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THEORY OF SELF-CONTACT IN DNA MOLECULES
MODELED AS ELASTIC RODS

PREFACE

A DNA molecule contains two complementary polynucleotide strands joined together in a duplex structure, i.e., a Watson-Crick double helix. Each of the strands has a sugar-phosphate chain to which there are attached nucleotide bases of four types: A, T, C, G, with A complementary to T, and C complementary to G. The duplex structure forms when the bases on one strand bind to their complements on the other. The resulting base pairs are, in an approximate sense, flat, rigid, rectangular objects, which are stacked with their mid-planes separated by 3.4 Å and their centers on a curve called the *duplex axis*. In the form DNA assumes under conditions that mimic those in living cells, each base pair is approximately perpendicular to that axis and is rotated relative to its predecessor by circa 34°.

In a rough sketch, the DNA duplex structure appears as a tube with an approximate diameter of 20 Å and with two parallel indentations, called the major and minor grooves, which are helical with a pitch of circa 36 Å and a common axis coinciding with the duplex axis. The base pairs are in the interior of the tube, while the sugar-phosphate chains lie on its surface and constitute the material between the two helical grooves. The base pairs, or, equivalently, the bases on one of the two complementary strands, are the units of the genetic code.

A segment of DNA that is closed, in the sense that each strand forms a closed curve, is called a *plasmid*. A bacterium has no nucleus and its entire genome is in a single plasmid. A cell with a nucleus generally has about a meter of DNA in a nucleus that is less than 1 micron in diameter; this DNA is in chromosomes and is anchored at several sites in such a way that the segments between the sites are topologically equivalent to plasmids.

Throughout the life of a cell, its compacted DNA is in a state of rapid, yet controlled, activity. Regulation of life functions requires repeated transcription of

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appropriate portions of the genetic code into strands of RNA. Reproduction of the cell requires that the duplex structure of its DNA be unwound to permit replication of each of the two DNA strands. Moreover, in all species there occur processes of recombination in which the DNA is broken in a controlled way and rearranged.

The attainment of an understanding of the way in which highly compacted DNA is made available for the processes of transcription, replication, and recombination is, in part, a problem in theoretical mechanics. This becomes clear once one notes that the configuration, and hence the compaction, of a plasmid depends on a topological parameter, \mathcal{L} , defined as the Gauss linking number of two closed curves: (i) the duplex axis and (ii) an arbitrarily chosen one of the two strands that form the DNA double helix. Plasmids that have the same size and base-pair sequence, but differ in such topological properties as the knot type of the duplex axis and the linking number \mathcal{L} , are called *topoisomers*. The enzymes that convert one topoisomer into another are called *topoisomerases*. One such enzyme, called eukaryotic topoisomerase I, can bring a mixture of topoisomers into an equilibrium state in which the ratio of the concentrations of two topoisomers with different \mathcal{L} is given, in accord with the laws of chemical equilibrium, by a function of their free energy difference. Other topoisomerases are DNA gyrases that change \mathcal{L} only in one direction. (There are topoisomerases that change both linking number and knot type, but here we are primarily concerned with the dependence of the equilibrium

configurations of a plasmid and hence its accessibility as a function of its \mathcal{L} and knot type, with unknotted DNA an important special case.) The point

make is that changes in \mathcal{L} induced by topoisomerases cause changes in configurations and hence affect the accessibility of compacted DNA.

Thus the matter of relating equilibrium plasmid configurations and equilibrium linking number has become of importance. It is often treated using *elastic rod models* that are based on the assumption that for study of the mechanics of compacted DNA changes one can model a DNA segment of appropriate length as an elastic rod in the theory of Kirchhoff. In such a model, the rod axis \mathcal{C} is identified with the duplex axis and the vectors \mathbf{d} that are embedded in the rod's cross-sections and used to define twist density (as in equation (2) below) are identified with vectors normal to the duplex axis and point from that axis to the sugar-phosphate backbone of one of the two DNA strands.

In early attempts to employ elastic rod models to calculate the equilibrium configurations of DNA on \mathcal{L} a difficulty was encountered. The configurations of interest are "supercoiled configurations" in which the DNA makes contact with itself and, for even the simplest case of Kirchhoff's nonlinear theory of elastic rods, the problems of finding equilibrium configurations in which self-contact occurs and analyzing their stability were open. Much of the recent research on the mechanics of DNA supercoiling grew out of the need to understand the mechanics of DNA supercoiling.

Just as is the case for Signorini's problem in the linear theory of three-dimensional elastic bodies, the self-contact problem in non-linear rod

to a consideration of variational inequalities. As many major contributions to the development of the theory of variational inequalities in general, and to the formulation and resolution of Signorini's problem in particular, were made by Italian mathematicians, we have thought it not inappropriate to give here an overview of research on the self-contact problem for a class of elastic rods. Although rods of the type we consider are commonly employed as models for DNA molecules, for the remainder of this paper emphasis will be placed on the mathematical theory, rather than on its applications in molecular biology.

As he did in his talk at the Convegno, Coleman would like to mention here his 40 year old happy memory of the academic year that he spent at the University of Bologna, where he enjoyed the kind hospitality of Professor Dario Graffi and did his early research on the thermodynamics of materials with memory. During that year he followed the lectures of Professor Graffi and on occasion had a chance to discuss with him the mathematical topics of the day, among them the status and implications of research on Signorini's problem.

