometry, neglecting excluded volume effects.

Closed polymer rings are of biological relevance, and topological objects such as knots are better defined on such closed curves, meaning that such a system is of interest in describing the physics of entangled plasmids [6]. We describe and implement here a numerical simulation protocol, allowing us to compare our results with [4, 5].

THE SADOWSKY FUNCTIONAL

The geometry of a curve in space is defined by the position of its centerline $\{\mathbf{r}(s)\}$ where s is the curvilinear coordinate. From the function $\mathbf{r}(\mathbf{s})$ derives the kinematic tangent vector to the curve $\mathbf{t}(s) = \mathrm{d}\mathbf{r}/\mathrm{d}s$. The kinematic unit normal vector to the curve is $\mathbf{n}(s) = \kappa^{-1}\mathrm{d}\mathbf{t}/\mathrm{d}s$, where $\kappa = |\mathrm{d}^2\mathbf{r}/\mathrm{d}s^2|$ is the curvature. The *Frenet* frame $(\mathbf{t}, \mathbf{n}, \mathbf{t}\times\mathbf{n})$ defines the orientation of the curve at each point s. In the case of a ribbon we also need to specify in which direction the "flat" side is facing: To give a simple description of this, we provide a simplified geometric solution by defining on top of the kinematic Frenet frame a material frame $(\mathbf{t}, \mathbf{b}, \mathbf{t}\times\mathbf{b})$ sharing the same tangent vector but where $\mathbf{b}$ is rotated by an angle $\phi(s)$ from $\mathbf{n}(s)$ around $\mathbf{t}(s)$, giving $\mathbf{b}(s) = \cos\phi(s)\mathbf{n}(s) + \sin\phi(s)\mathbf{t}\times\mathbf{n}$. Physically, ϕ is the *twist angle*, gauging how much the ribbon is deformed from its natural pitch. With such a frame, we define the material torsion as $\tau(s)^2 = a^{-2}|\mathbf{n} - \mathbf{b}|^2 = 2a^{-2}(1-\cos\phi(s))$, where a is a twisting persistence length, assumed to be small with respect to the bending persistence length.

A classic result in differential geometry established by Sadowsky [7] gives a simple expression for the that the elastic energy cost of a curved and twisted configuration of a developable ribbon of length L with negligible width and thickness $w, h \ll L$ is given by

$$\beta H = \frac{1}{2}\frac{Dw}{kT}\int \mathrm{d}s \frac{(\kappa^2 + \tau_f^2)^2}{\kappa^2} \tag{1}$$

where $\tau_f(s)$ is the ribbon geometrical torsion in the Frenet description $\tau_f = |\mathrm{d}(\mathbf{t}\times\mathbf{n})/\mathrm{d}s|$ $D = h^3E/[12(1-\nu^2)]$ is the bending rigidity, with E and ν the Young and Poisson moduli respectively. The *bare* (bending) persistence length is then $\ell_0 = Dw/kT$. A developable surface can be seen as one which could be created by moving a straight line through space: our characterization of the ribbon by the couple $(\mathbf{r}(s), \phi(s))$ is not compatible with this geometrical constraint; however we commit to a geometrical approximation and approximate $\tau_k = \tau$. This approximation effectively allows us to consider the characterization $(\mathbf{r}(s), \phi(s))$ as representative of the ribbon, while still introducing a non-linear coupling between twisting and bending. In this sense, our model is a middle ground between the true Sadowsky functional and decoupled twist as studied by *eg* [3].

NUMERICAL SIMULATION OF A CLOSED RIBBON

To bring the statistical conformations of a closed ribbon of length L amenable to numerical simulation, we consider a discretization of the Sadowsky functional on a chain of $N = L/a$ elements ('beads') at positions $\{\mathbf{r_1}, \ldots, \mathbf{r_N}\}$, with a periodic closure $\mathbf{r}_{i+N} = \mathbf{r}_i$. We adopt a 'soft' inextensibility constraint by imposing an harmonic energy penalty $K(|\mathbf{r}_{i+1} - \mathbf{r}_i| - a)^2/2$ with large K. We can write down a discrete analog of the tangent vector $\mathbf{t}_i = a^{-1}(\mathbf{r}_{i+1} - \mathbf{r}_i)$, allowing us to write the local curvature $\kappa_i^2 = a^{-2}|\mathbf{r}_{i+1} - 2\mathbf{r}_i + \mathbf{r}_{i-1}|^2 = a^{-2}|\Delta \mathbf{r}_i|^2$ where Δ is the discrete Laplacian operator. The torsion τ_i^2 can be likewise discretized as $a^{-2}|\mathbf{n}_i - \mathbf{b}_i|^2 = 2a^{-2}(1 - \cos\phi_i)$

