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Approximating ideal shapes with tight elements

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Abstract: A variational approach is applied to the problem of finding the shortest curves in space separated by constant distance. Among particular extremal solutions are straight line, circular arc and double helix. Various knots and links may be assembled from these elements. It turns out that the structures so created may serve as very good approximations of the ideal shapes. Explicit construction of the trefoil knot and link 4_1^2 furnishes the examples.

Keywords: ideal knots and links

1 Introduction

An ideal (or tight) knot or link is a configuration of one or several closed non-overlapping tubes of constant uniform thickness such that the ratio of the centreline(s) length to thickness is minimal for given topology [23]. It is believed that this ratio is a parameter that can help to classify knots and links. The properties of the ideal shapes relate to various physical systems and models ranging from behaviour of DNA in gel to glueballs (e.g. [8, 14, 2]). No analytical description of any ideal knot except the unknot is currently known and only few ideal links are characterized explicitly, though approximate configurations can be computed numerically [18, 12, 15, 1, 5].

If one looks at a numerical approximation of the ideal trefoil [11, 5], several features stand out. In particular, the shape has 3-fold symmetry and there are large fragments which look like circular arcs. On the other hand, if we take a short piece of the tight double helix [18, 24] it seems to be very close to two pieces of circular tubes touching each other like in the Hopf link which is known to be ideal as the solution of the Gehring link problem [6, 17] (see also Ref. [4] and references therein). Both circular arc (plus its central point) and double helix are extremal solutions to the problem of finding the shortest curves in space separated by constant distance. These two observations suggest an attempt to build a shape from the elements of these two types. Surprisingly, the result turned out to be very close to the numerical approximation (though with a little greater length-to-radius ratio).

Since the trefoil is a torus knot, another simple analytical approximation of the ideal trefoil is a curve lying on the surface of a torus [19]. It also gives the value of the ratio worse than both numerics and our shape, and the difference between that toroidal configuration and ours is much bigger than between ours and numerics.

2 Variational approach

Let $\mathbf{r}_i(\sigma), i = 1, \ldots, n, n \geq 2$, be the curves in $\mathbb{R}^3$ of class C^2, σ being a *common* parameter, $\sigma \in [0, \Lambda]$. We assume that the curves $\mathbf{r}_i$ represent the centrelines of n pieces of an incompressible rope of the constant thickness diameter D. The i-th and $(i+1)$-st pieces touch each other continuously so that, for every $\sigma_0 \in [0, \Lambda]$, the points $\mathbf{r}_i(\sigma_0)$ and $\mathbf{r}_{i+1}(\sigma_0)$ are the closest ones, i.e. the distance between them is equal to D. We assume that the global curvature [7] for all the curves does not exceed $2/D$. Without loss of generality we may set $D = 1$.

We are seeking shapes of the curves $\mathbf{r}_i$ connecting two sets of n points such that the sum of their lengths is minimal and the minimal distance between every pair of curves $\mathbf{r}_i, \mathbf{r}_{i+1}$ is constant:

$$\begin{gathered} L = \int_0^\Lambda \sum_{i=1}^n \|\mathbf{r}_i'(\sigma)\| \, d\sigma \to \min; \\ \mathbf{r}_i'(\sigma) \cdot (\mathbf{r}_i(\sigma) - \mathbf{r}_{i+1}(\sigma)) = 0, \quad i = 1, \ldots, n-1, \quad \sigma \in [0, \Lambda]; \\ \mathbf{r}_i'(\sigma) \cdot (\mathbf{r}_i(\sigma) - \mathbf{r}_{i-1}(\sigma)) = 0, \quad i = 2, \ldots, n, \quad \sigma \in [0, \Lambda]. \end{gathered} \tag{1}$$

