Stability analysis of kinked DNA in $\mathcal{F}(K, \tau)$ model

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(Dated: June 9, 2009)

Abstract

We phenomenologically analyze short DNA rings’ stability by discussing the second variation of its elastic free energy. Through expanding the perturbation functions as Fourier series, we obtain DNA rings’ stability condition in a general case. By reviewing the relationship between the Kirchhoff model and the worm-like road chain (WLRC) model, we insert a spontaneous curvature term which can partly reflect the twist angle’s contribution to free energy in the WLRC model and name this extended model the EWLRC model. By choosing suitable spontaneous curvature, stability analysis in this model provide us with some useful results which are consistent with the experimental observations.

PACS numbers:

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I. INTRODUCTION

An important biological function for DNA loops is that it has abundant deformations under different conditions. This deformations are mostly due to the interaction between the DNA chain and the environment. For instance, protein operation \[1\], ion concentration \[2, 3\] and temperature change \[4\] all can induce deformations. Since it has been found that DNA shapes and deformations can be investigated by the Kirchhoff elastic theory, much work have been done based on this theory \[5, 6, 7, 8, 9, 10, 11, 12, 13, 14\]. However, modern experimental techniques, such as optical tweezers \[15\], micromanipulation \[16, 17, 18\] and other techniques \[19, 20, 21\], indicate that DNA has abundant mechanic characteristics which cannot be explained by classical Kirchhoff theory. For example, under different pulling force, DNA has different stretching ability \[15\]. Thus, several different models have been suggested to describe DNA chain in different conditions. For instance, the wormlike chain (WLC) model \[22\] was used to describe DNA under a small external force. And the WLRC model \[23, 24, 25\] is appropriate to describe DNA with its double-helix structure under a moderate force. Further, following the increase of external force, new energy terms are introduced \[26\], and the results are highly consistent with the experimental observations.

Based on the Kirchhoff theory, the free energy density of duplex DNA chain can be written as

\[
F = \frac{1}{2} a_1 (K_1 - \bar{K}_1)^2 + \frac{1}{2} a_2 (K_2 - \bar{K}_2)^2 + \frac{1}{2} a_3 (K_3 - \bar{K}_3)^2, \quad (1)
\]

where \(K_1 = -x_2 \cdot (dx_3 / ds)\), \(K_2 = x_1 \cdot (dx_3 / ds)\), \(K_3 = x_2 \cdot (dx_1 / ds)\) and \(\{x_1, x_2, x_3\}\) denotes the basis of the local coordinates on DNA chain \[25, 27\], and \(s\) is the arc length of DNA centreline, \(a_1, a_2\) and \(a_3\) are constants. \(\bar{K}_1\) and \(\bar{K}_2\) are spontaneous curvature and \(\bar{K}_3\) is spontaneous tension. Let \(\phi = \phi(s)\) be the angle between \(x_1\) and the main normal \(n\), we have

\[
K_1 = K \cos \phi, \quad K_2 = K \sin \phi, \quad K_3 = \tau + \dot{\phi}, \quad (2)
\]