VARIATIONAL INEQUALITIES FOR EQUILIBRIUM CONFIGURATIONS OF IMPENETRABLE RODS

We here treat the self-contact problem for the case of an impenetrable rod of circular cross-section that is inextensible, homogeneous, intrinsically straight, and transversely isotropic in elastic response [1-3]. The configuration of a rod \mathcal{R} of that type is characterized by giving: (i) the *axial curve* \mathcal{C} , which is described by a function $\mathbf{x}(\cdot)$ with $\mathbf{x}(s)$ the spatial location of the material point on the rod axis with arc-length parameter s , and (ii) the *twist density* Ω , which is defined by the relation

$$(1) \quad \Omega = \Omega(s) = \mathbf{d}(s) \times \mathbf{d}'(s) \cdot \mathbf{t}(s), \quad 0 \leq s \leq L,$$

in which L is the length of \mathcal{C} , $\mathbf{t}(s) = \mathbf{x}'(s)$ is the unit tangent vector for \mathcal{C} at s , and $\mathbf{d}(s)$ is a unit vector imbedded in the cross-section of \mathcal{R} at s . If the rod is closed, i.e., is a ring or is modeling a DNA plasmid, then in each of its configurations, $\mathbf{x}(L) = \mathbf{x}(0)$, $\mathbf{t}(L) = \mathbf{t}(0)$, $\mathbf{d}(L) = \mathbf{d}(0)$.

We write Ω_0 for the twist density in a stress-free reference configuration of \mathcal{R} . For an arbitrary configuration, the total twist \mathcal{T} and the excess twist $\Delta\mathcal{T}$ (in turns) are

$$(2) \quad \mathcal{T} = \mathcal{T}(\Omega(\cdot)) = \frac{1}{2\pi} \int_0^L \Omega(s) ds, \quad \Delta\mathcal{T} = \frac{1}{2\pi} \int_0^L \Delta\Omega(s) ds,$$

where $\Delta\Omega = \Omega - \Omega_0$ is the *density of excess twist*. As we assume that \mathcal{R} is an inextensible, intrinsically straight, transversely isotropic rod obeying Kirchhoff's theory, its elastic energy Ψ is the sum of a bending energy that depends on the curvature κ of \mathcal{C} and a twisting energy that depends on $\Delta\Omega$:

$$(3) \quad \Psi = \Psi_B + \Psi_T, \quad \Psi_B = \frac{A}{2} \int_0^L \kappa(s)^2 ds, \quad \Psi_T = \frac{C}{2} \int_0^L \Delta\Omega(s)^2 ds.$$

Here, as we take the rod to be homogeneous, the coefficients of flexural and torsional rigidity, A and C , are constants. We further assume that (i) \mathcal{R} is impenetrable, (ii) cross-sections of \mathcal{R} are circular with uniform diameter D , and (iii) when self-contact occurs, the contact forces are frictionless reactive forces normal to the surface of \mathcal{R} .

A closed rod is subject to the constraint that all of its configurations give the same value to \mathcal{L} , the Gauss linking number for two closed curves: \mathcal{C} and the curve $\mathcal{C}^\#$ obtained by displacing each point $\mathbf{x}(s)$ of \mathcal{C} along $\mathbf{d}(s)$ by a fixed distance less than $D/2$. It follows from a result of White [4] and Calugareanu [5] that the integral topological constant \mathcal{L} obeys the relation

$$(4) \quad \mathcal{L} = \mathcal{W} + \mathcal{T}$$

in which \mathcal{W} , the *writhe* of the (closed) curve \mathcal{C} equals the average, over all orientations of a plane, of the sum of the signed self-crossings of the projection of \mathcal{C} on the plane [6]. Equivalent to equation (4) is the relation

$$(5) \quad \Delta\mathcal{L} = \mathcal{W} + \Delta\mathcal{T}$$

in which $\Delta\mathcal{L}$, called the *excess link* is, by definition, $\mathcal{L} - \mathcal{T}(\Omega_u(\cdot))$ and is a topological constant that need not be an integer.

Once end conditions are specified, a pair $(\mathcal{C}, \Delta\Omega)$ is called a *configuration* only if it obeys the constraints imposed on the rod (which include the assumption of impenetrability and the specified end conditions). A homotopy $\mathcal{H}: \eta \mapsto (\mathcal{C}_\eta, \Delta\Omega_\eta)$ of configurations is said to be *admissible* if it is compatible with the constraints and, in the case of a closed rod, the requirement that the value of $\Delta\mathcal{L}$ be preserved. The familiar definition of an *equilibrium configuration*, in which a configuration $(\mathcal{C}, \Delta\Omega)$ is said to be in equilibrium if, for each smooth admissible homotopy \mathcal{H} with a domain containing the point $\eta = 0$ in its interior and with

$$(6) \quad (\mathcal{C}_\eta, \Delta\Omega_\eta)|_{\eta=0} = (\mathcal{C}, \Delta\Omega),$$

there holds

$$(7) \quad \left. \frac{d}{d\eta} \Psi(\mathcal{C}_\eta, \Delta\Omega_\eta) \right|_{\eta=0} = 0,$$

is not appropriate when $(\mathcal{C}, \Delta\Omega)$ is a configuration in which the rod makes contact with itself. Such a configuration is in equilibrium if, for each admissible homotopy \mathcal{H} obeying (6) for which the domain is $0 \leq \eta < \varepsilon$, there holds

$$(8) \quad \left. \frac{d}{d\eta} \Psi(\mathcal{C}_\eta, \Delta\Omega_\eta) \right|_{\eta=0+} \geq 0.$$

When $(\mathcal{C}, \Delta\Omega)$ is in equilibrium according to this criterion, (7) holds for those homotopies that can be smoothly extended from $0 \leq \eta < \varepsilon$ to $-\varepsilon < \eta < \varepsilon$.