The prime denotes the derivative with respect to σ. The first order necessary condition for $\mathbf{r}_i(\sigma), i = 1, \ldots, n$, to be a solution to the problem (1) is that there are the Lagrange multipliers $\lambda_i^+(\sigma), i = 1, \ldots, n-1$, and $\lambda_i^-(\sigma), i = 2, \ldots, n$, such that the functional

$$\int_0^\Lambda \left(\sum_{i=1}^n \|\mathbf{r}_i'(\sigma)\| - \right. \\ \left. - \sum_{i=1}^{n-1} \lambda_i^+ \mathbf{r}_i'(\sigma) \cdot (\mathbf{r}_i(\sigma) - \mathbf{r}_{i+1}(\sigma)) - \sum_{i=2}^{n} \lambda_i^- \mathbf{r}_i'(\sigma) \cdot (\mathbf{r}_i(\sigma) - \mathbf{r}_{i-1}(\sigma)) \right) d\sigma \tag{2}$$

is stationary. The corresponding Euler-Lagrange equations are

$$\mathbf{t}_1' - (\lambda_1^+)'(\mathbf{r}_1 - \mathbf{r}_2) + (\lambda_1^+ - \lambda_2^-)\mathbf{r}_2' = \mathbf{0}, \tag{3}$$

$$\begin{gathered} \mathbf{t}_i' - (\lambda_i^+)'(\mathbf{r}_i - \mathbf{r}_{i+1}) - (\lambda_i^-)'(\mathbf{r}_i - \mathbf{r}_{i-1}) + (\lambda_i^+ - \lambda_{i+1}^-)\mathbf{r}_{i+1}' - \\ -(\lambda_{i-1}^+ - \lambda_i^-)\mathbf{r}_{i-1}' = \mathbf{0}, \quad i = 2, \ldots, n-1, \end{gathered} \tag{4}$$

$$\mathbf{t}_n' - (\lambda_n^-)'(\mathbf{r}_n - \mathbf{r}_{n-1}) - (\lambda_{n-1}^+ - \lambda_n^-)\mathbf{r}_{n-1}' = \mathbf{0}, \tag{5}$$

where by $\mathbf{t}_i$ we denoted the unit tangent vectors to the curves $\mathbf{r}_i$. Now we project Eq. (3) onto $\mathbf{r}_1'$, Eq. (4) onto $\mathbf{r}_i'$ and Eq. (5) onto $\mathbf{r}_n'$. Since $\mathbf{t}_i' \cdot \mathbf{r}_i' = 0$ for any $i = 1, \ldots, n$, the resulting system reduces to $n-1$ equations

$$(\lambda_i^+ - \lambda_{i+1}^-) \, \mathbf{r}_i' \cdot \mathbf{r}_{i+1}' = 0, \quad i = 1, \ldots, n-1. \tag{6}$$

The i-th Eq. (6) is satisfied if at least one of the two conditions holds:

(a) $\lambda_i^+ = \lambda_{i+1}^-$,

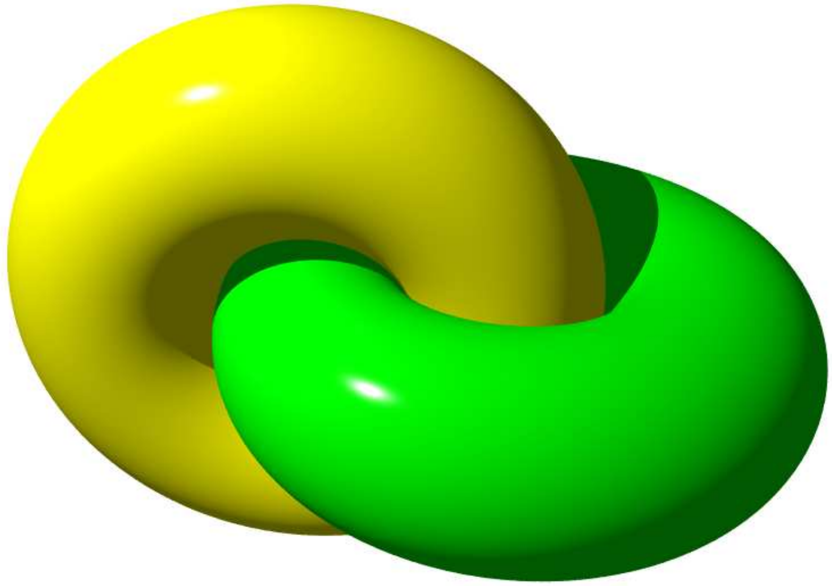

Figure 1: The ideal Hopf link.

