Helices

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Helices are among the simplest shapes that are observed in the filamentary and molecular structures of nature. The local mechanical properties of such structures are often modeled by a uniform elastic potential energy dependent on bending and twist, which is what we term a rod model. Our first result is to complete the semi-inverse classification, initiated by Kirchhoff, of all infinite, helical equilibria of inextensible, unshearable uniform rods with elastic energies that are a general quadratic function of the flexures and twist. Specifically, we demonstrate that all uniform helical equilibria can be found by means of an explicit planar construction in terms of the intersections of certain circles and hyperbolas. Second, we demonstrate that the same helical centerlines persist as equilibria in the presence of realistic distributed forces modeling nonlocal interactions as those that arise, for example, for charged linear molecules and for filaments of finite thickness exhibiting self-contact. Third, in the absence of any external loading, we demonstrate how to construct explicitly two helical equilibria, precisely one of each handedness, that are the only local energy minimizers subject to a nonconvex constraint of self-avoidance.

biomolecules | differential geometry | elasticity | filaments | rods

Scientists have long held a fascination, sometimes bordering on mystical obsession, for helical structures in nature (1, 2). Helices arise in nanosprings, carbon nanotubes, α-helices, DNA double and collagen triple helices, lipid bilayers, bacterial flagella in *Salmonella* and *Escherichia coli*, aerial hyphae in actynomycetes, bacterial shape in spirochetes, horns, tendrils, vines, screws, springs, and helical staircases (3–13). Helical structures can be understood from a discrete point of view as a regular, periodic stacking of rigid blocks, such as the bases in DNA strands (14), the tail sheaths of bacteriophages (15), the packing of flagellin subunits (16), or simply the stairs in spiral staircases (1). However, it also can be beneficial to adopt a continuous description in which a filamentary structure is represented by a central space curve along with a frame that captures the orientation of the material cross sections at each point along the curve. Although this description neglects some fine features of deformations in the cross section, it is nevertheless suitable to describe the large-scale geometrical and physical properties of long, thin structures. If the deformations are small enough with respect to the appropriate characteristic length scales of the problem, the physical attributes of the filament such as the stresses acting across cross sections can be averaged and represented as a resultant force and moment acting on the centerline. We will refer to such a description of a filamentary structure as a rod model (see, for instance, refs 5, 7, 8, and 10–13 for examples of such rod theories).

In continuum mechanics, a semi-inverse problem is generally taken to mean the study of a special class of solutions with certain features specified *a priori*, as opposed to the study of, for example, all solutions to a particular boundary value problem. Kirchhoff (17–19) first proposed the semi-inverse problem of determining all equilibrium configurations of a uniform rod whose centerlines were a helix, i.e., a curve with constant curvature and torsion (see also ref. 20). In addition, Kirchhoff himself found all helical solutions in the particular case of what is now called an isotropic Kirchhoff rod, i.e., an inextensible, unshearable rod with a quadratic bending and twisting energy that has equal response to bending in any material direction.

After Kirchhoff, the semi-inverse classification of helical equilibria of rods was resolved for more general classes of nonlinear constitutive relations, and also for models encompassing effects of shear and extension, by Whitman and DeSilva (21) and Antman (22), but still only in isotropic cases. More recently, the general classification of helical equilibria for nonisotropic rods has been discussed in ref. 23, where a necessary and sufficient set of conditions that must be satisfied by uniform helical equilibria was obtained, and various conclusions about multiplicities of such solutions were reached. It is here important to distinguish between uniform helical structures, in which the orientation of the material cross section is fixed with respect to the Frenet frame of the helical centerline so that the geometrical torsion and physical twist coincide, and nonuniform helical structures.

After brief introductions to the kinematics and mechanics of rods in the first two sections, our first original contribution is to demonstrate that when specialized to the particular Kirchhoff case of inextensible and unshearable rods with quadratic bending and twist energy, the necessary conditions derived in ref. 23 allow a complete, explicit, and elementary classification of all uniform helical equilibria. The additional progress possible in the classification for the particular case of a nonisotropic quadratic energy is of some practical importance because it is precisely this case that arises in many modeling applications. We further show, in the rather technically detailed *Supporting Text*, which is published as supporting information on the PNAS web site, that, with the exception of some very particular and well characterized energies and equilibria, all helical equilibria of a nonisotropic rod are in fact uniform helical equilibria. Thus, in a certain sense we here complete the classification of all helical equilibria started by Kirchhoff.

Our second set of results concerns nonlocal central interactions. We demonstrate that any helical equilibrium of an inextensible, unshearable rod in the absence of nonlocal interactions remains as an equilibrium in the presence of nonlocal interactions that arise from central pairwise forces, as is the case for either electrostatics or self-contact. The geometry of the helical equilibrium is unmodified, while the tangential component of force or tension in the rod is appropriately incremented to satisfy the balance laws.

Our third set of results concerns the possible minimum energy states of a uniform elastic rod of prescribed tubular thickness when subject to a self-avoidance requirement and in the absence of any external loading. For such rods the actual state of least energy may not be accessible because of the self-avoidance constraint. We show that, again with the exception of certain very special and classifiable cases, there are always precisely two helical states, one left-handed and one right-handed, that realize the only two local minima of the elastic energy subject to self-avoidance.