where \(K = K(s)\) and \(\tau = \tau(s)\) are the curvature and torsion of the DNA centreline. An overdot denotes a differential with respect to \(s\). Then the energy density in \[11\] can be
changed into
\[
\mathcal{F} = \mathcal{F}(K, \tau, \phi, \dot{\phi}) = \frac{1}{2} K^2 (a_1 \cos^2 \phi + a_2 \sin^2 \phi) - K (a_1 \bar{K}_1 \cos \phi + a_2 \bar{K}_2 \sin \phi) + \frac{1}{2} a_3 (\tau + \dot{\phi} - \bar{K}_3)^2 + \text{constant},
\]
and the shape equations are shown in [27]. Considering the energy density in (3) contains \(\phi\), thus, any \(\mathcal{F}(K, \tau)\) model, such as the Helfrich model [28], the WLRC model [23, 24, 25] and the WLC model [22], cannot be equal to the classical Kirchhoff model, because they cannot give any information about the twist angle \(\phi\). But specially choose \(a_1 = a_2 = A\) and \(a_3 = C\), and let \(\dot{\phi} = c = \text{constant}\), the energy density in (3) is reduced to
\[
\mathcal{F} = \frac{A}{2} K^2 - t_0 AK + \frac{C}{2} (\tau - c - \bar{K}_3)^2 + \text{constant},
\]
where \(t_0 = \bar{K}_1 \cos \phi + \bar{K}_2 \sin \phi\). If \(t_0 \equiv 0\), we get the WLRC model. But in this paper we choose \(t_0 = \text{constant}\) and \(\dot{\phi} = c = \text{constant}\), and name this model the extended worm-like road chain (EWLRC) model. We think the EWLRC model with \(t_0 = \text{constant}\) is better than the WLRC model to a certain extent because the arbitrary constant \(t_0\) can partly reflect that the twist angle \(\phi\) and spontaneous curvatures \(\bar{K}_1\) and \(\bar{K}_2\) influence DNA shapes. Then we choose energy density as the form
\[
\mathcal{F} = \frac{A}{2} (K - t_0)^2 + \frac{C}{2} (\tau - \omega_0)^2,
\]
where \(\omega_0 = \bar{K}_3 - c\) and we also name it the spontaneous tension. Clearly, the EWLRC model is different from the model discussed in [29] by choosing \(a_1 = a_2, \bar{K}_2 = 0\) and \(\bar{K}_3 = 0\) in (1).

By studying the second variation of DNA’s free energy, Zhao et al. [28] found that the chiral term in energy function could induce abundant shape transformations of DNA rings in the Helfrich model, which is in good agreement with the experimental observations in [2, 3]. In [29], Zhou et al. showed that the spontaneous curvature plays a significant role in the stability of kinked DNA. By choosing Euler angles as variable for the free energy function, Panyukov and Rabin [30] generally investigated the effects of thermal fluctuations on elastic rings and pointed out that spontaneous curvature is important in affecting the spatial configurations of the ring. In this paper, we discuss the second variation of the \(\mathcal{F}(K, \tau, \dot{K}, \dot{\tau})\) model and give stability condition of ring solution in Sec. II. In Sec. III
we take the EWLRC model as an example and obtain some useful results which are very consistent with experimental observations. Finally, a short discussion is given in Sec. IV.

II. SECOND VARIATIONS OF FREE ENERGY AND STABILITY CONDITION OF DNA RINGS

We choose the free energy for the closed duplex DNA with the form [31, 32]

\[ F = \oint \mathcal{F}(K, \tau, K', \tau') ds + \lambda \oint ds, \]  

(6)

where \( \mathcal{F} \) is an arbitrary function and \( ds \) is the element of the arclength \( s \), and \( \lambda \) is the Lagrange multiplier. The central axis \( \mathbf{R}(s) \) of duplex DNA chain under small perturbations can be written as

\[ \mathbf{R}'(s) = \mathbf{R}(s) + \psi(s)\mathbf{n} + \varphi(s)\mathbf{\beta}, \]  

(7)

where \( \psi(s) \) and \( \varphi(s) \) are two small smooth functions, and \( \mathbf{\beta} \) and \( \mathbf{n} \) are the binormal vector and the main normal vector, respectively. Under the perturbations, the general shape equations of DNA are attained in [32] by studying \( \delta F = 0 \). For the shape equations, a ring solution with radii \( R = 1/K \) and \( \tau = 0 \) induces

\[ \lambda = R^{-1}\mathcal{F}_1^0 - \mathcal{F}_0^0. \]  

(8)

Here we define \( \mathcal{F}_1 = \frac{\partial F}{\partial K}, \mathcal{F}_2 = \frac{\partial F}{\partial \tau}, \mathcal{F}_3 = \frac{\partial F}{\partial K'}, \mathcal{F}_4 = \frac{\partial F}{\partial \tau'}, \) and an up note ( )\(^0\) means in the case \( K = 1/R \) and \( \tau = 0 \), such as \( \mathcal{F}_1^0 = \mathcal{F}_1\big|_{(K=1/R, \tau=0)} \).

