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Comment on "General equilibrium shape equations of polymer chains"

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In this Comment, we point out that the Euler-Lagrange equations, which are referred to as the general equilibrium shape equations presented by Zhang *et al.* [Phys. Rev. E **70**, 051902 (2004)] are incorrect, along with equations derived from them. The correct equations are provided here and they are cross-checked using certain energy functions previously presented in the literature. Further, with the use of the correct equations, we present new numerical results, which for the values of the constants given by Zhang *et al.* do not give rise to the physical behavior observed for DNA by those authors. However, the correct equations can be consistent with sensible behavior for different values of the constants.

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To determine the shape of polymer chains, such as proteins and DNA, Zhang *et al.* [1] adopt a variational principle for an energy density, and obtain in [1] the Euler-Lagrange equations, which are referred to as general equilibrium shape equations. Here, we point out that these equations are incorrect, and we state the correct version of these equations and those equations derived from them.

For the free energy density $\mathcal{F}=\mathcal{F}(\kappa(s),\tau(s),\kappa'(s))$, which is a function of the curvature $\kappa(s)$, the torsion $\tau(s)$, and the derivative of the curvature, $\kappa'(s)=d\kappa(s)/ds$, where s is the arclength of the polymer chain, the correct Euler-Lagrange equations are derived by Thamwattana *et al.* [2], and in a comparable form to those presented by Zhang *et al.* [1], are given by

$$\frac{d^2}{ds^2}\left(\frac{2\mathcal{F}_2'\tau}{\kappa}+\mathcal{F}_1'\right)+\frac{d}{ds}\left(\frac{2\mathcal{F}_2'\kappa'\tau}{\kappa^2}-\frac{3\mathcal{F}_2'\tau'}{\kappa}\right)+\mathcal{F}_1'(\kappa^2-\tau^2) + \mathcal{F}_2'\left(2\kappa\tau-\frac{\kappa'\tau'}{\kappa^2}+\frac{\tau''}{\kappa}\right)-\mathcal{F}\kappa+\mathcal{F}_3'(3\kappa\kappa'-2\tau\tau') - \frac{d}{ds}[\mathcal{F}_3'(\kappa^2-\tau^2)]-\frac{d^3}{ds^3}\mathcal{F}_3'=0, \quad (1)$$

$$\frac{d^3}{ds^3}\left(\frac{\mathcal{F}_2'}{\kappa}\right)+\frac{d^2}{ds^2}\left(\frac{\mathcal{F}_2'\kappa'}{\kappa^2}\right)+\frac{d}{ds}\left(\frac{\mathcal{F}_2'}{\kappa}(\kappa^2-\tau^2)-2\mathcal{F}_1'\tau\right)+\mathcal{F}_1'\tau' - \mathcal{F}_2'\left(\frac{\kappa'\tau^2}{\kappa^2}-\frac{2\tau\tau'}{\kappa}\right)+\mathcal{F}_3'\tau''-\frac{d}{ds}(3\mathcal{F}_3'\tau')+\frac{d^2}{ds^2}(2\mathcal{F}_3'\tau) =0, \quad (2)$$

where $\mathcal{F}_1'=\partial\mathcal{F}/\partial\kappa$, $\mathcal{F}_2'=\partial\mathcal{F}/\partial\tau$, and $\mathcal{F}_3'=\partial\mathcal{F}/\partial\kappa'$. We note that, for convenience, we adopt the same notation as that in [1], except that here we use only $\kappa'=d\kappa/ds$ and $\tau'=d\tau/ds$, whereas Zhang *et al.* [1] use both κ' and κ_s to denote $d\kappa/ds$ and τ' and τ_s to represent $d\tau/ds$. The incorrect Euler-Lagrange equations given by Zhang *et al.* [1] originate from Eqs. (2.27) and (2.29) in [1] which are incorrect, and this therefore leads to the mistakes in the Euler-Lagrange equations (2.31) and (2.32) as given in [1]. We comment that the incorrect Eq. (2.27) in Zhang *et al.* [1] is also employed in another paper by some of the same authors (Zhao *et al.* [3]). We refer to Eqs. (B6) and (B7) in Appendix B of Thamwattana *et al.* [2] for the correct versions of Eqs. (2.27) and (2.29), respectively.