To have an illustration of this theory of impenetrable rods let us consider the case of a closed rod \mathcal{R} of length L . The excess link $\Delta\mathcal{L}$, which obeys equation (5), is

a natural measure of the amount that the rod was pre-twisted before it was closed to form a ring. For each value of $\Delta\mathcal{L}$ there will be an equilibrium configuration for which

\mathcal{C} is a circle and hence $\mathcal{W} = 0$ in (5). For $\Delta\mathcal{L}$ sufficiently large, there will be equilibrium configurations with $\mathcal{W} \neq 0$ in which the ring makes contact with itself. At a point of self-contact, say, that at which the cross-section with $s = s^*$ touches the cross-section with $s = s^{**} \neq s^*$, there holds

$$(9) \quad |\mathbf{x}(s^*) - \mathbf{x}(s^{**})| = D, \quad \mathbf{t}(s^*) \cdot (\mathbf{x}(s^*) - \mathbf{x}(s^{**})) = 0.$$

We shall here confine attention to cases in which a given cross-section is in contact with at most one other. As we assume that the contact force, \mathbf{f}^* (i.e., the force exerted on the cross-section at s^* by that at s^{**}) is a reactive force that is frictionless (and hence normal to the surface of the rod at $s = s^*$), we have

$$(10) \quad \mathbf{f}^* = f^* \frac{\mathbf{x}(s^*) - \mathbf{x}(s^{**})}{D}.$$

It can be shown that our present definition of equilibrium with Ψ as in (3) implies that throughout intervals of values of s corresponding to contact-free subsegments, there hold the equations,

$$(11) \quad \mathbf{F}' = \mathbf{0}, \quad \mathbf{M}' = \mathbf{F} \times \mathbf{t},$$

in which $\mathbf{M}(s)$, the resultant of moments of the internal forces acting on a cross-section, is given by

$$(12) \quad \mathbf{M} = A\mathbf{t} \times \mathbf{t}' + C\Delta\Omega\mathbf{t},$$

and $\mathbf{F}(s)$, the resultant of the internal forces, is a reactive force not given by a constitutive relation. In an early work on the subject, Kirchhoff [7] observed that equations (11) and (12) are mathematically equivalent to Euler's equations for the motion of a symmetric top, a fact which has been employed in research on DNA configurations [8, 9]. It is known that use of a particular cylindrical coordinate system greatly simplifies the problem of obtaining an exact and explicit expression for a contact-free configuration of a rod segment obeying (3).⁽¹⁾

Contact can occur at isolated points or along contact curves. If s^* is an isolated value or an endpoint of an interval \mathcal{J} of values of s characterizing contact points, \mathbf{f}^* , the contact force at s^* , is a concentrated force, and balance of forces and moments yields

$$(13) \quad \mathbf{F}(s^* + 0) - \mathbf{F}(s^* - 0) + \mathbf{f}^* = \mathbf{0}, \quad \mathbf{M}(s^* + 0) - \mathbf{M}(s^* - 0) = \mathbf{0}.$$

In the interior of \mathcal{J} the contact force has a continuous density \mathbf{f} , equation (12) holds, and in place of (11) one has

$$(14) \quad \mathbf{F}'(s^*) + \mathbf{f}(s^*) = \mathbf{0}, \quad \mathbf{M}'(s^*) = \mathbf{F}(s^*) \times \mathbf{t}(s^*),$$

⁽¹⁾ See, e.g., references [10–12].

with \mathbf{M} and \mathbf{F} again smooth functions of s . The relations (13) and (14), like (11), are consequences of (8) and (3).

In a contact-free subsegment, the equations (11), with \mathbf{M} as in (12), are a system of differential equations for \mathcal{C} and $\Delta\Omega$ with solutions that can be expressed in terms of elliptic functions (and integrals) and 6 parameters [3, 12].

In cases in which \mathcal{R} contains a pair of subsegments \mathcal{R}^* , \mathcal{R}^{**} that meet at a contact curve c , the relations (14) hold in the interior of the interval of values of s corresponding to the axial curve \mathcal{C}^* of \mathcal{R}^* . If for one of these values of s we write $\mathbf{v}(s^*)$ for the unit vector along the line connecting the centroids of two cross-sections in contact and $\mathbf{u}(s^*)$ for the unit tangent vector for c and put $\mathbf{w} = \mathbf{u} \times \mathbf{v}$, then μ in the equation

$$(15) \quad \mathbf{t}(s^*) = \mathbf{u}(s^*) \cos \mu(s^*) - \mathbf{w}(s^*) \sin \mu(s^*)$$

is the *angle of winding* of \mathcal{C}^* about c . There are cases which one can combine this last equation with equations (9), (10), (12), and (14) to obtain a tractable differential equation for μ .