For different DNA models, they have different energy density functions : \( \mathcal{F}(K, \tau, K', \tau') \). For an arbitrary function \( \mathcal{F} \), we have

\[ \delta F = \delta (K) \mathcal{F}_1 + \delta (\tau) \mathcal{F}_2 + \delta (K') \mathcal{F}_3 + \delta (\tau') \mathcal{F}_4, \]  

(9)

\[ \delta (K) \mathcal{F} = \delta (K) \mathcal{F}_1 + \delta (\tau) \mathcal{F}_2 + \delta (K') \mathcal{F}_3 + \delta (\tau') \mathcal{F}_4 + \delta (K) \mathcal{F}_1 + \delta (\tau) \mathcal{F}_2 + \delta (K') \mathcal{F}_3 + \delta (\tau') \mathcal{F}_4 \]  

(10)
The first and second variations of total energy are
\[
\delta^{(1)} F = \oint \left[ (\mathcal{F} + \lambda)\delta^{(1)} \sqrt{\gamma} + \frac{1}{2} \delta^{(1)} \mathcal{F} \right] g^{-\frac{1}{2}} ds, \\
\delta^{(2)} F = \oint \left[ (\mathcal{F} + \lambda)\delta^{(2)} \sqrt{\gamma} + \frac{1}{2} \delta^{(2)} \mathcal{F} + \delta^{(1)} \mathcal{F} \delta^{(1)} \sqrt{\gamma} \right] g^{-\frac{1}{2}} ds.
\]

To obtain \(\delta^{(1)} F\) and \(\delta^{(2)} F\), those variations: \(\delta^{(1)} K, \delta^{(2)} K, \delta^{(1)} \dot{K}, \delta^{(2)} \dot{K}, \delta^{(1)} \tau, \delta^{(2)} \tau, \delta^{(1)} \tau\) and \(\delta^{(2)} \tau\) are indispensable. We give a method in Appendix A to obtain those useful terms.

For a planar ring with \(K = 1/R\) and \(\tau = 0\), we expand the two arbitrary functions \(\psi\) and \(\varphi\) as the following Fourier series
\[
\psi = c_0 + \sum_{n=1}^{\infty} c_n \cos(nKs) + \sum_{n=1}^{\infty} d_n \sin(nKs), \\
\varphi = e_0 + \sum_{n=1}^{\infty} e_n \cos(nKs) + \sum_{n=1}^{\infty} h_n \sin(nKs),
\]
and after a lengthy calculation, we get the second variation, it reads
\[
\delta^{(2)} F = p_0 + \sum_{n=1}^{\infty} \left[ p_n (c_n^2 + d_n^2) + q_n (e_n^2 + h_n^2) + 2m_n (c_n h_n - d_n e_n) + 2s_n (c_n e_n + d_n h_n) \right],
\]
with
\[
p_0 = \frac{\pi}{2} R^{-3} c_0^2 \mathcal{F}_{11}, \\
p_n = \frac{\pi}{2} R^{-3} (n^2 - 1)^2 (n^2 R^{-2} \mathcal{F}_{33}^0 + \mathcal{F}_{11}^0), \\
q_n = \frac{\pi}{2} R^{-2} n^2 (n^2 - 1) \left[ R^{-1} (n^2 - 1) (R^{-2} n^2 \mathcal{F}_{44}^0 + \mathcal{F}_{22}^0) + \mathcal{F}_{11}^0 \right], \\
m_n = \frac{\pi}{2} R^{-2} n (n^2 - 1) \left[ R^{-1} (n^2 - 1) (R^{-2} n^2 \mathcal{F}_{33}^0 + \mathcal{F}_{12}^0) - \mathcal{F}_{22}^0 \right], \\
s_n = \frac{\pi}{2} R^{-4} n^2 (n^2 - 1)^2 (\mathcal{F}_{23}^0 - \mathcal{F}_{14}^0).
\]
It is easy to find that \(n = 1\) is corresponding to a trivial translation. In the Eq. (13), if we don’t know whether \(p_n\) and \(q_n\) are positive or not, it seems difficult to discuss \(\delta^{(2)} F > 0\). Specially, if \(p_n\) and \(q_n\) are nonnegative, such as the Helfrich model \[28\], stability condition \(\delta^{(2)} F > 0\) yields
\[
p_n q_n - m_n^2 - s_n^2 > 0.
\]
For the Helfrich model and any \(F(K, \tau)\) model, we have \(\mathcal{F}_{23}^0 = \mathcal{F}_{14}^0 = 0\), then condition (15) is reduced to \(p_n q_n - m_n^2 > 0\). However, if \(p_n\) and \(q_n\) are nonnegative, only \(2m_n (c_n h_n - d_n e_n)\)
and $2s_n(c_ne_n + d_nh_n)$ in (13) have the possibility to be negative. So any stable deformations need

