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General equilibrium shape equations of polymer chains

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The general equilibrium shape equations of polymer chains are analytically derived in this paper. This provides a unified description for many models, such as the well-known wormlike chain (WLC) model, the wormlike rod chain (WLRC) model, carbon nanotubes, and so on. Using the WLC model, we find that the pitch-to-radius ratio of coils, 4.443, agrees with Z-DNA, and the pitch-to-radius ratio from WLRC agrees with the data of B-DNA qualitatively. Using the general shape equations, we discuss a chiral model in which the solutions of straight, helical, and circular biopolymers are given, respectively. We also find that the model suggested by Helfrich [Langmuir **7**, 567 (1991)] is very appropriate to describe B-DNA (or other biopolymers) if we choose the four phenomenological parameters as $A=50$ nm, $C=60$ nm^2, $\alpha=40$ nm^3, and $\beta=50$ nm^2.

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I. INTRODUCTION

The shapes and topological properties of polymer chains (such as proteins and DNA) play a significant role during processes such as replication and transcription [1,2]. Experimentally, a lot of techniques are available to study the conformation of polymer chains by bending or twisting them [2]. And theoretically, many models have been suggested to describe polymer chains. For example, the wormlike chain (WLC) model [3] was established to describe the DNA under a small external force [<10 picoNewton (pN)] and torque or semiflexible biopolymers such as actin, with a single elastic constant as the bending modulus. Another model, the wormlike rod chain (WLRC) model [4] is appropriate to describe DNA with its double-helix structure under a moderate force. The conformations of polymer chains are approached by using Lagrangian mechanics [5–9]. However, although considerable work has been done on various equilibrium properties (for instance, the force-extension relation of DNA) of all these models, the general equilibrium shape equations of polymer chains have not been determined so far. It plays a crucial role in understanding the properties of polymer chains. On the other hand, equilibrium shape equations of vesicle membranes were derived [10] over ten years, by which some characters of membranes have been studied theoretically. It is significant to determine the equilibrium shape equations of polymer chains. From them, the properties of polymer chains can be studied theoretically and their behaviors can be understood well.

Generally, the shape of a polymer chain is characterized by its curvature and torsion. The effects of bending, twisting, and the bend-twist coupling of the polymer chain are described by a free energy functional [11]. For simplicity, the contribution of the torsion is often neglected in the free energy [12,13]. However, the contribution of the torsion plays an important role in the conformation of polymer chains [14]. It is necessary to study the general equilibrium shape equations of polymer chains and the corresponding physical effects.

In this paper, we consider the free energy density as a functional of curvature and torsion of a polymer chain to study its general equilibrium equations. In Sec. II, by making use of differential geometry and calculating the variation of the free energy functional, we obtain the precise form of the general equilibrium shape equations of a polymer chain. In Sec. III, we bring the WLC model, the WLRC model, and the results obtained by Feoli *et al.* [12] into the present theory as special examples. The typical solutions of the corresponding equilibrium shape equations are investigated, and conformations of the polymer chains such as DNA are discussed in detail. In Sec. IV, we study the equilibrium equations of a chiral model derived in Ref. [14]. The conformations of DNA are discussed in the model. Section V is the conclusion.

II. THE GENERAL EQUILIBRIUM SHAPE EQUATIONS OF POLYMER CHAINS

Taking into account the one-dimensional nature of many polymer chains, we may write the free energy F as a functional defined on smooth curves $X(s)$ in three-dimensional Euclidean space,

$$F=\int \mathcal{F}[X(s)]ds,$$

where s is the length of a polymer chain and $\mathcal{F}$ is a scalar free energy density functional, which depends on the position vector $X(s)$ which describes the spatial shape of polymer chains. In three-dimensional ambient space, a smooth curve has two local invariants: curvature $\kappa(s)$ andtorsion $\tau(s)$.