As also shown by Thamwattana *et al.* [2], Eqs. (1) and (2) can be simplified to yield

$$\frac{d^2}{ds^2}\left(\mathcal{F}_1'-\frac{d}{ds}\mathcal{F}_3'\right)+\frac{2\tau}{\kappa}\frac{d^2}{ds^2}\mathcal{F}_2'+\left(\frac{\tau'}{\kappa}-\frac{2\kappa'\tau}{\kappa^2}\right)\frac{d}{ds}\mathcal{F}_2'+(\kappa^2-\tau^2) \times\left(\mathcal{F}_1'-\frac{d}{ds}\mathcal{F}_3'\right)+2\kappa\tau\mathcal{F}_2'+\kappa\kappa'\mathcal{F}_3'-\kappa\mathcal{F}=0, \quad (3)$$

$$\frac{1}{\kappa}\frac{d^3}{ds^3}\mathcal{F}_2'-\frac{2\kappa'}{\kappa^2}\frac{d^2}{ds^2}\mathcal{F}_2'-2\tau\frac{d}{ds}\left(\mathcal{F}_1'-\frac{d}{ds}\mathcal{F}_3'\right) -\left(\frac{\tau^2}{\kappa}+\frac{\kappa''}{\kappa^2}-\frac{2\kappa'^2}{\kappa^3}-\kappa\right)\frac{d}{ds}\mathcal{F}_2'-\tau'\left(\mathcal{F}_1'-\frac{d}{ds}\mathcal{F}_3'\right)+\kappa'\mathcal{F}_2' =0. \quad (4)$$

In Thamwattana *et al.* [2], the Euler-Lagrange equations are presented for the more general case $\mathcal{F}=\mathcal{F}(\kappa,\tau,\kappa',\tau')$. We note that the case of $\mathcal{F}=\mathcal{F}(\kappa)$ has been investigated previously by Feoli *et al.* [4]. By substituting $\mathcal{F}=\mathcal{F}(\kappa)$ into Eqs. (1) and (2), the Euler-Lagrange equations reduce to

$$\frac{d^2}{ds^2}\mathcal{F}_1'+\mathcal{F}_1'(\kappa^2-\tau^2)-\kappa\mathcal{F}=0, \quad 2\frac{d}{ds}(\tau\mathcal{F}_1')-\tau'\mathcal{F}_1'=0, \quad (5)$$

respectively, which are as shown in [4]. We point out that using Eq. (2.32) in Zhang *et al.* [1] will not result in the second of equations (5), even though they state it correctly in Eq. (3.2) of [1].

For a particular energy density given by

$$\mathcal{F}(\kappa,\tau,\kappa')=\frac{A}{2}\kappa^2+\frac{C}{4}\kappa^4-\frac{\alpha}{2}\kappa^2\tau+\frac{\beta}{2}(\kappa'^2+\kappa^2\tau^2)+\lambda, \quad (6)$$

Zhang *et al.* [1] claim that substitution of Eq. (6) into their general equilibrium shape equations, which are Eqs. (2.31) and (2.32) in [1], yields the two resultant equations presented by Wei *et al.* [5], namely,

$$
\begin{aligned}
&2A(\kappa^3-2\kappa\tau^2+2\kappa'')-4\lambda\kappa-2\alpha(3\kappa^3\tau-2\kappa\tau^3+6\kappa'\tau'+2\kappa\tau'' \\
&\quad +6\kappa''\tau)+C(3\kappa^5-4\kappa^3\tau^2+24\kappa\kappa'^2+12\kappa^2\kappa'') \\
&\quad +2\beta(5\kappa^3\tau^2-2\kappa\tau^4+\kappa\kappa'^2-2\kappa^2\kappa''-2\kappa'''' \\
&\quad +12\kappa''\tau^2+24\kappa'\tau\tau'+8\kappa\tau\tau''+6\kappa\tau'^2)=0,
\end{aligned}
\tag{7}
$$

$$
\begin{aligned}
&4A(2\kappa'\tau+\kappa\tau')-2\alpha(6\kappa'\tau^2+6\kappa\tau\tau'-3\kappa^2\kappa'-2\kappa''') \\
&\quad +C(4\kappa^3\tau'+24\kappa^2\kappa'\tau)+4\beta(4\kappa'\tau^3+6\kappa\tau^2\tau' \\
&\quad -3\kappa^2\kappa'\tau-\kappa^3\tau'-4\kappa'\tau''-6\kappa''\tau'-4\kappa'''\tau-\kappa\tau''')=0.
\end{aligned}
\tag{8}
$$

