The Kirchhoff elastic rod, the nonlinear Schrödinger equation, and DNA supercoiling

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We have derived a time-independent, one-dimensional nonlinear Schrödinger equation for the stationary state configurations of supercoiled DNA. The effect of DNA self-contact has been included analytically. For the cases of non-self-contact and periodic boundary conditions, closed-form solutions have been obtained which describe the stationary state configurations of supercoiled DNA.

I. INTRODUCTION

The mathematics of elastic rods has been studied for over two centuries since the days of Daniel Bernoulli and Euler in the 1730's. In 1859 Kirchhoff discovered that the equations that describe the thin elastic rod in equilibrium are mathematically identical to those used to describe the dynamics of the heavy top. The problem of the heavy symmetric top (now known as the Lagrange top) was solved exactly by Lagrange in 1788.

Although it was very successful, Kirchhoff's analogy only solved the initial value problem of the thin symmetric rod in equilibrium, but not the boundary value problem where the Cartesian coordinates are specified at both ends and the direction of the force in the rod is unknown. Besides the boundary value problem, stability and bifurcation problems have been and continue to be of considerable interest to many people. The literature of elasticity theory has also moved on to more sophisticated integrable (or nonintegrable) models that describe effects of shear and compression as well as bend and twist etc.

Because the thin elastic rod is often used as a model for the DNA molecule, there has been a recent resurgence of interest in applying the theory for the Kirchhoff elastic rod to the phenomenon of DNA supercoiling. In particular, the mathematics of closed DNA molecules with a linking number deficit or excess, $\Delta L_k$, has become important. According to the rules of topology, such a linking number deficit or excess must manifest itself as a combination of writhe of the axis of the DNA duplex helix as a space curve, $W_r$, and twist excess or deficit of the DNA duplex helix, $\Delta T_w$. In vivo, DNA is always found with an average linking number deficit of $-0.05$ turns per turn of DNA duplex helix. This linking number deficit is very important in reducing the number of configurational states allowed to DNA in nature, resulting in a substantial reduction of the volume occupied by the genetic carrier in vivo. The low entropic state is nevertheless capable of conformational transitions which are suspected of being important in gene regulation and cell cycle dynamics. It is thus essential that an appropriate mathematics be developed to model the high linking number deficit states of DNA.

A variety of techniques has been used to model these systems, including Monte Carlo calculations, finite element analysis, Euler angle method, while providing numerical solutions, lack parametric closed solutions for most of the interesting physical properties. Little physical insight and expendability are provided by these techniques.

Euler angle method provides a method for writing down differential equations describing such systems. These equations are usually highly nonlinear, in terms of Euler angles $[\theta(s), \phi(s), \psi(s)]$, and thus closed solutions to these equations have been elusive. In this manuscript, we demonstrate that focusing on curvature $\kappa(s)$ and geometric torsion $\tau(s)$, as opposed to focusing on the Euler angles $[\theta(s), \phi(s), \psi(s)]$, leads to well known differential equations with known solutions for the simplest cases. It is likely that this insight will provide a path to the solutions of the more difficult problems as well.

Organization and scope. In Sec. II we begin with a brief classical overview of the equilibrium equations of a thin elastic rod in a stationary state. We also discuss the two approaches that can be used in solving the equilibrium equations; the conventional Euler angle approach and the curvature-torsion approach.

In Sec. III we present a derivation of the time-independent one-dimensional nonlinear Schrödinger equation which can be used to describe the stationary states of the supercoiled DNA. The DNA self-contact effect has been included analytically by introducing an extra potential term in the equation.

In Sec. IV we present the closed-form solutions of the coordinates of DNA in cylindrical coordinates for the cases of non-self-contact. The methods described in Sec. IV also provide the closed-form expressions for the configurational energies, $U_{\text{bend}}$ and $U_{\text{twist}}$. The more complex cases of chains with self-contact will be considered in a future manuscript.

In Sec. V we limit ourselves to the case of toroidal helices where the closed DNA wraps periodically around a torus (doughnut). We also obtain the closed mathematical expressions for the writhe number $W_r$ and twist number $T_w$ of the toroidal helix. Other special solutions of Sec. IV, e.g., the helix-on-a-linear-helix, and the knotted toroidal helix, will be considered in manuscripts which will follow this work shortly.
II. STRATEGY FOR SOLVING THE EQUILIBRIUM EQUATIONS

A. Equilibrium equations

We treat the DNA duplex as an inextensible and unshearable thin elastic rod with circular cross section, characterized by a twist constant, C, a bending constant, A, and a radius of cross section, r_{DNA}. Here and elsewhere in this manuscript "DNA" and "rod" have the same meaning, as do "centerline of the rod" and "axis of DNA."

At each point s on the centerline, R(s), of the thin rod, a localized Cartesian coordinate frame (rod frame) \{e_1(s), e_2(s), e_3(s)\} is affixed with e_3(s)=\hat{e}_3(s) (the unit tangent vector) and with e_1(s) and e_2(s) in the directions of principal axes of inertia of its cross section. The variable, s, is a contour parameter analogous to time for the Lagrange (heavy symmetric) top. The localized coordinate frame at s+\Delta s is obtained by an infinitesimal rotation \Delta \Theta of the coordinate frame at s. The deformed state of the axis of the thin rod is determined by the curvature vector \omega(s) = (\omega_1, \omega_2, \omega_3) = \lim (\Delta \Theta/\Delta s)\), which is analogous to the angular velocity of the Lagrange top.

At a given position (say, s=s_0) along the centerline, there is a cross section upon which internal forces are exerted. One side of the cross section (s<s_0) acts on the other side (s>s_0) and vice versa. The internal forces are resolvable into a force F(s_0) and a torque M(s_0). At each cross section such a force and torque may be found, giving rise to functions F(s) and M(s) describing a system of stresses on the rod. The force, F, is analogous to gravity in the Lagrange top problem, whereas the torque, M, is analogous to the angular momentum. For a recent complete comparison of the thin elastic rod and the Lagrange top, see Table I of Ref. 5(a).

If \textit{F}^{(e)}(s) and \textit{M}^{(e)}(s) are the externally applied force and torque per unit length, then the stationary state conditions, in the body fixed frame (or rod frame or material frame), are\textsuperscript{11}

\[ \text{\textit{F}}(s) + \omega(s) \times \text{\textit{F}}(s) + \text{\textit{F}}^{(e)}(s) = 0, \quad (2.1a) \]
\[ \text{\textit{M}}(s) + \omega(s) \times \text{\textit{M}}(s) + \text{\textit{t}}(s) \times \text{\textit{F}}(s) + \text{\textit{M}}^{(e)}(s) = 0, \quad (2.1b) \]

where dot means the derivative with respect to contour parameter s and \textit{t}(s) is a unit vector along the centerline. The case [\textit{F}, \textit{F}^{(e)}]=\{0,0,0\} is analogous to that of a freely spinning top.

Since the force, F, will be shown to directly relate to the change of curvature and (geometric) torsion but not to the Cartesian coordinates \{x,y,z\} of the centerline of the rod in the space-fixed frame (or lab frame, or inertial frame), F=0 can be used to describe the centerline of the rod of uniform curvature and zero torsion such as a closed circle in the x-y plane. F=0 can also be used to describe the centerline of the rod of uniform curvature and nonzero constant torsion such as a linear helix, where the nonzero constant torsion gives rise to the linear translation of the centerline of the rod in the z direction. We should point out that not all circle and linear helix solutions are corresponding to F=0. In Appendix A we shall analyze the solutions of constant curvature and constant torsion and nonzero twist that associate with F\neq 0.

For small deformations local of the thin rod, the torque \textit{M}(s) is related to the curvature vector \omega(s) by linear constitutive relation (Hooke's law).

\[ \text{\textit{M}}(s) = I \left[ (\omega(s) - \omega^{(0)}) \right], \quad (2.2) \]

where I denotes the stiffness tensor of the thin rod and is diagonal in the rod frame, namely, I=AE_1 e_1+AE_2 e_2+C e_3 e_3. The \omega^{(0)}=\omega_3^{(0)} e_3 is the intrinsic constant curvature vector expressed in the rod frame. In other words, the relaxed state of DNA is assumed to be straight but is twisted by \omega_3^{(0)} radian per unit length. (The DNA duplex helix contains 10.4 base pairs per turn for which \omega_3^{(0)}=0.178 rad/nm.)

B. The choice between two approaches: Euler angles vs curvature and torsion

In the absence of an intrinsic constant curvature and external force and torque, i.e. \{\omega^{(0)}, \textit{F}^{(e)}(s), \textit{M}^{(e)}(s)\}=(0,0,0), system (2.1) is dynamically equivalent, by Kirchhoff kinematic\textsuperscript{2} to that describing the motion of a Lagrange top.\textsuperscript{3} The conventional method for solving these equations is (1) to express the curvature vector \omega_1, \omega_2, \omega_3 in terms of three Euler angles (\theta,\phi,\psi) with respect to the laboratory frame; (2) to construct a Lagrangian, Z, and find two constants of motion (conjugate momenta) by noting that angles (\phi,\psi) are cyclic coordinates (that is, they occur only in their derivatives with respect to the contour distance, s); (3) to solve for \{\theta,\phi,\psi\} in terms of \{\text{\textit{t}},\text{\textit{r}}\cos \theta\} from the two constants of motion and substitute them into the third integral of motion (constant energy), obtaining an equation which involves \{\theta,\cos \theta\} only; (4) to solve that equation for \textit{u}=\cos \theta as a function of the contour length parameter, s, in terms of elliptical functions and then solve for angles (\phi,\psi) in terms of \textit{u}=\cos \theta; (5) to determine the laboratory position of the DNA axis by quadratures; namely, x(s)=\int_0^s \sin \theta(s) \cos \phi(s) ds, y(s)=\int_0^s \sin \theta(s) \sin \phi(s) ds, and z(s)=\int_0^s \cos \theta(s) ds.