(b) $\mathbf{r}'_i \cdot \mathbf{r}'_{i+1} = 0$.

Under assumption of the case (a) for $i = 1, \ldots, n-1$, summation of all Eqs. (3)–(5) leads to the vector integral

$$\sum_{i=1}^{n} \mathbf{t}_i = \mathbf{const}. \tag{7}$$

For $n = 2$, Eq. (7) immediately implies either a double helix or two parallel straight lines or a circle (if the constant is zero). The latter forms the centreline of a bialy [10], a torus with no hole which is the unknot, the only proven ideal shape among knots. There is a particular case of the double helix when the pitch angle equals $\pi/4$ which means that $\mathbf{r}'_1 \cdot \mathbf{r}'_2 = 0$, i.e. both conditions (a) and (b) are satisfied [18, 24, 16]. The ideal Hopf link (Fig. 1) may be also viewed as a configuration for which the tangents at the closest-approach points are orthogonal.

Equation (7) can be interpreted as the equilibrium equation for the tensile forces in the ropes touching each other continuously [13].

The structure of contact sets obtained by numerical computations [5] suggests that the sequence of the correspondence points may be cycled or infinite which can make solving the Euler-Lagrange equations extremely hard even in topologically simple cases. Still, postulating certain symmetry properties may help find a solution to the problem. For example, let the sequence of four closest approach points form a cycle for every $\sigma \in [0, \Lambda]$. Further let the first and the third points lie in the same constant plane and the other two points belong to the orthogonal

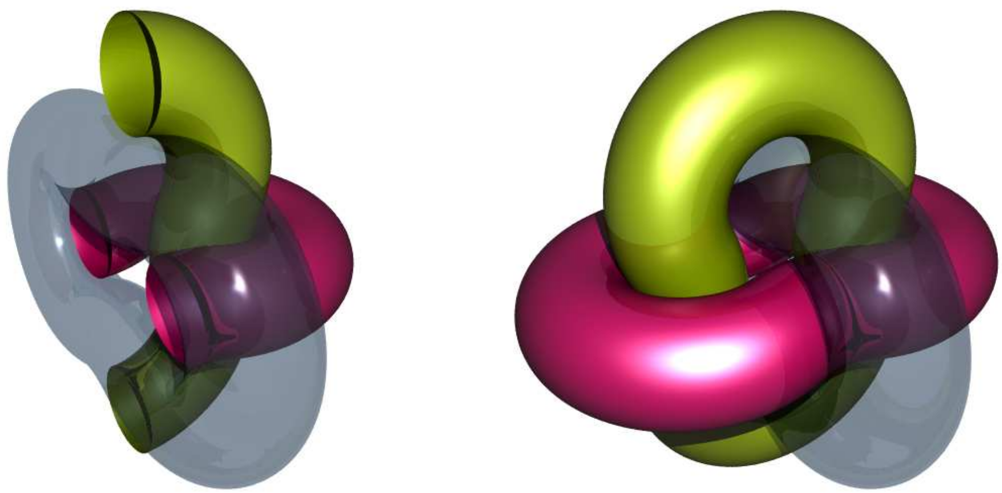

Figure 2: The piecewise circular approximation of the ideal Borromean rings.

plane, also constant. Then, the Euler-Lagrange equations may be solved analytically to obtain an explicit expression of a new extremal solution which is neither straight line nor circle nor helix [21, 22]. The pieces of that extremal curve may be used in assembling the conjectured tight configuration of clasped rope, periodic chains, 2D fabric-like periodic structures and the Borromean rings [21, 3].