Throughout, we consider only the semi-inverse problem for helical solutions. In particular, we consider only helical equilibria of infinite extent. Finite segments of these solutions will satisfy certain two-point boundary value problems, but only for rather special

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boundary data, and, for the case of nonlocal interactions, in the presence of specific distributed external loadings close to the boundary.

Kinematics

A configuration of an inextensible, unshearable rod (22) is defined by its centerline $\boldsymbol{r}(s)$ and an associated orthonormal framing of directors $\{\boldsymbol{d}_i(s)\}$, $i = 1, 2, 3$, where s is the arc length, $-L \le s \le L$. The kinematics of the frame are encapsulated in

$$\boldsymbol{d}_i' = \boldsymbol{u} \times \boldsymbol{d}_i, \quad i = 1, 2, 3, \qquad [1]$$

where $(\,)'$ denotes the derivative with respect to s, and $\boldsymbol{u} = u_1\boldsymbol{d}_1 + u_2\boldsymbol{d}_2 + u_3\boldsymbol{d}_3$. The components $\mathbf{u} := (u_1, u_2, u_3)$ are the strains of the rod; u_1 and u_2 are associated with bending, whereas u_3 describes physical twist. Inextensibility and unshearability are manifested in the vector constraint $\boldsymbol{r}' = \boldsymbol{d}_3$. Thus, the two vector fields $(\boldsymbol{d}_1(s), \boldsymbol{d}_2(s))$ span the normal plane to $\boldsymbol{r}(s)$; their directions encode the orientation of the material cross section of the filament at s and therefore provide more information than that contained in the curve $\boldsymbol{r}(s)$ itself.

In contrast, the classic intrinsic framing of $\boldsymbol{r}(s)$ is provided by the Frenet frame $\boldsymbol{F} := \{\boldsymbol{\nu}, \boldsymbol{\beta}, \boldsymbol{\tau}\}$ of principal normal, binormal, and tangent $\boldsymbol{\tau} \equiv \boldsymbol{d}_3$ that is defined purely in terms of the centerline $\boldsymbol{r}(s)$ wherever $\boldsymbol{r}'' \neq 0$ (see, e.g., ref. 24). The Frenet–Serret equations are

$$\boldsymbol{\tau}' = \kappa\boldsymbol{\nu}, \qquad [2a]$$

$$\boldsymbol{\nu}' = -\kappa\boldsymbol{\tau} + \tau\boldsymbol{\beta}, \qquad [2b]$$

$$\boldsymbol{\beta}' = -\tau\boldsymbol{\nu}, \qquad [2c]$$

where $\kappa(s) \ge 0$ is the curvature, and $\tau(s)$ is the (geometric) torsion of the curve. Because $\boldsymbol{\tau} = \boldsymbol{d}_3$ the directors $(\boldsymbol{d}_1(s), \boldsymbol{d}_2(s))$ are a rotation of $\{\boldsymbol{\nu}, \boldsymbol{\beta}\}$ through an angle $\varphi(s)$ about the tangent

$$\boldsymbol{d}_1 = \boldsymbol{\nu}\cos\varphi + \boldsymbol{\beta}\sin\varphi, \qquad [3a]$$

$$\boldsymbol{d}_2 = -\boldsymbol{\nu}\sin\varphi + \boldsymbol{\beta}\cos\varphi. \qquad [3b]$$

Following a nomenclature introduced in the study of DNA (25), we call the angle φ the register. The strains $\mathbf{u}$ are related to the curvature κ, torsion τ, and register φ through (see ref. 18, p. 383)

$$u_1 = \kappa\sin\varphi, \quad u_2 = \kappa\cos\varphi, \quad u_3 = \tau + \varphi'. \qquad [4]$$

Curves with constant curvature and torsion are helices, which, after elimination of a rigid-body motion, can be given the arc-length parametric form $\boldsymbol{r}(s) = r\cos(\eta_1 s)\boldsymbol{e}_1 + r\sin(\eta_1 s)\boldsymbol{e}_2 + p\eta_1 s\boldsymbol{e}_3$, where $\{\boldsymbol{e}_i\}$ is a fixed basis, r is the radius of the helix, $2\pi p$ is the pitch, and $\eta_1 = 1/\sqrt{r^2 + p^2}$. The constant curvature, torsion, radius, and pitch are related by

$$r = \frac{\kappa}{\kappa^2 + \tau^2}, \quad p = \frac{\tau}{\kappa^2 + \tau^2}. \qquad [5]$$

Of particular importance here is the geometric fact that at each point along a helix the principal normal is $\boldsymbol{\nu}(s) = -\cos(\eta_1 s)\boldsymbol{e}_1 - \sin(\eta_1 s)\boldsymbol{e}_2$, i.e., it is oriented inward and perpendicular to the helical axis $\boldsymbol{e}_3$.

Consideration of Eq. **4** reveals that provided the register $\varphi(s)$ is not constant, the configuration of a rod can have a constant curvature and torsion, i.e., a helical axis $\boldsymbol{r}$, without the strains $\mathbf{u}$ being constant. However, the helical configurations for which $\mathbf{u}$ is constant play a central role in the analysis and will be referred to as uniform helices. The centerline of such a configuration is a helix, and the register is constant. Uniform helices are completely characterized by a point in three-dimensional (3D) $\mathbf{u}$ space. Moving along rays $\gamma\mathbf{u}$ from the origin in this space traverses uniform helices with, from Eq. **4**, constant register and curvature and torsion $(|\gamma|\kappa, \gamma\tau)$ and, from Eq. **5**, radius and pitch $(r/|\gamma|, p/\gamma)$. Thus, the helices dilate as $\gamma \to 0$, and the origin in $\mathbf{u}$-space is a rather singular limit.

