1-1-2013

Comment on "equilibrium conformation of polymer chains with noncircular cross section"

Alexander Gerhardt-Bourke
University of Wollongong

Ngamta Thamwattana
University of Wollongong, ngamta@uow.edu.au

Abstract

In this Comment, we point out that the Euler-Lagrange equations, which are referred to as the general equilibrium equations by Zhao are incorrect along with the equations which are derived from them. The correct equations are provided in this Comment. We produce new numerical results with the use of the correct equations. © 2013 American Physical Society.

Keywords

polymer, conformation, equilibrium, comment, section, cross, noncircular, chains

Disciplines

Engineering | Science and Technology Studies

Publication Details

Gerhardt-Bourke, A. & Thamwattana, N. (2013). Comment on "equilibrium conformation of polymer chains with noncircular cross section". Physical Review E: Statistical, Nonlinear, and Soft Matter Physics, 87 (4), 046601-1-046601-3.

Comment on "Equilibrium conformation of polymer chains with noncircular cross section"

Alexander Gerhardt-Bourke and Ngamta Thamwattana*

School of Mathematics and Applied Statistics, University of Wollongong, Wollongong, New South Wales 2522, Australia

(Received 20 December 2012; published 19 April 2013)

In this Comment, we point out that the Euler-Lagrange equations, which are referred to as the general equilibrium equations by Zhao *et al.* [Phys. Rev. E **74**, 032801 (2006)] are incorrect along with the equations which are derived from them. The correct equations are provided in this Comment. We produce new numerical results with the use of the correct equations.

DOI: 10.1103/PhysRevE.87.046601 PACS number(s): 36.20.Fz, 46.25.Cc, 36.20.Ey

In Zhao *et al.* [1], we see a model of polymer chains with noncircular cross sections, which is used to discuss elastic ribbons. Zhao *et al.* consider the free energy density as a general functional of the curvature, torsion, and twist angle of a general polymer chain. Equilibrium conformation equations are then obtained by minimizing the free energy functional by calculating variations. However, the obtained equations are incorrect and, hence, so is their analysis of elastic ribbons. Here, we give the correct versions of these equations and complete the same analysis using new equations.

For the free energy density $\mathcal{F} = \mathcal{F}[\kappa(s),\tau(s),\alpha(s),\alpha'(s)]$, which is a function of the curvature $\kappa(s)$, the torsion $\tau(s)$, the twist angle $\alpha(s)$, and the derivative of the twist angle $\alpha'(s)$ with respect to s, where s is the arc length of the polymer chain, the correct Euler-Lagrange equations are given by

$$\frac{d^2}{ds^2}\left(\mathcal{F}_1 + \frac{2\tau}{\kappa}\mathcal{F}_2\right) + \frac{d}{ds}\left(\frac{2\kappa'\tau}{\kappa^2}\mathcal{F}_2 - \frac{3\tau'}{\kappa}\mathcal{F}_2\right) + [\kappa^2 - \tau^2]\mathcal{F}_1 + \left[2\kappa\tau + \frac{\tau''}{\kappa} - \frac{\kappa'\tau'}{\kappa^2}\right]\mathcal{F}_2 + \alpha'\kappa\mathcal{F}_4 - \kappa\mathcal{F} = 0, \tag{1}$$

$$-\frac{d^3}{ds^3}\left(\frac{1}{\kappa}\mathcal{F}_2\right) - \frac{d^2}{ds^2}\left(\frac{\kappa'}{\kappa^2}\mathcal{F}_2\right) + \frac{d}{ds}\left(2\tau\mathcal{F}_1 + \frac{\tau^2}{\kappa}\mathcal{F}_2 - \kappa\mathcal{F}_2\right) - \tau'\mathcal{F}_1 + \left[\frac{\kappa'\tau^2}{\kappa^2} - \frac{2\tau\tau'}{\kappa}\right]\mathcal{F}_2 = 0, \tag{2}$$

and

$$\mathcal{F}_3 - \frac{d}{ds}(\mathcal{F}_4) = 0, \tag{3}$$

where $\mathcal{F}_1 = \partial\mathcal{F}/\partial\kappa$, $\mathcal{F}_2 = \partial\mathcal{F}/\partial\tau$, $\mathcal{F}_3 = \partial\mathcal{F}/\partial\alpha$, and $\mathcal{F}_4 = \partial\mathcal{F}/\partial\alpha'$. We have adopted the same notation as Ref. [1] for convenience, however, we use α' to represent $d\alpha/ds$ as opposed to α_s. We note that $\alpha'(s) = d\alpha(s)/ds$ is the rate of rotation of the cross section along the centerline of the polymer chain [1].