This claim is not true, or in other words use of the two general equilibrium shape equations of Zhang *et al.* [1] does not give rise to Eqs. (7) and (8). By using the correct Eqs. (3) and (4) provided here, we confirm that by substituting Eq. (6) into Eqs. (3) and (4) we obtain Eqs. (7) and (8) exactly. We note that the constants A, C, $-\alpha/2$, and β used in [1] correspond, respectively, to the elastic moduli k_2, k_{22}, k_3, and k_4 shown in [5].

We may further check the two Euler-Lagrange equations Eqs. (3) and (4) by considering the well-known Sadowsky functional [6–8], which has the form

$$
\mathcal{F}(\kappa,\tau)=\kappa^2(1+\omega^2)^2, \tag{9}
$$

where $\omega=\tau/\kappa$. We note that the Sadowsky energy function is used to determine the shape of a narrow thin elastic band, such as Möbius strips [6–8]. Upon substituting Eq. (9) into Eq. (4), we obtain

$$
\begin{aligned}
&2\kappa^{-1}\omega(1+\omega^2)\kappa'''+2(1+3\omega^2)\omega'''+[-6\kappa^{-2}\omega(1+\omega^2)\kappa' \\
&\quad +4\kappa^{-1}(1+3\omega^2)\omega']\kappa''+[2\kappa^{-1}(1+3\omega^2)\kappa'+36\omega\omega']\omega'' \\
&\quad +4\kappa^{-3}\omega(1+\omega^2)\kappa'^3-4\kappa^{-2}(1+3\omega^2)\kappa'^2\omega' \\
&\quad +12\kappa^{-1}\omega\omega'^2\kappa'+12\omega'^3+\kappa\omega(1+\omega^2)^2\kappa' \\
&\quad +\kappa^2(1+\omega^2)(1+3\omega^2)\omega'=0,
\end{aligned}
\tag{10}
$$

which is exactly Eq. (4) in Hangan and Murea [7]. Next, we substitute Eq. (9) into Eq. (3) and obtain

$$
\begin{aligned}
&2(1+\omega^2)(1+3\omega^2)\kappa''+8\omega\kappa(1+2\omega^2)\omega''+8\omega(2+3\omega^2)\omega'\kappa' \\
&\quad +4\kappa(1+9\omega^2)\omega'^2-4\kappa^{-1}\omega^2(1+\omega^2)\kappa'^2 \\
&\quad +\kappa^3(1+\omega^2)^2(1+2\omega^2)=0.
\end{aligned}
\tag{11}
$$

By differentiating Eq. (11) with respect to the arclength parameter s, we deduce

$$
\begin{aligned}
&2(1+\omega^2)(1+3\omega^2)\kappa'''+8\omega\kappa(1+2\omega^2)\omega'''+[16\omega(2+3\omega^2)\omega' \\
&\quad -8\kappa^{-1}\omega^2(1+\omega^2)\kappa']\kappa''+[8\kappa(2+15\omega^2)\omega' \\
&\quad +8\omega(3+5\omega^2)\kappa']\omega''+[4(5+27\omega^2)\omega'^2+3\kappa^2(1+2\omega^2) \\
&\quad \times(1+\omega^2)^2]\kappa'+[-8\kappa^{-1}\omega(1+2\omega^2)\kappa'^2+4\kappa^3\omega(1+\omega^2) \\
&\quad \times(2+3\omega^2)]\omega'+72\kappa\omega\omega'^3+4\kappa^{-2}\omega^2(1+\omega^2)\kappa'^3=0.
\end{aligned}
\tag{12}
$$

Now we introduce the quantities

TABLE I. Helical pitch p and coil radius r_0 of A-, B-, and Z-DNA (Dickerson *et al.* [9] and Bates and Maxwell [10]), and $\omega_0=2\pi/p$ and the relations between p and r_0 and r_0 and h for each type of DNA.