Mechanics

The stresses acting across the cross section at $\boldsymbol{r}(s)$ can be averaged to yield a resultant force $\boldsymbol{n}(s)$ and moment $\boldsymbol{m}(s)$. Balance of forces and moments then yields (19)

$$\boldsymbol{n}' + \boldsymbol{f} = \mathbf{0}, \quad \boldsymbol{m}' + \boldsymbol{r}' \times \boldsymbol{n} + \boldsymbol{l} = \mathbf{0}, \qquad [6]$$

where $\boldsymbol{f}(s)$ and $\boldsymbol{l}(s)$ are, respectively, the body force and couple per unit length applied on the cross section at s. Different functional forms of these body forces and couples can be used to model different effects such as gravity, interaction with solvent, or interactions between different parts of the rod via electrostatics or self-contact, for example.

Because of the inextensibility and unshearability constraint, the force $\boldsymbol{n}(s)$ is a basic unknown, but to close the system a constitutive relation relating the moment and strains must be given. We assume a uniform, hyperelastic rod, i.e., there exists a convex, coercive strain-energy density function $W(\mathbf{w})$ with $W_{\mathbf{w}}(\mathbf{0}) = 0$ that generates the constitutive relations $\mathbf{m} = \partial_{\mathbf{u}}W(\mathbf{u} - \hat{\mathbf{u}})$. Here the constants $\hat{\mathbf{u}}$ are the strains in the uniform, unstressed reference configuration at which $\mathbf{m} = \mathbf{0}$.

It will be of importance to distinguish between isotropic and nonisotropic rods. The strain-energy function W is said to be isotropic if $W(w\cos\varphi, w\sin\varphi, w_3)$ is independent of φ for all w and w_3. The rod is said to be isotropic if in addition $\hat{u}_1 = \hat{u}_2 = 0$. Physically, an isotropic rod has no preferred bending direction.[‖]

We will be particularly concerned with one of the most important cases for applications in which the strain-energy density is well-approximated by a quadratic function of the strains, i.e.,

$$W(\mathbf{u} - \hat{\mathbf{u}}) = \frac{1}{2}(\mathbf{u} - \hat{\mathbf{u}})\cdot K(\mathbf{u} - \hat{\mathbf{u}}), \qquad [7]$$

where $\boldsymbol{K}$ is a symmetric 3×3 positive-definite matrix, which, by a rotation about $\boldsymbol{d}_3$ of the embedding of the frame $\{\boldsymbol{d}_i\}$ in the material of the rod, may without loss of generality be assumed to be of the form

$$\boldsymbol{K} = \begin{pmatrix} K_1 & 0 & K_{13} \\ 0 & K_2 & K_{23} \\ K_{13} & K_{23} & K_3 \end{pmatrix}, \quad K_1 \le K_2. \qquad [8]$$

For a quadratic strain energy, the constitutive relation for $\mathbf{m}$ is linear $\mathbf{m} = \boldsymbol{K}(\mathbf{u} - \hat{\mathbf{u}})$, which implies $\mathbf{u} = \hat{\mathbf{u}} + \boldsymbol{K}^{-1}\mathbf{m}$. The quadratic strain-energy Eq. **7** is isotropic precisely when $K_2 - K_1 = K_{23} = K_{13} = 0$, with the associated rod being isotropic when in addition $\hat{u}_1 = \hat{u}_2 = 0$.

Helical Equilibria in the Absence of Body Forces

In this section we consider the classic Kirchhoff problem of classifying helical equilibria in the absence of distributed body forces and couples, i.e., $\boldsymbol{f} = \boldsymbol{l} = \mathbf{0}$ in Eqs. **6**. Our starting point is the

‖In general, nonisotropic rods have the property that if the uniform, i.e., s-independent, constitutive relations are rewritten with respect to another reference framing, then the transformed constitutive relations will be nonuniform unless the old and new reference frames are related by means of a simple constant rotation. Thus, for nonisotropic rods there is a family of preferred choices of $\hat{u}$ leading to uniform constitutive relations, and the notion of uniform helices introduced above is with respect to any of these preferred coordinate systems. However, for isotropic rods the constitutive relations will remain uniform for any choice of $\hat{u}_3$, even though the different reference framings are not related through a constant rotation. Thus, for isotropic rods, the notion of which helical configurations are uniform and which are not, is coordinate system dependent and is accordingly not of physical importance. Because the set of helical configurations for isotropic rods is so well understood, the ambiguity in the isotropic case will turn out to be of no practical significance (see text below).

analysis of uniform helical equilibria presented in ref. 23, which we briefly summarize.

First, there are two limiting and exceptional 1D families of uniform helices with either $\mathbf{u} = \mathbf{0}$ or $\mathbf{n} = \mathbf{0}$ that can straightforwardly be verified to be equilibria through a direct consideration of the balance laws in Eqs. **6**. When $\mathbf{u} = \mathbf{0}$, the director frame steadily translates, the centerline is a straight line, i.e., a degenerate helix, the moment $\mathbf{m}$ is given by the constitutive relations, and the force $\mathbf{n}$ is parallel (or antiparallel) to the helix centerline with arbitrary magnitude. The second family of singular equilibria with $\mathbf{n} = \mathbf{0}$ have $\mathbf{m}$ and $\mathbf{u}$ parallel, with the vector $\mathbf{m}$ constant and parallel to the axis of the helical centerline. The absolute energy minimizer $\mathbf{u} = \hat{\mathbf{u}}$ at which $\mathbf{m} = \mathbf{0}$ is always a member of the second family. In addition, the two families intersect at the unique uniform helical equilibrium for which $\mathbf{u} = \mathbf{0} = \mathbf{n}$.