We note that Eqs. (1) and (2) are comparable to those given in Thamwattana *et al.* [2]; we see (1) has only one extra added term which is involving α', and (2) is unchanged when compared to Eqs. (2.1) and (2.2) of Ref. [2]. The incorrect Euler-Lagrange equations given by Zhao *et al.* [1] originate from employing incorrect equations given by Zhang *et al.* [3], which have since been corrected by Thamwattana *et al.* [2] and Thamwattana and Hill [4]. Comparing the equations given by Zhao *et al.* [1] to those given by Zhang *et al.* [3], we see that Eq. (6) in Ref. [1] is the correct version of Eq. (2.31) of Ref. [3] with the added term $\alpha'\kappa\mathcal{F}_4$. However, we see that Eq. (7) in Ref. [1] is identical to Eq. (2.32) of Ref. [3], which is incorrect. We note that Eq. (8) of Zhao *et al.* is correct and is given here as (3).

Furthermore, Eqs. (1) and (2) can be simplified to yield

$$\frac{d^2}{ds^2}(\mathcal{F}_1) + \frac{2\tau}{\kappa}\frac{d^2}{ds^2}(\mathcal{F}_2) + \frac{d}{ds}(\mathcal{F}_2)\left(\frac{\kappa\tau' - 2\kappa'\tau}{\kappa^2}\right) + \mathcal{F}_2(2\kappa\tau) + \mathcal{F}_1[\kappa^2 - \tau^2] + \mathcal{F}_4\alpha'\kappa - \kappa\mathcal{F} = 0, \tag{4}$$

and

$$-\frac{1}{\kappa}\frac{d^3}{ds^3}(\mathcal{F}_2) + \frac{d^2}{ds^2}(\mathcal{F}_2)\left(\frac{2\kappa'}{\kappa^2}\right) + \frac{d}{ds}(\mathcal{F}_2)\left(\frac{\kappa\kappa'' - 2(\kappa')^2}{\kappa^3} + \frac{\tau^2}{\kappa} - \kappa\right) - \kappa'\mathcal{F}_2 + 2\tau\frac{d}{ds}(\mathcal{F}_1) + 2\tau'\mathcal{F}_1 = 0. \tag{5}$$

We now follow the process of applying the Euler-Lagrange equations to the case of an elastic ribbon. As given in Zhao *et al.* [1], the free energy density of an elastic ribbon is given by

$$\mathcal{F}(\kappa,\tau,\alpha,\alpha') = \frac{A}{2}\kappa^2\cos\alpha + \frac{B}{2}\kappa^2\sin\alpha + C(\tau + \alpha' - \tau_0)^2, \tag{6}$$

where τ_0 is the spontaneous torsion and A, B, and C are constants depending on the elastic properties of materials and the geometry of the cross section. Using (3)–(6) and considering the case where the curvature and torsion of the curve $\mathbf{x}(s)$ do not depend on s, we derive the corresponding equilibrium equations to be

$$\kappa\left[\alpha''(B\cos\alpha - A\sin\alpha) - \left((\alpha')^2 - \frac{\kappa^2}{2} + \tau^2\right)(A\cos\alpha + B\sin\alpha) + C(\tau + \alpha' - \tau_0)(3\tau - 3\alpha' + \tau_0)\right] + \frac{4C\tau\alpha'''}{\kappa} = 0, \tag{7}$$

*Corresponding author: ngamta@uow.edu.au

$$-\frac{1}{\kappa}\left[2C\alpha^{(4)}+2C\alpha''\left(\frac{\tau^2}{\kappa}-\kappa\right)\right] + 2\tau\alpha'\kappa(B\cos\alpha - A\sin\alpha) = 0, \tag{8}$$

and

$$-\frac{A}{2}\kappa^2\sin\alpha+\frac{B}{2}\kappa^2\cos\alpha-2C\alpha''=0. \tag{9}$$

Thus, the equilibrium conformation of typical polymer chains with noncircular cross sections are determined by (7)–(9). We comment that (7)–(9) are completely different from Eqs. (10)– (12) given in Zhao *et al.* [1].