This gives a discretized energy functional

$$U = \sum_i \frac{Dw}{2}(\kappa_i^2 + 2\tau_i^2 + \frac{\tau_i^4}{\kappa_i^2}) + \frac{K}{2}(|\mathbf{r_{i+1}} - \mathbf{r_i}| - a)^2 \quad (2)$$

To study this system, we adopt a two-staged stochastic simulation step [8]: each step starts by updating the positions of the beads $\{\mathbf{r}_i\}$ by solving the overdamped Langevin equation,

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{F}_i(\{\mathbf{r_j}, \phi_j\}) + \sqrt{2kT}\eta(t). \quad (3)$$

which simulates the movement of the polymer in a thermal bath of surrounding particles, where $\mathbf{F}_i$ is the force deriving from the potential of the polymer conformation and $\eta(t)$ is a Langevin force satisfying $\langle \eta(t) \rangle = 0$ and $\langle \eta(t')\eta(t) \rangle = \delta(t - t')$. The advantage of using such a scheme to move the chain lies in that the energy is analytic in the $\{\mathbf{r}_i\}$ variables, leading to a convenient analytic expression of the deterministic force $\mathbf{F}_i = -\partial U/\partial \mathbf{r}_i$

$$\begin{aligned}\mathbf{F}_i = &-Dw\Delta^2\mathbf{r_i} + Dw\Delta\left(\frac{\tau_i^4}{\kappa_i^4}\Delta\mathbf{r_i}\right) \\ &- K(|\mathbf{r_{i+1}} - \mathbf{r_i}| - a)\frac{\mathbf{r_{i+1}} - \mathbf{r_i}}{|\mathbf{r_{i+1}} - \mathbf{r_i}|} \\ &- K(|\mathbf{r_{i-1}} - \mathbf{r_i}| - a)\frac{\mathbf{r_{i-1}} - \mathbf{r_i}}{|\mathbf{r_{i-1}} - \mathbf{r_i}|}\end{aligned}$$

This allows us to benefit from a fast method to reach thermal equilibrium for the position variables.

Once the positions are updated, we update the twist angles ϕ_i through a Metropolis-Hastings Monte Carlo method: two indices i, j and an angle $\delta \in [0, 2\pi[$ are randomly chosen, and the configuration with angles $(\phi_i, \phi_j) \leftarrow (\phi_i + \delta, \phi_j - \delta)$ is adopted with probability $\min(1, e^{-\beta\Delta U})$. This move keeps the total twist $\mathrm{Tw} = \sum_i \phi_i = 2\pi k$ constant, $k \in \mathbb{Z}$, allowing us to maintain the periodic conditions. The Metropolis-Hastings algorithm is well-suited for those local changes in energy.

The data on which the discussion below is based is based on stochastic simulations of a chain of $N = 50$ elements, each simulation first covering 5 10^5 steps to reach approximate thermal equilibration, then thermally averaging observables by averaging 10^4 samples taken every successive $2N$ steps.

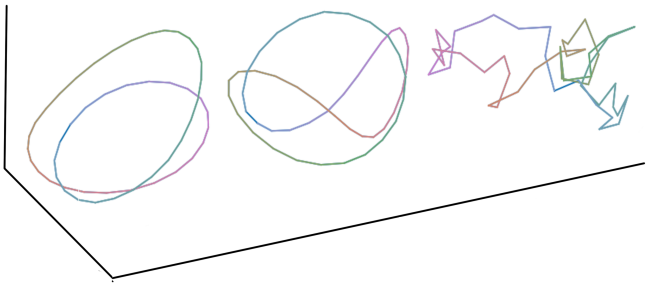

FIG. 1. Typical conformations of a closed ribbon after 10^6 simulation steps, with Tw = 0. (Left) $kT = 0.001$ (center) $kT = 0.1$, (right) $kT = 1$. Color for clarity. At lower temperatures the ribbon favours smooth configuration with a steady pitch