All remaining uniform helical equilibria can be characterized as follows. For each freely prescribed curvature $\kappa = \sqrt{u_1^2 + u_2^2} > 0$ and torsion $\tau = u_3$, there are two or more corresponding uniform helical equilibria with constant registers φ^* that need to be computed. Specifically the equilibrium registers φ^* are determined, through Eq. **4** with $\varphi' = 0$, from critical points $\mathbf{u}^*$ of the energy $W(\mathbf{u} - \hat{\mathbf{u}})$, subject to the constraints

$$\frac{1}{2}\,\mathbf{u}\cdot\mathbf{u} = \frac{1}{2}\,\eta_1^2, \quad u_3 = \eta_1\eta_2. \qquad \textbf{[9]}$$

In $\mathbf{u}$-space, and for $0 < \eta_1 < \infty$ and $-1 < \eta_2 < 1$, the constraints of Eq. **9** define the intersection of a sphere centered at the origin and a plane normal to the u_3-axis, i.e., a circle. On this circle, the continuous real-valued function W must have at least two critical points, namely a maximum and a minimum. Thus, there exists a discrete number of two or more families of uniform helical equilibria $\mathbf{u}^*(\eta_1, \eta_2)$ parameterized by the constants η_1 and η_2 with curvature $\kappa^2 = \eta_1^2(1 - \eta_2^2)$ and torsion $\tau = \eta_1\eta_2$. It can be shown that for these equilibria the force $\boldsymbol{n}$ is parallel to the helical axis, whereas the moment $\boldsymbol{m}$ lies in the tangent-binormal plane (which also contains the helix axis).

In the case of an isotropic rod, the function W is constant along the constraint circle, and consequently all of $\mathbf{u}$-space generates uniform helical equilibria. Moreover, as already found in refs. 21 and 22, the symmetry of isotropy generates further nonuniform helical equilibria of arbitrary constant curvature and torsion in which the register evolves linearly $\varphi(s) = c_0 + c_1 s$. According to Eq. **4**, c_1 represents the excess twist, i.e., the difference between the geometrical torsion τ and the physical twist u_3. Thus, in the case of an isotropic rod the discrete number of two-parameter families of uniform helical equilibria arising for nonisotropic rods is replaced by a single four-parameter family of nonuniform helical equilibria with arbitrary curvature, torsion, phase c_0 in register, and excess twist c_1.[††]

The main tool in the analysis of ref. 23 is to demonstrate that on uniform helical equilibria the balance laws of Eq. **6** are equivalent to the first-order necessary conditions for the constrained variational principle, namely,

$$\mathbf{m}{:} = \frac{\partial W}{\partial \mathbf{u}}(\mathbf{u} - \hat{\mathbf{u}}) = \mu_1\mathbf{u} + \mu_2\mathbf{d}_3, \qquad \textbf{[10]}$$

where $\mathbf{d}_3 = (0, 0, 1)^T$, and the constants μ_1 and μ_2 are undetermined Lagrange multipliers associated with the constraints of Eq. **9**.

We now move to an extension of the analysis presented (23). We first note that although the Lagrange multiplier approach of Eq. **10** is naturally related to balance of forces and moments, the constraint set of Eq. **9** for $\eta_1 > 0$ is actually 1D, specifically a circle, with tangent $\boldsymbol{\xi}{:} = (u_2, -u_1, 0)$. Consequently, the Lagrange multipliers can be eliminated, and the first-order necessary conditions can instead be written explicitly as

$$\boldsymbol{\xi}\cdot\frac{\partial W}{\partial \mathbf{u}} = 0, \qquad \textbf{[11]}$$

which is a single scalar algebraic equation that generically defines a 2D manifold in $\mathbf{u}$-space containing all uniform helical equilibria. In particular, the surface always passes through the absolute energy minimizer $\hat{\mathbf{u}}$. It also contains the entire u_3 axis. In the case that W is the quadratic energy Eq. **7**, Eq. **11** takes the particularly simple and explicit form

$$2u_1u_2(K_2 - K_1) + 2u_3(u_1K_{23} - u_2K_{13}) - (K_2\hat{u}_2 + K_{23}\hat{u}_3)u_1 + (K_1\hat{u}_1 + K_{13}\hat{u}_3)u_2 = 0. \qquad \textbf{[12]}$$

