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Statistical topology and knotting of fluctuating filaments

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HIGHLIGHTS

- What is a knot and how it can be detected in random chains.
- What is the probability that a given random ring is knotted.
- How to measure the size of a knot.
- How big are knots in random chains.

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ABSTRACT

The aim of these notes is to provide an introduction to the topic of statistical topology. With this name we refer to a combination of ideas and techniques from statistical mechanics and knot theory used to study the entanglement properties of fluctuating filaments. Some questions that we are going to address are the following: (i) What is a knot and how can we identify it? (ii) Which is the probability of finding a random curve that is knotted? (iii) How complex are these knots? (iv) How big are they? To try to partially answer these questions we will make use of few paradigmatic problems and try to investigate them by providing some "state of the art" theoretical and numerical techniques. Exercises and lists of open problems will be provided too.

1. Introduction

Knots belong to everyday life. They are very useful in practical issues such as secure boats and mountaineers, tie shoelaces. Sometimes, however, they are unwanted and very annoying events to handle. Notorious examples are the knots mysteriously formed in disorderly stored garden hoses or headphones' cables that require a lot of effort and patience to be removed.

Knots can also occur at much smaller length scales. They are very important in biology where ropes are replaced by biomolecules such as DNA and proteins [1,2]. In particular DNA molecules, being typically very long, can be knotted and this form of entanglement can affect the efficiency of cellular processes such as replication, transcription and recombination [3,4]. In physical contexts, knots can be generated as disclination defect lines in liquid crystals with colloidal inclusions, turning them into soft metamaterials with unconventional physical properties [5]. Knots can also be formed in propagating laser beams as singularities of the wave's phase (optical vortices) and in fluid or quantum vortices [6,7]. In chemistry, the synthesis of knotted molecules is one of the most active topics, with potential applications in the design of molecular machinery with complex functionality and self-assembling capabilities [8–12]

Since these knots form and evolve in environments where thermal fluctuations are important, a statistical approach to their study is natural. In the last two decades there has been a lot of work concerning the entanglement complexity of fluctuating filaments within the statistical mechanics framework. This effort has produced many interesting results on this

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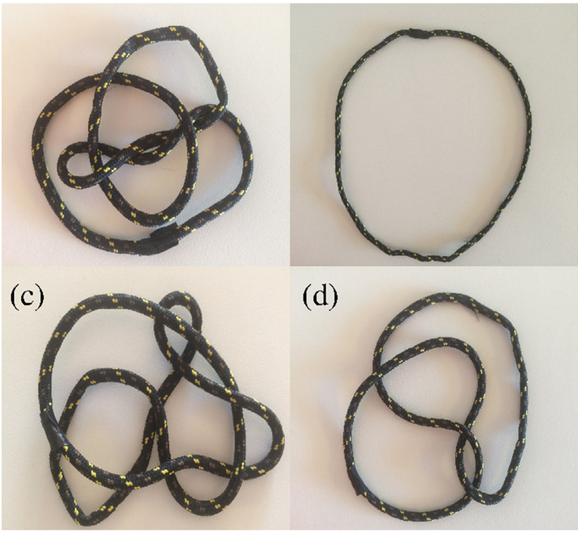

Fig. 1. Unknotted closed rope before (a) and after (b) a simplification of the geometrical entanglement obtained by smooth manipulations. A trefoil knotted rope before (c) and after simplification.

problem as well as novel investigational tools that are combination of techniques coming from different disciplines such knot theory, statistical mechanics and probability theory. In this respect this research topic, that we call *Statistical topology of fluctuating filaments*, is intrinsically multidisciplinary and spread over different disciplines.

The aim of these notes is to give an introduction of this topic by stressing the main results achieved so far as well as describing the tools most used in these investigations. This will be carried out by trying to answer at the following (apparently) simple questions:

- What is a knot and how can we detect it in a random closed chain?
- What is the probability that a given random ring is knotted?
- Can we measure the size of a knot?
- How big are the knots?

Given the limited amount of space available I will focus on knots in polymer chains but some of the notions and approaches we will discuss can be extended also to other form of topological entanglement (i.e. links) and to different filamentous systems. Open problems and exercises are given in the text.

2. What is a knot?

Although everyone is able to recognise whether a rope has a knot tied in, its rigorous definition is not as trivial as one would expect. Let us start with the following example: suppose to entangle a torsionally relaxed rope in space and then connect its extremities to form a closed chain. One can then lay the ring on a table and try to remove as much of its entanglement by a sequence of deformations. If the outcome of this procedure is a ring that can be fully flattened on the table, one can say that the rope is a *trivial knot* or is *unknotted* (see Fig. 1(a), (b)). If this is not possible, either we are not clever enough or the rope, once closed, has trapped its original entanglement into a knot and any smooth deformation gives rise to configurations having the same *knot type* (see Fig. 1(c), (d)). In this case the only way to convert the closed rope into a trivial knot and flatten it on the table is by cutting the rope in proximity of the crossings and perform appropriate strand passages. Two things are worth noticing: First the assumption of a torsionally relaxed rope is essential. In fact, a torsionally stressed rope, once converted into a ring it can coil on itself several times (as a telephone cord often does) and, even if unknotted, it cannot be flatten on a table with no crossings. Second, if the rope is left open it is sufficient to thread one extremity through the entanglement and remove any knot without resorting to traumatic (singular) operation such as cutting and re-joining. With this operative definition all open ropes are topologically equivalent. Note also that in 4D all closed curves are unknotted since one can use the fourth dimension to perform smooth strand passages. In this respect knots are genuine 3D objects. To have an analogue of knots in 4D one has to consider 2-spheres [13].

Inspired by this example one can state a mathematical definition of knotted curves as follows [14,15]. A knot is any regular embedding of a simple closed curve in three dimensional space. By regular embeddings we mean either curves of class C^1 or simple polygonal curves (see Fig. 2(a)). In both cases the knot is a *tame* knot, otherwise is a *wild* knot (see an example in Fig. 2(b)). Since wild knots cannot be representative of knots occurring in nature it is convenient to focus on