This procedure has been extensively studied by Benham\textsuperscript{5}, LeBret\textsuperscript{6}, and Wadati and Tsuru\textsuperscript{7(b),7(c)}. The disadvantage of this conventional approach is that it is very hard in general to get analytical expressions for the Cartesian coordinates \{x(s),y(s),z(s)\}. Thus it is even harder to relate the parameters, which determine the shape of the centerline of the rod, to known physical quantities, such as the total length L, the bending constant A, the twist constant C, and the linking number difference \Delta k if the rod is closed. In addition, this treatment cannot be applied to another class of DNA supercoiled structures which involve self-contact and which are typified by the plectonemic (interwound) conformation. Although they have been analyzed by numerical simulations, these conformations are very difficult to treat analytically.

In this paper we approach this problem from a different direction. There is a fundamental theorem for space curve in differential geometry\textsuperscript{12}

A three-dimensional space curve is determined (up to a rigid body motion in space) by its curvature \kappa(s) and torsion \tau(s).

For a thin rod the curvature and torsion of its centerline are given by\textsuperscript{13}
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\[ \kappa(s) = |\dot{t}(s)| = \sqrt{[\omega_1(s)]^2 + [\omega_2(s)]^2} \geq 0, \]  
\[ \tau(s) = [\dot{t}(s) \times \mathbf{n}(s)] \cdot \mathbf{\dot{n}}(s) = \omega_3(s) - \frac{d}{ds} \left[ \arctan \frac{\omega_1(s)}{\omega_2(s)} \right], \]

where \( \mathbf{n}(s) \) is the unit principal normal vector at \( s \). Therefore if we find solutions of \( \omega(s) = [\omega_1(s), \omega_2(s), \omega_3(s)] \) as functions of the contour parameter, \( s \), the centerline is determined. The advantage of our approach is that, in the absence of external force and torque, we can obtain mathematical expressions for the cylindrical coordinates of the centerline of the rod and for its total elastic energy in closed form. In general this "inverse problem" of curves (to reconstruct a curve from its curvature and torsion) is computationally very difficult, because infinite series are involved.12

### III. DERIVATION OF NONLINEAR SCHRÖDINGER EQUATION

#### A. Introduction of frictionless external forces

We now consider that the thin elastic rod may have self-contact, and that some frictionless forces are exerted which help to maintain the stationary configurations. The self-contact force will be in the direction perpendicular to the tangent direction \( \mathbf{t}(s) \).

For convenience we define \( \mathbf{N} = \mathbf{F}/A \) and \( \mathbf{N}^e = \mathbf{F}^e/A \).

Let \( \mathbf{b}(s) = \mathbf{t}(s) \times \mathbf{n}(s) \) be the binormal unit vector at \( s \), then we may express the most general self-contact force as

\[ \mathbf{N}^e = N_b^e \mathbf{b} + N_n^e \mathbf{n}, \]

where the force components \( N_b^e \) and \( N_n^e \) are real and where \( \mathbf{n}(s) \) and \( \mathbf{b}(s) \) are related to \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \) via

\[ \mathbf{b} = \frac{\omega_1 \mathbf{e}_1 + \omega_2 \mathbf{e}_2}{\sqrt{\omega_1^2 + \omega_2^2}}, \]

and

\[ \mathbf{n} = \frac{\omega_2 \mathbf{e}_1 - \omega_1 \mathbf{e}_2}{\sqrt{\omega_1^2 + \omega_2^2}}. \]

Since the forces are frictionless, the resulting self-contact torques are, of course, taken to be zero, \( M_1^e - M_2^e - M_3^e = 0 \).

We now substitute Eqs. (3.1) and (3.2) into Eq. (2.1) and rewrite them in component form, obtaining six first order differential equations for six unknowns

\[ \dot{\mathbf{N}}_b + \omega_3 \mathbf{N}_2 - \omega_5 \mathbf{N}_3 = \frac{N_b^e \omega_1 + N_n^e \omega_2}{\sqrt{\omega_1^2 + \omega_2^2}} = 0, \]

\[ \dot{\mathbf{N}}_2 + \omega_3 \mathbf{N}_1 - \omega_1 \mathbf{N}_3 + \frac{N_b^e \omega_2 - N_n^e \omega_1}{\sqrt{\omega_1^2 + \omega_2^2}} = 0, \]

\[ \dot{\mathbf{N}}_3 + \omega_1 \mathbf{N}_2 - \omega_2 \mathbf{N}_1 = 0, \]

\[ \omega_1 - \omega_2 \omega_3 + \lambda \omega_2[\omega_3 - \omega_3^{(0)}] = N_2, \]

\[ \omega_2 + \omega_1 \omega_3 - \lambda \omega_1[\omega_2 - \omega_2^{(0)}] = N_1. \]

#### B. Constants of motion

It is well known that there are three constants of motion for the Lagrange top.3 The Lagrange top can be equivalently described by Eq. (3.3) when the self-contact forces \( N_b^e \) and \( N_n^e \) are set to zero. We shall show that these constants of motion also exist for the case in which the force \( N_b^e \) is zero, but the force \( N_n^e \) is not zero. The first constant of motion is obvious in view of Eq. (3.3f). It is the scalar product of the internal torque \( \mathbf{M}(s) \) and the unit tangent vector \( \mathbf{t}(s) \),

\[ C[\dot{\omega}_3 - \omega_3^{(0)}] = \text{constant} = AD. \]

Physically this equation says that excess twist is uniformly distributed over the centerline of the rod. This leaves us only two components of curvature, namely \( \omega_1 \) and \( \omega_2 \), to be determined. We can also substitute Eqs. (3.3d) and (3.3e) into Eq. (3.3c), finding the second constant of motion

\[ \frac{1}{2} (\omega_1^2 + \omega_2^2) + N_3 = \text{constant} = B. \]

Thus \( N_3 \) is related to \( \omega_1 \) and \( \omega_2 \), and this still leaves us two components of the internal force to be determined.

The scalar product of the internal torque \( \mathbf{M}(s) \) and the internal force \( \mathbf{N}(s) \) is

\[ \omega_1 N_1 + \omega_2 N_2 + \lambda [\omega_3 - \omega_3^{(0)}] N_3 = \text{constant} = \int M_b^e \sqrt{\omega_1^2 + \omega_2^2} ds. \]

This result can be verified by differentiation of Eq. (3.6) and substitution of \( (\omega_1, \omega_2, \omega_3, \dot{N}_1, \dot{N}_2, \dot{N}_3) \) from Eq. (3.3).

It is interesting to notice that \( \mathbf{M}(s) \cdot \mathbf{N}(s) \) is still a constant of motion when the self-contact force is applied only in the principal normal direction [i.e., \( N_b^e \neq 0 \) but \( N_n^e = 0 \)]. However, in this case, the internal force \( \mathbf{N}(s) \) is a constant vector in the laboratory frame only in the region where there is no self-contact.

When self-contact forces \( N_b^e \) and \( N_n^e \) are both zero, we denote the constant of Eq. (3.6) by \( PN \), where \( N = ||\mathbf{N}(s)|| \) is the length of a constant vector in the laboratory frame.

#### C. Complex curvature and nonlinear Schrödinger equation

A strategy of this paper is to define a complex curvature \( \xi(s) = \xi_0(s) + i \omega_2(s) \) and a complex force \( \mathbf{N}(s) = \mathbf{N}(s) + i \lambda \mathbf{N}(s) \). From Eqs. (3.3d) and (3.3e), we get

\[ \xi + i \omega_2 \xi - i \lambda \xi = 0. \]

Likewise from Eqs. (3.3a) and (3.3b), we obtain

\[ \dot{\xi} + i \omega_2 \xi - i \lambda \xi = 0. \]

where Eq. (3.5) is used.
We can eliminate $J(s)$ from Eqs. (3.7a) and (3.7b), obtaining
\begin{equation}
\xi + ia\xi - b\xi + \frac{1}{2} [\xi|^2 \xi - [N_a^{(s)} + iN_b^{(s)}] \frac{\xi}{|\xi|} = 0, \tag{3.8}
\end{equation}
where real parameters $a$ and $b$ are defined as
\begin{equation}
a = 2\omega_3^{(Q)} + (2 - \lambda)(Q/\lambda), \tag{3.9a}
b = \frac{\omega_3^{(Q)}}{2} + (2 - \lambda)\omega_3^{(Q)}(Q/\lambda) + (1 - \frac{3}{2}\lambda)(Q/\lambda)^2. \tag{3.9b}
\end{equation}

We now change the dependent variable $\xi(s) = \eta(s)e^{-ia s^2/2}$, and obtain a simplified equation for $\eta(s)$ as
\begin{equation}
\ddot{\eta} - c \eta + \frac{1}{2} |\eta|^2 \eta - [N_a^{(s)} + iN_b^{(s)}] \frac{\eta}{|\eta|} = 0, \tag{3.10}
\end{equation}
where the real parameter $c$ is given by
\begin{equation}
c - b - \frac{a^2}{4} = -\kappa - \frac{1}{4} Q^2. \tag{3.11}
\end{equation}

Equation (3.10) is a time-independent cubic nonlinear Schrödinger equation with an extra potential term. This equation is one of the main conclusions of this paper. Let $\eta(s) = \kappa(s)\exp[i\chi(s)]$, where $\kappa(s) > 0$ and $\chi(s)$ are two real functions of $s$. Then the complex curvature becomes
\begin{equation}
\xi(s) = \kappa(s)\exp\left[i \left(\chi(s) - \frac{a}{2} s\right)\right]. \tag{3.12}
\end{equation}

The angle between the two unit vectors $b(s)$ and $e_3(s)$ is nothing but $\chi(s) = (a/2)s$. From now on we will assume that $\kappa(s) > 0$ and that function $\chi(s)$ is well defined. The case of $\kappa(s) = 0$ for all $s$ (i.e., rod is linear) will be treated in Appendix A. The case of $\kappa(s) = 0$ with $l = 1, 2, ..., \infty$ (i.e., the centerline of the rod has isolated points of inflexion (zero curvature)) will be discussed in Appendix B. Substituting into the definition of $\xi(s)$, we obtain
\begin{equation}
\frac{\omega_1(s)}{\omega_2(s)} = \frac{\text{Re}[\xi(s)]}{\text{Im}[\xi(s)]} = \tan\left[\frac{\pi}{2} - \chi(s) + \frac{a}{2} s\right]. \tag{3.13}
\end{equation}

Hence torsion $\tau(s)$ is related to $\chi(s)$ via
\begin{equation}
\tau(s) = \omega_3(s) + \dot{\chi}(s) - \frac{1}{2} Q + \dot{\chi}(s). \tag{3.14}
\end{equation}
Thus we can write the complex curvature as
\begin{equation}
\xi(s) = \kappa(s)\exp\left[i \left(\chi(s) - \frac{a}{2} s\right)\right]. \tag{3.15}
\end{equation}

When $Q + a = 0$, the transformation $R(s) \rightarrow \xi(s)$ reduces to the famous Hasimoto transformation. The Hasimoto transformation has been used to transform the localized induction equation (LIE) for the position $R(s)$ of a vortex filament into the cubic nonlinear Schrödinger equation for $\xi(s)$ with $Q + a = 0$.