I. HELICAL RIBBONS

Helical ribbons, as outlined by Zhao *et al.* [1], have the property $\alpha = 0$. Furthermore, they are characterized by the radius r and the pitch $2\pi h$ in the sense that they have s-independent curvature and torsion given by $\kappa = r/(r^2+h^2)$ and $\tau = h/(r^2+h^2)$. In Zhao *et al.* [1], Eqs. (11) and (12) are identically satisfied with this information. However, upon substitution into the corrected equations, here, we find from (9) that

$$\frac{B}{2}\kappa^2 = 0, \tag{10}$$

and we, thus, conclude that $B = 0$. Furthermore, Eq. (13) of Zhao *et al.* [1] comes from substitution into Eq. (10) not Eq. (12) as outlined. Upon substitution into our Eq. (7), we find

$$3Ch^2+\frac{A}{2}(r^2-2h^2)-C\tau_0(r^2+h^2)[2h+\tau_0(r^2+h^2)]=0. \tag{11}$$

We note that the difference between Eqs. (11) and (13) in Ref. [1] is the multiplication by 1/2 in the second term. As a result, the following results are different from Ref. [1].

As Eq. (11) describes the conformation of helical ribbons, it is clear that this conformation depends on the elastic properties of the ribbon, that is, constants A and C. In the case of spontaneous torsion $\tau_0 = 0$, we find

$$\frac{r}{h}=\frac{\kappa}{\tau}=\left[\frac{2(A-3C)}{A}\right]^{1/2}, \tag{12}$$

and thus, we can calculate the pitch angle defined by $\phi = \arctan(h/r)$ to be

$$\phi = \arctan\left[\frac{1}{\sqrt{2(1-3C/A)}}\right]. \tag{13}$$

As in Zhao *et al.* [1], it has been shown that the value of the pitch angle depends on the ratio of constants C and A. However, we can see that the critical value of the ratio is $C/A = 1/3$ rather than 2/3. Therefore, helical ribbons with no spontaneous torsion cannot exist with $C/A > 1/3$. Figure 1 shows the pitch angle as a function of C/A as the value of C/A increases from 0 to 2/3; we see that the pitch angle increases from 35° to 90°.

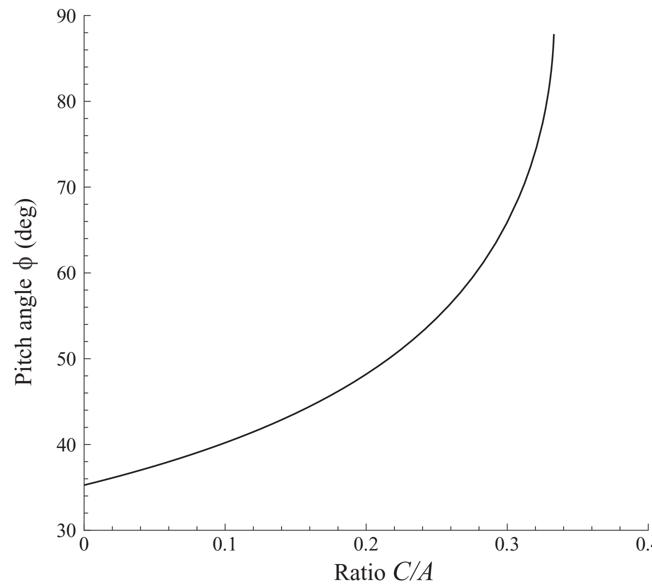

FIG. 1. Relationship between the pitch angle ϕ and the ratio C/A when $\tau_0 = 0$.

