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The Schrödinger equation for a Kirchhoff elastic rod with noncircular cross section

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The extended Schrödinger equation for the Kirchhoff elastic rod with noncircular cross section is derived using the concept of complex rigidity. As a mathematical model of supercoiled DNA, the Schrödinger equation for the rod with circular cross section is a special case of the equation derived in this paper. In the twistless case of the rod when the principal axes of the cross section are coincident with the Frenet coordinates of the centreline, the Schrödinger equation is transformed to the Duffing equation. The equilibrium and stability of the twistless rod are discussed, and a bifurcation phenomenon is presented.

Keywords: Kirchhoff elastic rod, Schrödinger equation, DNA model
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1. Introduction

The analysis of the equilibrium and stability of a thin elastic rod has a long tradition in classic mechanics since 1730 via Bernoulli and Euler. This theoretical problem has an important application in the study of chemical and biological fibres such as the supercoiled structure of DNA. In 1859 Kirchhoff found the dynamic analogue of equilibrium of a thin elastic rod and the motion of a rigid body about a fixed point, and constituted fundamental equations for the equilibrium of the thin elastic rod.[1,2] In 1994, on the basis of the Kirchhoff equation, Shi and Hearst derived the Schrödinger equation with the curvature and twisting as unknown variables.[3−6] As a new mathematical model of supercoiled DNA the Schrödinger equation is suitable for the rod with circular cross section only. In the present paper, using a concept of complex rigidity of the rod, we extend the Schrödinger equation to the more generalized case when the rod has a noncircular cross section. The Schrödinger equation derived by Shi and Hearst was a special case of the extended Schrödinger equation. As another special case of the extended Schrödinger equation, the equilibrium of a twistless rod is discussed when the principal axes of the cross section are coincident with the Frenet coordinates of the centreline, and the extended Schrödinger equation is transformed to the Duffing equation. A qualitative analysis can be made in this case to discuss the equilibrium and stability of the rod, and a pitchfork bifurcation is presented.

2. Derivation of nonlinear Schrödinger equation

We treat a thin elastic rod with noncircular cross section. Let P be an arbitrary point on the centreline with arc-coordinate s. Establish the Frenet coordinate frame (P-nbt), where n-, b-, t-axes are normal, binomial and tangent of the centreline at point P respectively. A principal coordinate frame (P-xyz) is fixed on the cross section, where the $z-$axis is along the tangent t-axis and χ is the angle between coordinate planes (n,b) and (x,y). Let $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$, and $\boldsymbol{e}_n$, $\boldsymbol{e}_b$, $\boldsymbol{e}_t$ be basis vectors of (P-xyz) and (P-nbt); it follows that

$$\begin{aligned} &\boldsymbol{e}_n \cdot \boldsymbol{e}_1 = \boldsymbol{e}_b \cdot \boldsymbol{e}_2 = \cos\chi, \\ &\boldsymbol{e}_t = \boldsymbol{e}_3. \end{aligned} \tag{1}$$

Denote the curvature vector of the cross section at point P by $\boldsymbol{\omega}$, of which the components ω_i (i=1, 2, 3) in (P-xyz) can be determined by the curvature κ,

torsion τ and twisting angle χ as follows:

$$\begin{aligned}\omega_1 &= \kappa \sin\chi,\\ \omega_2 &= \kappa\cos\chi,\\ \omega_3 &= \tau + \dot{\chi},\end{aligned} \tag{2}$$

where the dot means the derivative with respect to the arc-coordinate s. Introduce a complex variable ξ, defined as

$$\xi = \omega_1 + \mathrm{i}\,\omega_2 = \kappa \exp\left(\frac{\pi}{2} - \chi\right). \tag{3}$$

The rod is subjected to a self-contact force $\boldsymbol{F}^{\mathrm{e}} = F_n^{\mathrm{e}}\boldsymbol{e}_n + F_b^{\mathrm{e}}\boldsymbol{e}_b$, of which the components F_i^{e} (i=1, 2, 3) in (P-xyz) can be written as

$$\begin{aligned}F_1^{\mathrm{e}} &= \frac{1}{|\xi|}(F_b^{\mathrm{e}}\omega_1 + F_n^{\mathrm{e}}\omega_2),\\ F_2^{\mathrm{e}} &= \frac{1}{|\xi|}(F_b^{\mathrm{e}}\omega_2 - F_n^{\mathrm{e}}\omega_1),\\ F_3^{\mathrm{e}} &= 0,\end{aligned} \tag{4}$$