$$c_nh_n - d_ne_n < 0 \text{ or } c_ne_n + d_nh_n < 0. \tag{16}$$

It indicates that any deformations in this case are nonplanar, because we cannot choose $e_n = h_n = 0$. Then, tangential and normal deformations are coupled each other and they must occur simultaneously. Only when $p_n < 0$ in (13) can induce planar deformations ($c_n \neq 0, d_n \neq 0$ and $e_n = h_n = 0$).

### III. THE EWLRC MODEL

For the EWLRC model in (5) we assume $A > 0$ and $C > 0$, then the stability condition (15) is reduced to

$$\Delta = A(n^2 - 1)[A + C(n^2 - 1)] - A^2(n^2 - 1)t_0R - C^2\omega_0^2R^2 > 0. \tag{17}$$

By solving the above inequality, one gets the stable range of $R$. Here, we only show the upper boundary as an example

$$R < \frac{1}{2W^2\omega_0} \left[ \sqrt{(n^2 - 1)^2(t_0^2 + 4W^3) + 4W^2(n^2 - 1)} \right] + (n^2 - 1)\frac{t_0}{\omega_0}, \tag{18}$$

where $W = C/A$ and we let $\omega_0 > 0, t_0 > 0$. For DNA rings with fixed $R$, such as 168-bp DNA with $R \approx 9.1$ nm, inequality (18) implies that the lower states will be instable and rings will change into kinked shapes if $t_0$ decreases. Let $t_0$ be negatively related to the concentration of ion, this conclusion is consistent with the experimental results that complex deformations will emerge following the increase of ion concentration [3]. However, we have reverse conclusion for $\omega_0$ that it needs to be positively related to the concentration of ion. Specially, if $\omega_0 = 0$, we need that $t_0$ is positively related to the concentration of ion (we will see it in the late text).

Considering the helix solution $K = \frac{r_0}{r_0^2 + h^2}, \tau = \frac{h}{r_0^2 + h^2}$, the shape equations in [27, 31, 32] are reduced to ($\lambda = 0$)

$$A[(r_0^2 + h^2)t_0 - r_0][r_0^2(1 + r_0t_0) + h^2(r_0t_0 - 2)] + Cr_0[(r_0^2 + h^2)\omega_0 - h][(r_0^2 + h^2)\omega_0 + 3h] = 0. \tag{19}$$
TABLE I: The parameters for helix of A-, B-, and Z-DNA. Here $r_0$, $r_0/h$ and $\omega_0$ come from [33], $t_0$ is obtained by solving Eq. (19).