The first principal curvature $\kappa(s)$ of a curve characterizes the local bending of the curve at the point s. Hence, the dependence of the free energy density $\mathcal{F}$ on $\kappa(s)$ specifies the resistance of a polymer chain to be bent, while the second curvature or torsion $\tau(s)$ is determined by the relative rotation [13] around the tangent $dX(s)/ds$ at the point s of two-

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neighbor infinitely short elements of the polymer chain. Usually, people consider the free energy F as a functional only depending on curvature $\kappa(s)$, namely $\mathcal{F}=\mathcal{F}[\kappa(s)]$, because a rotation of a polymer chain results in only a small energy difference, allowing many overall conformations of a polymer chain to arise [13]. In this paper, considering the chirality and in order to obtain the precise form of the general shape equations of polymer chains, we add some terms regarding torsion and the derivative of curvature. Thus the free energy density $\mathcal{F}$ can be written as

$$\mathcal{F}=\mathcal{F}[\kappa(s),\tau(s),\kappa_s(s)]. \tag{2.1}$$

where $\kappa_s(s)=d\kappa(s)/ds$. Namely, the free energy density $\mathcal{F}$ is a function depending on curvature $\kappa(s)$, the derivative of curvature, and torsion $\tau(s)$. Thus the free energy F has the form

$$F=\int \mathcal{F}[\kappa(s),\tau(s),\kappa_s(s)]ds=\int \mathcal{F}(\kappa,\tau,\kappa_s)ds. \tag{2.2}$$

We use a natural parametrization of the curve $X(s)$ in three-dimensional Euclidean space $x^i(s), i=1,2,3$, to describe a polymer chain. In this parametrization,

$$\frac{dx^i}{ds}\frac{dx^i}{ds}=(X',X')=1$$

or

$$ds^2=dx^i dx^i=(dX,dX), \tag{2.3}$$

where (,) denotes the inner product. As usual, the sum over the repeated indexes is assumed in the corresponding range and, for convenience, differentiation with respect to the natural parameter s will be denoted by a prime. Thus the curvature $\kappa(s)$ can be defined as

$$\kappa^2(s)=\frac{d^2x^i}{ds^2}\frac{d^2x^i}{ds^2}=(X'',X''). \tag{2.4}$$

For an arbitrary functional F defined on smooth curves $x^i(s)$ in three-dimensional space, the Euler-Lagrange equations are a set of three equations

$$\frac{\delta F}{\delta x^i}=0, \quad i=1,2,3. \tag{2.5}$$

We shall use the orthonormal Frenet basis $\{e_a\}$ associated with the curve $X(s)$, where

$$(e_a,e_b)=\delta_{ab}, \quad a,b=1,2,3, \tag{2.6}$$

and the Frenet equations governing the motion of this basis along the curve $X(s)$,

$$\frac{de_a}{ds}=\omega_{ab}e_b, \quad \omega_{ab}+\omega_{ba}=0, \tag{2.7}$$

where

$$\omega_{1,2}=-\omega_{2,1}=\kappa(s), \quad \omega_{2,3}=-\omega_{3,2}=\tau(s). \tag{2.8}$$

The first vector, e_1, is directed along the tangent of the curve at the point s, or $e_1(s)=dX/ds=X'$. The variation of the space form of the polymer chain,

$$\delta X(s)=\varepsilon_a(s)e_a(s), \quad a=1,2,3, \tag{2.9}$$

results in the following variation of the free energy functional (2.2):

$$\delta F=\delta F_1+\delta F_2+\delta F_3+\delta F_4, \tag{2.10}$$

where

$$\delta F_1=\int ds\mathcal{F}_1'\delta k(s), \quad \delta F_2=\int ds\mathcal{F}_2'\delta\tau(s),$$

$$\delta F_3=\int ds\mathcal{F}_3'\delta k_s(s), \quad \delta F_4=\int \mathcal{F}\delta ds, \tag{2.11}$$

and $\mathcal{F}_1'=\partial\mathcal{F}/\partial k$, $\mathcal{F}_2'=\partial\mathcal{F}/\partial r$, and $\mathcal{F}_3'=\partial F/\partial\kappa_3$. The variation δds is calculated in a straightforward way,

$$\delta ds=\delta\sqrt{dx^i dx^i}=\frac{dx^i\delta dx^i}{ds}=\frac{dx^i}{ds}d(\delta x^i)=(X',d\delta X). \tag{2.12}$$

The substitution of Eq. (2.12) into δF_3 in Eqs. (2.11) and the subsequent integration gives

$$\delta F_4=-\int(\mathcal{F}_1'\kappa'+\mathcal{F}_2'\tau')(X',\delta X)ds-\int \mathcal{F}(X'',\delta X)ds. \tag{2.13}$$

By making use of the Frenet equations (2.7) and the variation (2.9), one can derive

$$(X',\delta X)=(e_1,\delta X)=\varepsilon_a(e_1,e_a)=\varepsilon_{1,}$$

$$(X'',\delta X)=(e_1',\delta X)=\omega_{12}(e_2,\delta X)=\kappa\varepsilon_2. \tag{2.14}$$

