Vol 17 No 7, July 2008
1674-1056/2008/17(07)/2361-05

Chinese Physics B

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Structure properties and Noether symmetries for super-long elastic slender rod*

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(Received 18 September 2007; revised manuscript received 25 December 2007)

DNA is a nucleic acid molecule with double-helical structures that are special symmetrical structures attracting great attention of numerous researchers. The super-long elastic slender rod, an important structural model of DNA and other long-train molecules, is a useful tool in analysing the symmetrical properties and the stabilities of DNA. This paper studies the structural properties of a super-long elastic slender rod as a structural model of DNA by using Kirchhoff's analogue technique and presents the Noether symmetries of the model by using the method of infinitesimal transformation. Based on Kirchhoff's analogue it analyses the generalized Hamilton canonical equations. The infinitesimal transformations with respect to the radial coordinate, the generalized coordinates, and the quasi-momenta of the model are introduced. The Noether symmetries and conserved quantities of the model are obtained.

Keywords: super-long elastic slender rod, Kirchhoff's analogue, Noether symmetry, conserved quantity

PACC: 0420M, 4600, 0320

1. Introduction

Elastic rod has been studied over 200 years since the days of Bernoulli and Euler.[1] Its applications range from the telephone cable and formation of sunspots,[2] to the three-dimensional scroll waves.[1] In the last 30 years, slender elastic rods have also been used to the structure model of a long train molecules such as DNA, which plays an important role in analysing their symmetric structure and stabilities. Various aspects of elastic structure of DNA have been analysed by applying the theory of elastic rod, and physical constants such as Young's modulus and Poisson ratio have been obtained by special experiments.[3,4]

Most elastic models of DNA simplify the molecules as super-long slender cylindrical elastic rods (Fig.1). One important super-long elastic rod model is based on the Kirchhoff's dynamic analogue,[2] in which the radial coordinate of the elastic rod centreline is treated as the time variable of rigid body dynamics. Therefore, the model has the similar structure of the dynamical system which can be described by the Hamilton equations.

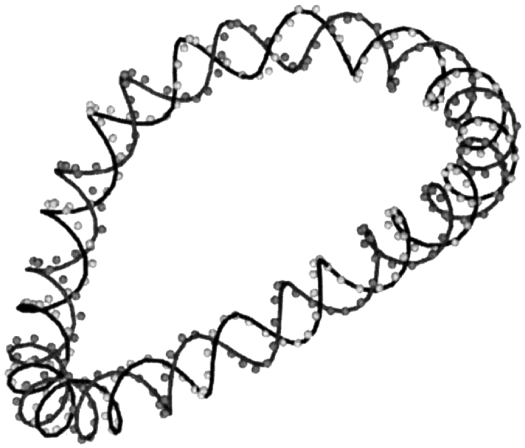


Fig.1. Discrete and continuous equilibrium configurations for the 12A09 DNA molecule (Robert S and John H 1996).

On the other hand, the theory of Lie group has been developed as a powerful tool for studying dynamical systems.[5−10] The symmetric theory has been widely used in mathematics, physics, mechanics and geometrical analysis of dynamical systems. A large body of literatures regarding the applications of Noether symmetries and Lie symmetries theory has been accumulated recently.[11−34]

In the symmetric theory, the transformation that

*Project supported by the National Natural Science Foundation of China (Grant Nos 10672143 and 60575055), the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences and the Natural Science Foundation of Henan Province Government of China (Grant No 0511022200).

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leaves the Hamilton action quantity invariant is called Noether symmetry, which induces conserved quantities. Taking the similarity of the structural models of super-long elastic slender rod and the dynamical models of mass points, we can borrow these concepts and theory to describe the Lie symmetrical properties of DNA along its central line.

In this paper, the Noether symmetries of a super long elastic round rod were studied. The generalized Hamilton canonical equations are established based on Kirchhoff theory. By means of infinitesimal transformation corresponding to radial coordinates, generalized coordinates, generalized momentum, the Noether symmetries, and the conserved quantities are derived.

