

## SOAP FILM SPANNING ELECTRICALLY REPULSIVE ELASTIC PROTEIN LINKS

GIULIA BEVILACQUA <sup>a</sup>, LUCA LUSSARDI <sup>b\*</sup>, AND ALFREDO MARZOCCHI <sup>c</sup>

**ABSTRACT.** We study the equilibrium problem of a mechanical system consisting of two Kirchhoff rods linked in an arbitrary way and also forming knots, constrained not to touch themselves by means of electrical repulsion and tied by a soap film, as a model to describe the interaction between an electrically charged protein and a biomembrane. We prove the existence of a solution with minimum total energy, which may be quite irregular, by using techniques of the Calculus of Variations.

### 1. Introduction

The existence of knotted proteins is widely known (see for instance Mansfield (1994)). In addition, they may also form links with other proteins or molecules. Such proteins are in general extremely complicated and made up by repeated subunits, so that a sort of “macroscopic modeling” as a filament is reasonable. Of course, since everything is immersed in a biological fluid, it is natural to take into account the action of a liquid film spanning the filament (see Figure 1). Therefore, we consider flexible filaments of the form of a closed loop spanned by a liquid film and we model our filament as a Kirchhoff rod (see for instance Antman (1995), Chap. 8). Moreover, in order to consider somewhat more complicated shapes, as the ones exhibited by proteins, we consider two thin elastic three-dimensional closed rods linked in a simple but nontrivial way: we impose that the midline of each rod has to have linking number equal to one with the other one: this implies that they form what is called a link (see Figure 2). This is not simply a generalization of the so-called *Plateau problem*, a centuries-old mathematical problem investigated by the Belgian physicist Joseph Plateau (Plateau 1873), but it is also a generalization of the Kirchhoff-Plateau problem with a single component, studied by Fried *et al.* in Giusteri *et al.* (2017), and with several Kirchhoff rods, studied by Bevilacqua *et al.* in Bevilacqua *et al.* (2018).

Since we want to give a more realistic, physical and biological background to take into account processes like the adsorption of a protein by a biomembrane (Huang 1986), we

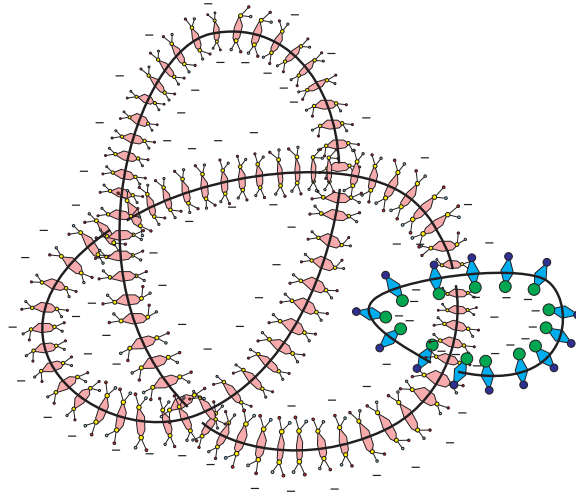


FIGURE 1. A schematic representation of a knotted protein linked to another one.

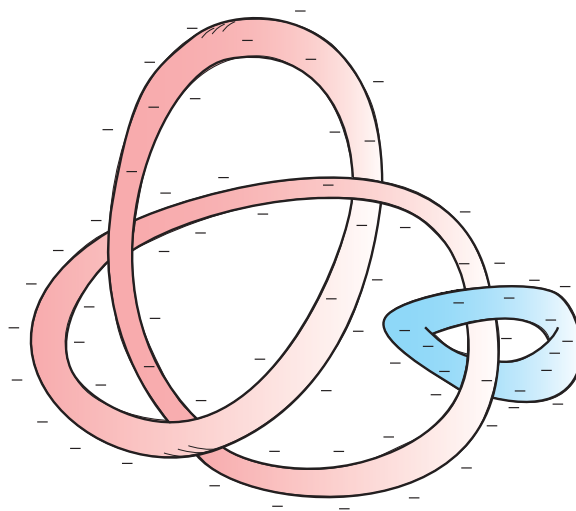


FIGURE 2. Geometry of the problem.

introduce an additional repulsional energy between the two rods. This idea is linked to the fact that the amino acids can link together by peptide bonds, but some of them, because of their chemical structure, can repel (see for instance Alberts *et al.* (2002), Chap. 3).

In order to consider a repulsion between the two loops, we would like to introduce an electrical potential energy on the surface on the loops. However, since a Kirchhoff rod can be entirely described only by one variable, the midline, the problem could be greatly simplified. Indeed, since the loops are longer than broad, putting the charges on the midline or on the surface may make a very little difference in a first approximation. The full problem with

charges on a surface will be investigated in a future paper. Hence, the major achievement with respect to Bevilacqua *et al.* (2018) is the introduction of a contribution into the energy functional of the system: we take into account the elastic and the potential energy for the link, the repulsion between the two loops and the surface tension energy of the film.

The most delicate point is the treatment of the definition of spanning surface. We use an approach presented by DeLellis *et al.* in De Lellis *et al.* (2017) but based on an idea by Harrison (Harrison and Pugh 2016): they formulate the Plateau problem in a particular notion of *spanning* and make use of Hausdorff topology for the convergence of surfaces (Reifenberg 1960; De Pauw 2009; David 2017). Hence, this approach has the advantage of considering also non-rectifiable, not fixed boundaries set in a particular configuration, which is exactly what we need. Hence, by using the Direct Method of the Calculus of Variations, we are able to prove the existence of the minimum, i.e. the solution of our problem.