Then we have

$$\delta F_4=-\int(\mathcal{F}_1'\kappa'+\mathcal{F}_2'\tau')\varepsilon_1(s)ds-\int \mathcal{F}\kappa\epsilon_2(s)ds. \tag{2.15}$$

In order to calculate the variation δF_1, we must find the variation of the curvature $\delta\kappa(s)$. Definition (2.3); and the Frenet equations (2.7) give

$$\kappa(s)\delta\kappa(s)=(X'',\delta X'')=(e_1',\delta X'')=\kappa(e_2,X'').$$

Hence

$$\delta\kappa=(e_2,\delta X''). \tag{2.16}$$

Applying Eq. (2.12), one can derive

$$\begin{aligned}\delta X'&=\delta\frac{dX}{ds}\\&=\frac{d}{ds}\delta X-\frac{dX(X',d\delta X)}{ds^2}\\&=\frac{d}{ds}\delta X-X'\left(X',\frac{d}{ds}\delta X\right)\\&=\frac{d}{ds}\delta X-e_1\left(e_1,\frac{d}{ds}\delta X\right),\end{aligned} \tag{2.17}$$

$$\begin{aligned}\delta X'' &= \delta\frac{dX'}{ds}\\ &= \frac{d}{ds}\delta X' - \frac{dX'(X',d\delta X)}{ds^2}\\ &= \frac{d^2}{ds^2}\delta X - 2e_1'\left(e_1,\frac{d}{ds}\delta X\right) - e_1\frac{d}{ds}\left(e_1,\frac{d}{ds}\delta X\right),\end{aligned} \tag{2.18}$$

$$\delta X''' = \delta\frac{dX''}{ds} = \frac{d}{ds}\delta X'' - X'''\left(X',\frac{d}{ds}\delta X\right). \tag{2.19}$$

In view of Eqs. (2.6) and (2.16), the last term in Eq. (2.18) does not contribute to $\delta\kappa$. Substituting Eq. (2.18) into Eq. (2.16) and using the Frenet equations (2.7) together with the variation (2.9), we obtain

$$\delta\kappa(s) = \varepsilon_2'' + \kappa'\varepsilon_1 + \varepsilon_2(\kappa^2-\tau^2) - 2\tau\varepsilon_3' - \tau'\varepsilon_3. \tag{2.20}$$

Substituting Eq. (2.20) into the first formula of Eq. (2.11), we have

$$\begin{aligned}\delta F_1 = \int F_1'\delta\kappa ds = \int F_1'[\varepsilon_2'' + \kappa'\varepsilon_1 + \varepsilon_2(\kappa^2-\tau^2) - 2\tau\varepsilon_3'\\ - \tau'\ \varepsilon_3]ds.\end{aligned} \tag{2.21}$$

Now let us calculate the variation δF_2. When we have a curve $X=X(s)$ and s is the natural parameter, the formula of the torsion is $\tau=(X',X'',X''')/k^2$ where (,,) denotes a triple product. By a short calculation, we have

$$\begin{aligned}\delta\tau = -2\frac{\tau}{\kappa}\delta\kappa + \frac{1}{\kappa^2}[(\delta X',X'',X''') + (X',\delta X'',X''')\\ + (X',X'',\delta X''')].\end{aligned} \tag{2.22}$$

By making use of

$$X' = e_1, \quad X'' = \kappa e_2, \quad X''' = -\kappa^2 e_1 + \kappa' e_2 + \kappa\tau e_3, \tag{2.23}$$

and Eqs. (2.7), (2.17)–(2.19), and (2.23) together with the expansion (2.9), one can derive

$$(\delta X',X'',X''') = \kappa^3\left(e_3,\frac{d}{ds}\delta X\right) = \kappa^3(\varepsilon_3' + \varepsilon_2\tau), \tag{2.24}$$

$$\begin{aligned}(X',\delta X'',X''') &= \left(\frac{d^2}{ds^2}\delta X,P\right) - 2\kappa(e_2,P)\left(e_1,\frac{d}{ds}\delta X\right)\\ &= \kappa\tau[(\kappa^2-\tau^2)\varepsilon_2 - \tau'\varepsilon_3 - 2\tau\varepsilon_3' + \varepsilon_2'']\\ &\quad + \kappa'(\kappa^2\varepsilon_3 - \tau'\varepsilon_2 - 2\tau\varepsilon_2' - \varepsilon_3''),\end{aligned} \tag{2.25}$$