2. Generalized Hamilton canonical equations

Assuming that $O-xyz$ is the inertial coordinate frame, the central line of an elastic rod can be described by a curve

$$r = r(s) : [0, L] \to R^3, \tag{1}$$

where $r(s)$ is a smooth curve of order ≥ 2 with s being the radial coordinate parameter and L the length of the rod. At a given point P of the rod central line, a Frenet coordinate frame $P-NTB$ is established. The three vectors $\boldsymbol{T}$, $\boldsymbol{N}$ and $\boldsymbol{B}$ are the unit vectors in the curve tangential direction, respectively (Fig.2). According to Kirchhoff's assumption,[1] we assume: (1) the length and the curvature of the radius of the rod are far greater than the scale of its cross section; (2) the rod is inextensible and unshearable.

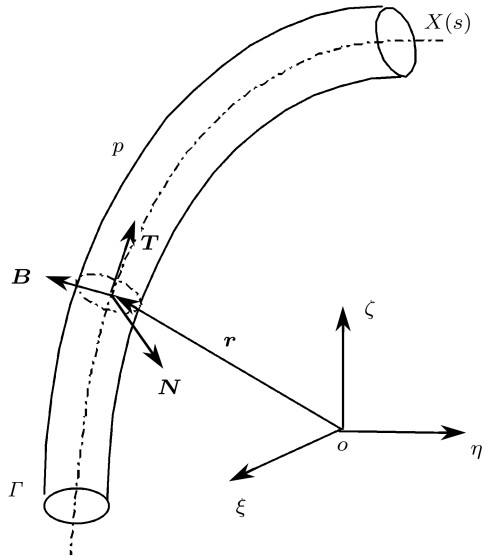


Fig.2. Sketch map of the elastic rod.

With these assumptions, the radial coordinate s can be considered as a quasi-time coordinate. The elastic rod surface was formed by a rigid closed plane curve Γ moving evenly along with 'time's. Let $X(s)$ be the position of moving curve Γ at time s, we move the original point O of inertial coordinate frame $O-xyz$ to its geometric centre P to set up a body fixed frame $P-xyz$ by using Euler angles (ψ, θ, φ) as the local variable of the curve $r(s)$. We have the equations depicting $r(s)$ under the frame,[1,4]

$$A\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\cos\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\sin\varphi\right)+(C-B)\left(-\frac{\mathrm{d}\theta}{\mathrm{d}s}\sin\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\cos\varphi\right)\left(\frac{\mathrm{d}\psi}{\mathrm{d}s}\cos\theta+\frac{\mathrm{d}\varphi}{\mathrm{d}s}\right)$$
$$-C\omega_0^3\left(-\frac{\mathrm{d}\theta}{\mathrm{d}s}\sin\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\cos\varphi\right)-F\sin\theta\cos\varphi=0, \tag{2}$$

$$B\frac{\mathrm{d}}{\mathrm{d}s}\left(-\frac{\mathrm{d}\theta}{\mathrm{d}s}\sin\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\sin\varphi\right)+(A-C)\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\cos\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\sin\varphi\right)\left(\frac{\mathrm{d}\psi}{\mathrm{d}s}\cos\theta+\frac{\mathrm{d}\varphi}{\mathrm{d}s}\right)$$
$$+C\omega_0^3\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\cos\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\sin\varphi\right)+F\sin\theta\sin\varphi=0, \tag{3}$$

$$C\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{\mathrm{d}\psi}{\mathrm{d}s}\cos\theta+\frac{\mathrm{d}\varphi}{\mathrm{d}s}\right)+(B-A)\left(\frac{\mathrm{d}\theta}{\mathrm{d}s}\cos\varphi+\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\sin\varphi\right)\left(\frac{\mathrm{d}\psi}{\mathrm{d}s}\sin\theta\cos\varphi-\frac{\mathrm{d}\varphi}{\mathrm{d}s}\sin\varphi\right)=0. \tag{4}$$

Introducing Hamilton like function,

$$H = \frac{1}{2}\Big[A\left(\theta\cos\varphi+\psi\sin\theta\sin\varphi\right)^2 +B\left(-\theta\sin\varphi+\psi\sin\theta\cos\varphi\right)^2 +C\left(\psi\cos\theta+\varphi\right)^2\Big]+F\cos\theta, \tag{5}$$

and denoting vectors $\boldsymbol{q}=(\psi,\theta,\varphi)^{\mathrm{T}}=(q_1,q_2,q_3)^{\mathrm{T}}$ and $\boldsymbol{p}=\boldsymbol{D}\boldsymbol{q}$ with