**2. Formulation of the problem**

We consider two continuous bodies whose reference configurations are two right cylinders of lengths  $L_1, L_2$ . The arc-length parameter  $s$  of the axis of each cylinder identifies a material (cross) section  $\mathcal{A}(s)$ , which consists of all points on a plane perpendicular to the axis at  $s$  ( see Antman (1995), Chap. 8). We describe each rod by three vector-valued functions  $[0, L_i] \rightarrow \mathbb{R}^3$  given by  $s \mapsto (r_i(s), u_i(s), v_i(s))$  ( $i = 1, 2$ ).

Now we fix a point  $O$  in the euclidean space  $\mathbb{E}^3$  and describe the position in space of each point of the  $i$ th rod. Setting  $G_i(s) - O = r_i(s)$  (the so-called *midline*), where  $G_i(s)$  is the center of mass of the cross-sections and considering  $u_i$  and  $v_i$  as applied vectors in  $G_i(s)$ , a generic point  $P_i$  of the rod in space is given by the knowledge of the vector

$$p_i(s, \zeta_1, \zeta_2) = P_i - O = r_i(s) + \zeta_1 u_i(s) + \zeta_2 v_i(s), \tag{1}$$

where  $(s, \zeta_1, \zeta_2) \in \Omega_i := \{(s, \zeta_1, \zeta_2) | s \in [0, L_i], (\zeta_1, \zeta_2) \in \mathcal{A}_i(s)\}$ .

More precisely,  $\zeta_1$  and  $\zeta_2$  are not completely free: there exists an  $R > 0$ , the maximum thickness, which has to be small compared to the length  $L_i$ , such that  $|\zeta_1| < R$  and  $|\zeta_2| < R$  for any  $(s, \zeta_1, \zeta_2)$ , i.e. we require that our body is “*longer than broad*”. We also assume that the rod is *unshearable*, so that  $u$  and  $v$  are orthogonal to the midline, and that this line is *inextensible*. Hence, our rods are exactly two Kirchhoff rods, a special case of Cosserat rods.

Given the function  $\mathcal{A}_i(s)$ , by three scalar parameters with a physical meaning, we can determine completely the position of the midline of each rod:  $k'_i$  and  $k''_i$  are the *flexural densities* and  $\omega_i$  the *twist density*. The vectors  $r_i, u_i, v_i$  satisfy the system of ordinary differential equations

$$\begin{cases} \dot{r}_i(s) = w_i(s), \\ \dot{u}_i(s) = -\omega_i(s)w_i(s) - k'_i(s)v_i, \\ \dot{v}_i(s) = k'_i(s)u_i(s) + k''_i(s)w_i(s); \end{cases} \tag{2}$$

where  $i = 1, 2$  and  $w = u \times v$  is tangent to the midline.

We now suppose that the first one is “clamped” by assigning an initial value to its system, i.e.

$$(r_1(0), u_1(0), v_1(0)) = (\hat{r}_1, \hat{u}_1, \hat{v}_1). \tag{3}$$

Since clearly

$$\dot{w}_1(s) = -\omega_1(s)u_1(s) - k_1''(s)v_1(s)$$

the triple  $(u_1, v_1, w_1)$  satisfies a non-autonomous linear system and therefore, by classical results (Hartman 2002), if the densities  $k_1', k_1''$  and  $\omega_1$  belong to  $L^p([0, L_1]; \mathbb{R})$  for some  $p \in (1, \infty)$ , then the initial-value problem has a unique solution, with  $r_1 \in W^{2,p}([0, L_1]; \mathbb{R}^3)$  and  $u_1, v_1 \in W^{1,p}([0, L_1]; \mathbb{R}^3)$ .

It is easy to verify that if  $(\hat{u}_1, \hat{v}_1, \hat{w}_1)$  is orthonormal, so is  $(u_1(s), v_1(s), w_1(s))$  for every  $s \in [0, L_1]$ . For every  $(\hat{u}_1, \hat{v}_1, \hat{w}_1) \in (\mathbb{R}^3)^3$  we then set

$$\mathbf{z}_1 = (k_1', k_1'', \omega_1) \in V_1 := L^p([0, L_1]; \mathbb{R}^3).$$

As for the second rod, since we do not know *a priori* its position in space, we need some information also on the orientation of one of its orthonormal frames. Therefore we seek a solution of the form

$$\mathbf{z}_2 = (k_2', k_2'', \omega_2, \hat{r}_2, \hat{u}_2, \hat{v}_2, \hat{w}_2) \in V_2 := L^p([0, L_2]; \mathbb{R}^3) \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3$$

where  $\hat{u}_2, \hat{v}_2, \hat{w}_2$  are orthonormal and  $\hat{r}_2$  gives their application point. We also set  $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2)$ .

Now the system (2)<sub>2,3</sub> and (3), together with the knowledge of  $\hat{r}_2$ , fully fixes the position in space of the second midline.

Obviously, since we want to deal with closed loops, we have to impose the closure of the midlines, *i.e.*

$$r_i(0) = r_i(L_i) \quad (i = 1, 2) \tag{4}$$

and, since we do not want interpenetration, we need to have also continuity of the tangent vectors, so that for  $i = 1, 2$

$$w_i(0) = w_i(L_i). \tag{5}$$

However, since the loops are three-dimensional, the simple determination of the midlines does not completely fix their shape. Indeed, the same midline may correspond to different bodies if the cross-sections  $\mathcal{A}_i(s)$  are rotated around the midline before being glued, and the final rotation angle depends on the shape of the cross-section. Hence, we introduce two definitions will be useful also later on.

