Tightening elastic \((n, 2)\)-torus knots

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Abstract. We present a theory for equilibria of elastic torus knots made of a single thin, uniform, homogeneous, isotropic, inextensible, unshearable rod of circular cross-section. The theory is formulated as a special case of an elastic theory of geometrically exact braids consisting of two rods winding around each other while remaining at constant distance. We introduce braid strains in terms of which we formulate a second-order variational problem for an action functional that is the sum of the rod elastic energies and constraint terms related to the inextensibility of the rods. The Euler–Lagrange equations for this problem, partly in Euler–Poincaré form, yield a compact system of ODEs suitable for numerical solution. By solving an appropriate boundary-value problem for these equations we study knot equilibria as the dimensionless ropelength parameter is varied. We are particularly interested in the approach of the purely geometrical ideal (tightest) limit. For the trefoil knot the tightest shape we could get has a ropelength of 32.85560666, which is remarkably close to the best current estimate. For the pentafoil we find a symmetry-breaking bifurcation.

Contact problems in the theory of elasticity have seen a surge of interest recently. They are challenging because of the one-sided constraints they introduce. Determining the topology and geometry of the contact set given the boundary conditions is probably the hardest part of any contact problem. Although great progress has been made in some of the 1D continua problems (Schuricht & von der Mosel, 2003; Gonzalez et al., 2002; van der Heijden et al., 2006) we are still far from a full understanding of the solutions of the Euler–Lagrange equations for general contact problems. Ideal knots (links) (Stasiak et al., 1998) deliver a particular example of a geometrical contact problem where ropelength (the length-to-thickness ratio of a tube embedded into space) is minimised instead of elastic energy. Here we consider an elastic version of the knot tightening problem by applying what seem to be the first equilibrium equations for elastic knots made of an incompressible tube. The theory of elastic braids (Starostin & van der Heijden, 2014) deals with a special type of (self-)contact problems of elastic rods. Our special case of contact involves only equality constraints and is in this sense simpler allowing progress to be made. We assume the topology of the contact set to be a circle, but we make no a priori assumption on the geometry. Rather, we obtain the shape of the contact curve as part of the solution.

We apply the theory of equilibria of braids made of two elastic rods (2-braids) (Starostin & van der Heijden, 2014) to compute tight elastic \((n, 2)\)-torus knots. We recall the essential equations, then formulate boundary conditions that smoothly seal the ends of the rods so that a knot is formed (Fig. 1) and after that discuss numerical solutions obtained when we inflate the incompressible tubes modelling the rods.
1. Theory of elastic braids made of two strands at constant distance

1.1. Jointly parametrised curves, reference frames and strains

Consider a pair of smooth curves \( r_1(s) \in \mathbb{R}^3, s \in [0, L_1], r_2(\sigma) \in \mathbb{R}^3, \sigma \in [0, L_2] \), both parametrised by arclength, that serve as centrelines of two inextensible elastic rods of length \( L := L_1 \) and \( L_2 \), respectively. We denote by \( t_1(s) = \frac{dr_1(s)}{ds} \) and \( t_2(\sigma) = \frac{dr_2(\sigma)}{d\sigma} \) the unit tangents to each of the curves. We define the point-to-point squared distance function \( D_2(s, \sigma) = \rho_2^2(s, \sigma) \), where \( \rho(s, \sigma) = r_2(\sigma) - r_1(s) \) is a chord vector connecting the two curves. We assume that there is a one-to-one mapping \( [0, L_1] \leftrightarrow [0, L_2] : s \leftrightarrow \sigma(s) \) between the two curves such that \( D_2 \) is bicritical at corresponding points, i.e.,

\[
\frac{\partial D_2}{\partial s}(s, \sigma) \bigg|_{\sigma=\sigma(s)} = -2\rho(s, \sigma(s)) \cdot t_1(s) = 0 \quad \text{and} \quad \frac{\partial D_2}{\partial \sigma}(s, \sigma) \bigg|_{\sigma=\sigma(s)} = 2\rho(s, \sigma(s)) \cdot t_2(\sigma(s)) = 0.
\]

Then \( D_2(s, \sigma(s)) \) is constant, say equal to \( \Delta^2 \), and the two curves are said to be at constant distance \( \Delta \). Moreover the chords \( \rho(s, \sigma(s)) \) are orthogonal to the curve tangents at both ends. Because of the one-to-one mapping there exists a common parametrisation for both curves. Taking arclength along the first curve as the common parameter, we can introduce the unit chord vector \( d_1(s) = \frac{\rho(s, \sigma(s))}{\Delta} = \frac{1}{\Delta} [r_2(\sigma(s)) - r_1(s)] \).