When c is a straight line, as is the case for contact curves in knot-free closed rods, \mathbf{u} is independent of s , and the differential equation for μ , which then takes the form [3]

$$(16) \quad \mu'' = \frac{8}{D^2} \sin^3 \mu \cos \mu + \frac{2C\Delta\Omega}{AD} \cos 2\mu,$$

has a solution,

$$(17) \quad \mu(s^*) = \operatorname{arc\,cot} \left(\frac{q \cot \mu_0 - p \tan^2(\operatorname{sn}((s^* - s_0)\sqrt{pq})/2) \cot \mu_1}{q - p \tan^2(\operatorname{sn}((s^* - s_0)\sqrt{pq})/2)} \right),$$

in which p, q , and the modulus of the elliptic function sn are functions of the constants $D, C/A, \mu_0, \Delta\Omega$, where μ_0 is the value of μ at a point where $\mu' = 0$. Thus, the configurations of the subsegments \mathcal{R}^* and \mathcal{R}^{**} can be expressed in terms of elliptic functions and 4 solution parameters, which are $\mu_0, \Delta\Omega$, and the arc-length coordinates of the endpoints of \mathcal{C}^* .

If \mathcal{R} has n isolated points and m straight contact curves, it has $2(n + m)$ contact-free subsegments and its configuration is determined when $12n + 16m$ solution parameters are specified. The equations (9), (10), and (13), the requirement that appropriate functions of s have period L , and the condition that $\Delta\mathcal{L}$ have its preassigned value yield $12n + 16m$ algebraic equations that can be solved for the $12n + 16m$ solution parameters [1-3]. Thus one obtains, for equilibrium configurations in which self-contact occurs at isolated points and intervals, (i) a value of $\Delta\Omega$ (which turns out to be constant throughout \mathcal{R}), (ii) a precise analytic representation for \mathcal{C} , and (iii) the value of \mathbf{f}^* at each contact point. It follows from (8) that in order for a solution of the equations (9)-(14) to correspond to an equilibrium configuration it must be such that when two cross-sections, at s^* and s^{**} , are in contact, \mathbf{f}^* in (10) is not negative; i.e., \mathbf{f}^* , if not zero, tends to push apart cross-sections in contact.

In the present theory, a configuration $(\mathcal{C}, \Delta\Omega)$ of a rod \mathcal{R} subject to appropriate end conditions is said to be *stable* if it gives a strict local minimum to Ψ in the class of configurations compatible with the imposed constraints. In other words, $(\mathcal{C}, \Delta\Omega)$ is stable when, for an appropriate topology, it has a neighborhood \mathcal{N} such that $\Psi(\mathcal{C}^\#, \Delta\Omega^\#) > \Psi(\mathcal{C}, \Delta\Omega)$ for each configuration $(\mathcal{C}^\#, \Delta\Omega^\#)$ in \mathcal{N} that is not equivalent⁽²⁾ to $(\mathcal{C}, \Delta\Omega)$ and, in addition, is accessible from $(\mathcal{C}, \Delta\Omega)$ by an admissible homotopy \mathcal{H} .

A configuration $(\mathcal{C}, \Delta\Omega)$ is *differentially stable*, if, for each admissible homotopy \mathcal{H} with domain $0 \leq \eta < \varepsilon$ and obeying (6), either

$$(18a) \quad \left. \frac{d}{d\eta} \Psi(\mathcal{C}_\eta, \Delta\Omega_\eta) \right|_{\eta=0+} > 0$$

or

$$(18b) \quad \left. \frac{d}{d\eta} \Psi(\mathcal{C}_\eta, \Delta\Omega_\eta) \right|_{\eta=0+} = 0 \quad \text{and} \quad \left. \frac{d^2}{d\eta^2} \Psi(\mathcal{C}_\eta, \Delta\Omega_\eta) \right|_{\eta=0+} \geq 0.$$

(A differentially stable configuration obeys (8) and hence is in equilibrium.)

Tobias, Swigon, and Coleman showed [1] that if $(\mathcal{C}, \Delta\Omega)$ is a member of a one-parameter family E of equilibrium configurations for which $\Delta\mathcal{L}$ is a function of \mathcal{W} (as in Figures 1 and 2 below), then: *in order for $(\mathcal{C}, \Delta\Omega)$ to be stable it is necessary that, for the family E , the slope of the graph of $\Delta\mathcal{L}$ versus \mathcal{W} , i.e., $d\Delta\mathcal{L}^E/d\mathcal{W}$, be not negative at $(\mathcal{C}, \Delta\Omega)$.* This condition, called “condition E”, is necessary but not sufficient for even differential stability.

A sufficient condition for stability of $(\mathcal{C}, \Delta\Omega)$, called “condition S”, is given in the following proposition [1]:

If for an equilibrium configuration $(\mathcal{C}, \Delta\Omega)$ in E , $d\Delta\mathcal{L}^E/d\mathcal{W} > 0$ at $(\mathcal{C}, \Delta\Omega)$ and, in addition, $(\mathcal{C}, \Delta\Omega)$ has a neighborhood \mathcal{N} such that, for each configuration $(\mathcal{C}^E, \Delta\Omega^E)$ in \mathcal{N} and E , there holds $\Psi_B(\mathcal{C}^\#) > \Psi_B(\mathcal{C}^E)$ for every accessible configuration in \mathcal{N} for which $\mathcal{C}^\#$ has the same writhe as, but is not congruent to, \mathcal{C}^E , then $(\mathcal{C}, \Delta\Omega)$ is stable.

This proposition enables one to determine the stability of a configuration that gives a global minimum to Ψ_B in the class of configurations with the same writhe.

For families of configurations that are not global minimizers of bending energy, the determination of stability is a more difficult matter. The following proposition, proven in reference [1], gives a necessary condition for stability, called “condition θ ”, that is stronger than condition E:

⁽²⁾Two configurations, $(\mathcal{C}^\#, \Delta\Omega^\#)$ and $(\mathcal{C}, \Delta\Omega)$, are equivalent if they have congruent axial curves and equal distributions of excess twist density.