**Definition 1.** Let  $\eta_i : [a, b] \rightarrow \mathbb{R}^3$ , with  $i = 1, 2$ , be two continuous curves with  $\eta_i(a) = \eta_i(b)$ .  $\eta_1$  and  $\eta_2$  are said to be *isotopic*,  $\eta_1 \simeq \eta_2$ , if there are open neighborhoods  $N_1$  of  $\eta_1([a, b])$ ,  $N_2$  of  $\eta_2([a, b])$  and a continuous mapping  $\Phi : N_1 \times [0, 1] \mapsto \mathbb{R}^3$  such that  $\Phi(N_1, \tau)$  is homeomorphic to  $N_1$  for all  $\tau \in [0, 1]$ ,  $\Phi(\cdot, 0)$  is the identity,  $\Phi(N_1, 1) = N_2$  and  $\Phi(\eta_1([a, b]), 1) = \eta_2([a, b])$ .

**Definition 2.** Let  $\eta_1, \eta_2$  be two absolutely continuous disjoint closed curves in  $\mathbb{E}^3$ . The number

$$L(\eta_1, \eta_2) = \frac{1}{4\pi} \int_a^b \int_a^b \frac{\eta_1(s) - \eta_2(t)}{|\eta_1(s) - \eta_2(t)|^3} \cdot (\eta_1'(s) \times \eta_2'(t)) ds dt$$

is called the *linking number* between  $\eta_1$  and  $\eta_2$ .

The first one defines the *knot type*, since the isotopy class is stable with respect to diffeomorphism, while the second one introduces the integer  $L$  (see Munkres (1963)), which is invariant in the isotopy class of the two curves. By imposing that every midline and a sufficiently close nearby curve preserve this number, the position of every cross section is

completely defined<sup>1</sup> and thus also the shape of the loops, which we will indicate by  $\Lambda[\mathbf{z}]$  (see Figure 4.)

Finally, we want to impose that the two loops form a link: we suppose that they are linked with a given linking number  $L_{12} \in \mathbb{Z}$ . As they are closed sets, they admit disjoint neighbourhoods, which we can suppose tubular without loss of generality ((Mukherjee 2015) pp. 199–223). By a further shrinking to the diameter of  $\mathcal{A}(s)$  we have that both rods are disjoint and linked one each other with the given linking number.

At this point, the shape of the two solids is assigned once we know  $\mathbf{z}_1, \mathbf{z}_2$ . However, since we are describing a physical problem, we have to avoid local and global interpenetration. To do this, we first introduce the elastic, potential and electrical energy stored in the loops.

Following Schuricht (2002), the elastic energy is supposed to be of the classical form (see for instance Dacorogna (1989), Chap. 2)

$$E_{el_1}[\mathbf{z}_1] := \int_0^{L_1} f_1(\mathbf{z}_1(s), s) ds \tag{6}$$

where  $f_i(\cdot, s)$  are continuous and convex for any  $s \in [0, L_i]$  and  $f_i(a, \cdot)$  is measurable for any  $a \in \mathbb{R}^3$ . Since we are going to apply the Direct Method of the Calculus of Variations, we suppose that there exist positive constants  $C_i, D_i$  such that

$$f_i(a, s) \geq C_i |a|^p + D_i \quad \forall (a, s) \in \mathbb{R}^3 \times [0, L_i]. \tag{7}$$

In view of this, the total elastic energy

$$E_{el}[\mathbf{z}] = E_{el_1}[\mathbf{z}_1] + E_{el_2}[\mathbf{z}_2] := \int_I f(\mathbf{z}(\xi), \xi) d\xi,$$

where  $I = [0, L_1] \times [0, L_2]$ ,  $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2)$  and  $\xi$  is a vector variable, is easily seen to be coercive on  $V := V_1 \times V_2$ .

As for the potential energy of the weight, it is given for each loop by

$$E_{g_i}[\mathbf{z}_i] = - \int_0^{L_i} \rho_i(s) g \cdot (G_i(s) - \mathcal{O}) ds$$

where  $\rho_i > 0$  stand for the mass of each section of the rod and  $g$  denotes the acceleration of gravity.

Moreover, since we want to avoid the possibility for the two loops to touch themselves, we introduce a kind of electrical potential energy which, physically, encodes the repulsion between the two rods.

$$E_{rep}[\mathbf{r}] := \int_0^{L_1} \int_0^{L_2} \frac{c}{h(\|r_1(s_1) - r_2(s_2)\|)} ds_1 ds_2, \tag{8}$$

where  $\mathbf{r} = (r_1, r_2)$ ,  $s_1 \in [0, L_1]$ ,  $s_2 \in [0, L_2]$ ,  $c$  is a constant and  $h$  is an increasing nonnegative and continuous function. A possible choice for  $h$  is represented in Fig. 3. Notice that with this choice we are introducing a positively unbounded energy, which may be infinite if the midlines are sufficiently close (this happens if the set where  $\|r_1 - r_2\| < \varepsilon$  is large enough). However, notice also that we cannot take  $\varepsilon$  too large otherwise we do not get any linked rods with finite repulsion energy. Since we are only assuming that  $h$  is increasing, nonnegative and continuous for  $r > \varepsilon$  we will also assume that  $\varepsilon$  is small enough so that the rods have finite repulsion energy.

<sup>1</sup>Up to a set of  $L^1$ -zero measure which is irrelevant.