where $|\xi| = \kappa$. Denote the resultant force and torque on the cross section at point P, respectively, by $\boldsymbol{F}$ and $\boldsymbol{M}$ with components F_i and M_i (i=1, 2, 3) in (P-xyz), and assume that the rod has an intrinsic twisting ω_3^0 in the relaxed state, then the following relationship should be satisfied:

$$\begin{aligned}M_1 &= A\omega_1,\\ M_2 &= B\omega_2,\\ M_3 &= C(\omega_3 - \omega_3^0),\end{aligned} \tag{5}$$

where A, B, C are the bending and twisting rigidities of the cross section about x-, y-, z-axes, respectively. Introduce a complex torque $M = M_1 + \mathrm{i}M_2$, and a complex rigidity D as

$$\begin{aligned}D &= D_1 + \mathrm{i}\,D_2,\\ D_1 &= A\sin^2\chi + B\cos^2\chi,\\ D_2 &= (B - A)\sin\chi\cos\chi,\end{aligned} \tag{6}$$

then the first two terms of Eq.(5) can be written in complex form,

$$M = D\xi. \tag{7}$$

The Kirchhoff equation of the rod in vector form is

$$\dot{\boldsymbol{F}} + \boldsymbol{\omega}\times\boldsymbol{F} + \boldsymbol{F}^{\mathrm{e}} = 0, \tag{8a}$$

$$\dot{\boldsymbol{M}} + \boldsymbol{\omega}\times\boldsymbol{M} + \boldsymbol{e}_t\times\boldsymbol{F} = 0, \tag{8b}$$

in which the derivatives with respect to the arc-coordinate s are performed in the (P-xyz). Defining complex forces $F = F_1 + \mathrm{i}F_2$ and $F^{\mathrm{e}} = F_n^{\mathrm{e}} + \mathrm{i}F_b^{\mathrm{e}}$, we can write the components of Kirchhoff equations (8a) and (8b) on x-, y-axes in complex form,

$$\dot{F} + \mathrm{i}(\omega_3 F - F_3\xi) - \mathrm{i}\frac{\xi}{|\xi|}F^{\mathrm{e}} = 0, \tag{9}$$

$$\dot{M} + \mathrm{i}(D\omega_3 - M_3)\xi + \mathrm{i}F = 0. \tag{10}$$

The components of Kirchhoff equations (8a) and (8b) on the z-axis can be written as

$$\dot{F}_3 + \mathrm{Im}(F\xi) = 0, \tag{11}$$

$$C\dot{\omega}_3 + D_2|\xi|^2 = 0. \tag{12}$$

In the case without contact force when $F^{\mathrm{e}} = 0$, the Kirchhoff equation permits a Jacobi integral as

$$\frac{1}{2}(D_1\kappa^2 + C\omega_3^2) + F_3 = H, \tag{13}$$

where the constant H is determined by values of ω_i and F_3 at initially given arc-coordinate s.

We solve F from Eq.(10) and obtain

$$F = \mathrm{i}\dot{M} - (D\omega_3 - M_3)\xi. \tag{14}$$

Substituting Eq.(14) and its derivative with respect to s into Eq.(9), in which M is expressed by Eq.(7), we obtain a complex differential equation as

$$D\ddot{\xi} + \mathrm{i}k_1\dot{\xi} + \frac{D_1}{2}|\xi|^2\xi + k_2\xi - \frac{\xi}{|\xi|}F^{\mathrm{e}} = 0, \tag{15}$$

where k_1 and k_2 are defined as

$$k_1 = 2D\omega_3 - C(\omega_3 - \omega_3^0) - 2\mathrm{i}\dot{D}, \tag{16a}$$

$$\begin{aligned}k_2 = &-H - C\omega_3^0\omega_3 + \left(\frac{3}{2}C - D\right)\omega_3^2\\ &+ \ddot{D} + \mathrm{i}[2\dot{D}\omega_3 - (C - D)\dot{\omega}_3].\end{aligned} \tag{16b}$$

Equation (15) is the Schrödinger equation for an elastic rod with non-circular cross section. The set of equations (15) and (12) is closed about complex variable ξ and real variable ω_3.