Now the separation of real part and imaginary part of Eq. (3.10) leads to
\begin{equation}
\dot{\kappa} + 2\kappa(\tau - \frac{1}{2} Q) = N_a^{(s)} \tag{3.16a}
\end{equation}
\begin{equation}
N_b^{(s)} \tag{3.16b}
\end{equation}

Thus we have obtained two coupled equations for $\kappa(s)$ and $\tau(s)$ in which the self-contact forces have also been included.

**IV. THE CLOSED-FORM EXPRESSIONS FOR $\rho(s)$, $\phi(s)$, AND $z(s)$ IN THE ABSENCE OF THE SELF-CONTACT FORCE**

**A. Solutions for $\kappa(s)$, $\tau(s)$, and $\chi(s)$**

In the absence of external forces and contacts [i.e., $N_a^{(s)} = N_b^{(s)} = 0$], system Eq. (3.3) has three constants of motion, namely, $Q$, $\xi$, $P$. If we also know the mechanical parameter, $\lambda$, the total length, $L$, and the strength of the “gravitation force,” $N$, then the solutions to system (3.3) are uniquely determined.

Equations (3.16) in this case become the following Euler–Lagrange equations:
\begin{equation}
\kappa - \kappa(\tau - \frac{1}{2} Q)^2 - c\kappa + \frac{1}{4} k^3 = 0, \tag{4.1a}
\end{equation}
\begin{equation}
k^2(\tau - \frac{1}{2} Q) = J. \tag{4.1b}
\end{equation}

A curve with curvature $\kappa$ and torsion $\tau$ which satisfies the $Q = 0$ version of (4.1) is called twist free elastica. The classical term twist free elastica (or elastic curve) refers to a curve in a plane or in three-dimensional space which has the minimum total squared curvature among curves which have the same length and which obey first-order boundary conditions. A curve with curvature $\kappa$ and torsion $\tau$ satisfying (4.1) is then called elastica.

System (4.1) with $Q = 0$ has been extensively studied by Langer and Singer. They have obtained a closed form solution for $R(s) = (d/ds)R(s)$ in terms of cylindrical coordinates $[\rho(s), \phi(s), z(s)]$. They have also obtained the constraints that must be satisfied in order to close the rod [i.e., $R(0) = R(L)$]. System (4.1) has also been studied by Langer and Singer. They have obtained three first order differential equations for $[\rho(s), \phi(s), z(s)]$. The explicit expressions for $[\rho(s), \phi(s), z(s)]$ can be obtained by quadratures but are not presented in their paper.

The true knowledge of the cylindrical coordinates $[\rho(s), \phi(s), z(s)]$ is essential to the study of DNA supercoiling. Therefore, in the remainder of Sec. IV we will use a simple integration procedure to analyze the system (4.1). This procedure has been extensively developed by Langer and Singer.

Equations (4.1) have a solution of the form
\begin{equation}
\kappa^2(s) = \alpha \left[1 - \frac{\mu}{\nu} \text{sn}^2(ws|\mu)\right], \tag{4.2a}
\end{equation}
\begin{equation}
\tau(s) = \frac{1}{2} Q + \frac{J}{\kappa^2(s)}, \tag{4.2b}
\end{equation}
where $\text{sn}(ws|\mu)$ is the Jacobi sinus amplitudeinus elliptic function, and where $\mu$ is the modulus of the elliptical function and $w$ is a nonzero real parameter. The integration of $\tau(s)$ is given by
\[
\int_0^s \tau(t) dt = \frac{1}{2} Q s + \frac{j}{\omega \alpha} \prod \left( \frac{\mu}{\nu} ; w s \right) \mu \]
(4.3a)

and consequently
\[
\chi(s) = \frac{j}{\omega \alpha} \prod \left( \frac{\mu}{\nu} ; w s \right) \mu ,
\]
(4.3b)
\[
\int_0^s \omega_3(t) dt = \int_0^s \tau(t) dt - \left[ \chi(s) - \frac{\alpha}{2} s \right],
\]
(4.3c)

where
\[
\Pi(x; s) = \int_0^s \frac{dt}{1 - x \sin^2(t/\mu)}
\]
(4.4)

is a standard function known as the incomplete elliptic integral of the third kind.18

It is well known that the centerline of the rod is solely determined, up to a rigid body motion, by its curvature \( \kappa(s) \) and torsion \( \tau(s) \). We emphasize that it is the angle \( \chi(s) - (a/2)s \) that helps to make \( [\kappa(s), \tau(s), \chi(s) - (a/2)s] \) a representation of the thin elastic rod.

Substitution of Eq. (4.2) into Eq. (4.1) leads to
\[
\alpha = 4 w^2 \nu ,
\]
(4.5a)
\[
c = w^2 (1 - \mu + 3 \nu) ,
\]
(4.5b)
\[
J^2 = 16 w^6 \nu (1 - \nu) (\nu - \mu) .
\]
(4.5c)

Since \( \kappa^2 > 0, J^2 > 0 \), we must require that \( 0 \leq \mu \leq \nu \leq 1 \) and \( w = \text{real number} \).

We remark that the case of isolated inflexion points, which will be discussed in Appendix B, is corresponding to the requirement \( 0 < \mu = \nu < 1 \). The case of \( \kappa(s) = 0 \) for all \( s \) (i.e., rod is linear), which will be discussed in Appendix A, is corresponding to the requirement \( \mu = \nu = 0 \).

Integration of Eq. (4.1a) gives rise to the useful relation
\[
\frac{(\dot{\kappa})^2}{2} + \frac{J^2}{2 \kappa^2} - \frac{c \kappa^2}{2} + \frac{\kappa^4}{8} = B = \frac{J^2}{2 \alpha} - \frac{c \alpha}{2} + \frac{\alpha^2}{8} .
\]
(4.6)

Substitution of Eq. (4.5) into Eq. (4.6) leads to
\[
B = 2 w^4 [\mu (2 \nu - 1) + \nu (2 - 3 \nu)] .
\]
(4.7)

It is known that the elliptical function \( \sin(s/\mu) \) has a real period of \( 4K \), where \( K = K(\mu) \) is the complete elliptical integral of the first kind.18 Therefore \( \kappa(s), \tau(s), \chi(s) \), which depend on \( \sin^2(s/\mu) \), have periods of \( 2K/w \).

### B. Solutions for \( M(s) \) and \( N(s) \)

Once the complex curvature \( \dot{\xi}(s) \) is solved, the internal torque \( M(s) \) is given by
\[
M(s) = A \kappa(s) b + A Q t .
\]
(4.8)

The complex internal force \( \dot{J}(s) = N_1(s) + i N_2(s) \) can also be solved by using Eq. (3.7a). The result can be expressed in terms of known functions \( \kappa(s), \tau(s), \chi(s) \), and their derivatives or integrations, namely,
\[
\dot{J}(s) = \kappa(s) \exp \left[ \frac{i}{2} (Q + a) s + i \int_0^s \tau(t) dt \right]
\]

Since \( N_1(s) = \text{Re} [J'(s)] \) and \( N_2(s) = \text{Im} [J'(s)] \), after some calculation we obtain,
\[
N(s) = N_1 e_1 + N_2 e_2 + N_3 e_3 - \left[ 2 \pi \frac{1}{2} \kappa^2(s) \right] t - \kappa(s)n + \kappa(s) [Q - \tau(s)] b .
\]
(4.10)

We also obtain the useful relation
\[
N^2 = 2B - JQ + \dot{\tau}^2 .
\]
(4.11)

It is obvious that \( \Phi(s) \neq 0 \) implies (1) \( N(s) \neq 0 \) and (2) \( M(s) \neq 0 \) and \( N(s) \) are not parallel or antiparallel to each other. The case of \( \Phi(s) = 0 \) for all \( s \) will be considered in Appendix A. The case of \( \Phi(s_0) = 0 \) for isolated points \( s_0 \) will be considered in Appendix B. Since vector \( N \) is a nonzero constant vector in the laboratory with unknown direction and unknown norm, we can define the \( z \) direction unit vector of the lab frame as
\[
e_z = -N/|N| .
\]
(4.14)

Finally the unit vector in the \( \rho \) direction can be defined as
\[
e_\rho = \Phi/|\Phi| .
\]
(4.15)

Finally the unit vector in the \( \rho \) direction can be defined as
\[
e_\rho = e_\rho \times e_z = -(\Phi \times N)/|\Phi \times N| .
\]
(4.16)

Since \( R = \rho e_\rho + z e_z \), we can write the unit tangent vector as
\[
t = \dot{R} = \dot{\rho} e_\rho + \rho \ddot{\rho} e_\rho + \dot{z} e_z .
\]
(4.17)

We note that this expression is different from that of Langer and Singer,15 where they have a constant, instead of \( \rho \), in front of \( \rho e_\rho \) in Eq. (4.17). Taking the dot product of \( t \) with
(e_p, e_φ, e_z) defined above, and setting v(s) = κ^2(s), we obtain

$$\dot{p} = \frac{v}{2N(v + Q^2 - P^2)^{1/2}},$$

(4.18a)

$$\rho \dot{\phi} = \frac{P(2 \zeta - v) - 2QN}{2N(v + Q^2 - P^2)^{1/2}},$$

(4.18b)

$$\dot{z} = \frac{1}{2N}(v - 2\zeta).$$

(4.18c)

It is interesting to note that when Q is set to zero, the expressions of Eq. (4.18) are identical to those given in Ref. 15, although a different expression for the unit tangent vector t has been used.