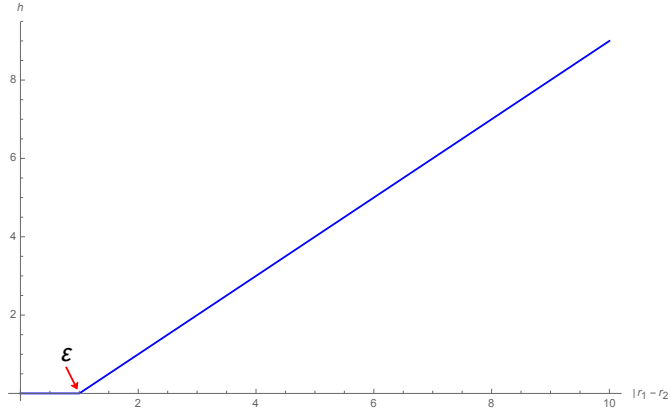


FIGURE 3. A possible choice of  $h$

We also set <sup>2</sup>

$$E_{\text{loop}}[\mathbf{z}] = E_{\text{el1}}[\mathbf{z}_1] + E_{\text{g1}}[\mathbf{z}_1] + E_{\text{el2}}[\mathbf{z}_2] + E_{\text{g2}}[\mathbf{z}_2] + E_{\text{rep}}[\mathbf{r}]$$

and look for sufficient conditions for the local and global non-interpenetration of our configuration.

As for the first, we only need to introduce the natural growth conditions on the elastic energy as

$$f_i(\mathbf{z}_i(s), s) \rightarrow +\infty \quad \text{as} \quad g_i(k'_i(s), k''_i(s), s) \rightarrow 1, \quad (i = 1, 2), \tag{9}$$

such as the elastic energy approaches infinity under complete compression (remember that  $f_i$  may depend on  $g_i$ ) and where  $g_i$  are two functions related to our geometry, see for instance Antman (1995), Theorem 6.2, p.276, which satisfy the inequality

$$g_i(k'_i(s), k''_i(s), s) \leq 1 \quad \text{for a.e. } s \in [0, L_i], \quad (i = 1, 2). \tag{10}$$

As for the global injectivity, we must distinguish each loop and their union. First of all, Ciarlet and Nečas (Ciarlet and Necas 1987) proved that if the following condition holds,

$$\int_{\Omega_i} \det \frac{\partial p_i(s, \zeta_1, \zeta_2)}{\partial (s, \zeta_1, \zeta_2)} d(s, \zeta_1, \zeta_2) \leq \mathcal{L}^3(p_i[\mathbf{z}_i](\Omega_i)), \tag{11}$$

then the global injectivity is true. Moreover, in our case it can be rewritten as

$$\int_{\Omega_i} (1 - \zeta_1 k'_i(s) - \zeta_2 k''_i(s)) d(s, \zeta_1, \zeta_2) \leq \mathcal{L}^3(p_i[\mathbf{z}_i](\Omega_i)). \tag{12}$$

Hence, assuming (12) true, one has the global injectivity of the functions  $p_i$  on each rod. At this point, for the union of the two, we notice that by the introduction of the repulsive component in the loop energy, i.e.  $E_{\text{rep}}$ , with an appropriate choice of  $\epsilon$ , we ensure not only the possibility of non-interpenetration between the two rods but also we avoid the contact.

So, we can prove the

<sup>2</sup>In principle,  $r$  does not belong to  $\mathbf{z}$ , but, once the tangent vectors are known, also  $r$  can be reconstructed.

**Theorem 1.** Let  $\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2) \in V = V_1 \times V_2$  satisfy (10),  $f_i$  with  $i = 1, 2$  satisfy (9) and  $E_{\text{loop}}[\mathbf{z}] < +\infty$ .

Then the mapping  $(s, \zeta_1, \zeta_2) \mapsto p[\mathbf{z}](s, \zeta_1, \zeta_2) = (p_1, p_2)[\mathbf{z}_1, \mathbf{z}_2](s, \zeta_1, \zeta_2)$  is locally injective and open on  $\text{int}\Omega$ . Moreover, if  $\mathbf{z}_i$  satisfies (12), the mapping  $(s, \zeta_1, \zeta_2) \mapsto p[\mathbf{z}](s, \zeta_1, \zeta_2)$  is globally injective on  $\text{int}\Omega$ .

*Proof.* Essentially, the proof is based on Schuricht (2002). Precisely, on a hand, for the first statements, the proof is exactly a little modification of the one presented in Giusteri *et al.* (2017). On the other one, for the second result, the proof is similar to the one of Theorem 2 in Bevilacqua *et al.* (2018). However, by the introduction of the new energy contribution, we don't have to consider configurations which allow contact between the two rods.  $\square$

Finally, the energy stored in a film that will deform the link is defined as

$$E_{\text{film}}(S) = 2\sigma \mathcal{H}^2(S), \tag{13}$$

where  $\mathcal{H}^d$  represents the  $d$ -dimensional Hausdorff measure. When a soap film is in stable equilibrium, as in eq. (13), any small change in its area,  $S$ , will produce a corresponding change in its energy  $E$ , provided that  $\sigma$  remains constant. As  $E_{\text{film}}$  is minimized when the film is in stable equilibrium,  $S$  will be minimized.

Anyway, we still cannot provide the final expression for the energy since we have not yet specified how the film is attached to each loop. To formulate the idea of a solution we have to give a good definition of the terms *surface*, *area* and *contact*, which we will call *span*. To this end, we give some recalls of topology.

**Definition 3.** Let  $H = \bigcup_{j \in J} H_j$  be a closed compact 3-dimensional submanifold of  $\mathbb{E}^3$  consisting of connected components  $H_j$ . We say that a circle  $\gamma$  embedded in  $\mathbb{E}^3 \setminus H$  is a *simple link* of  $H$  if there exists  $i \in J$  such that the linking numbers  $L(\gamma, H_j)$  verify

$$|L(\gamma, H_i)| = 1, \quad L(\gamma, H_j) = 0 \quad j \neq i.$$

Clearly, a simple link 'winds around' only one component<sup>3</sup> of  $H$  (see Figure 4).

