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Matched asymptotic expansions for twisted elastic knots: A self-contact problem with non-trivial contact topology

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ABSTRACT

We derive solutions of the Kirchhoff equations for a knot tied on an infinitely long elastic rod subjected to combined tension and twist, and held at both endpoints at infinity. We consider the case of simple (trefoil) and double (cinquefoil) knots; other knot topologies can be investigated similarly. The rod model is based on Hookean elasticity but is geometrically nonlinear. The problem is formulated as a nonlinear self-contact problem with unknown contact regions. It is solved by means of matched asymptotic expansions in the limit of a loose knot. We obtain a family of equilibrium solutions depending on a single loading parameter $\overline{U}$ (proportional to applied twisting moment divided by square root of pulling force), which are asymptotically valid in the limit of a loose knot, $\varepsilon \to 0$. Without any *a priori* assumption, we derive the topology of the contact set, which consists of an interval of contact flanked by two isolated points of contacts. We study the influence of the applied twist on the equilibrium.

1. Introduction

Knots are found in everyday life, shoe lacing being probably the most common example. They are also essential in a number of activities such as climbing and sailing. In science, knots have long been studied in the field of mathematics, the main motivation being to propose a topological classification of the various knot types, see the review by Tabor and Klapper (1994). Recently, there has been an upsurge of interest in knots in the biological context: knots form spontaneously in many long polymers chains such as DNA (Katritch et al., 1996) or proteins, and have been tied on biological filaments (Arai et al., 1999). Knotted filaments have a lower resistance to tension than unknotted ones and break preferably at the knot (Saitta et al., 1999; Pieranski et al., 2001a). Despite a wide range of potential applications, the mechanics of knots is little advanced. The present paper is an attempt to approach knots from a mechanical perspective by using a well-established model of thin elastic rods.

The problem of finding so-called ideal knot shapes has received much attention in the past decade (Katritch et al., 1996; Stasiak et al., 1998). In this geometrical description of tight knots, an impenetrable tube with constant radius is drawn around an inextensible curve in Euclidean space and one seeks, for each knot type, the configurations of the curve such that the radius of the tube is maximum. The case of open knots, where the curve does not close upon itself, has been studied by Pieranski et al. (2001b) in connection with the breakage of knotted filaments under tension (Pieranski et al., 2001a).

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To go beyond a purely geometrical description of knots, it is natural to formulate the problem in the framework of the theory of elasticity. The case of tight knots, or even of moderately tight knots, leads to a problem of 3D elasticity with geometrical nonlinearities (finite rotations), finite strains, and self-contact along an unknown surface: there is no hope to derive analytical solutions. Numerical solution of this problem raises considerable difficulties too, which have not yet been tackled to the best of our knowledge. In the present paper, we study the limit of *loose* knots, when the total contour length captured in the knot is much larger than the radius of the filament. In this limit, it is possible to use a Cosserat type model and describe the rod as an inextensible curve embedded with a material frame, obeying Kirchhoff equations; as we show, the equilibria of open knots can be solved analytically in this limit.

Self-contact in continuum mechanics, and in the theory of elastic rods in particular, leads to problems that are both interesting and difficult. This comes from the fact that the set of points in contact is not known in advance—in fact, not even the topology of this set is known. This paper builds up on prior work by von der Mosel (1999) and Schuricht and von der Mosel (2003), who characterize the smoothness of the contact force in equilibria of elastic rods, and by Coleman and Swigon (2000), who write down the Kirchhoff equations for rods in self-contact explicitly, including the unknown contact force. These equations have been solved by numerical continuation in specific geometries by Coleman and Swigon (2000), van der Heijden et al. (2003) and Neukirch (2004). In these papers, the authors simultaneously solve for the nonlinear Kirchhoff equations and for the unknown contact forces. In the present paper, we show that, *under the same set of assumptions that warrant applicability of the Kirchhoff equations*, one can in fact neglect the geometrical nonlinearities in the region of self-contact. As a result, nonlinearities and contact can be addressed in well-separated spatial domains. This brings in an important simplification and, as the result, we are able for the first time to derive analytical solutions of a self-contact problem for rods undergoing finite displacement, exhibiting a non-trivial contact set topology.

Our solution is constructed by matched asymptotic expansions with respect to a small parameter ε which is zero for a perfectly thin rod. As is done routinely in boundary layer analysis, we use qualitative reasonings (dimensional analysis) to justify how the various quantities scale with the small parameter ε. We emphasize that our final solution is exact and does not involve any other assumption than the smallness of the parameter ε: it is *asymptotically* exact. Our presentation is based on formal expansions; proofs of convergence are beyond the scope of the present paper and can hopefully be established in the future. For an introduction to matched asymptotic expansions, see the book by Hinch (1991) or Audoly and Pomeau (2009).

The mechanical problem considered here is the following. We solve the Kirchhoff equations for an infinite rod, with clamped boundary conditions at both endpoints at infinity. The rod is inextensible, unshearable and its weight is neglected; bending and twisting moments are related to curvature and twist by a linear constitutive law given in Eq. (3) but geometric non-linearities are retained. Topology of the centerline is a prescribed knot shape (we consider trefoil and cinquefoil knots). This knotted shape is enforced by self-contact forces, which are taken into account in the equations of equilibrium. The rod is loaded under combined tension force T and twisting moment U at its endpoints; this loading is captured by a single dimensionless parameter, $\overline{U}$, defined in Eq. (19). We derive a family of solutions of the boundary-value problem depending on the loading parameter $\overline{U}$, which is asymptotically valid for small ε. In a previous short paper (Audoly et al., 2007), we have announced some of the results reported here, for the case of a purely tensile loading, $U = 0$; in addition to presenting a justification of these results, we address here the influence of twist on the knot shape.

The outline of the present paper is as follows. In Section 2, we introduce the Kirchhoff equations for rods in equilibrium, including the contact forces relevant for the knotted geometry; we discuss the equivalent formulation as a minimization problem with topological constraints. In Section 3, we discuss the singular limit of vanishing thickness when the region of contact collapses to a point connecting a circular loop and two straight tails. In Section 4, we propose a perturbation scheme of the original equations in powers of ε. Following the general methodology of matched asymptotic analysis, the solution is given by different expansions in different regions—here we have three regions, namely a loop, two tails and a braid. The form of these expansions is motivated by dimensional analysis for small but non-zero thickness. Next the expansion is carried out by solving the equations in the various regions: the tails are solved in Section 5, the loop in Section 6. The solution in the braid region is the most challenging as this is where contact occurs, and in Section 7 we obtain a universal solution describing the shape of the rod in this region. In Section 8 we build a global solution by matching the solutions derived previously in each region. Thereby, we obtain a unique equilibrium solution for any given value of the loading parameters (pulling force and twisting moment). In Section 9, this theory is validated by experiments. Appendix A discusses the topology of the contact set in more details.

2. Model

We seek equilibrium solutions of a thin elastic rod bent into an open[1] knot with a prescribed type, and subjected to tensile end force and torsional end moment, as shown in Fig. 2. In the present paper, we focus on two specific knot types, which are open trefoil knots, also called *simple* knot and noted 3_1, and open cinquefoil knots, also called *double* knot and noted 5_1, see Fig. 1. Other knot types can be handled similarly. The rod is infinitely long and the loading is applied at infinity.

[1] In topology, a knot is defined as a closed, non-self-intersecting curve. Here we consider curves having two infinite tails, hence the name 'open knots'.