$$\boldsymbol{D}=\begin{pmatrix}\left(A\left(\sin\varphi\right)^2+B\left(\cos\varphi\right)^2\right)\left(\sin\theta\right)^2+C(\cos\theta)^2 & (A-B)\sin\theta\cos\varphi\sin\varphi & C\cos\theta\\ (A-B)\sin\theta\cos\varphi\sin\varphi & A(\cos\varphi)^2+B\left(\sin\varphi\right)^2 & 0\\ C\cos\theta & 0 & C\end{pmatrix}, \tag{6}$$

then we obtain

$$\begin{aligned}p_1 &= \psi\left[\left(A\sin^2\varphi+B\cos^2\varphi\right)\sin^2\theta+C\cos^2\theta\right]\\ &\quad+(A-B)\theta\sin\theta\cos\varphi\sin\varphi+C\varphi\cos\theta,\\ p_2 &= (A-B)\psi\sin\theta\cos\varphi\sin\varphi+A\theta\cos^2\varphi\\ &\quad+B\theta\sin^2\varphi,\\ p_3 &= C\psi\cos\theta+C\varphi.\end{aligned} \tag{7}$$

Equations (2)–(4) can be rewritten in generalized Hamilton canonical forms

$$\begin{aligned}&\dot{q}_1=\dot{\psi}=\frac{\mathrm{d}\psi}{\mathrm{d}s}=\frac{\partial H}{\partial p_1},\quad \dot{q}_2=\dot{\theta}=\frac{\mathrm{d}\theta}{\mathrm{d}s}=\frac{\partial H}{\partial p_2},\\ &\dot{q}_3=\dot{\varphi}=\frac{\mathrm{d}\varphi}{\mathrm{d}s}=\frac{\partial H}{\partial p_3},\quad \dot{p}_1=\frac{\mathrm{d}p_1}{\mathrm{d}s}=-\frac{\partial H}{\partial \psi},\\ &\dot{p}_2=\frac{\mathrm{d}p_2}{\mathrm{d}s}=-\frac{\partial H}{\partial \theta},\quad \dot{p}_3=\frac{\mathrm{d}p_3}{\mathrm{d}s}=-\frac{\partial H}{\partial \varphi}.\end{aligned} \tag{8}$$

Analogous to the dynamical descriptions, we call $\boldsymbol{p}$ the quasi-momentum. The parameters A and B are respectively the bending rigidity on the rod cross sections around axis x and y, while C is the twisting rigidity of the cross section around axis z. The variable of the Hamilton canonical form is s. Although the equations are not dynamical (in terms of time), we can still use existing techniques to discuss its Noether symmetries and conserved quantities.

For the circular cross section $A=B$, the generalized Hamilton canonical equations are

$$\begin{aligned}\dot{q}_1 &= \frac{\partial H}{\partial p_1}=\frac{p_1-p_3\cos q_2}{A\sin^2 q_2},\\ \dot{q}_2 &= \frac{\partial H}{\partial p_2}=\frac{p_2}{A},\\ \dot{q}_3 &= \frac{\partial H}{\partial p_3}=\frac{p_3}{C}-\frac{(p_1-p_3\cos q_2)\cos q_2}{A\sin^2 q_2},\\ \dot{p}_1 &= -\frac{\partial H}{\partial q_1}=0,\\ \dot{p}_2 &= -\frac{\partial H}{\partial q_2}=\frac{(p_1-p_3\cos q_2)(p_3-p_1\cos q_2)}{A\sin^3 q_2}\\ &\quad -F\sin q_2,\\ \dot{p}_3 &= -\frac{\partial H}{\partial q_3}=0.\end{aligned} \tag{9}$$

3. Noether symmetries and conserved quantities

Similar to the techniques used in analysing dynamical systems, we introduce the action of the Hamiltonian

$$S=\int_{s_1}^{s_2}\left[\sum_{i=1}^{3}p_i\dot{q}_i-H\left(s,\boldsymbol{q},\boldsymbol{p}\right)\right]\mathrm{d}s. \tag{10}$$