Substituting the exponential expression of ξ into complex equation (15) and separating them into real and imaginary parts, we obtain

$$D_1\ddot{\kappa} + 2(\dot{D}_1 - D_2\tau)\dot{\kappa} + \frac{1}{2}D_1\kappa^3 - \frac{\mu_1}{2}\kappa = F_n^{\mathrm{e}}, \tag{17a}$$

$$D_2\ddot{\kappa} + \mu_2\dot{\kappa} + \mu_3\kappa = F_b^{\mathrm{e}}, \tag{17b}$$

where

$$\begin{aligned}\mu_1 =&2[H + D_2\dot{\tau} - \ddot{D}_1 + (C\omega_3^0 + 2\dot{D}_2 - 2C\dot{\chi})\tau]\\ &- (3C - 2D_1)\tau^2 - C\dot{\chi}^2,\\ \mu_2 =&C(\omega_3^0 - \tau - \dot{\chi}) + 2(D_1\tau + \dot{D}_2),\\ \mu_3 =&(2\dot{D}_1 - D_2\tau)\tau + D_1\dot{\tau} + \ddot{D}_2 - C(\dot{\tau} + \ddot{\chi}).\end{aligned} \tag{18}$$

Equation (12) can be written as

$$C(\dot{\tau}+\ddot{\chi})+D_2\kappa^2=0. \tag{19}$$

The set of real differential equations (17) and (19) is closed about the curvature κ, torsion τ and twisting angle χ.

3. Special cases

3.1. A rod with circular cross section

For a rod with circular cross section, let $A=B$, then $D_1=A$, $D_2=0$, and Eq.(12) or Eq.(19) has a first integral as

$$\omega_3=\omega_{30} \quad \text{or} \quad \dot{\chi}=\omega_{30}-\tau, \tag{20}$$

which means that the twisting density ω_3 of the rod is constant. The coefficients of Schrödinger equations (15) and (17) become

$$\begin{aligned}
&k_1=2D\omega_3-C(\omega_{30}-\omega_3^0),\\
&k_2=-H-C\omega_3^0\omega_{30}+\left(\frac{3}{2}C-D\right)\omega_{30}^2,\\
&\mu_1=2(H+A\tau^2)-C\omega_{30}^2,\\
&\mu_2=C(\omega_3^0-\omega_{30})+2A\tau,\\
&\mu_3=A\dot{\tau}.
\end{aligned} \tag{21}$$

Substituting these into Eqs.(15) and (17), we obtain the Schrödinger equation derived by Shi and Hearst for a rod with circular cross section,[3,7,8]

$$\ddot{\xi}+\mathrm{i}\tilde{k}_1\dot{\xi}+\frac{1}{2}|\xi|^2\xi+\tilde{k}_2\xi-\frac{\xi}{|\xi|}\tilde{F}^{\mathrm{e}}=0, \tag{22}$$

or

$$\ddot{\kappa}-\kappa\left(\tau-\frac{Q}{2}\right)^2-c\kappa+\frac{1}{2}\kappa^3=\tilde{F}_n^{\mathrm{e}}, \tag{23a}$$

$$\kappa\dot{\tau}+2\dot{\kappa}\left(\tau-\frac{Q}{2}\right)=\tilde{F}_b^{\mathrm{e}}, \tag{23b}$$

where $\tilde{k}_i=k_i/A\ \ (i=1,2)$, $\tilde{F}^{\mathrm{e}}=F^{\mathrm{e}}/A$, and

$$\begin{aligned}
&c=\frac{H}{B}-\frac{Q^2}{4}-\frac{\lambda}{2}\left(\frac{Q}{\lambda}+\omega_0\right)^2,\\
&Q=\lambda(\omega_{30}-\omega_3^0),
\end{aligned} \tag{24}$$

where $\lambda=C/A$ is the ratio of rigidities.

