Stiff Knots

Relating topology to geometry and mechanics

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Abstract : We analyze the energy and the geometry of closed knotted strings. We focus on the properties of the ground state (the state of lowest energy). We point out the important role of the the bridge number n. Indeed, the energy of the ground state exhibits upper and lower bounds which both scale as n^2. The geometry of the knot in the ground state is found explicitly in some special cases. Finally, we mention some additional results on the role of torsional elasticity, on the multiplicity of contact points and on the size of the knot.

1 Introduction

The analysis of the shape of a string with a bending rigidity can be traced back to Bernoulli and Euler[1]. But the fully explicit solution of the so-called Euler-Bernoulli elastica in 3D was given only in the 1980's by Langer and Singer[2]. A similar approach was developed for the so-called Kirchhoff elastica[3], where the string has both bending and twist rigidities.

The elastica approach does not account for self-contact of the strings, and therefore cannot account for physical knots and entanglements in strings and filaments. In the literature, this constraint was taken into account in numerical approaches, but a systematic analytical approach is still missing. A mathematical analysis of this problem was given by H. von der Mosel [4]. The same author has also provided some inequality on the multiplicity of contact points. Recently, a different approach was proposed[5], which allowed one to derive upper and lower bounds for the energy of the knot in the ground state (the state of lowest energy).

2 Model

We shall begin with a summary of the results of Refs.[5]. We start with the Kirchhoff elastica model. We consider a closed curve with the energy

$$\mathcal{E} = \frac{C}{2}\int ds\, \kappa^2 + \frac{D}{2}\int ds(\nabla^\perp \phi)^2, \tag{1}$$

where s is the arclength along the curve, C is the bending rigidity, κ is the curvature, D is the twist rigidity, and ϕ is the twist angle. The total length of the filament

$$\mathcal{L} = \int ds \tag{2}$$

is fixed. In addition, we consider an excluded volume tube of width w along the curve, and take the limit $w \to 0$. In this limit, crossings and multiple lines (coming from thin braids) are expected whereas localized knots and angles are forbidden because they lead to a divergence of the energy.

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3 Fundamental inequalities on the knot energy for $D = 0$

In order to proceed further, we have to define two knot invariants. The first one is the bridge number n. It is defined as the smallest number of maxima that a knot can exhibit in a given direction in space. The second invariant is based on Alexander's theorem, which states that any knot can be deformed to into a closed braid. The braid index i of a knot is defined as the smallest possible number of strands in this braid. One has in general $i \geq n$. Using these two invariants, one may derive some inequalities on the ground state energy $\mathcal{E}^*$ of a knot with $D = 0$:

$$2\pi^2 \frac{C}{\mathcal{L}} n^2 \leq \mathcal{E}^* \leq 2\pi^2 \frac{C}{\mathcal{L}} \min[\alpha n^2; i^2], \tag{3}$$

with $\alpha \approx 3.86...$

The first consequence of this result is that $\mathcal{E}^* \sim n^2$. Therefore, the bridge number n is the topological invariant which controls the ground state energy.

The second consequence, is that, $\mathcal{E}^* = 2\pi^2 n^2 C/\mathcal{L}$ when $n = i$. In this case, the geometry of the knot is a n-times covered circle. The condition $n = i$ defines a class of knots which includes torus knots. Some other knots belong to this class, as can be seen from an inspection of the standard knot tables. But to our knowledge, there is no information about how big this knot class is, and what types of knots belong to it.

4 Monte Carlo simulations

In order to gain more insights about the configuration of stiff knots, we have performed Monte Carlo (MC) simulations with a closed chain of $N = 150$ beads separated by segments of fixed length -equal to 1. The length-preserving elementary motion of the chain is implemented via the rotation (with angle $\pm\pi/100$) of one bead around the axis which runs through its neighbors. We use the Metropolis algorithm, with the energy:

$$\mathcal{E}_d = C \sum_{n=1}^{N} (1 - \mathbf{u_n}.\mathbf{u_{n+1}}) , \tag{4}$$

where $\mathbf{u_n}$ is a unit vector along the nth segment. The closure of the chain imposes:

$$\sum_{n=1}^{N} \mathbf{u}_n = 0 , \tag{5}$$

$$\mathbf{u_{N+1}} = \mathbf{u}_1 . \tag{6}$$

At low temperatures, the chain length $\mathcal{L} = N$ is much smaller than the persistence length $L_p = C/k_B T$, where T is the temperature, and k_B is the Boltzmann constant. Then, the curve is smooth, and $\mathcal{E}_d \to \mathcal{E}$. Non-crossing conditions are imposed with spheres of excluded volumes around each bead: we forbid beads to get closer than $1/\sqrt{2}$. This leads to an excluded volume tube with a non-constant width w, varying between 1 and $\sqrt{2}$.