Let us introduce the infinitesimal transformations with respect to the radial coordinate, the generalized coordinate and the quasi-momentum respectively

$$\begin{aligned}&s^*=s+\Delta s,\\ &q_i^*(s^*)=q_i(s)+\Delta q_i,\\ &p_i^*(s^*)=p_i(s)+\Delta p_i,\qquad i=1,2,3,\end{aligned} \tag{11}$$

which can be expanded as

$$\begin{aligned}&s^*=s+\varepsilon\xi_0(s,\boldsymbol{q},\boldsymbol{p}),\\ &q_i^*=q_i+\varepsilon\xi_i(s,\boldsymbol{q},\boldsymbol{p}),\\ &p_i^*=p_i+\varepsilon\eta_i(s,\boldsymbol{q},\boldsymbol{p}),\quad i=1,2,3,\end{aligned} \tag{12}$$

where ε is a small parameter, ξ_0, ξ_s and η_s are infinitesimal generators. Substituting Eq.(12) into the variation of Eq.(10), we obtain

$$\begin{aligned}\Delta S &= \delta S+\dot{S}\Delta s=\int_{s_1}^{s_2}\left(p_i\delta\dot{q}_i+\dot{q}_i\delta p_i-\frac{\partial H}{\partial q_i}\delta p_i-\frac{\partial H}{\partial p_i}\delta q_i\right)\mathrm{d}s+(p_i\dot{q}_i-H)\Delta s\\ &= \int_{s_1}^{s_2}\left\{\frac{\mathrm{d}}{\mathrm{d}s}[p_i\delta q_i+(p_i\dot{q}_i-H)\Delta s]+\left(-\dot{p}_i-\frac{\partial H}{\partial p_i}\right)\delta q_i+\left(\dot{q}_i-\frac{\partial H}{\partial p_i}\right)\delta p_i\right\}\mathrm{d}s,\end{aligned} \tag{13}$$

and

$$\Delta S = \int_{s_1}^{s_2} \left\{ \Delta(p_i\dot{q}_i - H) + (p_i\dot{q}_i - H)\frac{\mathrm{d}}{\mathrm{d}s}(\Delta s) \right\} \mathrm{d}s$$
$$= \int_{s_1}^{s_2} \left\{ p_i\Delta\dot{q}_i + \dot{q}_i\Delta p_i - \frac{\partial H}{\partial s}\Delta s - \frac{\partial H}{\partial q_i}\Delta q_i - \frac{\partial H}{\partial p_i}\Delta p_i + (p_i\dot{q}_i - H)\frac{\mathrm{d}}{\mathrm{d}s}(\Delta s) \right\} \mathrm{d}s, \tag{14}$$

since

$$\Delta s = \varepsilon\xi_0(s, \boldsymbol{p}, \boldsymbol{q}),$$
$$\delta q_i = \Delta q_i - \dot{q}_i\Delta s = \varepsilon(\xi_i - \dot{q}_i\xi_0),$$
$$\delta p_i = \Delta p_i - \dot{p}_i\Delta s = \varepsilon(\eta_i - \dot{p}_i\xi_0). \tag{15}$$

Equation (13) can be reduced to

$$\Delta S = \int_{s_1}^{s_2} \varepsilon \left\{ \frac{\mathrm{d}}{\mathrm{d}s}[p_i(\xi_i - \dot{q}_i\xi_0) + (p_i\dot{q}_i - H)\xi_0] + \left(-\dot{p}_i - \frac{\partial H}{\partial q_i}\right)(\xi_i - \dot{q}_i\xi_0) + \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right)(\eta_i - \dot{p}_i\xi_0) \right\} \mathrm{d}s. \tag{16}$$

Now, we give the following definition and criteria of Noether symmetry for a super-long elastic slender rod by using Mei's method.[25]

Definition If the action ΔS of the Hamiltonian remains invariant under the Lie group of the transformation (12), the invariance is called the Noether symmetry of the system.

Criterion 1 If the infinitesimal transformation (11) satisfies

$$p_i\Delta\dot{q}_i + \dot{q}_i\Delta p_i - \frac{\partial H}{\partial s}\Delta s - \frac{\partial H}{\partial q_i}\Delta q_i - \frac{\partial H}{\partial p_i}\Delta p_i + (p_i\dot{q}_i - H)\frac{\mathrm{d}}{\mathrm{d}s}(\Delta s) = 0, \tag{17}$$

then the transformation is Noether symmetric for the system.

Criterion 2 If the infinitesimal transformation (12) satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[p_i\left(\xi_i - \dot{q}_i\xi_0\right) + \left(p_i\dot{q}_i - H\right)\xi_0\right] + \left(-\dot{p}_i - \frac{\partial H}{\partial q_i}\right)(\xi_i - \dot{q}_i\xi_0) + \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right)(\eta_i - \dot{p}_i\xi_0) = 0, \tag{18}$$

then the transformation is Noether symmetric for the system.