We shall henceforth write expressions like \( r_2(s) \) instead of \( r_2(\sigma(s)) \).

Figure 1. Elastic pentafoil knot as a closed 2-braid with two ‘strands’ (of unequal length) painted in different colours. The ropelength is 49.01152520.

Along each curve we define two moving frames as follows (Fig. 2). We define \( u_1 := t_1 \times d_1 \) so that the vectors \( t_1, d_1, u_1 \) form an orthonormal frame that we call the first braid frame. We also define an orthonormal material frame on the first rod: \( \{t_1, d_0, v_1\} \) (\( d_0 \) along arbitrary normal direction). The two frames differ by a rotation about \( t_1 \) through an angle \( \xi_1 \) measured from \( d_0 \) to \( d_1 \). Correspondingly, we define two moving orthonormal frames on the second curve \( r_2 \). The first one (called the second braid frame) is made up of the vectors \( t_2, d_1, u_2 := t_2 \times d_1 \), while the second one (called the second material frame) is \( \{t_2, d_2, v_2\} \). They differ by a rotation about the tangent vector \( t_2 \) through an angle \( \xi_2 \), measured from \( d_1 \) to \( d_2 \).

After choosing a coordinate system we may identify the orientations of the above four
reference frames with elements of the group of orthogonal $3 \times 3$ matrices:

$$R_{ij}(s) := (t_j(s), d_i(s), \beta_{ij}(s)) \in SO(3), \quad \beta_{ij}(s) = t_j(s) \times d_i(s) = i(2-i)u_j(s) + |i-1|v_j(s),$$

where $i \in \{0, 1, 2\}$, $j \in \{1, 2\}$, $ij \neq 02, 21$. These define four skew-symmetric $3 \times 3$ matrices in the Lie algebra $\mathfrak{so}(3)$ as follows:

$$\hat{\omega} = R_{11}^T R_{11}', \quad \hat{\Omega} = R_{12}^T R_{12}', \quad \tilde{\omega} = R_{01}^T R_{01}', \quad \tilde{\Omega} = R_{22}^T R_{22}'$$ \hspace{0.5cm} (1)

where we have introduced the ‘hat’ isomorphism between skew-symmetric matrices $\hat{w} = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}$ in $\mathfrak{so}(3)$ and axial (rotation) vectors $w = (w_1, w_2, w_3)^T$ in $\mathbb{R}^3$. \(^1\)

Here and in the following a prime denotes differentiation with respect to $s$. Thus we have defined four axial vectors $\omega, \Omega, \hat{\omega}, \hat{\Omega}$, where $\omega = (\omega_1, \omega_2, \omega_3)^T$ is the rotation vector of the braid frame $\{t_1, d_1, \hat{u}_1\}$, $\Omega = (\Omega_1, \Omega_2, \Omega_3)^T$ is the rotation vector of the braid frame $\{t_2, d_1, u_2\}$, $\tilde{\omega} = (\tilde{\omega}_1, \tilde{\omega}_2, \tilde{\omega}_3)^T$ is the rotation vector of the material frame $\{t_1, d_1, v_1\}$ and $\tilde{\Omega} = (\tilde{\Omega}_1, \tilde{\Omega}_2, \tilde{\Omega}_3)^T$ is the rotation vector of the material frame $\{t_2, d_2, v_2\}$.