**Definition 4.** We say that a compact subset  $K \subseteq \mathbb{E}^3$  *spans*  $H$  if every simple link of  $H$  intersects  $K$ .

This idea is crucial: we need spanning sets (in simple cases, surfaces) crossing every simple link: in this way it is impossible for  $K$  to be "detached" from  $H$ . However, in our problem  $H$  is not given a priori since  $H = \Lambda[\mathbf{z}]$ , i.e. it depends on the considered configuration, we need a still more general definition.

Now let  $H$  be a closed subset of  $\mathbb{E}^3$  and consider the family

$$C_H = \{\gamma: \mathbb{S}^1 \rightarrow \mathbb{E}^3 \setminus H : \gamma \text{ is a smooth embedding of } \mathbb{S}^1 \text{ into } \mathbb{E}^3\}.$$

A set  $C \subseteq C_H$  is said to be *closed by homotopy* (with respect to  $H$ ) if it contains all elements belonging to the same homotopy class.

---

<sup>3</sup>Precisely, the definition of the linking number between a closed subset and a curve is exactly the one given before (Definition 2) by considering the compactification of the  $\mathbb{E}^3$  (for more details see Rolfsen (2003), pp.132-136).

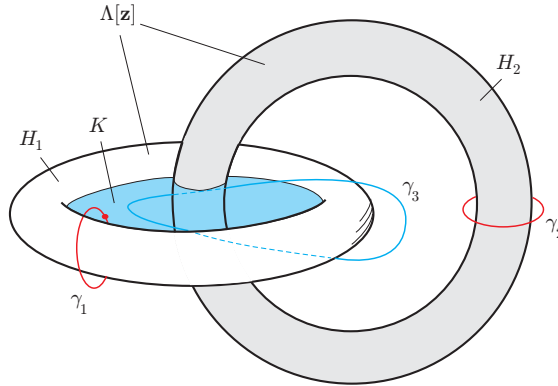


FIGURE 4.  $\gamma_i$  ( $i = 1, 2$ ) are simple links for  $H_i$  while  $\gamma_3 \in F(\Lambda[\mathbf{w}])$ . Even if  $K$  is not  $D$ -spanning for the whole system, notice how  $\gamma_1 \cap K \neq \emptyset$ .

**Definition 5.** Given  $C \subseteq C_H$  closed by homotopy, we say that a relatively closed subset  $K \subset \mathbb{E}^3 \setminus H$  is a  $C$ -spanning set of  $H$  if

$$K \cap \gamma \neq \emptyset \quad \forall \gamma \in C.$$

We denote by  $F(H, C)$  the family of all  $C$ -spanning sets of  $H$ .

Notice that the set spanned by the surface can be any closed set in  $\mathbb{E}^3$ , so we can consider  $H = \Lambda[\mathbf{z}]$  with finite cross-section, as in our case and not only a line as in the Plateau’s problem. Nevertheless, the spanning surface depends only on the choice of the homotopy class and not to the configuration  $\mathbf{z}$ . Hence, we give the following

**Definition 6.** We call a set  $D_{\Lambda[\mathbf{z}]} \subseteq C_{\Lambda[\mathbf{z}]}$  a  $D_{\Lambda[\mathbf{z}]}$ -spanning set of  $\Lambda[\mathbf{z}]$  if it contains all the smooth embeddings  $\gamma$  which are not homotopic to a constant and which have linking number one with both rods. For the sake of brevity, we will write  $D$  in place of  $D_{\Lambda[\mathbf{z}]}$ .

Finally, we denote  $F(\Lambda[\mathbf{z}], D)$  the family of  $D$ -spanning sets of  $\Lambda[\mathbf{z}]$  with linking number one with both components (see Figure 4). We are now in position to define the energy functional for our problem. We set

$$E_{KP}[\mathbf{z}] := E_{loop}[\mathbf{z}] + \inf\{E_{film}(S) : S \text{ is a } D\text{-spanning set of } \Lambda[\mathbf{z}]\}, \tag{14}$$

where  $\mathbf{z} \in V$  and verifies all the above-mentioned constraints. Precisely, the inf in the equation (14) is necessary since we want to eliminate the dependence on the spanning surface  $S$  and writing everything in the terms of the configuration  $\mathbf{z}$  only.

At this point a first important result holds.

**Theorem 2.** Let two circumferences  $\eta_i : [0, L_i] \rightarrow \mathbb{E}^3$  and  $M \in \mathbb{R}$  and  $n_1, n_2 \in \mathbb{Z}$  three constants be given. Then, the set

$$U_{M, n_1, \eta_i} := \{\mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2, \hat{r}_2, \hat{u}_2, \hat{v}_2) \in V = V_1 \times V_2 : E_{loop}[\mathbf{z}] < M; \tag{4), (5) \text{ and (12) hold } L(\mathbf{z}_i) = n_i; \tag{15}$$

$$L_{12} = 1 \text{ and } (r_1[\mathbf{z}_1], r_2[\mathbf{z}_2]) \simeq (\eta_1, \eta_2)\}$$

is weakly closed in  $V$ .

*Proof.* For the proof, one can refer to Bevilacqua *et al.* (2018). □

### 3. Main results

Now we want to prove the existence of a solution to the Kirchhoff-Plateau problem, *i.e.* the existence of a minimizer of  $E_{KP}$  given by (14) in the class  $U_{M,n_i,\eta_i}$ . As a first step we find a minimizer of each of its two terms.