3.2. Twistless rod

In the case of a rod with noncircular cross section, we rewrite Eq.(12) as

$$C\dot{\omega}_3=(A-B)\kappa^2\cos\chi\sin\chi. \tag{25}$$

As $A\neq B$, the twisting density ω_3 is constant only when $\chi\equiv j\pi/2$ (j=0, 1, ...), i.e. when the principal axes of the cross section are coincident with the Frenet coordinates of the centreline. Without loss of generality, let $\chi\equiv\pi/2$, then $\omega_1=\kappa$, $\omega_2=0$ and $D_1=A$, $D_2=0$. Since there is no twisting relative to the Frenet coordinates frame, $\dot{\chi}=0$, and the twisting density ω_3 is equivalent to the torsion τ. Let

$$\omega_3=\tau=\omega_{30}, \tag{26}$$

and the coefficient μ_1 is simplified to

$$\mu_1=2(H+C\omega_3^0\omega_{30})-(3C-2A)\omega_{30}^2. \tag{27}$$

Substituting Eq.(27) into Eq.(17a) and letting $F_n^{\mathrm{e}}=F_b^{\mathrm{e}}=0$, we obtain a Duffing equation of curvature κ,

$$\ddot{\kappa}-c\,\kappa+\frac{1}{2}\kappa^3=0, \tag{28}$$

where the coefficient c is defined as

$$c=\frac{H}{A}+\lambda\omega_3^0\omega_{30}+\left(1-\frac{3}{2}\lambda\right)\omega_{30}^2. \tag{29}$$

4. Stability analysis and bifurcation

The coefficient c of Duffing equation (28) can be written as

$$c=\left(\frac{3}{2}\lambda-1\right)(\mu-1)\,\omega_{30}^2, \tag{30}$$

where μ is a dimensionless parameter, depending on the initial condition of the rod

$$\mu=\left(\frac{3}{2}\lambda-1\right)^{-1}\left(\frac{H}{A\omega_{30}^2}+\frac{\lambda\omega_3^0}{\omega_{30}}\right). \tag{31}$$

Letting $\ddot{\kappa}=0$ leads to an equation of constant curvature κ_{s} as

$$\kappa_{\mathrm{s}}\left[(3\lambda-2)(1-\mu)\,\omega_{30}^2+\kappa_{\mathrm{s}}^2\right]=0. \tag{32}$$

Let $\lambda>2/3$ and $\mu\leq 1$, then Eq.(32) has only a trivial solution $\kappa_{\mathrm{s}}=0$, corresponding to a straight equilibrium of the rod. When $\mu>1$, as well as the trivial solution, there exist two nontrivial solutions $\kappa_{\mathrm{s}}=\pm\omega_{30}\sqrt{(3\lambda-2)(\mu-1)}$, corresponding to a helical equilibrium. The curvature κ_{s} of the rod has a pitchfork bifurcation at $\mu=1$, and a stability criterion of the straight equilibrium of the rod can be derived according to the theory of Poincaré as

$$\begin{aligned}
&\mu\leq 1: \quad \text{stable},\\
&\mu>1: \quad \text{unstable}.
\end{aligned} \tag{33}$$

In the case of straight equilibrium, let $\kappa_s = 0$, $F_3 = F_0$ and $\omega_{30} = M_0/C$, the constant H can be calculated from Eq.(13); and then substituting into Eq.(31), the stable condition $\mu \leq 1$ can be obtained:

$$F_0 \leq \frac{M_0^2}{C}\left(1 - \frac{A}{C} - \frac{\omega_3^0}{\omega_{30}}\right). \tag{34}$$

In a special case when $C = 2A$, $\omega_3^0 = 0$, the condition (34) is simplified to the same form as the Greenhill formula,[9]

$$F_0 \leq \frac{M_0^2}{4A}. \tag{35}$$

It is shown that the stability criterion for a straight rod with circular cross section under extension and torsion is effective for a twistless straight rod with noncircular cross section when the rigidities satisfy the Kovalevskaya condition $C = 2A$.

References

[1] Kirchhoff G 1859 *J. Reine Angew. Math.* **56** 285

[2] Love A E H 1944 *A Treatise on Mathematical Theory of Elasticity* 4th edn (New York: Dover) p381

[3] Shi Y and Hearst J E 1994 *J. Chem. Phys.* **101** 5186

[4] Tian Q and Ma B K 1999 *Acta Phys. Sin.* **48** 2125 (in Chinese)

[5] Liu J B and Cai X P 2001 *Acta Phys. Sin.* **50** 820 (in Chinese)

[6] Ruan H Y and Chen Y X 2001 *Acta Phys. Sin.* **50** 586 (in Chinese)

[7] Shi Y Borovi A E and Hearst J E 1995 *J. Chem. Phys.* **103** 3166

[8] Shi Y, Hearst J E *et al* 1998 *J. Chem. Phys.* **109** 2959

[9] Greenhill A G 1883 *Proc. Inst. Mech. Eng.* (London)