For each set of coefficients defining a quadratic energy, and except for the single degenerate case of isotropic rods for which $K_2 - K_1 = K_{23} = K_{13} = \hat{u}_1 = \hat{u}_2 = 0$, Eq. **12** defines a ruled quadric in $\mathbf{u}$-space (see Fig. 1). If $K_2 - K_1 \neq 0$, it can be factored further as

$$(u_1 - a - b\,u_3)(u_2 - c - d\,u_3) = (a + b\,u_3)(c + d\,u_3), \qquad \textbf{[13]}$$

where the constants a, b, c, and d are

$$a = \frac{K_1\hat{u}_1 + K_{13}}{K_2 - K_1}, \quad c = \frac{K_2\hat{u}_2 + K_{23}\hat{u}_3}{K_1 - K_2},$$

$$b = \frac{K_{13}}{K_2 - K_1}, \quad d = \frac{K_{23}}{K_1 - K_2}.$$

Now it can be observed that the set of all uniform helical equilibria with prescribed torsion $\tau = u_3$ lies on the hyperbola in (u_1, u_2)-space defined by Eq. **13**. For all u_3 the hyperbola has asymptotes parallel to the u_1 and u_2 axes, center at the point $(a + bu_3, c + du_3)$, and one branch of the hyperbola passes through the origin (compare Fig. 1 *Inset*). Consideration of small and large circles centered at the origin reveals that other than in the

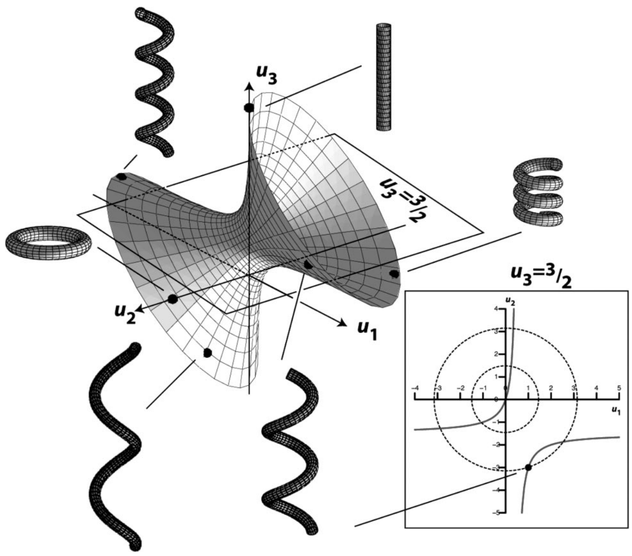

Fig. 1. The hyperboloid in curvature space (u_1, u_2, u_3) on which all helical solutions for a quadratic energy W are located (case shown: $K_1 = 1$, $K_2 = 3/2$, $K_{23} = K_{13} = 1/2$, $\hat{u}_1 = 1$, $\hat{u}_2 = \hat{u}_3 = 0$). We show various helical solutions for different points on the hyperboloid. (*Inset*) A planar horizontal section of the hyperboloid (case shown: $u_3 = 3/2$).

[††]Further to footnote ‖, we remark that the precise value of the excess twist c_1 on a given helical equilibrium depends on the choice of reference framing that has been made, so that in particular for an isotropic rod the subset of uniform helical equilibria, i.e., those with $c_1 = 0$, depends on the coordinate system chosen.

special case where the center of the hyperbola is itself at the origin, there will be precisely two uniform helical equilibria of the prescribed torsion and small curvature $\kappa = \sqrt{u_1^2 + u_2^2}$, whereas there will be precisely four helical equilibria for sufficiently large curvatures that the corresponding circle intersects both branches of the hyperbola.

The above analysis gives a rather explicit characterization of all uniform helical equilibria of a nonisotropic rod with quadratic strain-energy. Going back to Kirchhoff, the set of all helical equilibria for an isotropic rod has been known, and it includes many nonuniform helical equilibria. To complete the semi-inverse classification of helical equilibria for the nonisotropic case, it is therefore necessary to address the following question: Can a nonisotropic rod also have nonuniform helical equilibria? Perhaps somewhat surprisingly the answer is yes, but only for very special constitutive relations, and even then only for very special helices. The detailed analysis justifying these conclusions is presented in the *Supporting Text*, and a specific example is illustrated in Fig. 5, which is published as supporting information on the PNAS web site.

Nonlocal Central Interactions

Nonlocal interaction forces and contact forces between filamentary structures play an important role in many mechanical systems such as ropes and cables (26–28) and biological systems such as chromatin fibers (29), DNA structures (30), and myelin figures (31). The modeling of contact problems in rods and helical structures has been considered by many different authors in the mechanics, engineering, and physics literature (32–40); however, these analyses are restricted to rods in contact with external objects, rods in self-contact at discrete points, or very particular helical solutions. Here, we concentrate on self-interactions of uniform helices.

We first suppose that $(\boldsymbol{r}, \boldsymbol{d}_i, \boldsymbol{m}, \boldsymbol{n})$ is a uniform, i.e., $\mathbf{u}$ constant, helical equilibrium in the absence of any distributed loads ($\boldsymbol{l} \equiv \mathbf{0} \equiv \boldsymbol{f}$), as constructed in the previous section. Next we remark that if we introduce distributed loads in Eq. **6** of the special form

$$\boldsymbol{f} = \alpha \boldsymbol{\nu}, \quad \boldsymbol{l} = \mathbf{0}, \qquad [14]$$

for some constant α, where $\boldsymbol{\nu}(s)$ is the principal normal to the helix, then $(\boldsymbol{r}, \boldsymbol{d}_i, \boldsymbol{m}, \boldsymbol{n} + \frac{\alpha}{\kappa}\boldsymbol{\tau})$ is an associated uniform helical equilibrium; i.e., the effect of adding a distributed load of the form given in Eq. **14** to a uniform helical equilibrium is balanced merely by changing the force $\boldsymbol{n}$ with the addition of a tangential component that is proportional to the applied load and inversely proportional to the curvature. It is straightforward to verify this fact because the directors $\boldsymbol{d}_i$ and strains $\mathbf{u}$, and therefore also the moment $\boldsymbol{m}$ are all unchanged, whereas the balance laws of Eq. **6** are linear in both $\boldsymbol{n}$ and $\boldsymbol{l}$, the tangent $\boldsymbol{\tau}$ and principal normal $\boldsymbol{\nu}$ satisfy the Frenet–Serret Eqs. **2** with constant curvature κ, and because of the inextensibility and unshearability constraint the force $\boldsymbol{n}$ enters in no constitutive relation. Slight generalizations of this observation are possible, but we instead pursue the question of when a distributed loading of the particular form of Eq. **14** is of practical interest.