We can then solve for p(s), φ(s), and z(s) by integration, and the results are

$$p(s) = \frac{\sqrt{\alpha \nu}}{N} \left[ 1 - \frac{\nu'}{\nu} \, \text{sn}^2(ws|\mu) \right]^{1/2},$$

(4.19a)

$$\phi(s) = -\frac{P}{2} s + \frac{J'}{w \alpha} \Pi \left( \frac{\nu'}{\nu}; ws|\mu \right),$$

(4.19b)

$$z(s) = \frac{1}{N} \left[ \alpha + 2w^2(v-1) \right] s + \frac{2w}{N} E(ws|\mu).$$

(4.19c)

where

$$J' = P - QN + \frac{P}{2} (Q^2 - P^2),$$

(4.20a)

$$\alpha' = \alpha + Q^2 - P^2,$$

(4.20b)

$$\nu' = \frac{\alpha}{\alpha'}. \mu.$$  

(4.20c)

The function E(ws|μ) is the standard incomplete elliptical integral of the second kind,^{18} defined as

$$E(s|\mu) = s - \mu \int_0^s \text{sn}^2(t|\mu) \, dt.$$  

(4.21)

Langer and Singer^{15} have given a partial description of the twist free elastica, a curve Γ traced out by vector R(s)|_{Q=0}, based on the expression for R(s)|_{Q=0} of Eqs. (4.17) and (4.18). We now modify it as little as possible and give the following complete description of the elastica, a curve Γ traced out by vector R(s), by virtue of Eqs. (4.2) and (4.19).

The entire elastica Γ lies between two concentric cylinders (the inner cylinder possibly degenerating to a line). The critical points and periodicity of p(s), κ(s), and π(s) coincide; the three functions pass in one period from a minimum (on the inner cylinder) to a maximum (on the outer cylinder) and back to a minimum, with no other critical points. Meanwhile, the critical points of z(s) and φ(s) coincide, each having zero, one, or two critical points in each period of p(s). In addition, z(s) and φ(s) differ from periodic functions by linear functions in s.

The radii of the inner and outer cylinders are given by

$$\rho_{\text{min}} = \frac{1}{N} \alpha' \left( \frac{1 - \mu'}{\nu} \right), \quad \rho_{\text{max}} = \frac{1}{N} \sqrt{\alpha'}. $$

(4.22)

We note that the mathematical formulas in Eq. (4.19a)-(4.19c) are similar to those obtained by Kida^{19} to describe the vortex filament movement without change of form.

In an effort to visualize the geometric forms represented by Eqs. (4.19a)-(4.19c) we introduce the following equations:

$$p^2(s) = a_1 + b_1 f_1(s),$$

(4.19d)

$$\phi(s) = a_2 s + b_2 f_2(s),$$

(4.19e)

$$z(s) = a_3 s + b_3 f_3(s),$$

(4.19f)

where f_i(s) (i=1,2,3) are periodic functions of s (with the same period as that of \text{sn}^2(ws|μ)) and with values in the range [-1,1]. In Appendix D, we prove that Eqs. (4.19a) to (4.19c) are equivalent to Eqs. (4.19d) to (4.19f). Thus we say that the general solution (4.19) can be viewed as a helix-on-a-linear-helix, i.e., DNA wraps around a rod whose centerline is itself a linear helix. The first terms of the cylindrical coordinates, \{√a_1, a_2 s, a_3 s\}, describe the linear helix and the second terms, \{b_1 f_1(s), b_2 f_2(s), b_3 f_3(s)\}, describe the wrapping of DNA around the rod whose centerline is described by the first terms.

The elliptic function solutions (4.2), (4.3), (4.19), and (4.20) for the \{κ(s), π(s), χ(s), ρ(s), φ(s), z(s)\} are uniquely determined by six parameters (w, \mu, v, Q, λ, L). This is because parameters (\xi, P, N) can be expressed in terms of (c, J, B, Q) [cf. Eqs. (3.11), (4.11), and (4.12)] and then parameters (c, J, B) can be expressed in terms of (w, \mu, v) [cf. Eqs. (4.5b), (4.5c), and (4.7)]. The quantity α in Eqs. (4.2), (4.3), (4.19), and (4.20) is equal to 4w^2v [cf. Eq. (4.5a)].

Thus we have, in principal, expressed the curvature-torsion solutions (4.2) and (4.3) and cylindrical coordinate solutions (4.19) and (4.20) in terms of six parameters (w, \mu, v, Q, λ, L).

D. Euler rotation matrix

After considerable calculation using Eqs. (4.8), (4.10), (4.13)-(4.16), we obtain a relation between the Frenet frame and cylindrical lab frame, namely,

$$(n, b, t) = T(κ, ρ) \cdot (e_p, e_φ, e_z),$$

(4.23a)

$$(e_p, e_φ, e_z) = T^T(κ, ρ) \cdot (n, b, t),$$

(4.23b)

where \(T^T\) is the transpose of \(T\), and the transformation matrix \(T(κ, ρ)\) is given by
\[ T(\kappa, \rho) = \frac{1}{N^2 \rho} \begin{pmatrix} \frac{1}{\kappa} [\mathcal{J} Q + (\varepsilon - \frac{1}{2} Q^2) \kappa^2 - \frac{1}{2} \kappa^4], & -\mathcal{Q}, & \kappa \kappa \\ -P \kappa, & -JP + (N - \frac{1}{2} P Q) \kappa^2, & \left(\frac{\varepsilon - \frac{1}{2} \kappa^2}{\kappa}ight) P - N Q \\ N \rho \kappa, & \left(\frac{J}{\kappa} \frac{\mathcal{Q} \kappa}{2}\right) N \rho, & \left(\frac{1}{2} \kappa^2 - \varepsilon\right) N \rho \end{pmatrix}. \] (4.24)

Equations (4.23) and (4.24) are very useful when one wants to plot a thickened DNA molecule, because the surface of the thin elastic rod (DNA) with nonzero $r_{DNA}$ (radius of cross section) can be parameterized by

\[ S(s, s') = \rho(s - s')e(s) + z(s)\epsilon_z + r_{DNA}[n(s) \cos(s') + b(s) \sin(s')], \] (4.25)

where $s$ and $s'$ vary from 0 to $L$ and 0 to $2\pi$, respectively.

The cylindrical lab frame is related to Cartesian lab frame via

\[ (e_x, e_y, e_z) = \mathbf{V}(\phi) \cdot (e_x, e_y, e_z), \] (4.26)

similarly the rod frame is related to the Frenet frame via

\[ (e_1, e_2, e_3) = \mathbf{V}\left(\chi - \frac{a}{2} s - \frac{\pi}{2}\right) \cdot (n, b, t), \] (4.27)

where $\phi = \phi(s)$ is given by Eq. (4.19b) and $\chi = \chi(s)$ is given by Eq. (4.3b), and where the rotation matrix $\mathbf{V}(\beta)$ is defined as

\[ \mathbf{V}(\beta) = \begin{bmatrix} \cos \beta & \sin \beta & 0 \\ -\sin \beta & \cos \beta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \] (4.28)

Thus we obtain a closed-form expression for the Euler rotation matrix, which rotates the space-fixed (or lab) frame to the body-fixed (or rod) frame, namely,

\[ (e_1, e_2, e_3) = \mathcal{R} \cdot (e_x, e_y, e_z), \] (4.29)

\[ \mathcal{R} = \mathbf{V}\left(\chi - \frac{a}{2} s - \frac{\pi}{2}\right) \cdot T(\kappa, \rho) \cdot \mathbf{V}(\phi). \] (4.30)

The inverse of Euler matrix is given by $\mathcal{R}^{-1} = \mathbf{V}(-\phi) \cdot T^T(\kappa, \rho) \cdot \mathbf{V}(\pi/2 - \chi + a/2s)$.

\section*{E. Boundary conditions}

We may now impose different boundary conditions on the elliptical function of Eq. (4.19) to obtain different shapes of the centerline of a rod in a stationary state. Let $n$ be the number of periods of $\rho(s)$ when $s$ evolves from 0 to $L$.

1. If we require

\[ \rho(0) = \rho(L), \] (4.31a)

\[ \varepsilon(0) = \varepsilon(L), \] (4.31b)

\[ \phi(L) - \phi(0) = 2\pi l, \] (4.31c)

where $l$ is an integer, then we obtain a set of closed knotted toroidal helix solutions. These knotted toroidal helices can be characterized by two integers $(n, l)$.

2. If we require

\[ \rho(0) = \rho(L), \] (4.32a)

\[ \varepsilon(0) = \varepsilon(L), \] (4.32b)

\[ \phi(L) - \phi(0) = 2\pi l. \] (4.32c)

where $l$ is an integer, then we obtain a set of helix-on-a-linear-helix solutions. The helix on a linear helix may or may not be knotted and can be characterized by two integers $(n, l)$ and one positive number $s$ which satisfies $0 < s < 1$.

For all curves of these forms, the periodicity of the solutions assure that $[(d\rho/ds)R(s)]_{s=0} = [(d\rho/ds)R(s)]_{s=L}$, where $p = 1, 2, \ldots$.