For each ξ with $0 < \xi \leq L$, let $\theta(\xi)$ be the minimum value of $d\Delta\mathcal{L}/d\mathcal{W}$ at $(\mathcal{C}, \Delta\Omega)$ over the families of equilibrium configurations of \mathcal{R} that obey the added imposed constraint that the subsegment of \mathcal{R} with $\xi \leq s < L$ be held rigid. In order that an equilibrium configuration $(\mathcal{C}, \Delta\Omega)$ be stable, it is necessary that $\theta(\xi) \geq 0$ for each ξ , $0 < \xi \leq L$.

For equilibrium configurations with available explicit analytic representations, it is not difficult to determine whether condition θ holds.

The present authors have recently employed the well developed theory of conjugate point criteria for the stability of solutions of ordinary differential equations (cf., Manning, Rogers, & Maddocks [13]) to show that fulfillment of condition θ is sufficient for differential stability of a contact-free configuration and are currently working on an extension of that result to configurations with self-contact.

EXAMPLES OF CONFIGURATIONS AND BIFURCATION DIAGRAMS FOR CLOSED RODS

Recent research [1, 2] has shown that for discussion of stability it is useful to draw bifurcation diagrams as plots of $\Delta\mathcal{L}$ versus \mathcal{W} . Precise calculation of \mathcal{W} by numerical evaluation of its representation as a double integral over \mathcal{C} is notoriously difficult. In the present case, however, one can obtain an analytic representation for the integral along \mathcal{C} of the geometric torsion, and make use of the fact that \mathcal{W} plus the torsion integral is an integer, called the *self-link* of \mathcal{C} [5, 14], which, in practical cases, is not difficult to evaluate [12].

Figures 1 and 2 contain examples of bifurcation diagrams for a closed, knot-free, rod with $C/A = 2/3$ and with $L/D = 122$. The value used for C/A is appropriate to a rod (of circular cross-section) formed from a material that is isotropic and incompressible. It is also at the lower end of the range of values of C/A proposed for DNA molecules in solution. The chosen value of L/D corresponds to a DNA molecule with $D = 20 \text{ \AA}$ that has 718 nucleotides in each of its two strands. Here, for configurations on the trivial branch ζ , i.e., the branch for which \mathcal{C} is independent of $\Delta\mathcal{L}$, \mathcal{C} is a circle and hence $\mathcal{W} = 0$. Each point of ζ with

$$(19) \quad \Delta\mathcal{L} = (A/C)\sqrt{m^2 - 1}, \quad m = 2, 3, \dots,$$

is a bifurcation point at which a primary branch with $\mathcal{W} \neq 0$ originates. The primary branches with $m = 2, 3$, etc. are referred to as branch α , branch β , etc. In reference 2 it was observed that for each $m \geq 2$ the symmetry group of configurations in the primary branch with index m is the dihedral group D_m (which has order $2m$). Hence, whether or not self-contact is present, the curve \mathcal{C} for a configuration on the primary branch of index m has a single m -fold symmetry axis that is perpendicular to the plane \mathcal{P} containing the $2m$ points at which the curvature κ of \mathcal{C} has a local extremum.

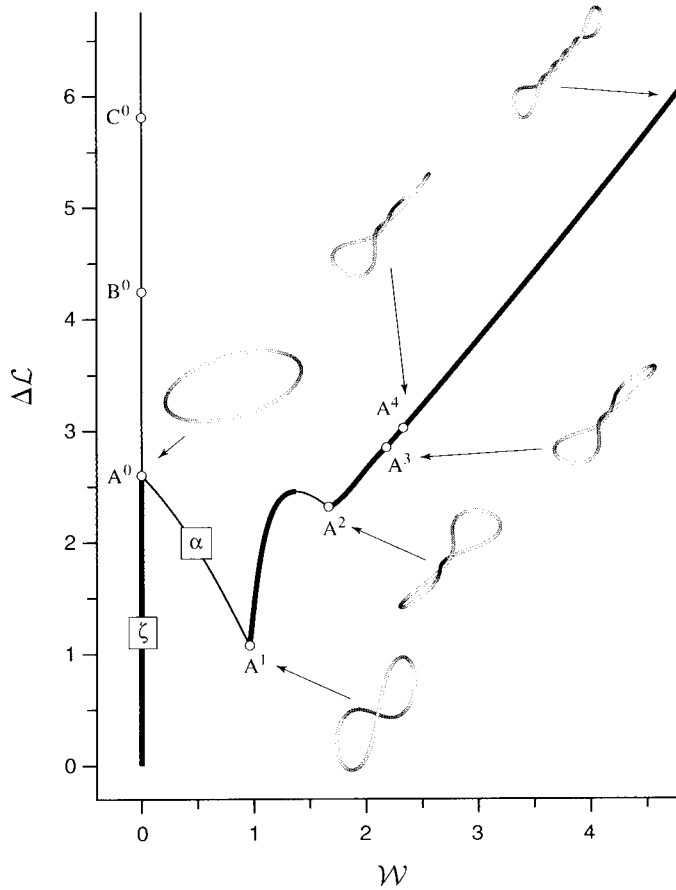


Fig. 1. — Graphs of excess link, $\Delta\mathcal{L}$, versus writhe, \mathcal{W} , for the primary branch α . For $n = 0, 1, 2, 3$, the configurations with n points of self-contact correspond to points between A^n and A^{n+1} . At values of $\Delta\mathcal{L}$ greater than that at A^4 , the configurations have an interval and two isolated points of self-contact (which are indiscernible at this scale of drawing); in the example shown of such a configuration, $\Delta\mathcal{L} = 6$. Families of stable configurations are shown as heavy curves. The configuration A^1 has been called the “figure-8 configuration”; those with $\mathcal{W} > \mathcal{W}(A^1)$ are said to be “plectonemically supercoiled”. At the points on branch ζ labeled A^0, B^0, \dots , the parameter $\Delta\mathcal{L}$ obeys equation (19).