DNA	p (nm)	r_0 (nm)	ω_0 (nm^{-1})	p/r_0	r_0/h
A-DNA	2.46	1.3	2.55	1.89	3.32
B-DNA	3.32	1.0	1.89	3.32	1.89
Z-DNA	4.56	0.9	1.38	5.07	1.24

$$
a=\frac{1}{2\kappa(1+\omega^2)},\quad b=-\frac{\omega}{(1+\omega^2)},\quad c=-\frac{\kappa'}{2\kappa^2(1+\omega^2)},
$$

and it can be shown that the linear combination $a\times$ (12)+b $\times$Eq. (10) +$c\times$Eq. (11) gives rise to

$$
\begin{aligned}
&\kappa^{-1}(1+\omega^2)\kappa'''+2\omega\omega'''+[-\kappa^{-2}(1+\omega^2)\kappa'+12\kappa^{-1}\omega\omega']\kappa'' \\
&\quad +[6\kappa^{-1}\omega\kappa'+8(1+\omega^2)^{-1}(1+3\omega^2)\omega']\omega''-8\kappa^{-2}\omega\kappa'^2\omega' \\
&\quad +8\kappa^{-1}(1+\omega^2)^{-1}(1+3\omega^2)\kappa'\omega'^2+24\omega(1+\omega^2)^{-1}\omega'^3 \\
&\quad +\kappa(1+\omega^2)^2\kappa'+3\kappa^2\omega(1+\omega^2)\omega'=0,
\end{aligned}
\tag{13}
$$

which is precisely Eq. (3) stated in Hangan and Murea [7].

For the energy density $\mathcal{F}$ of the wormlike chain (WLC) model studied in [1], which depends only on the curvature κ, namely

$$
\mathcal{F}(\kappa)=\kappa^2+\lambda, \tag{14}
$$

where λ is a constant representing external forces or constraints, we find from Eq. (5) that we also obtain Eq. (3.7) shown in [1], given by

$$
2\kappa''+\kappa^3-\lambda\kappa-2\kappa\tau^2=0,\quad \mathcal{C}=4\kappa^2\tau, \tag{15}
$$

where $\mathcal{C}$ denotes an arbitrary constant. Thus, for a coiled polymer chain which has the curvature and torsion given by

$$
\kappa=\frac{r_0}{r_0^2+h^2},\qquad \tau=\frac{h}{r_0^2+h^2}, \tag{16}
$$

where r_0 is the helical coiled radius and $h=p/(2\pi)$, where p is the helical pitch, we deduce from Eq. (15) that

$$
r_0^2-2h^2-\lambda(r_0^2+h^2)^2=0,\quad \mathcal{C}=\frac{4r_0^2h}{(r_0^2+h^2)^3}. \tag{17}
$$

We note that the first of equations (17) is in agreement with Eq. (3.10) in [1]. In the case of $\lambda=0$, we have from the first of equations (17) that $r_0=\sqrt{2}h$, which then gives rise to $\mathcal{C}=8/(27h^3)$. Since $p=2\pi h$, therefore $p/r_0=\sqrt{2}\pi\simeq 4.443$. Comparing this to the values for A-, B- and Z-DNA shown in Table I, we see that the WLC model with no external force or constraint applied gives a crude approximation to only the DNA of Z form.

In Zhang *et al.* [1], the free energy density for the wormlike rod chain (WLRC) model is also examined, which is given by