For both cases above, we may also impose a boundary condition on the complex curvature $\xi(s) = \kappa(s)e^{i[x(s) - (a/2)s]}$ of Eqs. (3.12) and (4.3b) to obtain a solution of a rod with certain winding number of the unit vector $e_x(s)$ with respect to the unit binormal vector $b(s)$ in the $n(s) - b(s)$ plane. If we require

\[ \kappa(0) = \kappa(L), \] (4.33a)

\[ \left[ x(s) - \frac{a}{2} s \right]_{s=L} - \left[ x(s) - \frac{a}{2} s \right]_{s=0} = -2\pi m, \] (4.33b)

then the unit vector $e_x(s)$ winds $m$ turns with respect to $b(s)$, when $s$ varies from 0 to $L$. We notice that Eq. (4.33a) is equivalent to Eqs. (4.31a) and (4.32a) since both $\kappa^2(s)$ and $\rho^2(s)$ are linear functions of $sn^2(ws / \mu)$.

\section*{V. TOROIDAL HELIX}

In this section we consider the special case of the unknot toroidal helix by setting $l = \pm1$. The corresponding curve for the centerline of the elastic rod is a simple (unknotted) toroidal helix, the most elementary solution of a helical rod closed at its ends.

\subsection*{A. Closure of the rod}

When $\rho(s)$ is a constant, the centerline of the rod is either a circle or a linear helix. Both of the cases will be considered in Appendix A. Thus we assume here that $\rho(s)$ is not a constant. The boundary conditions (4.31) and (4.33) are equivalent to

\[ wL = 2\pi K, \quad n = \text{nonzero integer}, \] (5.1a)

where sign(x) = 1 for x > 0, sign(x) = -1 for x < 0, and sign(x) = 0 for x = 0. Symbol \( E = E(K|\mu) \) is the complete elliptical integral of the second kind, and \( \Pi(x; K|\mu) \) is the complete elliptical integral of the third kind. In deriving Eq. (5.1), the following identities have been used:

\[ E(nK|\mu) = nE, \]
\[ \Pi(x; nK|\mu) = n\Pi(x), \]

where \( n \) is an integer.

### B. Wr, Tw, Lk of the toroidal DNA duplex helix

Let \( r_{DNA} \) denote the radius of the DNA circular cross section and let \( v(s) \) denote an arbitrary unit vector field perpendicular to the unit tangent vector \( t(s) \) of the centerline of the DNA. It is well known that for two closed space curves \( \Gamma \), traced out by vector \( R(s) \), and \( \Gamma_v \), traced out by vector \( R(s) + r_{DNA}v(s) \) (with \( r_{DNA} < L \)), the Călugăreanu relationship applies:

\[ Lk(\Gamma_v, \Gamma) = Wr(\Gamma) + Tw(\Gamma_v, \Gamma), \]

where \( Wr(\Gamma) \) is the writhe of curve \( \Gamma \), \( Lk(\Gamma_v, \Gamma) \) is the linking number of curves \( \Gamma \) and \( \Gamma_v \), and \( Tw(\Gamma_v, \Gamma) \) is the twist of curve \( \Gamma_v \) with respect to curve \( \Gamma \). In the rest of this subsection we will show that when \( v(s) = e_i(s) \), the linking number \( Lk(\Gamma_v, \Gamma) \) is related to the two integers \( n \) and \( m \) that we introduced in the boundary conditions (5.1).

First we set \( v(s) = n(s) \), and the relation (5.3) takes the form:

\[ SL(\Gamma) = Wr(\Gamma) + \frac{1}{2\pi} \int_0^L \tau(s)ds. \]

This is because \( Lk(\Gamma_v, \Gamma) \) is usually called the self-linking number, denoted by a special symbol \( SL(\Gamma) \), and the twist of the curve \( \Gamma_n \) with respect to the curve \( \Gamma \) becomes \((1/2\pi)\int_0^L \tau(s)ds\).

The calculation of the self-linking number \( SL(\Gamma) \) is relatively straightforward. If one projects the curve \( \Gamma \) into the \( x-y \) plane, then \( SL(\Gamma) \) is simply one-half the number of inflection points, or \( SL(\Gamma) \) is the number of self-crossings counted in an appropriate way.

By using Eqs. (3.9a) and (5.1d), (5.7), and (5.9a), we can express \( \Delta m/n \) as:

\[ \frac{\Delta Lk - n - \Delta m}{n} = \frac{1}{2\pi} \int_0^L \frac{Q}{K'} \left[ \omega_3 - \omega_1 \right] ds = \frac{1}{2\pi}\frac{Q}{K} L. \]

### C. Final assembly procedure

In Sec. IV A we have, in principle, expressed the curvature-torsion solutions (4.2) and (4.3) and cylindrical coordinate solutions (4.19) and (4.20) in terms of six parameters \( w, \mu, \nu, Q, \lambda, L \).

From Eqs. (5.1) and (5.10), we know that if the parameters \( (n, \Delta Lk, \lambda, L) \) are given, then the parameters \( (w, \mu, \nu, Q) \) are completely determined.

Furthermore we shall show that the parameters \( (\mu, \nu) \) as well as the shape of the toroidal helix are uniquely determined by the parameters \( (n, \Delta Lk, \lambda) \). The total length \( L \) only changes the scale of the whole figure of DNA. It also puts an upper physical limit on \( |\Delta Lk| \).

We begin with defining five dimensionless quantities as follows [cf. Eqs. (4.5), (4.7), (5.1c)]:

\[ \tilde{a} = a/|w|^2 = 4\nu, \]
\[ \tilde{c} = c/|w|^2 = (-1 - \mu + 3\nu), \]
\[ \tilde{J} = J/|w|^3 = 4\operatorname{sign}(J)[\nu(\nu - 1) - (\nu - \mu)]^{1/2}. \]
\[ \tilde{r} = R|w|^4 = 2[\mu(2v - 1) + \nu(2 - 3v)], \] (5.11d)

\[ \tilde{z} = z|w|^2 = 2 \left( -1 + \nu + \frac{E}{K} \right), \] (5.11e)

Using Eqs. (5.10b), (5.10e), and (3.11) we can define

\[ \tilde{Q} = Q|w|^2 = 2 \text{sign}(Q) \left( 1 + \frac{E}{K} + \mu - \nu - 1 \right)^{1/2}. \] (5.11f)

Other dimensionless quantities can be expressed in terms of these quantities and parameters \( \mu \) and \( \nu \) [cf. Eqs. (4.11), (4.12), (4.20)].

\[ N = N|w|^2 = (2B - JQ + \bar{\xi}^2)^{1/2}, \] (5.12a)

\[ \tilde{p} = P|w| = (\tilde{Q} - \bar{J})/\tilde{N}, \] (5.12b)

\[ \tilde{\eta}' = \eta'|w|^2 = \tilde{p} \tilde{Q} - \tilde{Q} + \frac{\tilde{p}}{2} (\tilde{Q}^2 - \tilde{p}^2), \] (5.12c)

\[ \mu' = \frac{4\nu}{4\nu + \tilde{Q}^2 - \tilde{p}^2} \mu. \] (5.12d)

For convenience we also define

\[ \tilde{g} = J/\alpha|w|^2 = \tilde{J}/4\nu, \] (5.13a)

\[ \tilde{g}' = J'/\alpha'|w|^2 = \tilde{J}'/4\mu \mu. \] (5.13b)

Substituting of Eqs. (5.11), (5.12), and (5.13) into Eqs. (5.1b) and (5.10), we obtain

\[ |n|^{-1} = \frac{\text{sign}(l)}{2\pi} \left[ \tilde{p} K - 2 \tilde{g}' \Pi \left( \frac{\mu'}{\nu} \right) \right], \] (5.14a)

\[ \frac{\Delta L_k - n}{|n|} = \frac{\Delta m}{|n|} = \frac{1}{2\pi} \left[ \frac{2}{\nu - 1} \tilde{Q} K - 2 \tilde{g} \Pi \left( \frac{\mu}{\nu} \right) \right]. \] (5.14b)

Equations (5.14a) and (5.14b) can be thought of as two implicit equations for parameters \( \mu \) and \( \nu \) when \((n, \Delta L_k, \lambda)\) are given. One may also notice the similarity between the quantities in the square brackets in Eqs. (5.14a) and (5.14b).

The lower limit for parameter \( \nu \) is \( \nu_{\text{min}}(\mu) = \mu \) [cf. the condition below (4.5e)]. The upper limit for parameter \( \nu \) is given by

\[ \nu_{\text{max}}(\mu) = 2 \frac{E(\mu)}{K(\mu)} + \mu - 1. \] (5.15)

This is because the quantity \( Q \) in Eq. (5.11f) is real. One can verify that \( 0 \leq \nu_{\text{max}}(\mu) \leq \mu \). When \( \nu_{\text{max}}(\mu) = \nu_{\text{min}}(\mu) \), we obtain, for parameter \( \mu \), the upper limit \( \mu_{\text{max}} \), which satisfies \( 2 E(\mu_{\text{max}}) = K(\mu_{\text{max}}) \), or \( \mu_{\text{max}} = 0.826 \). Therefore the possible values for parameter \( \mu \) and \( \nu \) are confined in a triangle in the \( \nu-\mu \) plane, which is determined by two straight lines \( \mu = 0 \), and \( \nu = \nu \) and a curve \( \nu(\mu) = \mu - 1 + 2 E(\mu)/K(\mu) \).

Now it is convenient for us to trade the dependent parameters \( \mu \) and \( \nu \) for two independent new parameters \( \tilde{\mu} \) and \( \tilde{\nu} \), via

\[ \mu = \tilde{\mu} \mu_{\text{max}}, \] (5.16a)

\[ \nu = \tilde{\nu} \nu_{\text{max}} + \frac{2 E(\tilde{\mu} \mu_{\text{max}})}{K(\tilde{\mu} \mu_{\text{max}})} - 1 \tilde{\nu}. \] (5.16b)

Thus, when parameters \( \tilde{\mu} \) and \( \tilde{\nu} \) vary independently from 0 to 1, the parameter \( \mu \) varies from 0 to \( \mu_{\text{max}} \) and the parameter \( \nu \) varies dependently from \( \mu \) to \( \nu_{\text{max}}(\mu) \). In other words, Eqs. (5.16) map a square in the \( \tilde{\mu}-\tilde{\nu} \) plane onto the triangle in the \( \mu-\nu \) plane.