The orthonormal frames form a sequence under consecutive rotations about $t_1, d_1$ and $t_2$. Thus

$$R_{11} = R_{01} R_1(\xi_1), \quad R_{12} = R_{11} R_2(\eta), \quad R_{22} = R_{12} R_1(\xi_2),$$

where

$$R_1(\xi_i) = \exp(\xi_i \hat{e}_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \xi_i & -\sin \xi_i \\ 0 & \sin \xi_i & \cos \xi_i \end{pmatrix}, \quad i = 1, 2, \quad e_1 = (1, 0, 0)^T,$$

$$R_2(\eta) = \exp(\eta \hat{e}_2) = \begin{pmatrix} \cos \eta & 0 & \sin \eta \\ 0 & 1 & 0 \\ -\sin \eta & 0 & \cos \eta \end{pmatrix}, \quad e_2 = (0, 1, 0)^T,$$

and $\eta$ is the angle, about $d_1$, from the first tangent, $t_1$, to the second, $t_2$ (see Fig. 2). From Eqs. (1), (2) it follows that the rotation vectors of the material and braid frames are related as

$$\hat{\omega} = R_1^T(\xi_1) \hat{\omega} R_1(\xi_1) + R_1^T(\xi_1) R_1(\xi_1),$$

$$\hat{\Omega} = R_2^T(\eta) \hat{\Omega} R_2(\eta) + R_2^T(\eta) R_2(\eta),$$

$$\tilde{\omega} = R_1^T(\xi_2) \tilde{\omega} R_1(\xi_2) + R_1^T(\xi_2) R_1(\xi_2).$$

Owing to the inextensibility condition $|\frac{d\sigma}{d\sigma}| = 1$, the arclength parameter $\sigma$ along the second centreline satisfies

$$\sigma' = \sqrt{(\Delta \omega_1)^2 + (\Delta \omega_3 - 1)^2}. \hspace{0.5cm} (6)$$

We express the angle $\eta$ as a function of the components of $\omega$ as

$$\sin \eta = -\Delta \omega_1 / \sigma', \quad \cos \eta = (1 - \Delta \omega_3 / \sigma'),$$

and hence

$$\omega_1 = \left( \omega_3 - \frac{1}{\Delta} \right) \tan \eta. \hspace{0.5cm} (8)$$

\(^1\) Throughout we adopt the notation that for any vector $v \in \mathbb{R}^3$ the sans-serif symbol $\nu$ denotes the triple of components $(v_1, v_2, v_3)^T = (v \cdot t_1, v \cdot d_1, v \cdot u_1)^T$ in the first braid frame. An exception is however made for sans-serif rotation vectors, which are always triples of components in their corresponding frames.
Eqs. (3)–(5) allow us to express the strand strains $\tilde{\omega}_1, \tilde{\omega}_2, \tilde{\omega}_3, \tilde{\Omega}_1, \tilde{\Omega}_2, \tilde{\Omega}_3$ in terms of the variables $(\omega_1, \omega_2, \omega_3, \xi_1, \xi_2)$, which we shall call the braid strains. In much of the following it will be convenient to use Eq. (8) to eliminate $\omega_1$ in favour of the angle $\eta$, which also has an intuitive physical meaning as braid angle. With either choice of variables we have an unconstrained description in which, by construction, the constant-distance constraint is automatically satisfied.

We note that if $\omega_1 = 0$ and $\omega_3 \neq 1/\Delta$, then $\eta = 0$ and the two strands are parallel (this condition does not restrict in any way the shape of the first centreline). When $\omega_3 = 1/\Delta$, and $\omega_1 \neq 0$, the second strand becomes orthogonal to the first one. If both $\omega_1 = 0$ and $\omega_3 = 1/\Delta$ then $\sigma' = 0$, i.e., the induced parametrisation of the second centreline is singular. The angle $\eta$ is then not defined. We need to rule out this case.

The tubes of radius $\Delta/2$ built around each of the centrelines should not overlap. Locally it means that the points connected by the bicritical chords must be the closest points of the centrelines. It may be shown that this requires $\eta \in (-\pi/2, \pi/2)$ (Starostin & van der Heijden, 2014).

1.2. Equations for the standard 2-braid

For the elastic energy we make the usual assumption of frame indifference, i.e., the energy is invariant under Euclidean motions. It will then depend only on the strains (and possibly arclength) and not, for instance, on the centreline $r_1$. We have already assumed both rods in the braid to be inextensible and unshearable, so there is no elastic energy on account of stretches. Apart from this restriction we allow for arbitrary hyperelastic rods (Antman, 2005) and write

$$U_1 = \int_0^{L_1} f_1(\tilde{\omega}) \, ds \quad \text{and} \quad U_2 = \int_0^{L_2} f_2(\tilde{\Omega}(\sigma)) \, d\sigma = \int_0^{L_1} f_2(\tilde{\Omega}/\sigma') \sigma' \, ds$$

for the strain energy of the first and second rod, respectively, where $f_1$ and $f_2$ are the strand strain energy densities, and the explicit argument of $\tilde{\Omega}$ in the $\sigma$ integral emphasises that $\tilde{\Omega}$ is to be regarded as a function of arclength $\sigma$ of the second rod in this integral.