The aim of this paper is different: it will be demonstrated that the already known particular types of solutions may be used to build good approximations of shapes for which we do not know exact solutions. Note that a fairly good approximation of the tight Borromean rings made up with circular arcs was proposed in Ref. [4] (Fig. 2).

3 Assembling procedure

The whole structure is to be composed from N (N = 3 or 4) circular tubes alternating with N tight double helices of the same length with pitch angle $\pi/4$. We fix the thickness radius of the tube to be $1/2$ in accordance with the chosen distance between their centrelines $D = 1$.

Let Oz be m-fold symmetry axis, $m = 3$ for $N = 3$ (Fig. 3) and $m = 2$ for $N = 4$. We direct the x-axis to the centre C_1 of the circular arc. The distance OC_1 is the first unknown parameter $a > 0$. The orientation of the plane P_1 of the circular arc is specified by the unit vector $\mathbf{e}_1$ which is tangent to the other piece of centreline at point C_1. To distinguish between the pieces of the knotted curve ($N = 3$) or the components of the link ($N = 4$), we call the fragment passing through C_1 the 1-st strand and the circular arc (and its helical extension) the 2-nd strand. In the plane P_1, the point A_1 is the end point of the circular arc and, in the same time, the starting point of the 2-nd strand of the double helix. The position of A_1 is specified

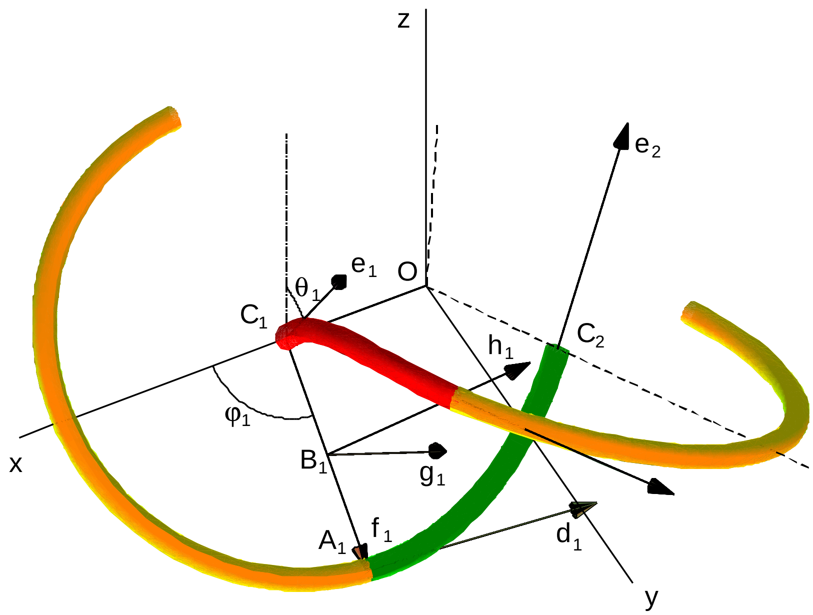

Figure 3: Construction of approximate ideal trefoil.

by the vector $C_1A_1 = \mathbf{f}_1 \in P_1$, $\|\mathbf{f}_1\| = 1$. Let $\mathbf{d}_1$ be the unit tangent to the 2-nd strand in point A_1. Thus we have an orthonormal triad $\{\mathbf{e}_1, \mathbf{f}_1, \mathbf{d}_1\}$. Generally, its orientation may be given by three Euler angles. However, we wish to find a solution that is symmetric with respect to rotation around the axis Ox through π. In other words, let $Ox \in P_1$. Then we need only two angles to orientate the triad $\{\mathbf{e}_1, \mathbf{f}_1, \mathbf{d}_1\}$:

$$\begin{aligned} \mathbf{e}_1 &= (0, \sin\theta_1, \cos\theta_1)^T, \\ \mathbf{f}_1 &= (\cos\phi_1, \sin\phi_1\cos\theta_1, -\sin\phi_1\sin\theta_1)^T, \\ \mathbf{d}_1 &= (-\sin\phi_1, \cos\phi_1\cos\theta_1, -\cos\phi_1\sin\theta_1)^T. \end{aligned}$$