Each of the m lines that intersect the m -fold symmetry axis and pass through 2 extrema of κ is a 2-fold symmetry axis.⁽³⁾

In reference 3 we show that a closed rod can have families of equilibrium configurations that are not on primary, secondary, or higher order branches, i.e., that are isolas in the sense that they are not connected to the trivial branch by a

⁽³⁾ For closed rods obeying the present assumptions, Domokos [15] proved that each contact-free equilibrium configuration has D_m symmetry, which is what was found in the present study. In the same paper he has conjectured that the symmetry group of an equilibrium configuration with self-contact contains C_2 as a subgroup, which is not the case for configurations on the tertiary branch β_{11}^* .

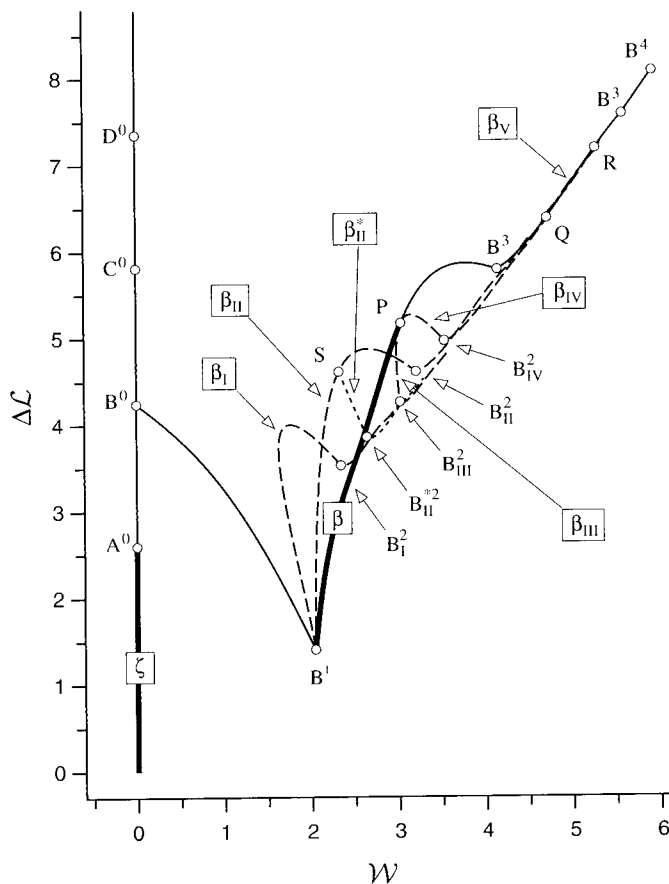


Fig. 2. — Graphs of $\Delta\mathcal{L}$ versus \mathcal{W} for the primary branch β (solid curve), the secondary branches, $\beta_I, \beta_{II}, \beta_{III}, \beta_{IV}$, (drawn with long dashes) originating at β , and the tertiary branch β_{II}^* (short dashes) originating at β_{II} . Configurations corresponding to selected labeled points are shown in Figure 3. The points B^0, B^1, P, Q, R are bifurcation points for β , S is a bifurcation point for β_{II} . For $n = 0, 1, 2, 3$, the configurations on branch β with $3n$ points of self-contact correspond to points between B^n and B^{n+1} . Not visible at this scale of drawing is a closed secondary branch β_V that meets β at the bifurcation points Q and R .

continuous path of equilibrium configurations that obey the constraints arising from impenetrability.

The configurations in the interior of intervals of regions of branch α that are drawn as heavy curves in Figure 1 obey condition S and hence are stable. As condition E does not hold on the intervals of branch α that are there drawn as light curves, the configurations in those intervals are not stable.

In Figure 2 one sees the primary branch β , the secondary branches that originate at points on β , and the tertiary branch β_{II}^* . On those branches, condition θ holds only for the configurations in the heavily drawn interval of branch β that runs from the bifurcation point B^1 to the bifurcation point P . No other configurations in those branches can be stable.

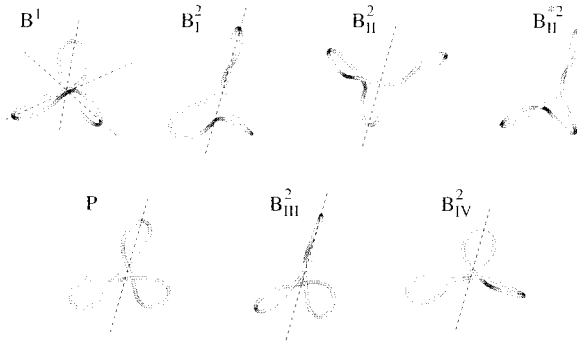


Fig. 3. — Selected configurations: B^1 and P are on branch β ; B_I^2 , B_{II}^2 , B_{III}^2 , B_{IV}^2 are on the secondary branches β_I , β_{II} , β_{III} , β_{IV} , respectively; B_{II}^{2*} is on the tertiary branch β_{II}^* . The configurations on branch β have D_2 symmetry; those on the secondary branches β_I – β_{IV} have C_2 symmetry; those on the tertiary branch β_{II}^* have no discernible symmetry. Here, and in Figure 5, axes of two-fold symmetry are shown as dashed curves.