Substituting Eq. (5.16) into Eq. (5.14), we can express \( (\Delta L_k, n) \) as functions of \( (\tilde{\mu}, \tilde{\nu}) \) and \( \text{sign}(\mu), \text{sign}(Q), \text{sign}(l), \lambda \). For each combination of \( \text{sign}(\mu), \text{sign}(Q), \text{sign}(l), \lambda \), Eqs. (5.14a) and (5.14b) represent two curves in the \( \tilde{\mu}-\tilde{\nu} \) plane for each integer pair \( (\Delta L_k, n) \). These two curves may or may not intersect. The parameters \( \tilde{\mu} \) and \( \tilde{\nu} \) are determined when two curves intersect, say, at \((\tilde{\mu}_i, \tilde{\nu}_i)\), where \( i \) is an index for the points of intersection. Once \( (\Delta L_k, n) \) and \( (\tilde{\mu}_i, \tilde{\nu}_i) \) are determined and the total length \( L \) is given, the parameter \( \mu \) is determined by Eq. (5.1a). The quantities \( (\mu, \nu, J, \alpha, \tilde{Q}, P, N) \) are similarly determined by Eqs. (5.16), (5.11), and (5.12). The excess twist is given \( \Delta T_w = (1/2\pi)(QL/\lambda) \) and the writhe is given by \( \text{Wr} = \Delta L_k - \Delta T_w \). Finally, the bending energy, twist energy, and total elastic energy can be expressed as

\[ U_{\text{Bend}} = \frac{A}{2} \int_0^L \kappa^2(s)ds = \frac{B}{2} AL, \] (5.17a)

\[ U_{\text{Twist}} = \frac{C}{2} \int_0^L [\omega_3 - \omega_3^{(0)}]^2 ds = \frac{1}{2\lambda} Q^2 AL, \] (5.17b)

\[ U_{\text{Total}} = U_{\text{Bend}} + U_{\text{Twist}}. \] (5.17c)

This completes the toroidal helix solution.

D. Numerical examples

In this subsection we shall show briefly some numerical examples of the toroidal helix. This numerical calculation has been carried out using the software program Mathematica which has built in all the elliptic functions and elliptic integrals.

(1) We choose \( \lambda = C/A = 1 \) and we assume that the DNA duplex helix contains 500 duplex turns for which the total length \( L \) is equal to 1768 nm \((=0.34 \text{ nm/base pair} \times 10.4 \text{ base pair/turn} \times 500 \text{ turn}) \) and the radius of the DNA duplex helix is 1 nm. We also assume that the linking number deficiency \( \sigma = \Delta L_k/L_k = 0.05 \). Thus \( \Delta L_k = 500 \times (0.05) = 25 \).

(2) There are four possible sign combinations for \( [\text{sign}(J), \text{sign}(Q)] \), namely, \((\pm, \pm)\) and \((\pm, \mp)\). For each combination of \( [\text{sign}(J), \text{sign}(Q)] \), since \( |n| > 0 \), we find numerically from Eq. (5.14a) that \( \text{sign}(l) \) is determined. For simplicity we consider here only the first two cases, i.e., \( \text{sign}(J) = \text{sign}(Q) = \text{sign}(l) = 1 \), which will result in \( \Delta T_w > 0 \), \( \text{Wr} > 0 \), and \( \text{Wr} = \Delta L_k + \Delta T_w > 0 \); (b) the mirror image of (a), i.e., \( \text{sign}(J) = \text{sign}(Q) = \text{sign}(l) = -1 \), which will result in \( \Delta T_w < 0 \), \( \Delta L_k > 0 \), and \( n > \Delta L_k - \Delta T_w < 0 \). Because we have already set \( \Delta L_k = 25 \), only case (b) needs to be considered.

(3) For case (b) we find out in the \( \tilde{\mu}-\tilde{\nu} \) plane that curve \( \Delta L_k = -25 \) intersects with curves \( n = -26, -27, -28, \ldots \), at points \( (\tilde{\mu}_i, \tilde{\nu}_i) \), which are tabulated in Table I.
TABLE I. Numerical values calculated follow the procedure outlined in part D of Sec. V.

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<th>i</th>
<th>$\tilde{\mu}_i$</th>
<th>$\tilde{\nu}_i$</th>
<th>$n$</th>
<th>$\Delta L_k$</th>
<th>$T_w/\Delta L_k$</th>
<th>$W_r/\Delta L_k$</th>
<th>$U_{\text{Total}}/U_{\text{Circle}}$</th>
<th>$U_{\text{Twist}}/U_{\text{Total}}$</th>
<th>$U_{\text{Bend}}/U_{\text{Total}}$</th>
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<tr>
<td>3</td>
<td>0.444444</td>
<td>0.766461</td>
<td>-40</td>
<td>-25</td>
<td>0.233539</td>
<td>0.766461</td>
<td>2.50487</td>
<td>0.021739</td>
<td>0.978261</td>
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<tr>
<td></td>
<td>(0.369642)</td>
<td>(0.961709)</td>
<td></td>
<td></td>
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<td></td>
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</tr>
</tbody>
</table>

(4) We then calculate and tabulate in Table I the following quantities for case (b): $U_{\text{Total}}/U_{\text{Circle}}$, $U_{\text{Twist}}/U_{\text{Total}}$, $U_{\text{Bend}}/U_{\text{Total}}$, $T_w/\Delta L_k$, $W_r/\Delta L_k$. The energy $U_{\text{Circle}}$ is the total elastic energy of the thin rod whose axis is a circle with radius $2\pi L$ and twist $\Delta T_w=\Delta L_k=-25$. It is given explicitly by Eq. (5.17).

(5) We make three plots (Figs. 1, 2, 3) for $n=-26$, $n=-30$, and $n=-40$ to show the basic features of the toroidal helices generated by the elliptic function solutions.

VI. CONCLUSIONS

The general solutions to the time independent nonlinear Schrödinger equation [Eq. (3.10)] represent the stationary...
FIG. 3. x-y plot and p-z plot for case (b) with \( AL_k = -25 \) and \( n = -40 \). The units of \( \{x, p, z, p\} \) are nanometers. The formulas for \( \{p, q, z\} \) (with \( x = p \cos \phi, y = p \sin \phi \)) are given in (4.19), whereas the parameters in (4.19) are given by \( \mu = 0.36964218030052302093, v = 0.96170883093623592605, w = -0.07964163029218922464, q = 0.009720401308497395265, Q = -0.02078496223560181204, N = 0.002495952822853953127, \) and \( P = 0.03859016748475215724 \).

states of the elastic rod with twist. Closed end boundary conditions without intersegmental contact of the DNA have led to toroidal stationary states, examples of which have been presented here. While these solutions are of considerable historical importance, they are not of immediate import to the representation of DNA, since plectonemic superhelical structures of the elastic rod are known to have lower energies than the corresponding toroidal forms.\(^{20d,8a}\) The plectonemic structures can also be determined from Eq. (3.10) and will be the topic of a subsequent manuscript.

DNA is a double helical polymer with a cross-sectional diameter of approximately two nanometers. In the case of small plasmid and viral genomes, DNA molecules have natural circular lengths of the order of microns. In higher cells, DNA molecules are linear and have lengths of the order of centimeters. In all cases the DNA is highly condensed \textit{in vivo}. For example, the centimeter lengths of DNA in higher cells are compacted into single chromatids with typical cylindrical dimensions of a micron in diameter and several microns in length.

There are several coiled structures which have been identified to be essential in the compaction process. First, there is a fiber, 11 nanometers in diameter, which consists of a linear chain of nucleosomes, protein core units around which DNA molecules are helically wrapped. Second, this 11 nanometer fiber itself wraps into a helical structure consisting of six nucleosomes per turn, with an overall diameter of 30 nm. This 30 nm fiber is the most prevalent structure observed by electron microscopy in the interphase nucleus. From the point of view of the DNA, the 11 nm fiber is a linear single helix which describes the position of the duplex cylindrical axis of the DNA. Such a linear helix can be represented by periodic boundary conditions applied to the ends of the helix.

The DNA molecule in the 30 nm fiber has the form of a helix-on-a-linear-helix, again with periodic boundary conditions. Both the linear helix and the helix-on-a-linear-helix are solutions to Eq. (3.10). In fact, with appropriate boundary conditions, Eqs. (4.2) readily represent the curvature and the torsion of such structures. While these structures are not the most stable structures accessible to free DNA, it is clear that, in the presence of external forces such as those exerted by the proteins in the 11 nm fibers, they can become stable.

Thus, the mathematical modeling of such structures reduces to judicious choices of \( N_n^{(e)} \) and \( N_p^{(e)} \) of Eq. (3.10), followed by the subsequent solution of the differential equation.

We thus consider Eq. (3.10) to be the route to the mathematical representation of all interesting DNA structures, subject to the constraint of the \textit{in vivo} linking number deficit. In this respect, the fundamental generality provided by Eq. (3.10), the nonlinear Schrödinger equation including external forces, has great potential.

Upon determination of the static solutions of Eq. (3.10) with certain choices of \( N_n^{(e)} \) and \( N_p^{(e)} \), the natural next step is the inclusion of time dependence. The solutions to the time-dependent equation will provide representation of local transitions from the chromatin 30 nm structure to the plectonemic DNA structure, perhaps free of protein cores. Such transitions may be at the heart of gene regulation. We expect that this mathematical model will play an important role in understanding the energetics and dynamics of such transitions.