**3.1. Energy minimizer for the bounding loop.** For the first term in (14), the functional  $E_{loop}$ , we use a quite straightforward application of the Direct Method of the Calculus of Variations. Recalling that its expression is

$$\begin{aligned} E_{loop}[\mathbf{z}] : V &\rightarrow \mathbb{R} \cup \{+\infty\} \\ \mathbf{z} &\mapsto E_{loop}[\mathbf{z}] = E_{el}[\mathbf{z}] + E_g[\mathbf{z}] + E_{rep}[\mathbf{r}] = \\ &= \int_I f(\mathbf{z}(\xi), \xi) d\xi + E_g[\mathbf{z}] + E_{rep}[\mathbf{r}], \end{aligned}$$

in order to verify if we can apply this method to  $E_{loop}$ , we follow the following steps.

First, we need to show that  $E_{loop}$  is bounded from below and proper, *i.e.*  $E_{loop} \neq +\infty$ . Now,  $E_{el}$  and  $E_g$  are proper by definition. Concerning  $E_{rep}$ , we assume that there is  $\mathbf{z} \in V$  such that  $L_{12} = 1$  and  $E_{rep}[\mathbf{z}] < +\infty$ . As for the boundedness, we can focus only on  $E_{el}$ , because  $E_g$  is always bounded from below, since the midline is bounded and  $E_{rep}$  is bounded from below by zero by the definition. Therefore, by (7) we immediately obtain

$$E_{el_i}[\mathbf{z}] \geq C_i \int_0^{L_i} |\mathbf{z}_i|^p ds + D_i L_i \geq D_i L_i > -\infty. \tag{16}$$

Hence,  $E_{loop}$  is bounded from below. Next, consider a sequence  $\{\mathbf{z}_k\}_{k \in \mathbb{N}}$  such that

$$\lim_k E_{loop}[\mathbf{z}_k] = \inf_{\mathbf{z} \in V} E_{loop}[\mathbf{z}] = m,$$

hence, it exists  $\bar{k}$  such that  $\forall k \geq \bar{k}$

$$E_{loop}[\mathbf{z}_k] \leq m + 1.$$

Precisely,  $E_{el}$  and  $E_g$  depend on  $\mathbf{z}_i$ , *i.e.* the configuration, while  $E_{rep}$  is an energy functional which depends on  $\mathbf{r} = (r_1, r_2)$ . Now, by the fact that a Kirchhoff rod is completely described by its midline, we can extract from  $\{\mathbf{z}_k\}$  a subsequence associated to the midline in order to minimize  $E_{loop}$  which, for sake of brevity, we will always indicate by  $\{\mathbf{z}_k\}$ . Now, we notice that this sequence is bounded: on a hand for the elastic and the potential component, this follows easily from the boundedness of the clamping parameters and by coercitivity, since

$$\int_0^{L_i} |\mathbf{z}_{i_k}|^p dx \leq \frac{1}{C_i} \int_0^{L_i} f_i(\mathbf{z}_{i_k}(s), s) ds - \frac{D_i L_i}{C_i} \leq \frac{1}{C_i} (m + 1) - \frac{D_i L_i}{C_i} \leq A,$$

where  $A > 0$  is a constant. So, since  $V$  and  $W^{2,p}([0, L_1]) \times W^{2,p}([0, L_2])$  are reflexive spaces (see for instance (Brezis 2010), Chap. 4),  $\{\mathbf{z}_k\}$  admits a weakly convergent subsequence, *i.e.* up to subsequences one has

$$\exists \mathbf{z} \in V : \quad \mathbf{z}_k \rightharpoonup \mathbf{z}.$$

Now we show that  $E_{\text{loop}}[\mathbf{z}]$  is weakly-lower semicontinuous (WLSC) in  $V$ . For  $E_{\text{el}}$  and  $E_{\text{g}}$ , this follows immediately from the hypotheses made on  $f_i$  and by noticing that  $E_{\text{g}}$  is a linear functional. For the repulsive part, get from Fatou’s lemma

$$\begin{aligned} E_{\text{rep}}[\mathbf{r}] &= \int_0^{L_1} \int_0^{L_2} \liminf_j \frac{c}{h(\|r_1^j(s_1) - r_2^j(s_2)\|)} ds_1 ds_2 \\ &\leq \liminf_j \int_0^{L_1} \int_0^{L_2} \frac{c}{h(\|r_1^j(s_1) - r_2^j(s_2)\|)} ds_1 ds_2 \\ &= \liminf_j E_{\text{rep}}[\mathbf{r}_j] = \lim_k E_{\text{rep}}[\mathbf{r}_k] \leq m. \end{aligned}$$

So, we obtain that the energy associated to the bounding loop is WLSC. Moreover, combining this previous result with the one of Theorem 2, we can state that if there is at least one admissible

$$\bar{\mathbf{z}} = (\bar{\mathbf{z}}_1, \bar{\mathbf{z}}_2) \in U_{M, n_i, \eta_i}$$

with  $M \in \mathbb{R}$ ,  $n_i \in \mathbb{N}$  and  $\eta_i : [0, L_i] \rightarrow \mathbb{E}^3$ , then the variational problem described above has a minimizer, i.e. there exists a minimizer  $\mathbf{z} \in U_{M, n_i, \eta_i}$  for the loop energy functional. Precisely, this statement is very easy to prove by using the fact that the constraints introduced are WLSC.