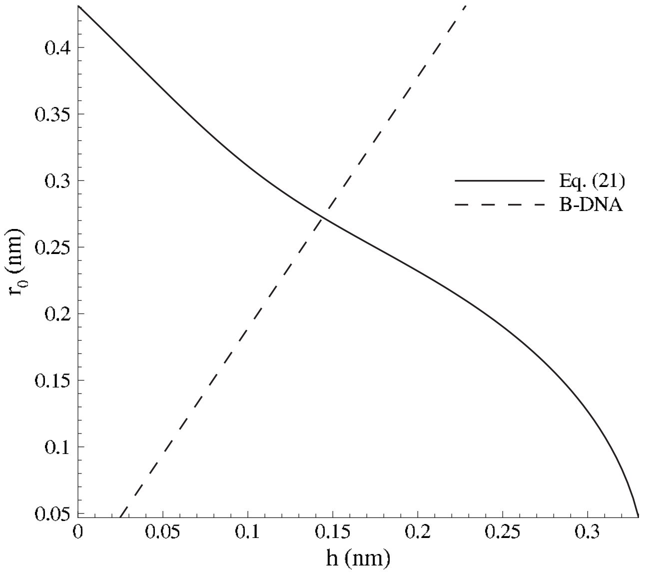

FIG. 1. Relation between the coil radius r_0 and h, where $h = p/(2\pi)$. The solid line is the WLRC model for B-DNA and the dashed line is the relation of r_0 and h for B-DNA from Table I.

$$\mathcal{F}(\kappa,\tau) = \frac{A}{2}\kappa^2 + \frac{C}{2}(\tau - \omega_0)^2, \tag{18}$$

where A is the bending rigidity, C is the twist rigidity, and ω_0 denotes the spontaneous twist of the helix given by $\omega_0 = 2\pi/p$, where p is the helical pitch. Since the general equilibrium shape equations (2.31) and (2.32) shown in Zhang *et al.* [1] are incorrect, Eqs. (3.13)–(3.15) in [1], which result from substituting (18) into Eqs. (2.31) and (2.32), are also incorrect. Here, we derive the correct equilibrium shape equations corresponding to the energy density (18) by using the correct Euler-Lagrange equations (3) and (4). From Eqs. (3), (4), and (18), we obtain

$$A\kappa^5 - \kappa^3[(2A-3C)\tau^2 + 2C\omega_0\tau + C\omega_0^2] + 2A\kappa^2\kappa'' - 4C\kappa'\tau\tau' + 2C\kappa(2\tau\tau'' + \tau'^2) = 0, \tag{19}$$

$$(A-C)\kappa^4\tau' + \kappa^3\kappa'[(2A-C)\tau + C\omega_0] + C\kappa^2(\tau^2\tau' - \tau''') + C\kappa(2\kappa'\tau'' + \kappa''\tau') - 2C\kappa'^2\tau' = 0. \tag{20}$$

Thus, for a coiled polymer chain which has the curvature and torsion given by Eq. (16) we deduce from Eqs. (19) and (20) the following relationship for r_0 and h:

$$(2A-3C)h^2 - Ar_0^2 + 2C\omega_0 h(r_0^2 + h^2) + C\omega_0^2(r_0^2 + h^2)^2 = 0. \tag{21}$$

We observe that two of the terms involving the constant C differ from those given in [1]. For the given values of A and C in [1] ($A = 50$ nm and $C = 1.5A$) and using $\omega_0 = 1.89\ \text{nm}^{-1}$ from Table I for B-DNA, as shown in Fig. 1 Eq. (21) gives a completely different physical behavior from that indicated in [1]. Upon comparing Eq. (21) with the behavior of B-DNA, it is very clear that, with these given constants, the WLRC model is not suitable for describing the properties of B-DNA. Furthermore, on using $A = 50$ nm and $C = 1.5A$ but changing the values of ω_0 for different DNA (see Table I), we obtain a similar behavior to that of Eq. (21), which is shown by the solid line of Fig. 1. Thus, we may conclude that the WLRC model with the present constants cannot be used to describe the properties of DNA. However, using values of the constants where C is much smaller than A, such as $A = 75$ nm and $C = 0.1$ nm, the correct equation may be used to predict the physical behavior of DNA. In fact, when C is much smaller than A, the behavior of Eq. (21) approaches that of $r_0 = \sqrt{2}h$, which is the case for the WLC model that can be used to approximate the physical behavior of Z-DNA (see Fig. 2).