Using

$$\Delta\dot{q}_i = \varepsilon(\dot{\xi}_i - \dot{q}_i\dot{\xi}_0), \tag{19}$$

and

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \tag{20}$$

we obtain the Noether equation

$$p_i\xi_i - \frac{\partial H}{\partial s}\xi_0 - \frac{\partial H}{\partial q_i}\xi_i - H\dot{\xi}_0 = 0. \tag{21}$$

From Eq.(21), we can obtain the Killing equations

$$p_i\frac{\partial\xi_i}{\partial q_1} - H\frac{\partial\xi_0}{\partial p_1} = 0, \quad p_i\frac{\partial\xi_i}{\partial q_2} - H\frac{\partial\xi_0}{\partial p_2} = 0, \quad p_i\frac{\partial\xi_i}{\partial q_3} - H\frac{\partial\xi_0}{\partial p_3} = 0,$$
$$p_i\frac{\partial\xi_i}{\partial s} + p_i\frac{\partial\xi_i}{\partial q_1}\frac{\partial H}{\partial p_1} - \frac{\partial H}{\partial s}\xi_0 - \xi_i\frac{\partial H}{\partial q_i} - H\frac{\partial\xi_0}{\partial s} - H\frac{\partial\xi_0}{\partial q_1}\frac{\partial H}{\partial p_1} = 0,$$
$$p_i\frac{\partial\xi_i}{\partial s} + p_i\frac{\partial\xi_i}{\partial q_2}\frac{\partial H}{\partial p_2} - \frac{\partial H}{\partial s}\xi_0 - \xi_i\frac{\partial H}{\partial q_i} - H\frac{\partial\xi_0}{\partial s} - H\frac{\partial\xi_0}{\partial q_2}\frac{\partial H}{\partial p_2} = 0,$$
$$p_i\frac{\partial\xi_i}{\partial s} + p_i\frac{\partial\xi_i}{\partial q_3}\frac{\partial H}{\partial p_3} - \frac{\partial H}{\partial s}\xi_0 - \xi_i\frac{\partial H}{\partial q_i} - H\frac{\partial\xi_0}{\partial s} - H\frac{\partial\xi_0}{\partial q_3}\frac{\partial H}{\partial p_3} = 0. \tag{22}$$

Noether theorem If the infinitesimal generators $\xi_0(t, \boldsymbol{q}, \boldsymbol{p}), \xi_i(t, \boldsymbol{q}, \boldsymbol{p})$ and $\eta_i(t, \boldsymbol{q}, \boldsymbol{p})$ satisfy Noether identical equation (21), then system (8) possesses a conserved quantity.

$$I = p_i\xi_i - H\xi_0 = \text{const}. \tag{23}$$

The Killing equations have the solutions

$$\xi_0 = 1, \quad \xi_1 = 0, \quad \xi_2 = 0, \quad \xi_3 = 0, \tag{24}$$

$$\xi_0 = 0, \quad \xi_1 = 1, \quad \xi_2 = 0, \quad \xi_3 = 0. \tag{25}$$

Substituting infinitesimal generators (24) into Eq.(23), we get the conserved quantity for the super-

long elastic slender rod Eqs.(1)–(3).

$$I = H = \frac{1}{2}\left[A\left(\theta\cos\varphi+\psi\sin\theta\sin\varphi\right)^2 + B\left(-\theta\sin\varphi+\psi\sin\theta\cos\varphi\right)^2 + C\left(\psi\cos\theta+\varphi\right)^2\right] + F\cos\theta = \text{const}, \quad (26)$$

and substituting infinitesimal generators (25) into Eq.(23), we get the conserved quantity of the system

$$I = p_1 = \psi\left(A\sin^2\varphi + B\cos^2\varphi + C\cos\theta\right) + (A-B)\,\theta\sin\theta\cos\varphi\sin\varphi + C\varphi\cos\theta = \text{const}. \quad (27)$$

4. Conclusion

In summary, we have generalized the existing Noether symmetry for dynamical systems to the structural model of super-long elastic slender rod. The infinitesimal transformations with respect to radial coordinate, generalized coordinates, and quasi-momenta are also introduced to the model. The Noether symmetries and conserved quantities are obtained for this system. We believe that this technique can be useful for further study of symmetrical structures in biomolecular systems, and the results along this line will be reported in the future.

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