**3.2. Area-minimizing spanning surface.** Up to now, we only proved the existence of an energy-minimizing configuration for the bounding loop in the absence of the liquid film. To show the existence of an area-minimizing spanning surface for the link, we use a result proved by DeLellis. However, before introducing this important result, we have to emphasize some aspects. We are dealing with approximating surfaces, so we need to specify the notion of convergence of surfaces. We do this following Fried *et al.* (Giusteri *et al.* 2017)

**Definition 7.** Let  $A, B$  be two nonempty subsets of a metric space  $(M, d_M)$ . The Hausdorff distance between  $A$  and  $B$  is defined by

$$d_H(A, B) := \max\{\sup_{a \in A} \inf_{b \in B} d_M(a, b), \sup_{b \in B} \inf_{a \in A} d_M(a, b)\}.$$

Moreover, the set  $K(M)$  of nonempty compact subsets of  $M$  is a metric space and the topology induced by  $d_H$  on all closed nonempty subsets of  $M$  does not depend on  $d_M$  and it is said Hausdorff topology.

Hence, since the closed subset  $\Lambda[\mathbf{z}_k] \subseteq \mathbb{R}^3$  occupied by the whole link changes along the minimizing sequence, we have to consider sequences of nonempty closed sets which possibly converge to a closed set, which might be our minimal link. This idea is the correct one: since  $\mathbf{z}_k \rightarrow \mathbf{z}$  in  $V$ , we can say that the sequence of corresponding midlines converge uniformly. Hence,  $\Lambda_k[\mathbf{z}_k]$  converges in the Hausdorff topology to  $\Lambda[\mathbf{z}]$ . So, it is reasonable to consider as an assumption of next theorem (which we introduce without proof being the same of Theorem 6 in Bevilacqua *et al.* (2018)) the existence of a sequence of subsets  $\Lambda_k$  which converge to  $\Lambda$  in the Hausdorff topology, i.e.  $\Lambda_k \xrightarrow{H} \Lambda$ .

**Theorem 3.** *Let  $\Lambda_k$  a sequence of closed non empty subsets of  $\mathbb{E}^3$  converging in the Hausdorff topology to a closed set  $\Lambda \neq \emptyset$ . Assume that*

- i)  $\forall k \in \mathbb{N}, S_k \in F(\Lambda_k[\mathbf{z}], D)$ , where  $F(\Lambda_k[\mathbf{z}], D)$  is a good class<sup>4</sup>;
- ii)  $S_k$  is a countably  $\mathcal{H}^2$ -rectifiable set;
- iii)  $\mathcal{H}^2(S_k) = \inf\{\mathcal{H}^2(S) : S \in F(\Lambda_k[\mathbf{z}], D)\} < +\infty$ .

*Then the sequence of measures  $\mu_k := \mathcal{H}^2 \llcorner S_k$  is a bounded sequence; moreover  $\mu_k \xrightarrow{*} \mu$  up to subsequences, and*

$$\mu \geq \mathcal{H}^2 \llcorner S_\infty,$$

*where  $S_\infty = (\text{supt } \mu) \setminus \Lambda$  is a  $\mathcal{H}^2$ -rectifiable set and it is an  $(M, 0, \infty)$ -minimal set in  $\mathbb{R}^3 \setminus \Lambda[\mathbf{z}]$  in the sense of Almgren<sup>5</sup>.*

However, this is still not enough. Up to now, we proved in a separate way that the two functionals, the one associated with the elastic link and the other with the film, admit global minimizers. In order to write the solution of our problem, i.e. making a balance of the two contributions, we have to rewrite the above result in terms of the configurations of our system. This follows immediately if we can find a link between the smooth embedding  $\gamma$  and the sequence of surfaces  $\{S_k\}$ . For example, as in Bevilacqua *et al.* (2018), if the intersection between the sequence of surfaces  $\{S_k\}$ , or large  $k$ , and a neighborhood of  $\gamma$  is not a point but a set with positive measure, we can state that the surface  $S_\infty$  belongs to  $F(\Lambda[\mathbf{z}], D)$ , and is the area minimal set (Theorem 3). This result is fundamental in order to rewrite everything in terms of the configuration  $\mathbf{z}$  only.

Now, in order to conclude, we have only to prove the existence of a minimum. This follows now easily by combining the fact that  $E_{\text{loop}}$  is WLSC as we proved above and also that the functional

$$\mathbf{z} \mapsto \inf\{\mathcal{H}^2(S) : S \in F(\Lambda[\mathbf{z}], D)\}$$

is WLSC, by using the result of Theorem 8 in Bevilacqua *et al.* (2018).

### Acknowledgments

The Authors wish to thank Marco Degiovanni, Eliot Fried and Giulio Giuseppe Giusteri for helpful suggestions and fruitful discussions. The work has been partially supported by INdAM groups G.N.F.M. (Bevilacqua, Marzocchi) and G.N.A.M.P.A. (Lussardi).

### References

- Alberts, B., Johnson, A., Lewis, J., Walter, P., Raff, M., and Roberts, K. (2002). *Molecular Biology of the Cell 4th Edition: International Student Edition*. Routledge.
- Almgren, F. J. (1968). “Existence and regularity almost everywhere of solutions to elliptic variational problems among surfaces of varying topological type and singularity structure”. *Annals of Mathematics* **106**(87). DOI: [10.2307/1970587](https://doi.org/10.2307/1970587).

<sup>4</sup>For a precise definition of *good class* see De Lellis *et al.* (2017). In our case the first one is just a family of subsets in which we can control their measures. Namely, it exists a selected and well-defined competitor  $L$  with finite 2-dimensional Hausdorff measure which controls the measure of each element of the class.

<sup>5</sup>For a precise definition of  $(M, 0, \infty)$ -minimal set in the sense of Almgren, see Almgren (1968). In our case it is a property of regularity on the subset  $S_\infty = (\text{supt } \mu) \setminus \Lambda$ .