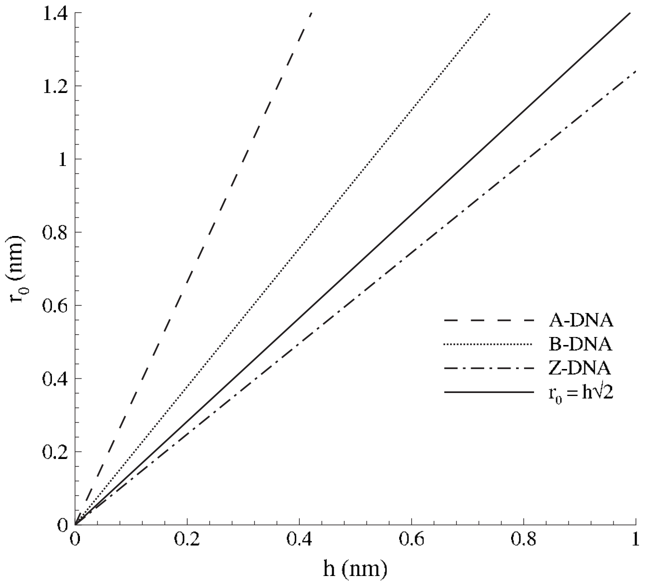

FIG. 2. Relation between the coil radius r_0 and h for A-, B-, and Z-DNA from Table I, compared with the limiting case $r_0 = \sqrt{2}h$ of Eq. (21).

Next, if we ignore the terms ω_0 in Eq. (18) for which the energy density for the WLRC model reduces to

$$\mathcal{F}(\kappa,\tau) = \frac{A}{2}\kappa^2 + \frac{C}{2}\tau^2, \tag{22}$$

then from Eq. (21) we may obtain

$$(2A-3C)h^2 - Ar_0^2 = 0,$$

which gives rise to

$$\frac{r_0}{h} = \sqrt{\frac{(2A-3C)}{A}},$$

assuming that A is greater than zero. Thus, for this model to be sensible, we need the condition that the values of A and C are such that $2A - 3C > 0$ and, since both A and C are positive, we have $0 \leq C/A < 2/3$. Furthermore, by prescribing $\mu = r_0/h$, we have

$$\frac{C}{A} = \frac{(2-\mu^2)}{3}. \tag{23}$$

Upon substituting the values of $\mu = r_0/h$ for A-, B-, and Z-DNA, which are given in Table I, into Eq. (23), we find

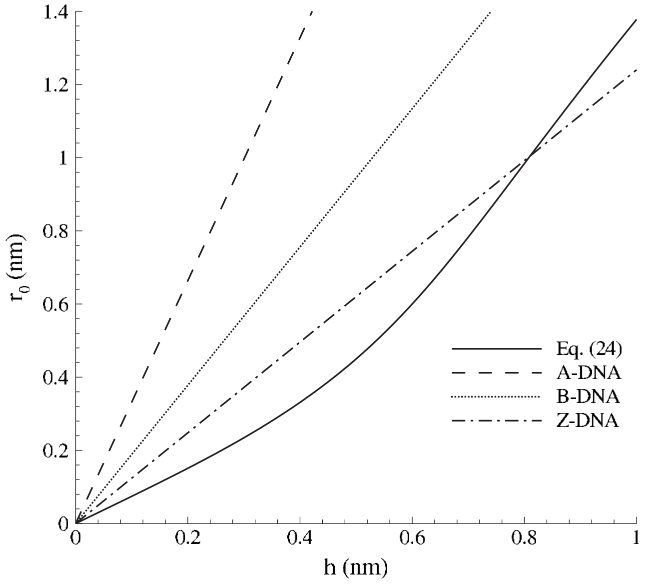

FIG. 3. Relation between the coil radius r_0 and h. The solid line is obtained from Eq. (24), which is based on the model proposed by [5]; the dashed, dotted, and dash-dotted lines, respectively, represent the relations of r_0 and h for A-, B-, and Z-DNA from Table I.

that $C/A=-3.007$, -0.524, and 0.154 for A-, B-, and Z-DNA, respectively. Therefore, we may conclude that the functional form (22) is appropriate only for describing the free energy density of Z-DNA, particularly when A and C satisfy $C/A=0.154$.