The point C_1 is the starting point of the 1-st strand of the double helix. The axis of the double helix is along $\mathbf{h}_1 = \frac{1}{\sqrt{2}}(\mathbf{d}_1 + \mathbf{e}_1)$. We also introduce another unit vector $\mathbf{g}_1 = \mathbf{h}_1 \times \mathbf{f}_1 = \frac{1}{\sqrt{2}}(\mathbf{d}_1 - \mathbf{e}_1)$. The points on the 2-nd strand of the helix are given by

$$\mathbf{r}_2(\gamma) = \mathbf{r}_{C1} + \frac{1}{2}(\mathbf{f}_1 + \gamma\mathbf{h}_1 + \mathbf{f}_1\cos\gamma + \mathbf{g}_1\sin\gamma), \tag{8}$$

where $\mathbf{r}_{C1} = (a, 0, 0)^T$ and γ is a parameter.

We require that for some value of γ the second strand come to the point C_2 which is the centre of the next circular arc, i.e. $\mathbf{r}_{C2} = \mathbf{r}_2(\gamma)$. Moreover we require that

$$\mathbf{r}_{C2}(\gamma) = R_N\mathbf{r}_{C1} \tag{9}$$

with

$$R_3 = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad R_4 \equiv R_4^{(a,b)} = \frac{b}{a} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad a, b \in \mathbb{R}^+.$$

Clearly, $R_3^3 = I$, I the identity matrix, and $(R_4^{(b,a)}\ R_4^{(a,b)})^2 = I$. It would be convenient to use the vector $\mathbf{a}_N = 2(R_N \mathbf{r}_{C1} - \mathbf{r}_{C1})$, namely, $\mathbf{a}_3 = (-3a, \sqrt{3}a, 0)^T$ and $\mathbf{a}_4 = (-2a, 2b, 0)^T$. Then Eqs. (8) and (9) imply

$$\mathbf{d}_1 \frac{\gamma + \sin\gamma}{\sqrt{2}} + \mathbf{e}_1 \frac{\gamma - \sin\gamma}{\sqrt{2}} + \mathbf{f}_1 (1 + \cos\gamma) = \mathbf{a}_N$$

or, in the coordinate form,

$$\cos\phi_1 (1 + \cos\gamma) - \sin\phi_1 \frac{\gamma + \sin\gamma}{\sqrt{2}} = a_{Nx}, \tag{10}$$

$$\cos\theta_1 \left[\sin\phi_1 (1 + \cos\gamma) + \cos\phi_1 \frac{\gamma + \sin\gamma}{\sqrt{2}} \right] + \sin\theta_1 \frac{\gamma - \sin\gamma}{\sqrt{2}} = a_{Ny}, \tag{11}$$

$$\sin\theta_1 \left[\sin\phi_1 (1 + \cos\gamma) + \cos\phi_1 \frac{\gamma + \sin\gamma}{\sqrt{2}} \right] - \cos\theta_1 \frac{\gamma - \sin\gamma}{\sqrt{2}} = 0. \tag{12}$$

Now compute the tangent vector to the second strand in point C_2:

$$\mathbf{e}_2(\gamma) = \frac{1}{\sqrt{2}} (\mathbf{h}_1 + \mathbf{g}_1 \cos\gamma - \mathbf{f}_1 \sin\gamma)$$

or

$$\mathbf{e}_2(\gamma) = \mathbf{d}_1 \frac{1 + \cos\gamma}{2} + \mathbf{e}_1 \frac{1 - \cos\gamma}{2} - \mathbf{f}_1 \frac{\sin\gamma}{\sqrt{2}}. \tag{13}$$

We further require that

$$\mathbf{e}_2(\gamma) = Q_N \mathbf{e}_1, \tag{14}$$

where $Q_3 = R_3$ and

$$Q_4 \equiv Q_4^{(1,2)} = \begin{bmatrix} 0 & -\frac{\sin\theta_2}{\sin\theta_1} & 0 \\ \frac{\sin\theta_2}{\sin\theta_1} & 0 & 0 \\ 0 & 0 & \frac{\cos\theta_2}{\cos\theta_1} \end{bmatrix},$$

so that $(Q_4^{(2,1)}\ Q_4^{(1,2)})^2 = I$.