Assuming fixed ends of the first strand, we add $-F \cdot [r_1(L) - r_1(0)] = -\int_0^L F \cdot t_1 \, ds$ as an isoperimetric constraint expression with $F$ a (constant) Lagrange multiplier (to become the internal force in the braid). Also, by inextensibility of the second rod we require the length of the second strand

$$L_2 = \int_0^{L_2} d\sigma = \int_0^L \sigma' \, ds = : \int_0^L f_\sigma(\omega_1, \omega_3) \, ds$$

(10)

to be constant, giving a second isoperimetric constraint.

We can express the arguments of the integrands in Eqs. (9) and (10) in terms of the braid strains $(\omega, \xi_1, \xi_2)$ and their derivatives by using Eqs. (3)–(5) and (6) and thus formulate a (second-order) variational problem for the reduced functional $l : 2\mathfrak{s}_0(3) \times \mathbb{R}^3 \times TS^1 \times TS^1 \to \mathbb{R}$,

$$l(\omega, \omega', F, \xi_1, \xi_1', \xi_2, \xi_2') = f_1(\tilde{\omega}) + f_2(\tilde{\Omega}(\sigma)) + h\sigma' - F \cdot t_1,$$

(11)

for variations that keep the end positions and orientations of the rods fixed; $h$ is a (constant) Lagrange multiplier.

The Euler–Lagrange equations are derived partly in Euler–Poincaré form and comprise (a) balance equations for the components of the overall braid force $F = (F_1, F_2, F_3)^T$ and braid moment $M = (M_1, M_2, M_3)^T$ expressed in the first braid frame (Starostin & van der Heijden, 2014)

$$F' + \omega \times F = 0,$$

(12)

$$M' + \omega \times M + t_1 \times F = 0,$$

(13)
(b) the ‘constitutive’ equations

\[ M_j = \frac{\partial l}{\partial \omega_j} - \frac{d}{ds} \frac{\partial l}{\partial \omega'_j}, \quad j = 1, 2, 3, \]  

(14)

and (c) the phase equations for the twist angles of the rods

\[ \frac{\partial l}{\partial \xi_i} - \frac{d}{ds} \frac{\partial l}{\partial \xi'_i} = 0, \quad i = 1, 2. \]  

(15)

Equations (12) and (13) are the familiar F\textsuperscript{\textsf{\textit{b}}} the ‘constitutive’ equations with the elastic energy density follows that |\textit{F}| and \textit{F} \cdot \textit{M} are first integrals.

Equations (15) can be written as a set of four first-order equations by introducing new variables \( T_i, i = 1, 2 \):

\[ T_i = \frac{\partial l}{\partial \xi'_i}, \quad T'_i = \frac{\partial l}{\partial \xi'_i}. \]  

(16)

If we eliminate the variable \( \omega_1 \) in favour of \( \eta \) by using \( \eta = \eta(\omega_1, \omega_3) \) given in Eq. (7), the reduced density \( l \) takes the form

\[ l = g(\omega_2, \omega_3, \eta, \eta', F_1, \xi_1, \xi_1', \xi_2, \xi_2'), \]  

(17)

while Eq. (14) transforms into (Starostin & van der Heijden, 2009)

\[ M_1 = \frac{\partial l}{\partial \omega_1} \xi_1'(g) = \Delta \cos^2 \eta \frac{\partial g}{\partial \omega_3} - 1 \left[ \frac{\partial g}{\partial \eta} - \left( \frac{\partial g}{\partial \eta'} \right)' \right], \]  

(18)

\[ M_2 = \frac{\partial g}{\partial \omega_2}, \]  