Further, Zhang *et al.* [1] also consider the solutions for helical biopolymers by substituting Eq. (16) into Eqs. (7) and (8) [which are Eqs. (4.2) and (4.3) in [1]]. We find that Eq. (4.4) in Zhang *et al.* [1] is incorrect. The correct equation is given by

$$Cr_0^2(4h^2-3r_0^2)+2A(2h^6+3r_0^2h^4-r_0^6) - 2\alpha h(2h^4-r_0^2h^2-3r_0^4)+2\beta h^2(2h^2-5r_0^2)+4\lambda(r_0^2+h^2)^4 = 0. \tag{24}$$

For the case of no external force or constraint ($\lambda=0$) and for particular values of the constants, namely, $A=50$ nm, $C=60$ nm^2, $\alpha=40$ nm^3, and $\beta=50$ nm^2, used in [1], we plot Eq. (24) (the solid line) showing the relation between r_0 and h in Fig. 3, together with the values of A-, B- and Z-DNA. Again, it is clear from Fig. 3 that with the given constants the above model does not describe the properties of any form of DNA, contradicting the claim made by Zhang *et al.* [1] that this model can be used for B-DNA. However, one might argue that, by choosing a set of appropriate constants, it may be possible to use this model to describe the features of DNA. For example, choosing $A=10$ nm, $C=60$ nm^2, $\alpha=1$ nm^3, and $\beta=1$ nm^2, we find from Fig. 4 that Eq. (24) agrees well with the behavior of Z-DNA. For $A=50$ nm, $C=20$ nm^2, $\alpha=40$ nm^3, and $\beta=10$ nm^2, Fig. 4 also shows reasonable agreement between the behavior of Eq. (24) and that of B-DNA.

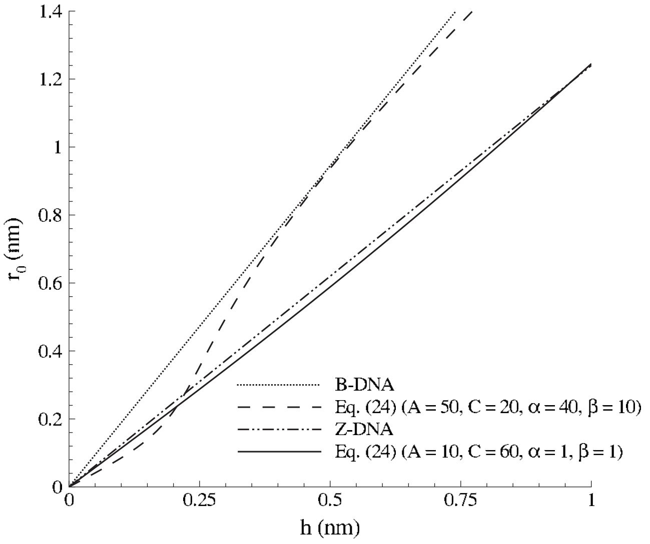

FIG. 4. Comparison between the behavior of B- and Z-DNA and Eq. (24) for two different sets of constants.

In summary, this Comment provides the correct Euler-Lagrange equations (3) and (4) which are cross-checked using certain energy functionals for which the resultant Euler-Lagrange equations have been given previously in the literature. We point out that Eqs. (2.27) and (2.29) in Zhang *et al.* [1] are incorrect, leading therefore to the incorrect Euler-Lagrange equations, namely (2.31) and (2.32) in [1]. We comment that since Eqs. (2.31) and (2.32) in Zhang *et al.* [1] are incorrect, all those results in [1] that are based on these equations are also incorrect. The correct results are provided here, and we find that for the numerical values of the constants given in [1] the WLRC model does not agree with the behavior of any form of DNA. We find that the free energy density, which arises from setting $\omega_0=0$ in the WLRC model, can be used to describe the physical behavior of Z-DNA when the constants A and C involved are chosen to satisfy $C/A=0.154$. For the energy density model proposed by Wei *et al.* [5], we discover that Eq. (4.4) in [1] is also incorrect. Again we give the correct equation here, namely, Eq. (24) and we also present new numerical results. With the numerical values of the constants used in Zhang *et al.* [1] we do not find any agreement between the behavior of the model based on [5] and any form of DNA. However, Eq. (24) may still be used for DNA, if appropriate numerical values of the constants are taken. Finally, although the WLC model with no external force or constraint can be used as a crude approximation, we do not find that it agrees well with Z-DNA as suggested in [1].

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