The bifurcation diagrams presented here and in references 1-3 are the first that have been obtained for impenetrable rods with nonzero cross-sectional diameter in a range of parameters in which self-contact occurs. After investigations by Le Bret [9] and Jülicher [16] of configurations with self-contact in the theory of impenetrable closed rods with zero cross-sectional diameter, investigators used approximate methods [17] to calculate, for rods of nonzero diameter, configurations in which lines of contact are present; those methods did not yield bifurcation diagrams or reveal such general features of self-contact as the following: when changes in $\Delta\mathcal{L}$ result in first 1 and then 2 isolated points of self-contact in a lobe, further change results in 3 isolated points and then a mixture of intervals and isolated points of self-contact.

Equation (17) was employed to calculate configurations on branch α with $\Delta\mathcal{L}$ and \mathcal{W} greater than their values at A^4 . The dependence on \mathcal{W} of the arc-length locations of the cross-sections that are in contact is shown in Figure 4, which illustrates the general observation that configurations on branch α with $\mathcal{W} > \mathcal{W}(A^4)$ have not only a contact line but also two isolated points of self-contact. These and other recent results [2, 3] show that, when impenetrability is taken into account, the equilibrium behavior of transversely isotropic rods of non-zero cross-sectional diameter is far more complex than one would anticipate, even though each equilibrium configuration of such a rod has an explicit representation.

For knotted closed rods one can find cases in which a contact curve c is not straight. We have obtained preliminary results for a closed rod for which the axial curve \mathcal{C} has the topology of a torus knot $(2, q)$, i.e., can be placed on the surface of a torus in such a way that, without intersecting itself, it cuts each meridian twice and each longitude q -times. For such a rod there is an interval \mathcal{J} of values of $\Delta\mathcal{L}$ for which the minimum energy configuration has a closed contact curve c that touches each cross-section and differs from a circle by terms that are $O((D/L)^2)$. Once c is taken to be a circle, the equations (9), (10), (12), (14), and (15) yield a differential equa-

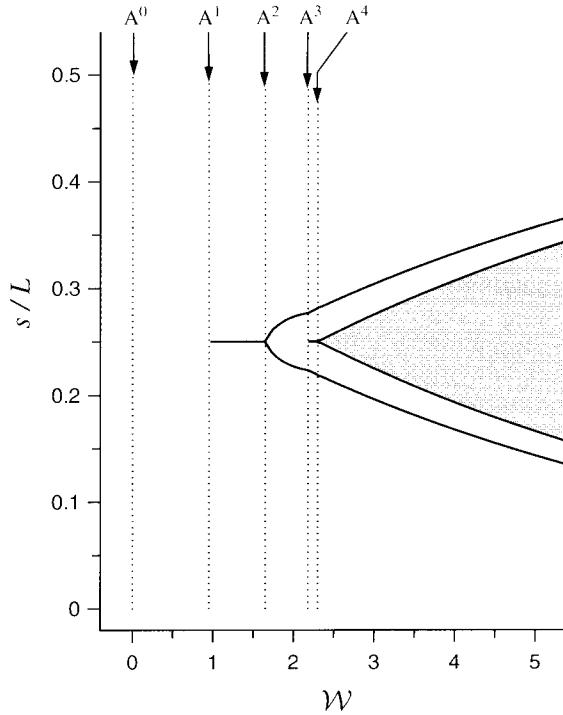


Fig. 4. — Dependence on W of the arc-length locations of cross-sections that are in contact when the configuration is on branch α . As these configurations have D_2 symmetry, results are shown only for $0 < s/L < 1/2$. The shaded area gives for each W the range of s/L that corresponds to the line of contact; the solid curves give s/L for isolated points of self-contact and endpoints of the line of contact.

tion for μ that is presently under study. For the case in which $q = 3$, i.e., in which \mathcal{C} is a trefoil knot, when $\Delta\mathcal{L}$ is away from \mathcal{J} , equilibrium configurations (including the minimum energy configuration) have analytic representations, for their contact points are either isolated or on straight contact lines (see Figure 5.) The goal of our study of knotted elastic rings is to arrive at a point where one can construct bifurcation diagrams for broad classes of knot types. The complexity of the problems to be faced

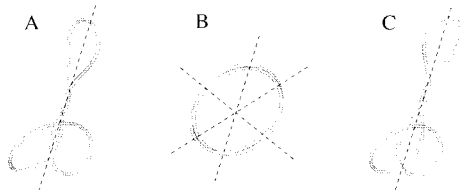


Fig. 5. — Minimum energy configurations of a knotted closed rod with trefoil topology and the following values of $\Delta\mathcal{L}$: for A, $\Delta\mathcal{L} = -5.879$; for B, $\Delta\mathcal{L} = -3.002$; for C, $\Delta\mathcal{L} = -0.568$. Here $C/A = 1.4$ and $L/D = 170$. Configurations A and C have only isolated contact points and were calculated using their analytic representations. Configuration B has $\Delta\mathcal{L}$ in \mathcal{J} and was calculated by numerical solution of the differential equation obeyed by μ when c is a circle; this configuration gives a global minimum to Ψ as $\Delta\mathcal{L}$ is varied and hence minimizes Ψ_B .

is indicated by the following considerations: (i) Bifurcation diagrams for knotted closed rods are not expected to have trivial branches. (ii) Low energy configurations of knotted rods can have self-contact with properties other than those normally considered, e.g., one cross-section can be in contact with two or more others, and such is expected to be the case for torus knots $(3, q)$.