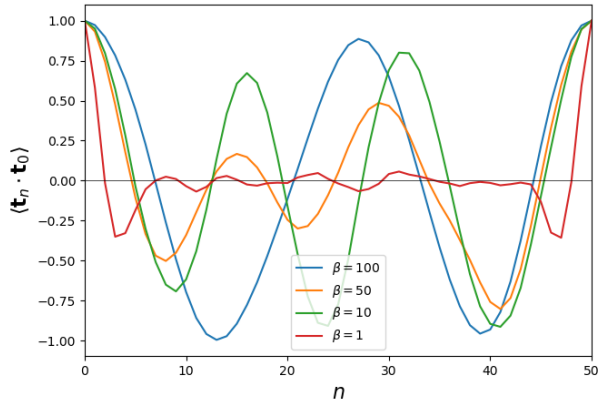

FIG. 2. Tangent-tangent correlation function for different typical temperatures, with Tw = 0. Note that the decay length and wavelength of oscillations is not monotonic.

COMPUTATIONAL RESULTS

Sample configurations obtained through this process are shown in Fig 1: Under a certain temperature $kT_c \approx 1$ the persistence length $\ell_P(T) > L/2$ and the ribbon takes a smoothed-out appearance, with an persistent helical structure, whereas for temperatures above T_c thermal noise breaks this form of short-range order.

To quantify this form of order, we introduce the tangent-tangent correlation function $\langle \mathbf{t}_n \cdot \mathbf{t}_0 \rangle$. Consistent with the analysis by Giomi and Mahadevan, we observe oscillations in the tangent-tangent correlation function at any finite temperature $\langle \mathbf{t}_n \cdot \mathbf{t}_0 \rangle \sim e^{-na/\ell_P} \cos kna$ – however, unlike their findings we do not find that k or

FIG. 3. Sample configuration of ribbons after 10^6 moves at $\beta = 100$, for (left) Tw = 5, (center) Tw = 0 (right) Tw = -5. The shapes on the left and center are unknotted, with a different number of kinematic curvature sign change. The shape on the right is a trefoil knot.

ℓ_P have a simple scaling with temperature (Fig 2). In particular, we would expect that at high temperature where $\ell_P \ll L$, the effects of periodicity would be negligible and that we would recover scaling results from open chain theory where an open Sadowsky ribbon sees $\ell_P \propto \beta$ and $k \propto \beta^{-1/2}$. Although the potential energy seems to reach equilibrium, the most likely hypothesis for this is the greater statistical noise at higher temperature, requiring more samples to effectively cull statistical deviations and get clean averages. Under the time and computing power limits available to the author, this will unfortunately remain an open question for now. A better analytical understanding of the critical behavior through a formal renormalization approach would be insightful.

At low temperatures, we investigated the effect of a non-zero twist number Tw $\neq 0$. The behavior of the tangent-tangent correlation function does not exhibit a clear trend with varying Tw; however visualizations of sample configuration suggest that the difference is probably more of a topological nature (Fig 3). Further work would focus on computing topological quantities such as the writhe of the curve, and studying their statistical properties. [9, 10]

CONCLUSION

The global constraint of periodicity in a closed ribbon proves to be a rich problem, with its specific computing challenges and physics that depart from the open chain regimes, and such a simple model misses notorious features of real ribbons, such as the apparition of characteristic plectomenes and toroids. This is a limitation of the phantom nature of our chains that can freely self-intersect to reduce their curvature, where material chains would wrap around themselves. The microscopic model dependence of open ribbons is strong, with both different quantitative and qualitative predictions from one model to another. This would also likely be a problem for the closed chain case, and it would be of interest to further explore the predictions coming from different descriptions in a closed geometry.

This project was a great opportunity to explore some computing methods and illustrate some analytical results in ribbon theory, providing the first steps to an *in silico* experimental platform to support further analytical work – no doubt that the materials developed here will be reused in subsequent studies.

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