(19)

\[ M_3 = \frac{\partial g}{\partial \omega_3} + \frac{\partial l}{\partial \omega_3} \xi_1'(g) = \frac{\partial g}{\partial \omega_3} - \Delta \sin \eta \cos \eta \frac{\partial g}{\partial \omega_3} - 1 \left[ \frac{\partial g}{\partial \eta} - \left( \frac{\partial g}{\partial \eta'} \right)' \right]. \]  

(20)

(cf. (Starostin & van der Heijden, 2007) )

We now specialise our theory to the case where the two strands are linearly elastic, uniform, isotropic, initially straight rods with bending stiffness \( B_1 \) and \( B_2 \) and torsional stiffness \( C_1 \) and \( C_2 \), respectively. We allow the strands to be intrinsically twisted with twist rates \( \omega_{01} \) and \( \omega_{02} \). We call this special case the standard 2-braid. The density \( g \) in Eq. (17) then takes the form

\[ g = g_e(\omega_2, \omega_3, \eta, \eta', \xi_1, \xi_2') + h(1 - \Delta \omega_3) / \cos \eta - F_1, \]  

(21)

with the elastic energy density \( g_e = f_1 + f_2 \), the sum of bending and torsional energy densities of the two strands, given by (using Eqs. (3)–(5))

\[ g_e = \frac{1}{2} \left[ B_1(\omega_2^2 + \omega_3^2) + \frac{B_2}{\sigma}(\Omega_2^2 + \Omega_3^2) + C_1(\omega_1 - \omega_{01})^2 + \frac{C_2}{\sigma} (\Omega_1 - \sigma \omega_{02})^2 \right] = \]

\[ = \frac{1}{2} \left( B_1(\omega_2^2 + \omega_3^2) + B_2 \left[ \frac{\cos \eta}{1 - \Delta \omega_3} (\omega_2 + \eta')^2 + \left( \omega_3 - \sin^2 \eta / \Delta \right)^2 \right] + \right. \]

\[ + C_1 \left[ \left( \omega_3 - \frac{1}{\Delta} \right)^2 \tan \eta - \xi_1' - \omega_{01} \right]^2 + \]

\[ + C_2 \left[ \frac{\cos \eta}{1 - \Delta \omega_3} \left( \frac{\sin \eta}{\Delta} - \xi'_2 \right)^2 + 2 \omega_{02} \left( \frac{\sin \eta}{\Delta} - \xi'_2 \right) + \omega_{02}^2 \frac{1 - \Delta \omega_3}{\cos \eta} \right] \right). \]  

(22)

This gives a system of 13 ODEs in \((F_1, F_2, F_3, M_1, M_2, M_3, \eta, \omega_2, \omega_3, \xi_1, T_1, \xi_2, T_2)\): Eqs. (12), (13), (16), (18), (19) and (20). The last three in fact contain two algebraic equations because \( g \) does not depend on \( \omega'_2 \) and \( \omega'_3 \), but these can be turned into ODEs by differentiation (and the algebraic equations used to solve for \( \eta' \) and \( h \)). Also note that since \( g \) does not depend on the phase angles \( \xi_1 \) and \( \xi_2 \), the \( T_i \) (the strand torques) are constants.
1.3. Kinematics equations

Reconstruction of the centreline of the first strand requires solving for the tangent \( t_1 \) and integrating this to get \( r_1 \). We choose a parametrisation of the first braid frame \( \{ t_1, d_1, u_1 \} \) in terms of four Euler parameters (or quaternions) \( q = (q_0, q_1, q_2, q_3) \) subject to the normalisation condition \( q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1 \) (Hanson, 1994) and write

\[
  t_1 = \left( \begin{array}{c} q_0^2 + q_1^2 - q_2^2 - q_3^2 \\ 2q_1q_2 + 2q_0q_3 \\ 2q_1q_3 - 2q_0q_2 \end{array} \right), \quad d_1 = \left( \begin{array}{c} 2q_1q_2 - 2q_0q_3 \\ q_0^2 - q_1^2 + q_2^2 - q_3^2 \\ 2q_2q_3 + 2q_0q_1 \end{array} \right), \quad u_1 = \left( \begin{array}{c} 2q_1q_3 + 2q_0q_2 \\ 2q_2q_3 - 2q_0q_1 \\ q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{array} \right).
\]