$$\begin{aligned}(X',X'',\delta X''') &= \kappa\left(e_3,\frac{d}{ds}\delta X''\right) + (e_3,X''')\left(e_1,\frac{d}{ds}\delta X\right)\\ &= \kappa[2\kappa^2\tau\varepsilon_2 - \tau^3\varepsilon_2 + 2\tau\kappa'\varepsilon_1\\ &\quad + \tau'(\kappa\varepsilon_1 - 3\tau\varepsilon_3 + 3\varepsilon_2') - 3\tau^2\varepsilon_3'\\ &\quad + \tau''\varepsilon_2 + 3\tau\varepsilon_2' + \varepsilon_3'''].\end{aligned} \tag{2.26}$$

Thus, using Eqs. (2.24)–(2.26) and (2.20), one can write $\delta\tau$ as follows:

$$\begin{aligned}\delta\tau = \frac{1}{\kappa^2}\{&\kappa'(\kappa^2\varepsilon_3 - \tau'\varepsilon_2 - 2\tau\varepsilon_2' - \varepsilon_3'')\\ &+ \kappa[2\kappa^2\tau\varepsilon_2 + \tau'(\kappa\varepsilon_1 - 2\tau\varepsilon_3 + 3\varepsilon_2')\\ &+ (\kappa^2-\tau^2)\varepsilon_3' + \tau''\varepsilon_2 + 2\tau\varepsilon_2'' - \varepsilon_3''']\}.\end{aligned} \tag{2.27}$$

Finally, let us calculate the variation δF_3. Using Eqs. (2.12), (2.14), and (2.17), it is easy to get

$$\delta\kappa_s = \frac{d}{ds}\delta\kappa - d\kappa\frac{\delta ds}{ds^2} = \frac{d}{ds}\delta\kappa - \kappa'(\varepsilon_1 - \kappa\varepsilon_2). \tag{2.28}$$

The substitution of Eq. (2.20) into Eq. (2.18) yields

$$\begin{aligned}\delta\kappa_s = (3\kappa\kappa' - 2\tau\tau')\varepsilon_2 + \kappa'\varepsilon_1' + (\kappa^2-\tau^2)\varepsilon_2'\\ - 3\tau'\varepsilon_3' + (\kappa'' - \kappa')\varepsilon_1 - \tau''\varepsilon_3\\ - 2\tau\varepsilon_3'' + \varepsilon_2'''.\end{aligned} \tag{2.29}$$

Noting the inextensibility of the polymer chain, one has that the variation of δF depends only on the normal variation of the curve $X(s)$, or more precisely, on the variation of $X(s)$ alongthe two normals e_2 and e_3. The terms in δF_1, δF_2, δF_3, and δF_4 do not depend on the variation $\varepsilon_1(s)$ along the tangent to the curve. Substituting Eqs. (2.15), (2.21), (2.27), and (2.29) into Eq. (2.10) and taking into account Eq. (2.11), we obtain

$$\begin{aligned}\delta F = \int ds\Bigg(\Bigg\{&\frac{d^2}{ds^2}\left(\frac{2F_2'\tau}{\kappa} + F_1'\right) + \frac{d}{ds}\left(\frac{2F_2'\kappa'\tau}{\kappa^2} + \frac{3F_2'\tau'}{\kappa}\right)\\ &+ \left[F_1'(\kappa^2-\tau^2) - F_2'\left(2\kappa\tau - \frac{\kappa'\tau'}{\kappa^2} + \frac{\tau''}{\kappa}\right)\right] - F\kappa\\ &+ F_3'(3\kappa\kappa' - 2\tau\tau') - \frac{d}{ds}[F_3'(k^2-r^2)] - \frac{d^3}{ds^3}F_3'\Bigg\}\varepsilon_2(s)\\ &- \Bigg\{\frac{d^3}{ds^3}\left(\frac{F_2'}{k}\right) + \frac{d^2}{ds^2}\left(\frac{F_2'k'}{k^2}\right) + \frac{d}{ds}\left[\frac{F_2'}{\kappa}(\kappa^2-\tau^2) - 2\tau F_1'\right]\\ &+ F_1'\tau' - F_2'\kappa' + \frac{F_2'\tau'\tau}{\kappa} + \frac{d^2}{ds^2}(2F_3'\tau) - \frac{d}{ds^2}(3F_3'\tau')\\ &+ F_3'\tau''\Bigg\}\varepsilon_3(s)\Bigg) = 0.\end{aligned} \tag{2.30}$$