Projecting Eq. (14) onto the directions $\mathbf{d}_1$, $\mathbf{e}_1$ and $\mathbf{f}_1$ and using the expression Eq. (13) for the tangent vector, we come to three equations

$$\mathbf{d}_1 \cdot Q_N \mathbf{e}_1 - \frac{\cos\gamma + 1}{2} = 0, \tag{15}$$

$$\mathbf{e}_1 \cdot Q_N \mathbf{e}_1 + \frac{\cos\gamma - 1}{2} = 0, \tag{16}$$

$$\mathbf{f}_1 \cdot Q_N \mathbf{e}_1 + \frac{\sin\gamma}{\sqrt{2}} = 0. \tag{17}$$

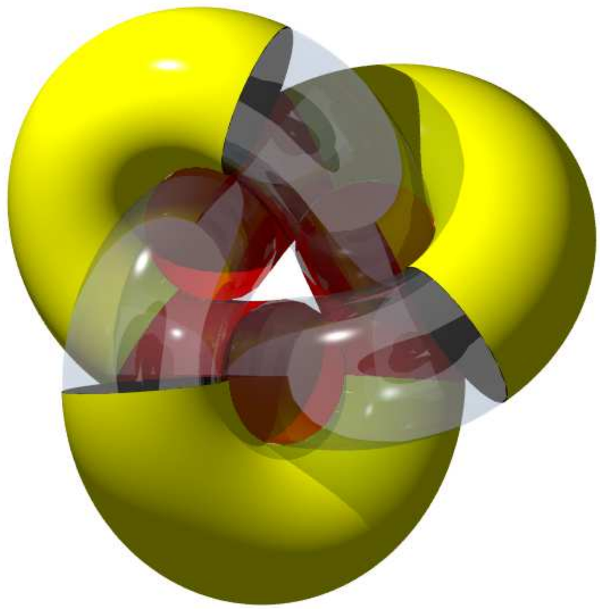

Figure 4: Approximation of ideal trefoil. One strand in each double helix pair is shown transparent.

Now we multiply the first equation by $\sin\phi_1$ and subtract it from the third one multiplied by $\cos\phi_1$ to obtain

$$(Q_N\mathbf{e}_1)_x + \frac{\sin\gamma}{\sqrt{2}}\cos\phi_1 + \frac{\cos\gamma+1}{2}\sin\phi_1 = 0. \tag{18}$$

4 Trefoil

For $N = 3$, Eq. (16) transforms into

$$\sin^2\theta_1 = \frac{1+\cos\gamma}{3} \tag{19}$$

and Eq. (18) into

$$-\sqrt{3}\sin\theta_1 + \sqrt{2}\sin\gamma\cos\phi_1 + (1+\cos\gamma)\sin\phi_1 = 0. \tag{20}$$

By means of Eq. (19), we can first exclude the angle θ_1 from Eq. (20) (assuming that $0 < \theta_1 < \pi/2$ and in doing so we fix the chirality of the knot)

$$-\sqrt{1+\cos\gamma} + \sqrt{2}\sin\gamma\cos\phi_1 + (1+\cos\gamma)\sin\phi_1 = 0 \tag{21}$$

and then from Eq. (12)

$$[\sqrt{2}(1+\cos\gamma)\sin\phi_1 + (\gamma+\sin\gamma)\cos\phi_1]\sqrt{1+\cos\gamma} - (\gamma-\sin\gamma)\sqrt{2-\cos\gamma} = 0. \tag{22}$$