We now consider helical ribbons with nonzero spontaneous torsion. We find that the pitch angle is given by

$$\phi = \arctan\left[\left(\frac{1}{2\left[2+\frac{C}{A}(\lambda+3)(\lambda-1)\right]}\right)^{1/2}\right], \tag{14}$$

where we have the defined parameter $\lambda = \tau_0/\tau$. Figure 2 shows the change in pitch angle as the ratio C/A increases for fixed values of λ. The solid line represents a plot of $\lambda = 0.8$; we see that, for this value, the pitch begins at approximately 26° and increases, and this will happen for any value in the range of $-3 < \lambda < 1$. The dashed line represents $\lambda = 2$; the value for the pitch begins again at 26° and approaches 0 as C/A increases, and this will be true for any value of $\lambda > 1$.

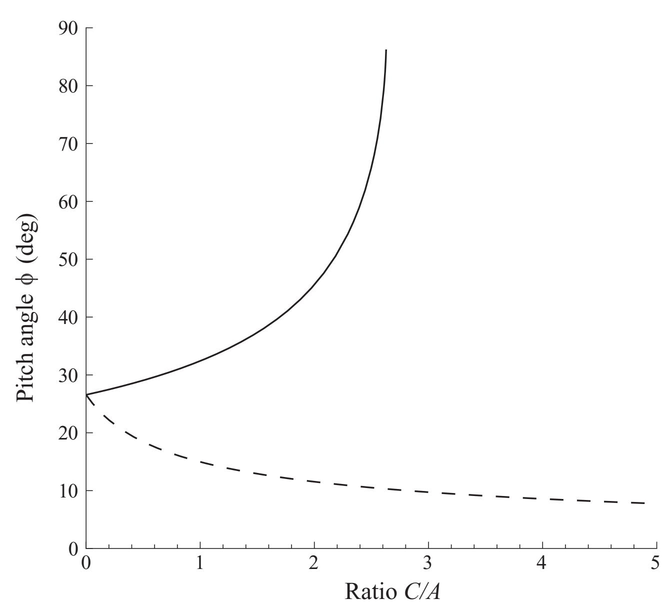

FIG. 2. Relationship between the pitch angle ϕ and the ratio C/A when τ_0 is nonzero.

In the case of $\tau = \tau_0$, we have $\lambda = 1$. From (14), we see that the pitch angle will be completely independent of C/A, and we have $\phi = \arctan(1/2)$.

II. TWISTED RIBBONS

For vanishing curvature and torsion ($\kappa = \tau = 0$), we see that (7) is identically satisfied. Furthermore, (9) yields the condition $C\alpha'' = 0$. Thus, we must have $C = 0$ or $\alpha'' = 0$, in either case, (8) is also identically satisfied.

In the case of $\alpha'' = 0$, we have $\alpha' = k$ for some constant k. Physically, this means that the rate of rotation is constant. With the extra information of $\kappa = \tau = 0$, the derivation of (3) produces the property that $\partial\mathcal{F}/\partial\alpha' = 0$. In this particular case of the twisted ribbon, this yields $\alpha' = \tau_0$. This physically implies that the rate of rotation is simply the spontaneous torsion. That is, for a distance x along the ribbon, the total angle of rotation along that distance will be $\alpha' x$.

To summarize, this Comment provides the correct Euler-Lagrange equations for the free energy density function $\mathcal{F} = \mathcal{F}[\kappa(s),\tau(s),\alpha(s),\alpha'(s)]$. For the case of an elastic ribbon, we find that (10)–(12) in Ref. [1] are incorrect, thus, all those results in Ref. [1] that are based on these equations are also incorrect. The correct equations are given here by (7)–(9). Furthermore, we provide new analysis for both helical and twisted ribbons.

ACKNOWLEDGMENT

The authors gratefully acknowledge financial support from the Faculty of Informatics, University of Wollongong.

[1] S. Zhao, S. Zhang, Z. Yao, and L. Zhang, Phys. Rev. E **74**, 032801 (2006).
[2] N. Thamwattana, J. A. McCoy, and J. M. Hill, Q. J. Mech. Appl. Math. **61**, 431 (2008).
[3] S. Zhang, X. Zuo, M. Xia, S. Zhao, and E. Zhang, Phys. Rev. E **70**, 051902 (2004).
[4] N. Thamwattana and J. M. Hill, Phys. Rev. E **78**, 013901 (2008).