From Eq. (2.30), two equations for principal curvatures follow:

$$\begin{aligned}\frac{d^2}{ds^2}\left(\frac{2F_2'\tau}{\kappa} + F_1'\right) + \frac{d}{ds}\left(\frac{2F_2'k'\tau}{\kappa^2} + \frac{3F_2'\tau'}{\kappa}\right) + \Bigg[F_1'(\kappa^2-\tau^2)\\ - F_2'\left(2\kappa\tau - \frac{k'\tau'}{k^2} + \frac{\tau''}{k}\right)\Bigg] - F\kappa + F_3'(3\kappa\kappa' - 2\tau\tau')\\ - \frac{d}{ds}[F_3'(\kappa^2-\tau^2)] - \frac{d^3}{ds^3}F_3' = 0,\end{aligned} \tag{2.31}$$

$$\frac{d^3}{ds^3}\left(\frac{F_2'}{\kappa}\right)+\frac{d^2}{ds^2}\left(\frac{F_2'k'}{\kappa^2}\right)+\frac{d}{ds}\left[\frac{F_2'}{\kappa}(\kappa^2-\tau^2)-2\tau F_2'\right]+F_1'\tau' - F_2'\kappa'+\frac{F_2'\tau'\tau}{\kappa}+\frac{d^2}{ds^2}(2F_3'\tau)-\frac{d}{ds}(3F_3'\tau')+F_3'\tau''=0. \tag{2.32}$$

The two equations are exactly the general shape equations of polymer chains, which provides a uniform description for the equilibrium shapes of polymer chains. If we can correctly construct the free energy density F of a polymer chain, we can always obtain its equilibrium shape equations immediately by substituting F into Eqs. (2.31) and (2.32). Furthermore, because the two equations are equations of mathematical physics, they are also fit for describing the shapes of carbon nanotubes [15,20] and even strings [12].

III. FEOLI'S FORMULISM AND EQUILIBRIUM SHAPE EQUATIONS OF WLC AND WLRC MODELS

From the equilibrium shape equations (2.31) and (2.32), many results can be derived. When the free energy density F depends only on the curvature $\kappa(s)$, one can write $F=F[\kappa(s)]$, and we have $F'=F_1'=\partial F/\partial\kappa, F_2'=0$, and $F_3'=0$. In view of the general shape equations (2.31) and (2.32), we obtain

$$\frac{d^2}{ds^2}F'+F'(\kappa^2-\tau^2)=Fk, \tag{3.1}$$

$$2\frac{d}{ds}(F'\tau)=F'\tau'. \tag{3.2}$$

We see that Eqs. (3.1) and (3.2) are exactly the results obtained by Feoli *et al.* [12]. From Eqs. (3.2) and (3.1), we obtain

$$\tau=\frac{C}{(F')^2}, \tag{3.3}$$

$$\frac{d^2}{ds^2}F'+F'\left(\kappa^2-\frac{C^2}{(F')^4}\right)-F\kappa=0, \tag{3.4}$$

where C is an integration constant.

We write the free energy density F of the WLC model as follows (having been rescaled) [13]:

$$F=F(\kappa)=\kappa^2+\lambda,$$

where λ is a constant denoting an external force or a constraint, κ is the curvature. Obviously we have $F'=F_1'=\partial F/\partial\kappa=2\kappa$. Then we obtain

$$2\kappa''+\kappa^3-\lambda k-\frac{C^2}{8\kappa^3}=0. \tag{3.5}$$

Using Eq. (3.3), we can easily obtain

$$\kappa^2\tau=\frac{C}{4}=C_1, \tag{3.6}$$

where C_1 is a constant. Therefore, Eq. (3.5) can be written as

$$0=2\kappa''+\kappa^3-\lambda\kappa-2\kappa\tau^2,$$

$$C_1=\kappa^2\tau. \tag{3.7}$$

Equations (3.7) are just the ones obtained by Langer *et al.* [13] with the Gauss curvature $G=0$, which is because the three-dimensional Euclidean space is a flat space.