It is expected that if one finds general rules in this complex field, one will be in a better position to address certain outstanding problems in molecular biophysics, such as that of understanding the mechanism of action of recombinases and type II topoisomerases which change the knot structure of DNA molecules.

OPEN RODS WITH SELF-CONTACT

There is a large literature dealing with the buckling of a straight rod subject to terminal forces and torques. (See, e.g., the expositions of Love [18] (Chap. XIX, §272), Antman [19] (Chap. IX, §5), and Antman & Kenney [20]). Nearly all of that literature is concerned with the determination of buckling points and calculation of contact-free configurations. Despite its importance in ocean engineering⁽⁴⁾ and the molecular biology of DNA⁽⁵⁾, the study of the problem of calculating equilibrium configurations and determining bifurcation diagrams for cases in which buckling under tension and torque leads to self-contact is in its early stages.

For impenetrable rods of circular cross-section obeying equations (9)-(14), the methods we have described here for obtaining exact analytic solutions of the governing equations and investigating their stability can be extended to cases in which the rod is open and subject to various types of end conditions, including those in which the applied twisting and tension are specified. Such a rod can contain plectonemic loops with isolated points and intervals of self-contact.

An example is shown in Figure 6, where Λ is the measure of twisting defined by the relation,

$$\Lambda = (\chi(L) - \chi(0) + \mu)/2\pi, \quad (20)$$

in which χ is the (oriented) angle between \mathbf{d} and $\mathbf{t} \times \mathbf{F}$, and μ is the dihedral angle between the planes perpendicular to $\mathbf{t}(0) \times \mathbf{F}$ and $\mathbf{F} \times \mathbf{t}(L)$. The loops shown are called plectonemic loops, or “plectonemes”, when they contain one or more points of self-contact (i.e., \mathcal{W} is greater than its value at A^1). The plectonemes with $\mathcal{W} > \mathcal{W}(A^1)$ show not only contact lines along which (17) holds, but also isolated contact points⁽⁶⁾.

⁽⁴⁾The formation of plectonemic loops can result in a damage to pipelines and undersea cables (including jacketed optical fibers); for references see Thompson & Champneys [21].

⁽⁵⁾Particularly for the interpretation of single-molecule torsion-stretching experiments (cf., reference 22).

⁽⁶⁾The published approximate calculations of plectonemic loops [17] do not reveal, as does the present exact theory, this simultaneous occurrence of intervals and isolated points of self-contact.

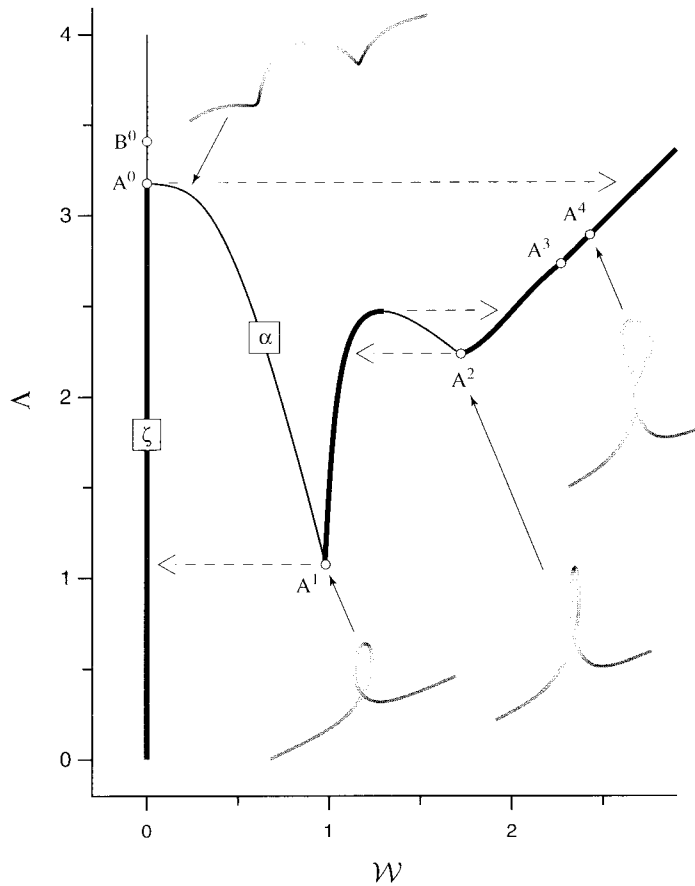


Fig. 6. — The trivial branch ζ and the primary branch α of the bifurcation diagram for an open rod subject to specified twisting Λ and a fixed tensile force F . Here $C/A=1.4$, $L/D = 170$, and $FL^2/A = 185$. As in Figure 1, for $n = 0, 1, 2, 3$, the configurations with n points of self-contact correspond to points between A^n and A^{n+1} . Configurations with $\Lambda > \Lambda(A^4)$ have an interval and isolated points of self-contact. The heavy curves denote families of stable configurations, and the dashed arrows indicate the hysteresis predicted for cycles of Λ .

Calculations have been made of configurations on bifurcation branches other than α , such as the branch β which originates at the point B^0 and the secondary and higher order branches that issue from it [23]. Studies of this type are expected to be useful in interpretation of hysteresis observed in torsion-stretching experiments on stiff rod-like molecules such as DNA.

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