ACKNOWLEDGMENTS

We would like to express our sincere gratitude to John Maddocks for his constructive comments on an early version of this work. Most of the material in Appendices A–D has been developed in response to his critique. We are grateful to Kathleen Rogers for correcting an error in plotting the figures in an earlier version of this manuscript. We also wish to extend our thanks to Robert A. Harris, Vaughan F. R. Jones, F. Alberto Grünbaum, Joel Langer, Craig J. Benham, Jerrold E. Marsden, and Joseph B. Keller for discussions and suggestions during the development of this theory. Y.S. was supported by National Institutes of Health Grant No. GM47945. J.E.H. was supported in part by National Institutes of Health Grant No. GM47945 and by the Office of Basic Energy Science in the Biological Energy Division of the Department of Energy under Contract No. DE-AC03-76SF000978.
APPENDIX A

In this Appendix, we consider all the special cylindrical coordinate solutions that are associated with the condition [cf. Eq. (4.13)]

\[ \Phi(s) = [N(s) \cdot M(s)]N(s) - |N(s)|^2 M(s) = 0 \quad (A1) \]

and therefore cannot be directly obtained by using the integration procedure of Part C of Sec. IV. Although these special solutions might be obtained from the general solutions after the limit \( \Phi(s) \to 0 \) is carefully taken, it is much easier to obtain them directly from the vector field expressions for \( N(s) \) and \( M(s) \). For convenience, we copy them from Sec. IV of the main text [Eqs. (4.10) and (4.8)] as follows:

\[ N(s) = \left[ \kappa - \frac{1}{2} \kappa^2(s) \right] t - \dot{k}(s) n + \kappa(s) [Q - \tau(s)] b, \quad (A2) \]

\[ M(s) = A \kappa(s) b + A Q t. \quad (A3) \]

There are three cases where \( \Phi(s) = 0 \): (1) \( M(s) = 0 \); (2) \( N(s) = 0 \); (3) \( N(s) \) and \( M(s) \) are nonzero and are parallel or anti-parallel to each other. We now consider them separately.

Case (1) \( M(s) = 0 \). We obtain, from (A3), that \( \kappa = \dot{\kappa} = 0 \). Comparison of this result with (4.2a) leads to \( \nu = \mu = 0 \). Thus the centerline of the rod becomes a straight line along the \( z \) axis, and the rod has no twist.

Case (2) \( N(s) = 0 \). We obtain, from (A1) to (A3), that \( \kappa = \dot{\kappa} = 0 \). Comparison of this result with (4.2a) leads to \( \nu = \mu = 0 \). It is well known that the linear helix is the only curve which has both constant curvature and constant torsion. Thus we can immediately write down the cylindrical coordinates for the linear helix

\[ (A4) \]

If we require that \( s \) be the arclength parameter and that the curvature \( \kappa \) and torsion \( \tau \) of the centerline of the rod satisfy \( \kappa = \sqrt{2} \kappa, \quad \tau = Q \), then we can readily obtain

\[ a = \frac{\sqrt{2} \kappa}{2 \kappa + Q^2}, \quad b = \pm \frac{\sqrt{2} \kappa - Q^2}{2 \kappa + Q^2}, \quad c = \pm \frac{Q}{\sqrt{2} \kappa + Q^2}. \quad (A5) \]

When \( Q = 0 \), we obtain \( \{a,b,c\} = \{(2 \kappa)^{1/2}, \pm (2 \kappa)^{1/2}, 0\} \), and the centerline of the rod becomes a planar circle in the \( x-y \) plane, and the rod has no twist. When \( \kappa = 0 \), we obtain \( \{a,b,c\} = \{0,0,\pm 1\} \) (where we need to take the \( Q \to 0 \) limit, because otherwise \( b \) is undetermined), and the centerline of the rod becomes a straight line along the \( z \) axis, and the rod has no twist.

Case (3) \( N(s) \) and \( M(s) \) are nonzero and are parallel or anti-parallel to each other. We obtain, from (A1), (A2), and (A3), that

\[ PN \left( \frac{\varepsilon - 1}{2} \kappa^2 \right) = N^2 Q, \quad \kappa = 0; \quad PN \kappa(Q - \tau) = N^2 \kappa, \quad (A6) \]

where we have used \( |N| = N \) and \( N \cdot M = A \). The centerline of the rod also takes the form of a linear helix of (A4) with parameters given also by (A5) but with the following replacements

\[ \varepsilon \to \varepsilon' = \varepsilon - Q \frac{N}{P}, \quad Q \to Q' = Q - \frac{N}{P}. \quad (A7) \]

Since the curvature in this case is a constant, we obtain from (4.2a) that \( \nu = \mu = 0 \). When \( Q' = 0 \), we obtain \( \{a,b,c\} = \{(2 \varepsilon' - 2 Q^2)^{1/2}, \pm (2 \varepsilon' - 2 Q^2)^{1/2}, 0\} \). The centerline of the rod becomes a planar circle in the \( x-y \) plane and the rod now has twist \( Q = N/P \). When \( \varepsilon' = 0 \), we obtain \( \{a,b,c\} = \{0,0,\pm 1\} \) (where we need to take the \( Q' \to 0 \) limit, because otherwise \( b \) is undetermined). The centerline of the rod becomes a straight line along the \( z \) axis, and the rod has twist \( Q = N/P \).

We now consider the case of the planar circle with twist in detail, because the total elastic energy for this case will be used as a comparison in Part D of Sec. V of the main text.

For a planar circle in the \( x-y \) plane with \( N \) in the \( z \) direction, we always have \( N \cdot t = N_z = 0 \). If the circumference of the circle is \( L \), then we obtain the curvature \( \kappa = 2 \pi L \), and we also obtain from (3.5) that \( \tau = 0 \). Comparison of this result with (4.2a) leads to \( \nu = \mu = 0 \). Since the writhe number \( W \) for a circle is zero, we obtain from (5.9a) that \( \Delta L k = \Delta w \). Consequently we have \( Q = 2 \pi L \Delta L k / L \) from (5.9b). Since \( \tau = 0 \), we obtain from (4.2b) that \( \tau = -\kappa^2 Q / 2 \).

Substitution of both (3.11) and of all of the results indicated in this paragraph into (4.6), (4.11), and (4.12) leads to

\[ P = \sigma(Q) \Delta L k / 2 \pi L \quad (A8) \]

and

\[ N = 4 \pi^2 \lambda \Delta L k / L^2. \quad (A9) \]

The total elastic energy is given by

\[ U_{\text{Total}} = A (2 \pi^2 / L^2)(1 + \lambda \Delta L k / L^2) = U_{\text{Circle}}. \quad (A10) \]

APPENDIX B

In this Appendix we will discuss the case of \( \kappa(s) = 0 \) with \( l = 1,2,\ldots,\infty \) [i.e., the centerline of the rod has isolated points of inflexion (zero curvature)].

As we remarked before, the case of isolated inflexion points corresponds to the requirement \( 0 < \mu = \nu \leq 1 \). By setting \( \nu = \mu \) in (4.2), (4.5), and (4.7) we obtain

\[ \kappa^2(s) = 4 w^2 \mu \cos^2(\pi s / \mu), \quad \tau = \frac{1}{2} Q, \quad (B1) \]

\[ c = w^2 (1 - 2 \mu), \quad J = 0, \quad B = 2 w^4 \mu (1 - \mu). \quad (B2) \]

As a consequence we set \( J = 0 \) in (3.11), (4.11), and (4.12)

\[ \varepsilon = c + \frac{1}{2} Q^2, \quad N^2 = B + \varepsilon^2, \quad P N = Q \Delta \varepsilon. \quad (B3) \]

There are only three independent real parameters in (B1); namely \( \{w, \mu, q\} \) where \( q = Q / |w| \). Equations (B2) and (B3) merely serve the purpose of defining parameters \( \{c, B, \varepsilon, N, P\} \) in terms of \( \{w, \mu, q\} \).

When \( \mu = 1 \), (B1) becomes

\[ \kappa(s) = 2 w \operatorname{sech}(w s), \quad \tau = \frac{1}{2} w q. \quad (w > 0). \quad (B4) \]

By setting \( \ell = 0 \) in Hasimoto’s single soliton solution to the localized induction equation for the motion of vortex filament,23 we readily obtain the Cartesian coordinate solution of (B4) (up to a rigid body motion):

\[ \varepsilon \to \varepsilon' = \varepsilon - Q \frac{N}{P}, \quad Q \to Q' = Q - \frac{N}{P}. \quad (A7) \]
\[ z(s) = s \left( 4w^2 + q^2 \right) \tanh(ws), \]
\[ x(s) + iy(s) = \rho(s) \exp[i\phi(s)], \quad (B5) \]

\[ \rho(s) = \frac{8}{(4+q^2)^{3/2}} \sech(ws), \quad \phi(s) = \frac{q}{2} ws. \]

When \( 0 < \mu < 1 \), we obtain, from (B2) and (B3), that \( N > 0 \), since \( B, C > 0 \). We also obtain, from (A1)–(A3), that

\[ |\Phi(s)|^2 = N^4 (|\mathbf{M}(s)|^2 - A^2 P^2) = A^2 N^4 (\kappa^2(s) + Q^2 - P^2). \]

Substitution of (B1)–(B3) into (B6) leads to

\[ |\Phi(s)|^2 \geq A^2 N^4 (Q^2 - P^2) = A^2 N^2 Q^2 (2B) > 0. \] 

Therefore the cylindrical coordinate solution to (B1) is still given by (4.19) with \( \nu = \mu \). Equations (B2), (B3), (4.5a), and (4.20) merely serve the purpose of defining parameters \{\( C, B, N, P, \alpha, J, \alpha', \alpha'' \}\] in terms of three independent parameters, \{\( \nu, \mu, q \]\].