| DNA  | $r_0$ (nm) | $r_0/h$ | $\omega_0$ (nm$^{-1}$) | $t_0$ (nm$^{-1}$) |
|------|------------|---------|------------------------|--------------------|
| A-DNA | 1.3        | 3.32    | 2.55                   | 0.69 or -0.56      |
| B-DNA | 1.0        | 1.89    | 1.89                   | 0.77 or -0.33      |
| Z-DNA | 0.9        | 1.24    | 1.38                   | 0.66 or 0.22       |

Choosing $A = 50$ nm, $C = 0.15$ nm and the values of $r_0, h, \omega_0$ in [33], we obtain the corresponding $t_0$ shown in Table I. Specifically, letting $h = 0, r_0 = R$, we get the equation for a ring

$$A(1 - R^2 t_0^2) - CR^2 \omega_0^2 = 0. \tag{20}$$

Solving the above equation, we get $t_0$ in Table II for 168-bp DNA and 126-bp DNA ($R \approx 6.8$ nm). However, these constants in Tables I and II only give us some coarse values, because the experimental observations require that $\omega_0$ and $t_0$ should relate to ion concentration. Actually, using these constants is difficult to explain the phenomena that 126-bp circles in 1 mM Zn$^{2+}$ mostly are not kinked but 168-bp circles mostly are kinked in the same condition [3].

Specially choosing $W = 0.154$ and $\omega_0 = 0$ suggested by Thamwattana et al. [33], condition (18) is reduced to

$$R < \frac{(n^2 - 1)W + 1}{t_0}. \tag{21}$$

Clearly, we need that $t_0$ is positively related to the concentration of ion to explain that high state deformation occurs following the increase of ion concentration [3]. Moreover, with the same $W$ and $t_0$, Eq. (21) indicates that a big DNA ring will have higher state deformation than a small one has. Supposing two rings with radius $R_1$ and $R_2$ ($R_1 < R_2$) are in the same...
TABLE II: The spontaneous curvature $t_0$ (nm$^{-1}$) obtained by solving Eq. (20) of A-, B-, and Z-DNA.

| DNA   | A-DNA | B-DNA | Z-DNA |
|-------|-------|-------|-------|
| 168-bp| 0.037 | 0.080 |       |
| 126-bp| 0.046 | 0.104 | 0.126 |

**FIG. 1:** Stable ranges of DNA rings with $W = 0.154$, $\omega_0 = 0$ and different $t_0$ (nm$^{-1}$). From a to b, elliptic shapes will emerge for 126-bp DNA; from c to d, there are trigonal shapes for 168-bp DNA, which is consistent with the value that the number of kinks per circle is 3.83 [3].

Condition (with the same $W$ and $t_0$), letting $T(n) = (n^2 - 1)W + 1$, we have

$$\frac{T(n_2)}{R_2} < t_0 < \frac{T(n_1)}{R_1},$$

(22)

where, $n_1$ and $n_2$ ($n_1 \leq n_2$) lie on the deformation level of the two rings with radius $R_1$ and $R_2$, respectively. Han et al. [3] find that 126-bp circles ($R_1 = 6.8nm$) in 1 mM Zn$^{2+}$ mostly are not kinked and have somewhat elliptical shapes ($n_1 < 3$) and 168-bp circles ($R_2 = 9.1nm$) in 1 mM Zn$^{2+}$ mostly are kinked, then we have

$$\frac{T(n_2)}{9.1} < t_0 < \frac{T(3)}{6.8},$$

(23)
We find that only $n_2 = 3$ can ensure $t_0$ is existent. So trigonal deformation will emerge for 168-bp DNA, which is consistent with the experimental result that the number of kinks is 3.83 per circler for 168-bp DNA in [3]. Then, we get $0.245 \, nm^{-1} < t_0 < 0.328 \, nm^{-1}$. Fig. 1 shows the stable range of two kinds of DNA rings with $W = 0.154$ and $\omega_0 = 0$ in (21), from which we can see that trigonal deformation will arise for 168-bp DNA rings and elliptic deformation will emerge for 126-bp DNA rings.