- Antman, S. S. (1995). *Nonlinear Problems of Elasticity*. Springer New York. DOI: [10.1007/978-1-4757-4147-6](https://doi.org/10.1007/978-1-4757-4147-6).
- Bevilacqua, G., Lussardi, L., and Marzocchi, A. (2018). “Soap film spanning an elastic link”. *Quarterly of Applied Mathematics*. DOI: [10.1090/qam/1510](https://doi.org/10.1090/qam/1510).
- Brezis, H. (2010). *Functional Analysis, Sobolev Spaces and Partial Differential Equations*. Springer New York. DOI: [10.1007/978-0-387-70914-7](https://doi.org/10.1007/978-0-387-70914-7).
- Ciarlet, P. G. and Necas, J. (1987). “Injectivity and self-contact in nonlinear elasticity”. *Archive for Rational Mechanics and Analysis* **97**(3). DOI: [10.1007/bf00250807](https://doi.org/10.1007/bf00250807).
- Dacorogna, B. (1989). *Direct Methods in the Calculus of Variations*. Springer Berlin Heidelberg. DOI: [10.1007/978-3-642-51440-1](https://doi.org/10.1007/978-3-642-51440-1).
- David, G. (2017). *Should We Solve Plateau’s Problem Again?* Princeton University Press. DOI: [10.23943/princeton/9780691159416.003.0006](https://doi.org/10.23943/princeton/9780691159416.003.0006).
- De Lellis, C., Ghiraldin, F., and Maggi, F. (2017). “A direct approach to Plateau’s problem”. *Journal of the European Mathematical Society* **19**(8). DOI: [10.4171/JEMS/716](https://doi.org/10.4171/JEMS/716).
- De Pauw, T. (2009). “Size minimizing surfaces”. *Annales scientifiques de l’Ecole normale superieure* **42**(1). DOI: [10.24033/asens.2090](https://doi.org/10.24033/asens.2090).
- Giusteri, G. G., Lussardi, L., and Fried, E. (2017). “Solution of the Kirchhoff-Plateau Problem”. *Journal of Nonlinear Science* **27**(3). DOI: [10.1007/s00332-017-9359-4](https://doi.org/10.1007/s00332-017-9359-4).
- Harrison, J. and Pugh, H. (2016). “Existence and soap film regularity of solutions to Plateau’s problem”. *Advances in Calculus of Variations* **9**(4). DOI: [10.1515/acv-2015-0023](https://doi.org/10.1515/acv-2015-0023).
- Hartman, P. (2002). *Ordinary Differential Equations*. Society for Industrial and Applied Mathematics. DOI: [10.1137/1.9780898719222](https://doi.org/10.1137/1.9780898719222).
- Huang, H. W. (1986). “Deformation free energy of bilayer membrane and its effect on gramicidin channel lifetime”. *Biophysical Journal* **50**(6). DOI: [10.1016/s0006-3495\(86\)83550-0](https://doi.org/10.1016/s0006-3495(86)83550-0).
- Mansfield, M. L. (1994). “Are there knots in proteins?” *Nature Structural and Molecular Biology* **1**(4). DOI: [10.1038/nsb0494-213](https://doi.org/10.1038/nsb0494-213).
- Mukherjee, A. (2015). *Differential Topology*. Springer International Publishing. DOI: [10.1007/978-3-319-19045-7](https://doi.org/10.1007/978-3-319-19045-7).
- Munkres, J. R. (1963). *Elementary Differential Topology*. Princeton University Press. DOI: [10.1515/9781400882656](https://doi.org/10.1515/9781400882656).
- Plateau, J. (1873). “Experimental and theoretical statics of liquids subject to molecular forces only”. *Gauthier-Villars, Paris*.
- Reifenberg, E. R. (1960). “Solution of the Plateau problem for  $m$ -dimensional surfaces of varying topological type”. *Bulletin of the American Mathematical Society* **66**(4). DOI: [10.1090/s0002-9904-1960-10482-x](https://doi.org/10.1090/s0002-9904-1960-10482-x).
- Rolfsen, D. (2003). *Knots and Links*. American Mathematical Society. DOI: [10.1090/chel/346](https://doi.org/10.1090/chel/346).
- Schuricht, F. (2002). “Global Injectivity and Topological Constraints for Spatial Nonlinearly Elastic Rods”. *Journal of Nonlinear Science* **12**(5). DOI: [10.1007/s00332-002-0462-8](https://doi.org/10.1007/s00332-002-0462-8).

- 
- <sup>a</sup> Politecnico di Milano  
MOX - Dipartimento di Matematica  
Via Bonardi 9, 20133 Milano, Italy
- <sup>b</sup> Politecnico di Torino  
Dipartimento di Scienze Matematiche 'Giuseppe Luigi Lagrange'  
Corso Duca degli Abruzzi 24, 10129 Torino, Italy
- <sup>c</sup> Università Cattolica del Sacro Cuore  
Dipartimento di Matematica e Fisica 'Niccolò Tartaglia'  
Via Musei 41, 25121 Brescia, Italy
- \* To whom correspondence should be addressed | email: [luca.lussardi@polito.it](mailto:luca.lussardi@polito.it)

Paper contributed to the workshop entitled "Mathematical modeling of self-organizations in medicine, biology and ecology: from micro to macro", which was held at Giardini Naxos, Messina, Italy (18–21 September 2017) under the patronage of the *Accademia Peloritana dei Pericolanti*

Manuscript received 20 March 2018; published online 30 November 2018



© 2018 by the author(s); licensee *Accademia Peloritana dei Pericolanti* (Messina, Italy). This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/) (<https://creativecommons.org/licenses/by/4.0/>).