A coiled polymer chain can be described by

$$\mathbf{r}(s)=(r_0\cos(\omega s),r_0\sin(\omega s),h\omega s), \tag{3.8}$$

where the coiled pitch $p=2\pi h$, r_0 is the coil radius, and $\omega=1/\sqrt{[r_0^2+h^2]}$. Substituting

$$\kappa=\frac{r_0}{r_0^2+h^2},\quad \tau=\frac{h}{r_0^2+h^2} \tag{3.9}$$

into Eq. (3.7), we obtain

$$r_0^2-2h^2-(r_0^2+h^2)^2\lambda=0. \tag{3.10}$$

This is the equation for helical chains. Letting $\lambda=m/a$, we see Eq. (3.10) is the result obtained in the study of conformations of multiwalled carbon nanotubes [15].

Furthermore, if $\lambda=0$, which means no external forces or constraints,we have $r_0=\sqrt{2}h$, and noting that for the pitch of coiled polymer chains $p=2\pi h$, we also have

$$\frac{p}{r_0}=\sqrt{2}\pi\approx 4.443, \tag{3.11}$$

which agrees well with Z-DNA [16] with $p=4.46$ nm and $r_0=0.90$ nm, thus $p/r_0\approx 4.96$. This result means that it is reasonable to approximately write the free energy density of Z-DNA as the form $F=(A/2)\kappa^2$.

For the WLRC model [4,9,17], the corresponding free energy density is given as follows:

$$F=F(\kappa,\tau)=\frac{A}{2}\kappa^2+\frac{C}{2}(\tau-\omega_0)^2, \tag{3.12}$$

where A is the usual bending rigidity, C is the twist rigidity, and $\omega_0=2\pi/p$ (p is the helical repeated length). For B-DNA [16], $A\approx 50$ nm, $C\approx 1.5$ A, and $\omega_0\approx 1.85\ \text{nm}^{-1}$.

Obviously, we have $F_1'=\partial F/\partial k=A\kappa$, $F_2'=\partial F/\partial r=C(\tau-\omega_0)$. In view of Eqs. (2.31) and (2.32), we obtain the corresponding equilibrium shapeequations as follows:

$$A\kappa^5-\kappa^3[(2A+5C)\tau^2-6C\omega_0\tau+C\omega_0^2]+2C(3\omega_0-5\tau)\kappa'\tau' + 2A\kappa^2\kappa''+2C\kappa[6(\tau')^2+(5\tau-3\omega_0)\tau'']=0, \tag{3.13}$$

$$-2A\kappa^4\tau\kappa'+6C(\omega_0-\tau)(\kappa')^3+(C-A)\kappa^5\tau'+6C\kappa\kappa'[\kappa'\tau' + (\tau-\omega_0)\kappa'']-C\kappa^2(-\tau^3\kappa'+\omega_0\tau^2\kappa'+3\tau'\kappa''+3\kappa'\tau'' + \tau\kappa'''-\omega_0\kappa''')+C\kappa^3(-2\tau^2\tau'+\omega_0\tau\tau'+\tau''')=0. \tag{3.14}$$

For the solutions of helical chains, substituting Eq. (3.9) into Eqs. (3.13) and (3.14), we obtain

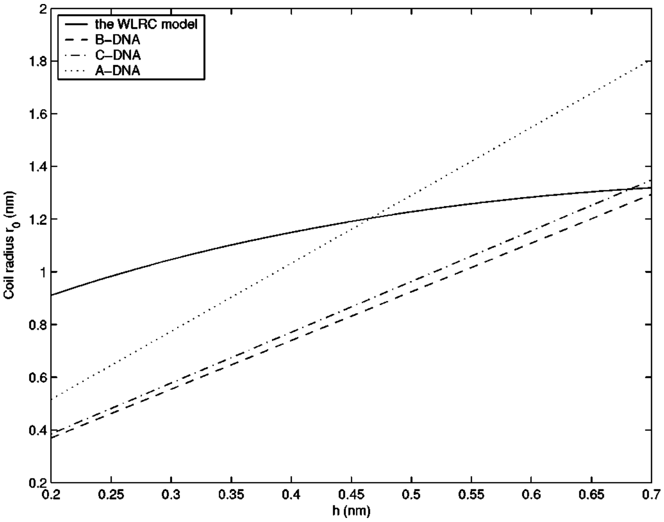

FIG. 1. The coil radius r_0 vs h of the WLRC model of B-DNA, where $h=p/2\pi$ and p is the helical pitch.The straight lines of B-DNA, C-DNA, and A-DNA are $r_0=1.848h$, $r_0=1.926h$, and $r_0=2.58h$, which are the experimental results [16].