These Euler parameters, unlike Euler angles, give a singularity-free description of arbitrary rotations in space and are therefore convenient for numerical computations. The kinematics equations are obtained by differentiating the above vectors and using Eq. (1):

\[
  \begin{pmatrix}
    q_0 \\
    q_1 \\
    q_2 \\
    q_3
  \end{pmatrix}' = \frac{1}{2} \begin{pmatrix}
    0 & -\omega_1 & -\omega_2 & -\omega_3 \\
    \omega_1 & 0 & -\omega_2 & \omega_3 \\
    \omega_2 & -\omega_3 & 0 & \omega_1 \\
    \omega_3 & \omega_2 & -\omega_1 & 0
  \end{pmatrix} \begin{pmatrix}
    q_0 \\
    q_1 \\
    q_2 \\
    q_3
  \end{pmatrix},
\]

where we recall from Eq. (8) that \( \omega_1 = (\omega_4 - \frac{1}{3}) \tan \eta \). It is straightforward to verify that \( q \cdot q' \) is a first integral of this system of equations. To find the centreline \( r_1 \) we solve Eq. (23) in conjunction with the equation \( r_1' = t_1 \). The second centreline is then given by \( r_2 = r_1 + \Delta d_1 \).

2. Numerical solution

In this section we present results obtained by numerically solving boundary-value problems for the standard 2-braid equations using the continuation and bifurcation code AUTO (Doedel, E. et al., 2007). AUTO solves ODEs using collocation and uses pseudo-arclength continuation to advance solutions as a control (or bifurcation) parameter is incremented. The code is also able to detect pitchfork or other bifurcation points along a solution branch where this branch intersects another solution branch and to switch to and compute this second branch. The thickness \( \Delta \) will be chosen as a bifurcation parameter.

Here we consider only the closed braid problem where the two rods form a \((n, 2)\)-torus knot. We start from an analytical solution (two linked rings) and perform continuations mimicking the cutting, twisting and resealing of the rings to obtain different torus knots (and links) (Starostin & van der Heijden, 2014). We compute solutions with different linking numbers for which we derive boundary conditions that ensure smooth closure of the braid into a knot (for semi-integer linking number of the braid).

For a 2-braid knot we define a linking number by following Fuller’s extension of the concept of a linking number to a (not necessarily closed) ribbon (Fuller, 1978). By a ribbon is here meant a curve with a field of normal vectors of constant length. First note that the contact curve of our knot \( \frac{1}{2}(r_1(s) + r_2(s)) = r_1(s) + \frac{1}{2}d_1(s), s \in [0, L], \) is a (smoothly) closed curve and the director \( \frac{1}{2}d_1(s) \) is an orthogonal vector defined for all \( s \in [0, L] \). It therefore forms a non-closed ribbon. We define the linking number of this ribbon as \( \mathcal{L}k = \mathcal{T}w + W_r \), where \( W_r \) is the writhing number of the contact curve and \( \mathcal{T}w = \frac{1}{2\pi} \int_0^L tw(s) \, ds \) is the total twist (the twisting number) of the braid with twist rate \( tw \). To have a closed single centreline, \( \mathcal{L}k \) has to be semi-integer, \( \mathcal{L}k = n/2, n \in \mathbb{Z} \). Alternatively, if we think of the ribbon as extended in both \( \pm \frac{1}{2}d_1 \) directions, we may say that, for our knots, this ribbon is one-sided (like a Möbius strip (Starostin & van der Heijden, 2007)) and its edge (given by the centreline of the rod) is a single knotted curve.

In addition to the 13-dimensional ODE derived in Section 1.2 we solve the 7 kinematics equations for \( q \) and \( r_1 \) of Section 1.3, so as to be able to apply displacement boundary conditions
To compute knot solutions of total length $L_{\text{tot}}$. Boundary conditions

The quaternion normalisation condition $|q| = 1$ can simply be imposed by choosing boundary conditions for the $q_i$ that satisfy it.

Given a solution of this 21D system of ODEs we can compute other properties such as the normal contact pressure $p$ or the curvature $\kappa_c$ of the contact curve. Frictionless hardcore contact is assumed. First integrals are monitored throughout to keep track of the numerical accuracy of solutions.