Equations (21) and (22) may be treated as a linear system with respect to $\sin\phi_1$ and $\cos\phi_1$. We may solve the system and find $\sin\phi_1$ and $\cos\phi_1$ as functions of the parameter γ and then exclude ϕ_1 from Eq. (21) (or Eq. (22)) to yield a single transcendental equation for γ. It is easy to localize the first root $\gamma > 0$, $\gamma \approx 1.7738716012$. Then $\phi_1 \approx 1.5006137011$ and $\theta_1 \approx 0.5420048264$ (Eq. (19)). The parameter a can be found from Eq. (10) or Eq. (11): $a \approx 0.6287060612$.

The total length of the trefoil is $L_3 = 3(L_{crc} + L_{hlx})$, where $L_{crc} = 2\phi_1$ is the length of the circular arc and $L_{hlx} = \sqrt{2}\gamma$ is the length of two strands of the helical part. Thus $L_3 = 3(2\phi_1 + \sqrt{2}\gamma) \approx 16.5438523491$. According to Ref. [1], the lowest known probable upper bound of the length is $L_{3num} \approx 16.3716932$. The relative error can be estimated as $\frac{L_3 - L_{3num}}{L_3} \approx 1.04\%$. Note that the constructed shape (Fig. 4) is much closer to the numerical result than the toroidal parametrization considered in Ref. [19] with length $L_{3tor} \approx 17.0883$.

5 Link 4_1^2

Now consider case $N = 4$. Equation (16) takes the form

$$\cos\theta_1 \cos\theta_2 = \frac{1 - \cos\gamma}{2} \tag{23}$$

and Eq. (18) becomes

$$\sin\theta_2 - \frac{\sin\gamma}{\sqrt{2}}\cos\phi_1 - \frac{1 + \cos\gamma}{2}\sin\phi_1 = 0. \tag{24}$$

By means of Eq. (24), we can eliminate θ_2 from Eq. (23)

$$\cos^2\theta_1 \left[1 - \left(\frac{\sin\gamma}{\sqrt{2}}\cos\phi_1 + \frac{1 + \cos\gamma}{2}\sin\phi_1\right)^2\right] = \frac{1}{4}(1 - \cos\gamma)^2. \tag{25}$$

The last equation allows us to express the angle θ_1 which we insert into Eq. (12). We can consider the result as an equation for the unknown ϕ_1, depending on the parameter γ:

$$\begin{aligned} &[4 - (\sqrt{2}\sin\gamma\cos\phi_1 + (1 + \cos\gamma)\sin\phi_1)^2] \times \\ &\times [2(1 + \cos\gamma)\sin\phi_1 + \sqrt{2}(\gamma + \sin\gamma)\cos\phi_1]^2 = \\ &= [2(\gamma - \sin\gamma)^2 + (2(1 + \cos\gamma)\sin\phi_1 + \sqrt{2}(\gamma + \sin\gamma)\cos\phi_1)^2](1 - \cos\gamma)^2. \end{aligned} \tag{26}$$

Knowing the solution of Eq. (26) $\phi_1(\gamma)$, we can find θ_1 by Eq. (25) and θ_2 by Eq. (24). After that, Eqs. (10) and (11) allow us to compute the distances a and b.

The length of the whole link is given by $L_4 = 2(L_{crc1} + L_{crc2} + 2L_{hlx})$, where $L_{crc1} = 2\phi_1$, $L_{crc2} = 2\phi_2$ and $L_{hlx} = \sqrt{2}\gamma$ as before.