We consider here the case where there is a distributed body force $\boldsymbol{f}(s)$ generated by nonlocal, pairwise central self-interactions. On a helical equilibrium the net body force at $\boldsymbol{r}(s)$ resulting from a pair of central interactions with upstream $\boldsymbol{r}(s + \delta)$ and downstream $\boldsymbol{r}(s - \delta)$ points, integrated over all δ is a force parallel to the principal normal $\boldsymbol{\nu}(s)$ of the form $\boldsymbol{f} = \alpha\boldsymbol{\nu}$ (see Fig. 2), i.e., is precisely of the form of Eq. **14**. This observation is a direct consequence of the assumed uniformity of the nonlocal interaction, the principle of equal but opposite action and reaction, and the discrete symmetry of rotating a helix through an angle π about the principal normal at s, which maps $\boldsymbol{r}(s + \delta)$ to $\boldsymbol{r}(s - \delta)$.

Our conclusion is that the semi-inverse classification of all uniform helical equilibria in the absence of nonlocal interactions trivially extends in the presence of central self-interactions. Note that the above symmetry arguments are only strictly valid in the bulk of the helix sufficiently far away from the ends. Exact solutions for finite helices would require a proper treatment of end effects in a region close to the boundary to take into account a varying body force density both in magnitude and deviation from the principal normal direction, and that seems to be an elusive computation.

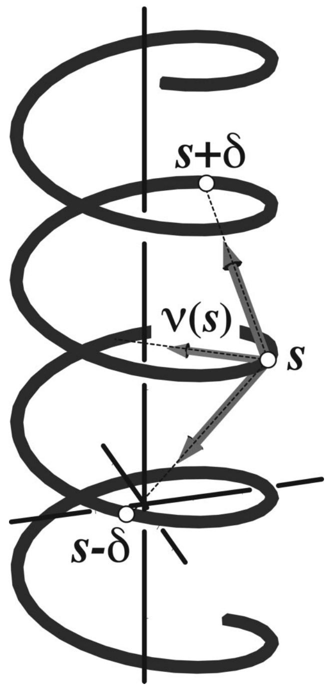

Fig. 2. With body forces created by pairwise central nonlocal interactions, the contributions to the total body force on the cross section at s by points located at $s \pm \delta$ is along the principal normal $\boldsymbol{\nu}(s)$.

Self-Contact

The rod theory described above is traditionally motivated as being a model of long, slender objects in which attention is focused on the deformations of the central curve $\boldsymbol{r}$, whereas deformations within the cross section are neglected. Nevertheless, the body has a nonvanishing cross section, and, for consistency within the rod model and in order that a configuration be admissible, the tube around the centerline $\boldsymbol{r}$ generated by the cross sections should be non-self-intersecting. This requirement implies both a local condition, namely that the radius of curvature of $\boldsymbol{r}$ should be everywhere larger than the dimension of the cross section, and a nonlocal condition, namely that no two points $\boldsymbol{r}(s_1)$ and $\boldsymbol{r}(s_2)$ corresponding to different arc lengths should be too close to each other in space. A general treatment of this self-avoidance problem for elastic rods is still a subject of current research (see e.g., refs. 41 and 42). However, the case of self-avoidance of helical configurations is much simpler, at least when each normal cross section is assumed to be circular of constant radius along the rod, as we describe next.

We scale all lengths such that the (constant) radius of each circular cross section is one. Then, helical configurations with no self-intersection exist only for values of the curvature and torsion in the no-contact regions illustrated in Fig. 3*A*. Self-contact is achieved for those special values on the contact curve defined as the boundary between the no-contact and the forbidden region. The analytic form of these one-parameter curves $(\kappa(\xi), \tau(\xi))$ is given in ref. 43 (based on refs. 31, 44, and 45; see also ref. 46, section 7.2). The vertical portion of the boundary corresponds to helices with large local curvature $\kappa = 1$ folding on themselves, a regime for which the validity of the rod model is questionable. In contrast, the curved segment of the boundary corresponds to helices resting on themselves, i.e., where contact is from remote parts of the helical