In (22) the existence of $t_0$ induces
\begin{equation}
W[(n_2^2 - 1)R_1 - (n_1^2 - 1)R_2] < R_2 - R_1.
\end{equation}
Choosing $R_1 = 6.8$ nm, $R_2 = 9.1$ nm and $n_1 = 3$, we find that the above condition can always be satisfied with any $W$ (note we assume $W > 0$) when $n_2 \leq 3$, because the left side of (24) is negative. This implies that 168-bp DNA rings with any $W$ will change into trigonal shapes when 126-bp DNA rings change into elliptic shapes in the same condition.

IV. CONCLUSIONS

We have generally investigated the second variation of DNA rings and shown the stability condition. However, only and if only $p_n \geq 0$ and $q_n \geq 0$ condition (15) is valid. The EWLRC model and the Helfrich model are satisfied with this condition, and deformations in those models are must nonplanar. If $\omega_0 = 0$, the stability condition (21) needs that $t_0$ is positively related to the ion concentration. Considering $t_0 = \bar{K}_1 \cos \phi + \bar{K}_2 \sin \phi$ and we choose $\phi = constant$, which is consistent the conclusion in [29] that the intercalation of Zn$^{2+}$ takes place mainly at the exposed side of the DNA ring hence causing an increase in its spontaneous curvature. In [3] Han et al. find that there are somewhat elliptic shapes for 126-bp DNA and that the number of kinks is 3.83 per circler for 168-bp DNA in 1 mM Zn$^{2+}$, by choosing $W = 0.154$, $\omega_0 = 0$ and $0.245 \, nm^{-1} < t_0 < 0.328 \, nm^{-1}$ in the EWLRC model, our results are very consistent with this phenomenon.
Acknowledgements

We thank Wang Jing for her helpful correction of our manuscript.

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Appendix A

In this appendix, we present a method to obtain $\delta^{(1)} K$, $\delta^{(2)} K$, $\delta^{(1)} \dot{K}$, $\delta^{(2)} \dot{K}$, $\delta^{(1)} \tau$, $\delta^{(2)} \tau$, $\delta^{(1)} \dot{\tau}$ and $\delta^{(2)} \dot{\tau}$. For simplicity, we only give the method and key steps. The variation of $R(s)$ is

$$\delta R = R' - R = \psi n + \varphi \beta.$$  \hspace{1cm} (25)

Let $g = R_{,x} \cdot R_{,x}$ ($R_{,x} = \frac{dR}{dx}$, $x$ is the variable in orthogonal coordinates), we have $ds = \sqrt{g} dx$ and

$$\delta g^\frac{1}{2} = -g^\frac{1}{2} K \psi + \frac{1}{2} g^\frac{1}{2} \left[ \psi^2 + (\psi^2 + \varphi^2) \tau^2 + \varphi^2 \right. \left. + 2(\psi \dot{\varphi} - \psi \varphi \tau) \right] + O(3),$$

$$\delta g^\frac{1}{2} = g^\frac{1}{2} K \psi - \frac{1}{2} g^\frac{1}{2} \left[ \psi^2 + (\psi^2 + \varphi^2) \tau^2 + \varphi^2 \right. \left. - 2\psi^2 K^2 + 2(\psi \dot{\varphi} - \psi \varphi \tau) \right] + O(3).$$  \hspace{1cm} (26)

Where $O(3)$ means the third and higher orders of $\psi$ and $\varphi$. For an arbitrary function $V = V(s)$, there is

$$\delta \dot{V} = (1 + g^\frac{1}{2} \delta g^\frac{1}{2}) (\delta V)_{,s} + g^\frac{1}{2} \dot{V} \delta g^\frac{1}{2}.$$  \hspace{1cm} (27)
Using above equation, we have

$$\delta \dot{R} = (1 + g^{\frac{1}{2}} g^{-\frac{1}{2}})(\delta R),_s + g^{\frac{1}{2}} \dot{R} g^{-\frac{1}{2}},$$

$$\delta \ddot{R} = (1 + g^{\frac{1}{2}} g^{-\frac{1}{2}})(\delta \dot{R}),_s + g^{\frac{1}{2}} \ddot{R} g^{-\frac{1}{2}}.$$