We use a simulated annealing method with a power law decrease of the temperature up to the low temperature regime. Repeated simulations with the same knot provide us with the ground state and sometimes also with metastable states.

The results of the simulations are given on Figure1. These simulations confirm the above mentioned predictions. An important result from the simulations is the existence of a meta-stable state for the 5_2 knot. This is the simplest knot which exhibits more than one locally-stable state. How meta-stable states proliferate as knot complexity increases is still an open question which would deserve an extensive investigation.

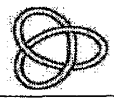
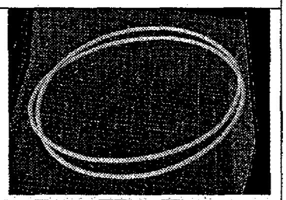
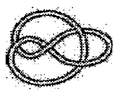
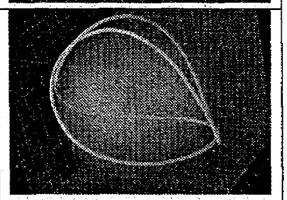
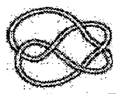
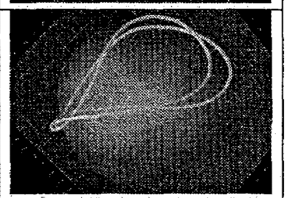
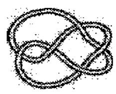
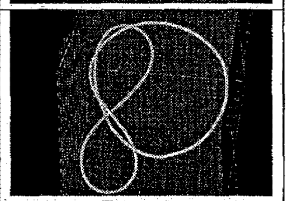
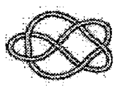
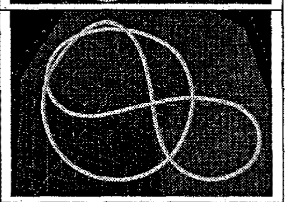
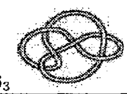
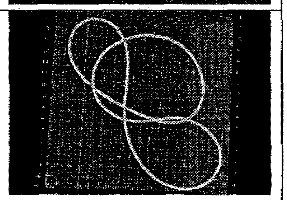
Knot and Diagram	n	i	Configuration	ϵ $w \to 0$ (theory)	ϵ_w $w \neq 0$ (MC)	Simlation (MC)
 3_1	2	2	Circular braid	$\epsilon^o_{CB} = 78.96$	80.9	
 4_1	2	3	4-fold cage	ϵ^o_{4C}	129.6	
 5_2	2	3	4-fold cage	ϵ^o_{4C}	157.5	
 5_2	2	3	80	$\epsilon^o_{80} = 142.1$	165.9	
 6_2	2	3	80	$\epsilon^o_{80} = 142.1$	163.5	
 6_3	2	3	80	$\epsilon^o_{80} = 142.1$	179.4	

Figure 1: Table of results for the MC simulations of closed stiff knots. Three different configurations are found: (i) the circular braid for the 3_1 knot; (ii) the 4-fold cage configuration for the 4_1 and 5_2 knots (the sphere is a guide for the eye, indicating that this configuration is approximately wrapped around a sphere); (iii) the "80" configuration for the 5_2, 6_2 and 6_3 knots.

5 Conclusions

In the above mentioned Monte Carlo simulations, the torsional rigidity was neglected, i.e. $D = 0$. The consequences of $D \neq 0$ are discussed in Ref.[6]. The central result is that, in the presence of a finite D, the upper bound related to n in (3) is twist-storing. Hence, this upper bound still valid when $D \neq 0$. But the upper bound related to i is not valid anymore because it exhibits a non-vanishing torsional energy.

The geometry of stiff knots is also investigated further in Ref.[6]. Two main results are obtained: (i) Following H. von der Mosel[4], upper bounds for the multiplicity of crossings, and braids can be derived; (ii) we derive upper and lower bounds for the radius of gyration of a stiff knot.

References

[1] L. Euler, Bousquet, Lausannae et Genevae **24**, E65A. O.O.Ser.I (1744).

[2] J. Langer and D.A. Singer, J. London Math. Soc. (2) **30** 512 (1984).

[3] S. Kawakubo, Osaka J. Math **37** 93 (2000).

[4] H. von der Mosel, Asymptotic Anal. **18**, 49 (1998).

[5] R. Gallotti and O. Pierre-Louis Phys. Rev. E **75**, 031801 (2007).

[6] O. Pierre-Louis, to be published.