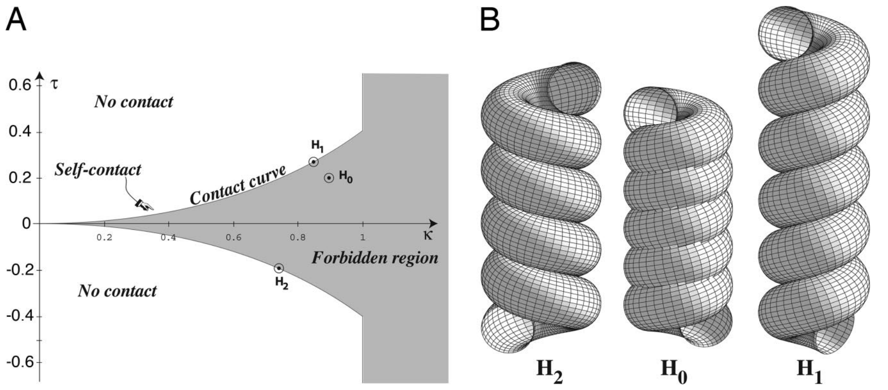

Fig. 3. The geometry of helical tubes with circular cross sections. (*A*) In the curvature–torsion plane, helices are in contact at the boundary between the clear and opaque region. (*B*) The helix H_0 corresponds to a helical tube with self-penetration while H_1 and H_2 are in self-contact. The configuration H_0 is the stress-free configuration for the elastic energy $W_1 = u_1^2 + (u_2 - 9/10)^2 + 3/4(u_3 - 2/10)^2$ when self-avoidance is not taken into account. Helical configurations H_1 and H_2 are two minimum energy configurations of opposite-handedness respecting self-avoidance. For reasons of geometric clarity, the point H_0 has been chosen comparatively close to the boundary $\kappa = 1$ where for some materials the validity of a rod model might already be considered questionable, but the same geometric phenomena persist for choices of H_0 arbitrarily close to the origin.

tube; the rod model is entirely consistent right up to this boundary. In the rest of this work, we only consider helices with such nonlocal self-contact.

The construction of helical equilibria described earlier remains unaltered for values of the curvature and torsion in the no-contact region. For helical configurations in self-contact, each point s interacts with a single pair of symmetrically located points via a pressure $P \geq 0$. Therefore, self-contact creates a uniform, distributed body force $\alpha\boldsymbol{\nu}$ with $\alpha \leq 0$ given in terms of P and the geometry of the helix. In addition, the contact pressure is balanced by an additional tangential component $(\alpha/\kappa)\boldsymbol{d}_3$ to the force $\boldsymbol{n}$, which corresponds to an increase in tension in the rod.

We reiterate that prescribing the curvature and torsion of a helical configuration does not specify the entire configuration. Rather it is necessary to determine the associated possible registers φ. For the particular case of uniform helices, this is equivalent to requiring that all three constants $\mathbf{u}$ be specified. Consequently, with the kinematic relations Eq. **4**, the noncontact region can be constructed in 3D $\mathbf{u}$-space merely by rotating the contact curve in Fig. 3*A* around the vertical axis (compare Fig. 4). One obtains two caps, one convex down and one convex up, that delimit the accessible configurations in $\mathbf{u}$-space.

We may now consider the following problem: Given a rod whose unstressed state is a helical configuration that cannot be achieved because of the self-avoidance restriction, what are the possible equilibrium configurations in the absence of any external loading? More precisely, given an unstressed reference configuration $\hat{\mathbf{u}}$ in the forbidden region, and a convex strain-energy density function $W(\mathbf{u} - \hat{\mathbf{u}})$, what is the minimum energy accessible uniform helix? Because the actual unstressed configuration $\hat{\mathbf{u}}$ cannot be achieved without self-penetration, we may consider the expanding level sets of the convex function W. These level sets are nested convex surfaces all centered at the point $\hat{\mathbf{u}}$. Accordingly, there will be a unique point $\mathbf{u}_-^*$ in the lower cap at which there is a tangential level set, and $\mathbf{u}_-^*$ will by construction provide the smallest value of the strain energy among self-avoiding uniform helices with negative torsion.

It is to be expected that this energy-minimizing configuration also will be an equilibrium, which can be verified explicitly as follows. Because the constraint set boundary is a surface of rotation about the vertical axis, the projection of any of its surface normals onto the (u_1, u_2)-plane is necessarily radial. At any tangency point the constraint surface normal and the energy level set normal are necessarily parallel. Consequently, at the tangency point $\mathbf{u}_-^*$ the projection of $W/\mathbf{u}$ onto the (u_1, u_2)-plane is radial. In other words, $\mathbf{u}_-^*$ is a solution of Eq. **10**, which for uniform helices is known to be equivalent to the balance laws of Eq. **6**. Interestingly, and following the analysis of the previous section, we see that neither the pressure P between the two strands, or equivalently the tangential component of force $\boldsymbol{n}$, are fixed by this argument. Instead, one of them should be specified by a condition at infinity or, in a more sophisticated analysis, from a matching condition close to a boundary.

Similarly, there will be a unique tangency of an energy level set to the top constraint cap at a configuration $\mathbf{u}_+^*$ with positive torsion. Both $\mathbf{u}_+^*$ and $\mathbf{u}_-^*$ realize local minima of the strain-energy among accessible helices, and the one corresponding to the lower energy will be the global such minimum. The curvature, torsion, and register of the helical state $\mathbf{u}_+^*$ will in general all be different from those of $\mathbf{u}_-^*$, which is a phenomenon that can be observed in telephone handset chords that have been tangled to have regions of opposite handedness. In fact, even if the unstressed state $\hat{\mathbf{u}}$ is in the accessible region allowed by self-avoidance with, say, positive torsion, there will generically still be a tangency and a touching helical solution to the self-contact boundary of negative torsion helices. (The case where the tangency arises at the singular point $\mathbf{u} = \mathbf{0}$ must be considered separately.) Thus, we see that accounting for self-avoidance, helical rods with no external loading and convex strain-energy density can still have multiple local energy minimizers. In addition to telephone cords, this phenomenon is frequently observed in the tendrils of plants where regions of helical shapes of opposite-handedness (either in the presence or absence of external loading) are separated by a bridging segment called a perversion (43).