$$(2A+5C)h^2-Ar_0^2-6C\omega_0 h(h^2+r_0^2)+C\omega_0^2(h^2+r_0^2)^2=0. \tag{3.15}$$

For B-DNA, we can plot the curve of r_0 versus h, shown as a solid curve in Fig. 1. We see that the value of r_0/h is not a constant. When $h\approx 0.54$ nm, $r_0\approx 1.26$ nm, which is larger than the experimental data of B-DNA, [16], $r_0=1$ nm. So it appears the WLRC model is not very appropriate to describe B-DNA. However, because the value of h of DNA is in the interval [16] (0.2,0.7), in which the extent of the curve of the r_0 versus h relation deviating from the straight lines is not very big, the WLRC model is somewhat appropriate to describe DNA.

If $\omega_0=0$, the corresponding free energy density has the form [17,18]

$$F=F(\kappa,\tau)=\frac{A}{2}\kappa^2+\frac{C}{2}\tau^2, \tag{3.16}$$

and we can easily get $p/r_0\approx 1.948$, which is much smaller than any one measured experimentally. For example, the corresponding values of p/r_0 of A-DNA, B-DNA, and C-DNA are 2.435, 3.4, and 3.263, respectively [16]. Therefore, it is not appropriate to describe the free energy density of DNA by Eq. (3.16).

IV. EQUILIBRIUM SHAPE EQUATIONS OF THE MODEL OF CHIRAL BIOPOLYMERS

Let us discuss a chiral model which favors special chirality, originally suggested by Helfrich [14]. The corresponding free energy density F reads [14,19]

$$F=F(\kappa,\tau)=\frac{A}{2}\kappa^2+\frac{C}{4}\kappa^4-\frac{\alpha}{2}\kappa^2\tau+\frac{\beta}{2}(\kappa_s^2+\kappa^2\tau^2)+\lambda, \tag{4.1}$$

where λ is a constant denoting a constraint or a force, and A, C, α, β are all non-negative constants. The term $-(\alpha/2)k^2\tau$ is associated with the chirality of biopolymers. In view of Eqs. (2.31) and (2.32), one can derive the corresponding shape equations as follows:

$$\begin{aligned}&2A(\kappa^3-2\kappa\tau^2+2\kappa_{ss})-4\lambda\kappa-2\alpha(3\kappa^3\tau-2\kappa\tau^3+6\kappa_s\tau_s\\&\quad+2\kappa\tau_{ss}+6\kappa_{ss}\tau)+C(3\kappa^5-4\kappa^3\tau^2+24\kappa\kappa_s^2+12\kappa^2\kappa_{ss})\\&\quad+2\beta(5\kappa^3\tau^2-2\kappa\tau^4+\kappa\kappa_s^2-2\kappa^2\kappa_{ss}-2\kappa_{ssss}+12\kappa_{ss}\tau^2\\&\quad+24\kappa_s\tau\tau_s+8\kappa\tau\tau_{ss}+6\kappa\tau_s^2)=0,\end{aligned} \tag{4.2}$$

$$\begin{aligned}&4A(2\kappa_s\tau+\kappa\tau_s)-2\alpha(6\kappa_s\tau^2+6\kappa\tau\tau_s-3\kappa^2\kappa_s-2\kappa_{sss})\\&\quad+C(4\kappa^3\tau_s+24\kappa^2\kappa_s\tau)+4\beta(4\kappa_s\tau^3+6\kappa\tau^2\tau_s-3\kappa^2\kappa_s\tau\\&\quad-\kappa^3\tau_s-4\kappa_s\tau_{ss}-6\kappa_{ss}\tau_s-4\kappa_{sss}\tau-\kappa\tau_{sss})=0.\end{aligned} \tag{4.3}$$

This result has also been derived previously by Zhao *et al.* in the study of kink instability in circular DNA [19].

Now let us make use of the equilibrium shape equations (4.2) and (4.3) to discuss some possible solutions.

A. Solutions of straight biopolymers

From Eqs. (4.2) and (4.3), we can easily obtain the vanishing curvature and torsion,

$$\kappa=0, \quad \tau=0,$$

as solutions of the shape equations. Obviously, the above solutions give a straight line, which corresponds to straight biopolymers.