(28)

Then, we get

$$\delta K^2 = 2 \ddot{R} \cdot \delta \ddot{R} + \delta \ddot{R} \cdot \delta \dot{R}.$$

Consequently, we attain

$$\delta K = \frac{1}{2} (K^2)^{-1/2} \delta K^2 - \frac{1}{8} (K^2)^{-3/2} (\delta K^2)^2 + \cdots$$

$$= (K^2 - \tau^2) \psi - \dot{\tau} \varphi - 2 \tau \dot{\varphi} + \ddot{\psi} + K \left[ K^2 \psi^2 - \frac{1}{2} \tau^2 (\varphi^2 + 6 \psi^2) - 2 \tau \varphi \psi - 6 \tau \dot{\varphi} \psi - \dot{\varphi}^2 + \frac{1}{2} \psi^2 + \ddot{\psi} + K \psi (\dot{\psi} - \tau \varphi) + \frac{1}{2} K^{-1} (\ddot{\varphi} + \dot{\tau} \psi + 2 \tau \dot{\varphi} - \tau^2 \varphi)^2 + O(3).$$

(29)

Now, we have

$$\delta K^{-1} = -K^{-2} \delta K + K^{-3} (\delta K)^2 + \cdots.$$  

(30)

The variation of \( n \) is

$$\delta n = K^{-1} \delta \dot{R} + \dot{\delta} K^{-1} + \ddot{\delta} K^{-1}.$$  

(31)

The variation of \( \dot{n} \) can be obtained by

$$\delta \dot{n} = (1 + g^{\frac{1}{2}} g^{-\frac{1}{2}})(\delta n),_s + g^{\frac{1}{2}} \dot{n} g^{-\frac{1}{2}}.$$  

(32)

The first variation of tension is

$$\delta^{(1)} \tau = K(2 \tau \psi + \dot{\varphi}) + K^{-2} \dot{K} \left( \tau^2 \varphi - \ddot{\tau} \psi - 2 \tau \dot{\psi} - \dot{\varphi} \right) + K^{-1} \left[ \ddot{\tau} \psi + 2 \tau \dot{\psi} - \tau^2 \dot{\varphi} + \varphi^{(3)} + 2 \tau (\ddot{\psi} - \varphi \dot{\tau}) \right].$$

(33)

Considering \( \dot{n} \cdot \ddot{n} = K^2 + \tau^2 \), we have

$$\delta^{(2)} \tau = \frac{1}{2} \tau^{-1} \left[ 2 \dot{n} \cdot \delta^{(2)} \ddot{n} + \left( \delta^{(1)} \dot{n} \right)^2 - \delta^{(2)} K^2 - \left( \delta^{(1)} \tau \right)^2 \right].$$

(34)
Inserting (29), (32) and (33) into (34), after a lengthy calculation, we get