The end point of the helix axis is $\mathbf{r}_{C1} + \frac{1}{2}(\mathbf{f}_1 + \gamma\mathbf{h}_1)$. The vector connecting this point with C_2 forms the angle ϕ_2 with the y-axis, hence, ϕ_2 can be found from the equation $(\mathbf{f}_1 + \gamma\mathbf{h}_1 - \mathbf{a}_4)_y = \cos\phi_2$ or

$$\cos\theta_1 \sin\phi_1 + \frac{\gamma}{\sqrt{2}}(\sin\theta_1 + \cos\theta_1\cos\phi_1) - 2b = \cos\phi_2.$$

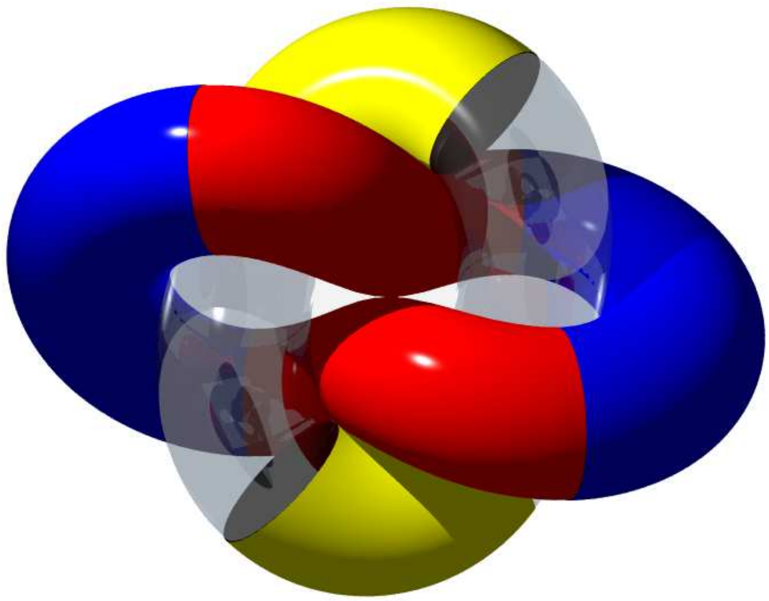

Figure 5: Approximation of ideal link 4_1^2. The helical parts of one component are shown transparent.

Finally, $L_4 = L_4(\gamma) = 4(\phi_1(\gamma) + \phi_2(\gamma) + \sqrt{2}\gamma)$.

Since the parameter γ has not been specified yet, we can vary it to look for the smallest L_4. The graph $L_4(\gamma)$ shows that the minimal length is achieved when one of the rings touches itself in the origin point, i.e. when either $a = 1/2$ or $b = 1/2$. For the definiteness sake, let us choose $a = 1/2$. Solution for γ yields $\gamma \approx 1.9234874489$. The other variables are $\theta_1 \approx 0.3553039796$, $\theta_2 \approx 0.7705487841$ and $b \approx 1.0011187376$. The assembled configuration is presented in Fig. 5.

Note that $\theta_1 \approx \pi/4$ which means that the circular arcs of the self-touching ring are almost orthogonal to each other. It is also interesting that the parameter b is very close to 1. The angles defining the lengths of the circular arcs are $\phi_1 \approx 0.8023098550$, $\phi_2 \approx 1.5395250794$ and the length of the whole link $L_4 \approx 20.2482278867$. The numerical approximation gives the length $L_{4num} = 20.0542$ [11] and the relative error $\frac{L_4 - L_{4num}}{L_4} \approx 0.96\%$ is at the same level of accuracy as for the trefoil.

6 Concluding remarks

For both the trefoil knot and the link 4_1^2, the approximations constructed have constant curvature and hence their centrelines, which are of class C^2, may serve as examples of closed space curves of constant curvature. Other examples of such curves can be found in Ref. [9].

Chronologically, the first numerical approximations of centrelines of ideal shapes were polygonal [18, 12, 15]. Indeed, the straight line is a solution of the Euler-Lagrange equations: to see this, just consider the case $n = 1$. Later, it was proposed to approximate ideal shapes with biarcs [20, 5], i.e. with circular arcs. Again, as we have seen, the circular arc is an exact solution in some cases. In view of this, widening the set of building blocks by adding the double helices is a natural step to keep moving in the same direction. In the configurations made up with polygonal lines or circular arcs, torsion is concentrated in junction points as distinct from the presented examples with helical intervals of constant torsion.

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