B. Solutions of helical biopolymers

The shape equations (4.2) and (4.3) possess a nonvanishing constant curvature and a torsion solution as Eq. (3.9). Substituting Eq. (3.9) into Eqs. (4.2) and (4.3), we obtain

$$\begin{aligned}&Cr_0^2(4h^2-3r_0^2)+2A(2h^6+3h^4r_0^2-r_0^6)-2\alpha h(2h^4-3h^2r_0^2\\&\quad-r_0^4)+2\beta h^2(2h^2+3r_0^2)+4\lambda(r_0^2+h^2)^4=0,\end{aligned} \tag{4.4}$$

which is the equation for helical biopolymers, corresponding to the free energy density Eq. (4.1).

Let $\lambda=0$, which means no external forces or constraints, and when $A=50$ nm, $C=60$ nm^2, $\alpha=40$ nm^3, $\beta=50$ nm^2, we find the value of $r_0/h(\approx 1.848)$ is almost a constant, which agrees well with the experimental value of B-DNA [16] (see Fig. 2). Therefore, we can expect that it is reasonable to describe properties of DNA by the above model with the corresponding parameters A, C, α, β.

C. Solutions of circular biopolymers

We know that the shape equations (4.2) and (4.3) possess a ring like solution with a vanishing torsion $\tau=0$ and a constant curvature κ. In view of this, from Eqs. (4.2) and (4.3)

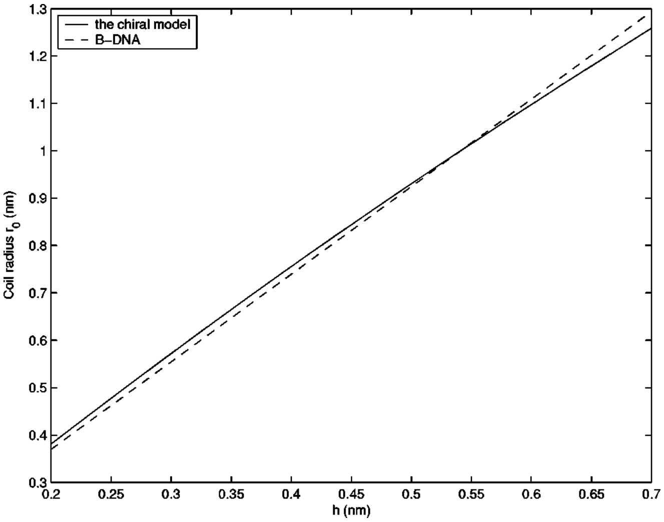

FIG. 2. The coil radius r_0 vs h of the theoretical model of B-DNA with $A=50$ nm, $C=60$ nm^2, $\alpha=40$ nm^3, and $\beta=50$ nm^2.

we obtain $3C\kappa^4+2A\kappa^2-4\lambda=0$, of which we can write out the solution κ as follows.

When $C=0$, we have

$$\kappa=\sqrt{\frac{2\lambda}{A}}, \tag{4.5}$$

and when C is nonzero, we have

$$\kappa=\left[\frac{-A+\sqrt{A^2+12C\lambda}}{3C}\right]^{1/2}. \tag{4.6}$$

From Eq. (4.5), if we let $A=2$, we have $\kappa=\sqrt{\lambda}=1/R$, where R is the radius of the circle. Furthermore, if we let $\lambda=m/\alpha$, we see the result is just the one obtained in the study of conformations of multiwalled carbon nanotubes [20].

V. CONCLUSION

To conclude, we have derived two rather general equilibrium shape equations (2.31) and (2.32) of a polymer chain. Also, the results of Feoli *et al.* have been generalized, and the equilibrium shape equations of the well known wormlike chain (WLC) model and the wormlike rod chain (WLRC) model have been obtained by making use of our general equilibrium shape equations. We find that the ratio of pitch and radius of coil is about 4.443 in the WLC model, which agrees well with Z-DNA [16]. And the ratio of the coil pitch to the radius from WLRC agrees with the data of B-DNA [16] qualitatively. We find that the model suggested by Ref. [14] is very appropriate to describe B-DNA (or other biopolymers) if we choose the four phenomenological parameters as $A=50$ nm, $C=60$ nm^2, $\alpha=40$ nm^3, and $\beta=50$ nm^2.

Our present approach does not take into account the conformation entropy of the chain because it is a phenomenological theory. Although the particular choice of the effective energy may represent entropic contributions, temperature effects, and fluctuations, it is necessary to consider the microscopic theory of polymer chains in future work.

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