2.1. Boundary conditions

To compute knot solutions of total length $L_{\text{tot}}$ we apply the following boundary conditions

\[
\begin{align*}
  x_1(0) &= 0, \quad x_1(L) - x_1(0) = \Delta, \quad (24) \\
  y_1(0) &= 0, \quad y_1(L) = 0, \quad (25) \\
  z_1(0) &= 0, \quad z_1(L) = 0, \quad (26) \\
  q_0(0) &= 0, \quad q_0(L) = q_3(L), \quad (27) \\
  q_1(0) &= -1/\sqrt{2}, \quad q_1(L) = -q_2(L), \quad (28) \\
  q_2(0) &= -1/\sqrt{2}, \quad 4q_0(L)q_1(L) = \sin \eta(L), \quad (29) \\
  q_3(0) &= 0, \quad \eta(L) = \eta(0), \quad (30) \\
  \xi_1(0) &= 0, \quad [M_2(0) - B_1\omega_2(0)]/B_2 = -\omega_2(L), \quad (31) \\
  \xi_2(0) &= 0, \quad (1 - \Delta\omega_3(0))/\cos \eta(0) = \cos \eta(L)/(1 - \Delta\omega_3(L)), \quad (32) \\
  T_1(0) &= t_{10}, \quad \sigma(L) = L_2, \quad (33) \\
  T_2(0) &= t_{20}, \quad L + L_2 = L_{\text{tot}}, \quad (34) \\
  \sigma(0) &= 0, \quad (35)
\end{align*}
\]

where $t_{10}$ and $t_{20}$ are constants.

The first nine of these conditions ensure smooth closure of the braid into a doubly-covered ring, smooth here meaning continuity up to second derivatives of $r_i$, i.e., curvatures. Conditions Eqs. (36)–(38) place the end of the first centreline $r_1$ at the beginning of the second centreline $r_2$, both strands thus forming a single closed rod. Conditions Eqs. (39) and (40) imply $d_1(L) = -d_1(0)$. Condition Eq. (41) guarantees that $t_1(L)$ makes an angle $\eta(L)$ with $t_1(0)$ of the same strand. Together with condition Eq. (42) this ensures matching of the tangents: the tangent at $s = L$ of the first strand aligns with the tangent at $s = 0$ of the second strand, and vice versa. Conditions Eqs. (42)–(44) are equivalent to $\Omega_1(0)/\sigma'(0) = \omega_1(L)$, $\Omega_2(0)/\sigma'(0) = -\omega_2(L)$ and $\Omega_3(0)/\sigma'(0) = -\omega_3(L)$, which ensure that the curvatures at the end of the first strand match the curvatures at the beginning of the second strand.

The total number of boundary conditions is 23 and the three free parameters required for solution branches are $L$, $L_2$ and $\Delta$. Since for a knot the two strands are part of a single closed rod, it only makes good sense to take $B_2 = B_1$, $C_2 = C_1$ and $t_{20} = -t_{10}$. Note that the material frames of these knot solutions will in general not be closed. Material closure requires $\xi_1(0) + \xi_2(L) = \pi \text{ (mod } 2\pi)\text{ and can be achieved by inserting the right amount of twist by varying } t_{10} \text{ and } t_{20}.$

3. Tightening the trefoil and pentafoil knots

There is considerable recent interest in the configuration and contact set of the tightest possible (tubular) knot within a given topological class, i.e., the closed tube embedded in 3D space of
shortest ropelength $2L_{vol}/\Delta$ (Stasiak et al., 1998). Note that local non-self-intersection requires that the radius of curvature of the centreline must be bounded from below by the radius $\Delta/2$ of the tube. These tightest knots, called ideal knots, appear naturally in various physical problems (Calvo et al., 2005). They allow, for instance, the prediction of electrophoretic mobility of DNA knots through gel (Stasiak et al., 1996). Large numerical efforts have in particular focused on the trefoil knot for which the best current upper bound for the shortest ropelength is 32.742934547 (Przybyl & Pieranski, 2014). It is known from numerical simulations that in the ideal configuration each point along the knot’s centreline has two (distant) closest-approach points. The best numerical results available also indicate that in the ideal shape the centreline curvature $\kappa$ attains its maximum allowed value, $\kappa = 2/\Delta$, over six arclength intervals. Our theory, assuming one-to-one arclength mapping, is of course not designed for situations with multiple points of contact. Nevertheless, it is instructive to see how close our elastic knots, not merely geometrical solutions but equilibria, can be inflated to the ideal shape.