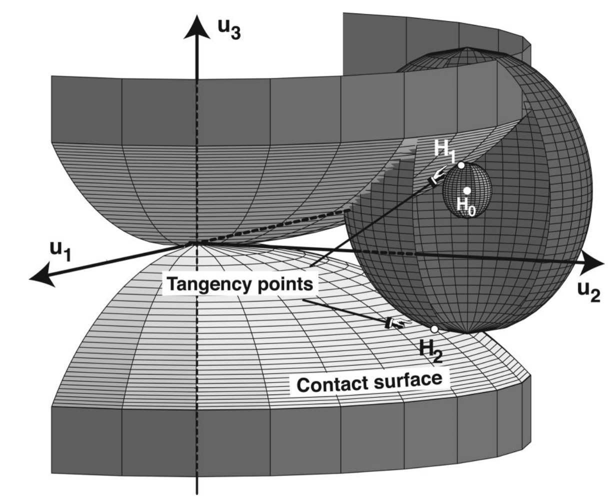

Fig. 4. The contact surface in **u**-space is obtained by rotating the curve in Fig. 3*A* around the vertical axis. Given an unstressed configuration in the forbidden region (due to self-penetration) represented by a point H_0, there exist two helices with self-contact and no external loading obtained by finding the tangency points of the contact surface with a level set of the energy $W_1 = C$ in the upper (right-handed) and lower (left-handed), half space. The two tangency points correspond to the solutions $H_{1,2}$ of Fig. 3.

Conclusions

We have presented a simple classification of all infinite, uniform helical equilibria of uniform, inextensible, unshearable, nonisotropic rods. The classification is entirely explicit in terms of simple quadrics in 3D strain space for the class of quadratic strain energies, which represent perhaps the most important case for many modeling applications. We also identified the rather surprising, and previously unobserved, possibility that nonisotropic rods may have equilibria with helical centerlines but nonuniform strains, albeit that these solutions are highly exceptional.

Whereas the classic theory of rods has mostly been explored assuming no nonlocal self-interaction, many helical filaments found in nature are either in contact with themselves or interact through nonlocal forces such as electrostatics. One problem is then to understand why helices persist in this more general context. As remarked here, and because of the discrete rotational symmetry of helices around any principal normal vector, any uniform, central self-interactions of an inextensible, unshearable rod can be balanced merely by appropriately modifying the tangential component of the force in a helical equilibrium without self-interaction. Consequently, our semi-inverse classification of all infinite uniform helical equilibria is essentially unaffected by the presence or absence of central, nonlocal self-interactions.

Central, nonlocal interactions include the case of a helix that is in self-contact, or in contact with multiple neighboring helices, or wound on a cylinder such as rods found in plies and cables (40). In this work, we discussed the particular case of a single self-avoiding helix in the absence of any external loading. In this problem, and with a single caveat, we concluded that there are always two helical equilibria, of opposite-handedness and at least one of which is in self-contact, that realize local minima of the strain energy subject to the self-avoidance constraint. The caveat concerns rods that have a level set of the strain energy that is tangent to the constraint set at the point $\mathbf{u} = \mathbf{0}$, in which case there may be a unique local minimum of the strain energy. Excluding this case is in some sense a genericity assumption. However, the exceptions include the case of rods with a straight unstressed state, i.e., $\hat{\mathbf{u}} = \mathbf{0}$, which is perhaps the single most studied case in rod mechanics.

Many questions remain open. For example, having in hand a complete semi-inverse classification of helical solutions of infinite length, it would be natural to attempt to construct solutions or approximate solutions to various finite boundary value problems. This process is in our opinion a nontrivial task, particularly so for problems with nonlocal interactions where our symmetry arguments certainly break down sufficiently close to the boundary. Similarly, it would certainly be of interest to better understand the stability properties of helical configurations in various senses, for example how sensitive is the dependence of helical equilibria to s-dependent perturbations in the material parameters of the rod, or what is the dependence of the solutions to changes in boundary conditions at one point. Studies of particular cases are certainly possible, but we are unaware of results in this direction that match the level of generality of our semi-inverse classification.

One natural notion of stability is to ask which among the constructed equilibria are actually local minima of the strain-energy under some admissible set of variations. Our construction of equilibria with self-contact means that we automatically find local minima, but the helical equilibria could merely be stationary points of the energy. To make this question precise, one must specify boundary conditions. One simple, yet general, observation is that if any rod equilibrium shape, including helices, is clamped at two points, i.e., the appropriate Dirichlet boundary conditions are imposed on both the centerline $\boldsymbol{r}(s)$ and directors $\{\boldsymbol{d}_i(s)\}$ at two points of arc lengths s_0 and s_1, then provided only that $|s_1 - s_0|$ is sufficiently small, i.e., the two clamping points are sufficiently close, the equilibrium will in fact be a local minimizer among variations respecting the boundary conditions. This conclusion is a standard result of the calculus of variations, and how close the points need to be can be determined on any particular equilibrium through a study of the conjugate points of the associated Jacobi fields. This approach is further discussed in the particular case of helical equilibria in ref. 47, but no simple and general conclusion was reached.

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