We note that when \( \tau = \frac{1}{4} Q \) is set to zero and \( w \) is set to \( 1 \) in (B1), the curve of (4.2) reduces to a famous planar curve with curvature \( \kappa^2(s) = 4 \mu \) known as Euler’s elastica with inflexion points. The expressions of its Cartesian coordinates can be readily found in Love’s monograph. \footnote{24}

\[ \kappa^2(s) = 4 \mu \]

When we set \( \tau = \frac{1}{4} Q \) to zero, the curve of (4.2) reduces to a famous planar curve with curvature \( \kappa^2(s) = 4 \mu \) known as Euler’s elastica without inflexion points; its Cartesian coordinates expressions can also be readily found in Love’s monograph. \footnote{24}

**APPENDIX C**

In this Appendix we will discuss the case of \( \Phi(s)=0 \) with \( i=1,2,3,\ldots,\infty \) \[ \text{i.e., the real vector function } \Phi(s) \text{ defined in (4.13) of the main text has isolated points of zeroes} \]. Our goals here are (1) to express the exact lower bound of \( |\Phi(s)|^2 \) in terms of four independent parameters \{\( w, \nu, \mu, q \)\} where \( q = |q|/w \); and (2) to find out the conditions that four independent parameters \{\( w, \nu, \mu, q \)\} should satisfy when the exact lower bound of \( |\Phi(s)|^2 \) takes the minimum value, zero. Here we need only to consider the case of \( 0 < \mu < \nu < 1 \). Therefore \( N > 0 \) (cf. Appendix A).

From (B6) and (4.2), and (4.5a), we can express the exact lower bound of \( |\Phi(s)|^2 \) as

\[ |\Phi(s)|^2 \geq A^2 N^4 \left[ 4w^2(\nu - \mu \sn^2(ws|\mu) + Q^2 - P^2 \right]. \] 

where dimensionless \( G \) is defined as

\[ G = w^6 N^2 (4w^2(\nu - \mu \sn^2(ws|\mu) + Q^2 - P^2). \]

We want to point out (as suggested by Maddocks) that \( \rho^2(s) \) of (4.19) and \( |\Phi(s)|^2 \) share the same exact lower bound. Furthermore, from (4.19a), (4.20), and (4.5a), we can rewrite \( \rho^2(s) \) as

\[ \rho^2(s) = N^{-2} \left[ 4w^2(\nu - \mu \sn^2(ws|\mu) + Q^2 - P^2 \right]. \] 

Comparison of (C3) with (C1) gives us

\[ \rho^2(s) = A^{-2} N^{-6} |\Phi(s)|^2. \] 

We now want to express \( G \) of (C2) in terms of four independent parameters \{\( w, \mu, v, q \)\}. We eliminate \( P \) in (C2) by substituting (4.12), (4.11), (3.11), (4.7), (4.5b) into (C2). For convenience we replace the parameter \( \mu \) throughout with

\[ \mu = \nu - w^{-6} J^2 [16w(1 - \nu)^{-1}], \quad (C5) \]

which is merely another version of (4.5c). After much calculation we obtain

\[ G = \frac{1}{10} \nu^{-5} (1 - \nu)^{-3} (\nu^2 - 1)^2 (\nu - \mu)^2, \] 

\[ j = 4^{-1} \nu^{-3} J = \text{sgn}(J) \sqrt{\nu(1 - \nu)(\nu - \mu)}, \] 

\[ c = 2[\nu(1 - \nu) \pm \sqrt{\nu(1 - \nu)(\nu - \mu)}]. \]

The exact lower bound of \( |\Phi(s)|^2 \) is always nonnegative, since \( G \) in (C6) is always nonnegative. Finally we notice from (C6)–(C8) that the roots of (C6) can be simply expressed as

\[ q = c/z = 2 \text{sgn}(J) \nu^{-1/2} \sqrt{\nu(1 - \nu) \pm \sqrt{\nu(1 - \nu)(\nu - \mu)}}. \]

In principle, the cylindrical coordinate solution, when \( |\Phi(s)|^2 \) has isolated points of zero, is still given by (4.19). However, only three independent parameters, say, \{\( w, \nu, \mu \)\}, are now involved, and the parameter \( Q = |q|/w \) is determined in terms of \{\( w, \nu, \mu \)\} [cf. Eq. (C5)]. In practice, care must be taken as one tries to numerically evaluate the cylindrical coordinates using (4.19), because when \( |\Phi(s)|^2 \) goes to zero, Eq. (4.19b) contains a term of zero times infinity.

In the remainder of this appendix, we prove that (4.19b) remains finite and valid in the limit of \( |\Phi(s)|^2 \rightarrow 0 \). From (4.22), (C2)–(C6) we obtain

\[ \alpha' \left( 1 - \frac{\mu^2}{\nu} \right) = N^{-2} w^6 G. \] 

Likewise we obtain from (4.20), (4.5a), and (C2) that

\[ \alpha' = 4 w^2 (G + \mu). \] 

Thus we have

\[ \left( 1 - \frac{\mu^2}{\nu} \right) = \frac{1}{4} w^4 N^{-2} (G + \mu)^{-1}. \] 

From Eq. (C12), when \( G \rightarrow 0^+ \) \[ \text{i.e., } G \text{ approaches zero from above} \], the ratio \( \mu^2/\nu \rightarrow 1^- \). Therefore, \( \Pi(\mu^2/\nu, w|\nu) \rightarrow \infty \) in this limit. We now write \( \Pi(x|w|\nu) \) as the product of a singular part (when \( x \rightarrow 1^- \) and \( 0 < \mu < x \leq 1 \)) and a regular part

\[ \Pi(x|w;\mu) = \delta_2(x, \mu)[\lambda(x, s, \mu) - 4m(x, \mu) n(s|s)]. \] 

\[ \delta_2(x, \mu) = [x(1 - x)^{-1} (x - \mu)^{-1}]^{1/2}. \]

The expressions for \( m(x, \mu) \) and \( n(s|s) \) as given explicitly in Ref. 24, are very complicated. Here we only write down their limiting forms; namely,
\[
\lambda(x, s, \mu), m(x, \mu)^{x-1} \rightarrow 0^+.
\] (C15)

It should be pointed out that \(\lambda(x, s, \mu)\) and \(m(x, \mu)\) approaches zero slower than \(1/\delta_2(x, \mu)\) approaches zero when \(x \rightarrow 1^-\) (otherwise \(\Pi(x; ws|\mu)\) would no longer diverge).

We now deal with the coefficient of \(\Pi(\mu'/v; x|\mu)\) in (4.19b); namely, \(J'w\alpha'\). Eliminating \(P, \gamma\) in (4.20c), as we did in deriving (C6), we obtain
\[
J' = \frac{1}{32} |w|^3 v^{-3}(1 - v)^{-3}(v - \mu)^{-1} |jq - 2v(1 - v)|
\times (jq - c_+)(jq - c_-).
\] (C16)

Substitution of (C11) and (C16) into \(J'/w\alpha'\) leads to
\[
\frac{J'}{w\alpha'} \propto (G + \mu)^{-1} \sqrt{G}.
\] (C17)

Substituting \(x = \mu'/v\), and (12) into (4.19b) \(\delta\), we obtain
\[
\frac{J'}{w\alpha'} \propto (G + \mu)^{-1} \sqrt{G}.
\] (C18)

Combining (C13), (C15), and (C18), we finally obtain
\[
\frac{J'}{w\alpha'} \Pi(\mu'/v; ws|\mu) \mu'/v^{-1} \rightarrow 0^+.
\] (C19)

The cylindrical coordinate solution of (4.19a) and (4.19b) in this case takes the following simplified form:
\[
\rho^2(s) \rightarrow 4w^2 \mu N^{-2} \text{sn}^2(ws|\mu),
\]
\[
\varphi(s) \rightarrow -\frac{p}{s}.
\] (C20)

In this limit, there is no change in \(z(s)\) of (4.19c).

### APPENDIX D

In this Appendix we define functions \(f_i(s)\) (\(i=1,2,3\)) which are used in Sec. IV. Functions \(f_i(s)\) (\(i=1,2,3\)) are periodic functions of \(s\) [with the same period as that of \(\text{sn}^2(ws|\mu)\)], having values in range \([-1,1]\) and defined explicitly as
\[
f_1(s) = 1 - 2 \text{sn}^2(ws|\mu),
\] (D1)
\[
f_2(s) = Y(\mu'/v; ws|\mu)/Y(\mu'/v; \xi_2|\mu),
\] (D2)
\[
f_3(s) = Z(ws|\mu)/|Z(\xi_3|\mu)|.
\] (D3)

The function \(Z(x|\mu)\), known as the Jacobi's zeta function, is defined as
\[
Z(x|\mu) \equiv E(x|\mu) - x \frac{E}{K},
\] (D4)

is the periodic version of the elliptic integral of the second kind, \(E(\phi|\mu)\). The parameter \(\xi_3\) is determined from
\[
\sin^2(\phi(\mu)) = \frac{1}{1 - E \kappa^{-1}}.
\] (D5)

which satisfies \(\max Y(\mu'/v; ws|\mu) = |Z(\xi_3|\mu)|\).

The function \(Y(p; x|\mu)\) is defined similarly as
\[
Y(p; x|\mu) = \Pi(p; x|\mu) \alpha - \frac{\Pi(p)}{K},
\] (D7)

i.e., it is the periodic version of the elliptic integral of the third kind, \(\Pi(p; x|\mu)\). The parameter \(\xi_2\) is similarly determined from \((\partial/\partial x)Y(\mu'/v; ws|\mu)|_{\xi_2} = 0\), with one of its values given explicitly by
\[
\xi_2(\mu) = F(\phi(\mu)|\mu),
\] (D8)

\[
\sin^2(\phi(\mu)) = \frac{v}{\mu} \left[ 1 - K \kappa^{-2} \left( \frac{\mu'}{v} \right) \right].
\] (D9)

In deriving (D5) and (D8), the following identities have been used:
\[
E(nK|\mu) = nE,
\] (D11)
\[
\Pi(x; nK|\mu) = n\Pi(x),
\] (D12)

where \(n\) is an integer.

---

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Reference 17, see Chap. 17.


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Reference 14. See Eqs. (3.19) and (3.20). Jacobi Amplitude

Reference 17, Chap. 17. See Eqs. (17.7.10) to (17.7.13).