Figure 3 shows an example of a trefoil knot solution. It is used as starting solution of a continuation run in which the thickness $\Delta$ is increased while applying the boundary conditions of Section 2.1. Two trefoil knots computed in this run are shown in Fig. 4. All computed

![Figure 3](image)

**Figure 3.** Trefoil 3\textsubscript{1} knot with $Lk = -\frac{3}{2}$ (left), the contact pressure $p$ (middle) and the curvature $\kappa_c$ of the contact curve (right). Ropelength 202.7096000, $L = 1$, $\Delta = 0.02$, $B_1 = B_2 = 1$, $t_{10} = t_{20} = 0$. The force vector is perpendicular to the plane of the figure.

![Figure 4](image)

**Figure 4.** Elastic trefoil knot. Individually adjusted colouring of the tubes shows the contact pressure (everywhere positive). Ropelength 39.50609870 (left) 32.85560666 (middle and right). Right: Contact set (pink) and trace of the closest-approach chord.
knots are untwisted ($t_{10} = t_{20} = 0$), so we are effectively only minimizing the bending energy of the centrelines (i.e., we may set $C_1 = C_2 = 0$). The solution in Fig. 4 with the ropelength of $2(L + L_2)/\Delta = 32.85560666$ is the tightest we could get. This value is remarkably close to the best current estimate given above. Careful examination reveals that the solution is free from self-intersections. Figure 5 (left) shows that the centreline curvature stays well below the maximum allowed value $2/\Delta = 16.2170$, Fig. 5 (middle) gives a plot of the torsion of the centreline, while Fig. 5 (right) shows the alternating steep-flat nature of the arclength mapping $s \rightarrow \sigma$ close to the limiting ideal state. For our elastic trefoil the contact set always remains a topological circle (see Fig. 4 (right), which also illustrates the arclength mapping by showing the closest-approach chords), while for the ideal shape the best available numerics suggests it is a trefoil knot (Przybyl & Pieranski, 2014).

![Figure 5](image1.png)

**Figure 5.** Normalised plots for the tight trefoil knot of Fig. 4, middle. Curvature (*left*) and torsion (*middle*) of the first strand. *Right:* Arclength $\sigma$ of the second strand against $s$.

We carried out similar numerical tightening of the pentafoil knot $5_1$. It is known that, contrary to the trefoil, its ideal shape lacks $D_5$ symmetry (Cantarella *et al.*, 2014). However, with increase of $\Delta$ the solution path bifurcates and we may follow either a $D_5$-symmetric or a $C_2$-symmetric branch. The bifurcation diagram is presented in Fig. 6. (The symmetry is checked up to numerical accuracy.) So, both $D_5$-symmetric and $C_2$-symmetric pentafoil knots are in equilibrium for some interval of thickness. We could keep tightening $D_5$-symmetric shapes up to ropelength 49.01152520 (Fig. 1) without self-overlapping of the tube. The tightest $D_5$-symmetric pentafoil computed in (Cantarella *et al.*, 2014) has ropelength 48.23. We see that

![Figure 6](image2.png)

**Figure 6.** Bifurcation diagram (*left*) for elastic pentafoil knots and two examples on the $C_2$-symmetric branch: • (*middle*) ropelength 65.90515002, no overlapping; ▲ (*right*) ropelength 49.73900556, the second strand tube (transparent) overlaps itself. ♦ marks the $D_5$-symmetric knot shown in Fig. 1.
we do not approach this value as closely as the limiting value for the trefoil. The code stops working for thicker shapes because the angle $\eta$ between strands approaches the singular value $\pi/2$. Nevertheless, for the pentafold $\eta$ gets substantially closer to $\pi/2$ than for the trefoil. This suggests that for the ideal $D_5$-symmetric pentafoil the two centrelines get closer to orthogonality than for the trefoil. This is not surprising as the braid axis of the $D_n$-symmetric knot becomes less curved as $n$ increases, in the limit reaching the tightest double helix with exactly orthogonal strands (Neukirch & van der Heijden, 2002). As to the non-symmetric equilibria (Fig. 6), they begin self-intersecting earlier, i.e., at larger ropelength.

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