\[ \delta^{(2)} \tau = K^2 \psi (3 \tau \psi + 2 \dot{\phi}) - \tau^3 (\psi^2 + \varphi^2) - 5 \tau \tau \psi \phi \]
\[ + \tau^2 (\dot{\psi} \phi - 5 \psi \dot{\phi}) + 2 \tau (\dot{\psi}^2 - \dot{\phi}^2 + 3 \psi \psi) \]
\[ + \tau (8 \ddot{\psi} \psi - \dot{\phi} \phi) + 2 \ddot{\psi} \psi^2 + 2 \varphi (\psi) \psi + 2 \psi \dot{\phi} \phi \]
\[ + 2 \dot{\phi} \psi + K^{-1} \left[ \dddot{K} \psi (\tau \psi + \phi) + \dddot{K} (\dot{\psi} \phi) \right] \]
\[ + \tau^2 \psi \psi \phi \right] + K^{-2} \left\{ - \dddot{K}^2 \psi (\dot{\phi} + \tau \psi) \right. \]
\[ + \tau^2 \left[ 2 \tau (\psi^2 - \varphi^2) + 3 \psi \dot{\phi} + 3 \psi \phi \right] + 2 \tau^3 (\psi^2 - \varphi^2 + \dddot{\psi} \psi - \dddot{\phi} \phi - 2 \dddot{\psi} \phi \psi) \]
\[ + \tau^2 (5 \ddot{\psi} \phi + 5 \ddot{\phi} \phi + \psi (3) \phi + \psi \phi (3)) \]
\[ + \tau (3 \ddot{\phi} \phi - 3 \dddot{\psi} \psi + \psi (3) \phi - \psi (3) \phi) \]
\[ + 2 \tau (\ddot{\phi}^2 - \dddot{\psi} \psi + \phi (3) \phi + \psi (3) \phi) \]
\[ + \tau^2 \dddot{K} (\psi \psi - \phi \phi) \]
\[ + 2 \tau \tau \psi \phi + 4 \tau \tau (\dddot{\psi} \phi + \dddot{\phi} \phi + 3 \dddot{\psi} \phi) \]
\[ + \tau \dddot{\phi} \phi - \dddot{\psi} \psi \phi) + 2 \tau \tau (\dddot{\psi} \phi + \dddot{\phi} \phi) \]
\[ - \psi (3) \phi - \dddot{\phi} \phi (3) - \tau^4 (\dddot{\psi} \phi + \dddot{\phi} \phi) \}
\[ + 2 K^{-3} \dddot{K} (\tau^2 \psi + \tau \phi + 2 \tau \phi - \psi) \]
\[ \times (\tau^2 \varphi - \tau \phi - 2 \tau \phi - \dddot{\phi}) \]. \tag{35} \]

Considering (27), we have

\[ \delta \dddot{K} = (1 + \frac{1}{2} \delta \dddot{g} - \delta \dddot{\tau}) (\delta K), + g \frac{1}{2} \dddot{K} \delta \dddot{g} - \delta \dddot{\tau}, \tag{36} \]
\[ \delta \dddot{\tau} = (1 + \frac{1}{2} \delta \dddot{g} - \delta \dddot{\tau}) (\delta \tau), + g \frac{1}{2} \dddot{\tau} \delta \dddot{g} - \delta \dddot{\tau}. \tag{37} \]

Here, for simplicity, we only give \( \delta \dddot{K} \) and \( \delta \dddot{\tau} \) for a planar ring with \( K = 1/R \) and \( \tau = 0 \), they are

\[ \delta^{(1)} \dddot{K} = R^{-2} \dddot{\psi} + \psi (3) \], \tag{38} \]
\[ \delta^{(2)} \dddot{K} = 3 R^{-3} \dddot{\psi} \dddot{\psi} + R^{-1} (3 \psi \dddot{\psi} (3) + 3 \dddot{\psi} \dddot{\psi} + 2 \dddot{\phi} \dddot{\phi}) + R \dddot{\phi} \dddot{\phi} (3), \tag{39} \]
\[ \delta^{(1)} \dddot{\tau} = R^{-1} \dddot{\phi} + R \varphi (4), \tag{40} \]
\[ \delta^{(2)} \dddot{\tau} = R^{-2} (3 \dddot{\phi} \dddot{\phi} + 2 \dddot{\phi} \dddot{\phi}) - R^2 (\dddot{\phi} \dddot{\phi} (4) + \dddot{\phi} \dddot{\phi} (4) + 2 \psi (3) \phi (3)) \]
\[ + 4 \dddot{\phi} \dddot{\phi} + 4 \dddot{\phi} \dddot{\phi} (3) + 3 \psi \dddot{\phi} (4) + 2 \psi (3) \phi. \tag{41} \]