Asymmetric elastic rod model for DNA

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In this paper we consider the anharmonic corrections to the anisotropic elastic rod model for DNA. Our model accounts for the difference between the bending energies of positive and negative rolls, which comes from the asymmetric structure of the DNA molecule. We will show that the model can explain the high flexibility of DNA at small length scales, as well as kink formation at high deformation limit.

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I. INTRODUCTION

Characterizing the elastic behavior of DNA molecule is of crucial importance in understanding its biological functions. In recent years, single-molecule experiments such as DNA stretching and cyclization [1,2] have provided us with valuable information about the elasticity of long DNA molecules. The results of these experiments can be described by the elastic rod model (also called wormlike-chain model) [3,4]. In this model it is assumed that the elastic energy is a harmonic function of the deformation [4,5]. The elastic rod model is very successful in explaining the elastic behavior of the micron-size DNA molecules.

Recently, modern experimental techniques have made it possible to study the elasticity of DNA at nanometer length scale [6–9]. In these experiments it is observed that short DNA molecules are much more flexible than predicted by the elastic rod model. Although there is some doubt about the results of some of these experiments [10], several different models have been presented by now that try to explain the origin of this discrepancy by considering the possibility of local DNA melting [9,11–13] or the occurrence of kinks in the DNA structure [14]. Also Wiggins *et al.* [[8] suggested an alternative form for the elastic energy [15].

Since the DNA is not a symmetric molecule, the energy required to bend the DNA over its major groove is not equal to the energy required to bend it over its minor groove. The model, which is introduced in this paper, takes this difference into account. The effect of asymmetric structure of DNA on its elastic energy has been discussed previously by Marko and Siggia [5], where they showed that there must be a coupling term between bend and twist in the harmonic elastic energy. We will discuss that the asymmetric structure of DNA can also be introduced as a correction to the harmonic elastic energy, which is of the third order. We shall show that our *asymmetric elastic rod model* can account for the high flexibility of short DNA molecules.

II. MODEL

In the elastic rod model DNA is represented by a continuous inextensible rod [3,4]. The curve, which passes through the rod center, determines the configuration of the DNA in three-dimensional (3D) space. This curve is denoted by $\vec{r}$ and is parametrized by the arc-length parameter s (Fig. 1). In addition, a local coordinate system with an orthonormal basis $\{\hat{d}_1,\hat{d}_2,\hat{d}_3\}$ is attached to each point of the rod. As depicted in Fig. 1, $\hat{d}_3(s)$ is tangent to the curve $\vec{r}$ at each point, $\hat{d}_3(s)=\mathrm{d}\vec{r}/\mathrm{d}s$, $\hat{d}_1(s)$ is perpendicular to $\hat{d}_3(s)$ and points toward the major groove, and $\hat{d}_2(s)$ is defined as $\hat{d}_2(s)=\hat{d}_3(s)\hat{d}_1(s)$. These three orthogonal vectors uniquely determine the three dimensional configuration of DNA. From classical mechanics we have

$$\dot{\hat{d}}_i=\vec{\Omega}\times\hat{d}_i \quad i=1,2,3, \tag{1}$$

where the dot denotes the derivative with respect to s and $\vec{\Omega}$ is called the spatial angular velocity. The components of $\vec{\Omega}$ in the local coordinate system are denoted by Ω_1, Ω_2, and Ω_3. The elastic energy of an inextensible DNA in the most general form can then be written as

$$E=\int_0^L \mathcal{E}[\Omega_1(s),\Omega_2(s),\Omega_3(s)]ds, \tag{2}$$

where L is the total length of DNA. $\mathcal{E}(s)$ is the energy per unit length of DNA, i.e., the energy density, at point s. For small deformations, the energy density can be written as a

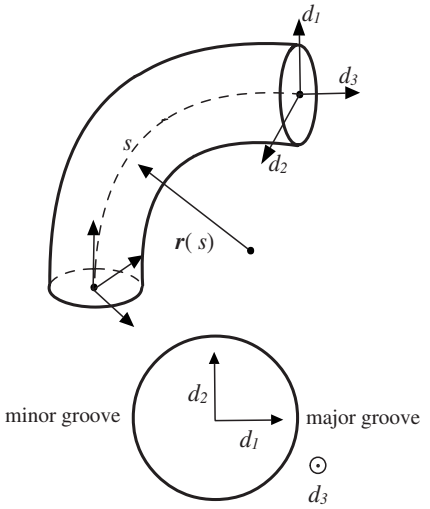

FIG. 1. Parametrization of the elastic rod. The local frame $\{\hat{d}_1,\hat{d}_2,\hat{d}_3\}$ is attached to the rod.

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Taylor expansion about the lowest-energy configuration [5]. For a DNA with no intrinsic curvature and a constant intrinsic twist ω_0, the lowest-energy configuration is given by $\vec{\Omega}_0=[0,0,\omega_0]^T$. Thus, at the lowest order, we arrive at a harmonic energy density in the form

$$\mathcal{E}_{\text{harm}}[\Omega_1,\Omega_2,\Omega_3]=\frac{1}{2}k_BT_r\vec{\omega}^T\mathbf{Q}\vec{\omega}, \tag{3}$$

where k_B is the Boltzmann constant, $T_r\simeq 300$ °K is the room temperature, and $\vec{\omega}$ is defined by $\vec{\omega}=\vec{\Omega}-\vec{\Omega}_0$. $\mathbf{Q}$ is a 3×3 symmetric matrix whose elements are the elastic constants of DNA [3,4,16]. Considering a short segment of DNA with the length ds at point s, this segment has a symmetry under 180° rotation about the local $\hat{d}_1$ axis at point s. Thus the odd powers of Ω_1 must not appear in the expansion of energy density, and the matrix $\mathbf{Q}$ has only four independent nonzero elements: $\mathbf{Q}_{11}$, $\mathbf{Q}_{22}$, $\mathbf{Q}_{33}$, and $\mathbf{Q}_{23}$. Therefore, the harmonic energy density can be written as [5]

$$\mathcal{E}_{\text{harm}}=\frac{1}{2}k_BT_r[A_1\Omega_1^2+A_2\Omega_2^2+C(\Omega_3-\omega_0)^2 + 2D\Omega_2(\Omega_3-\omega_0)]. \tag{4}$$

The first two terms in Eq. (4) correspond to the bending of DNA over its grooves (roll) and over its backbone (tilt), respectively. A_1 and A_2 are the corresponding bending constants. Since roll requires less energy than tilt [17–19], one expects that $A_2<A_1$. The third term indicates the energy needed for twisting the DNA about its central axis, with the twist constant C. Finally, the fourth term accounts for the coupling between roll and twist [20]. Although the elastic constants of DNA may depend on the sequence [16], in this paper we neglect sequence dependence and assume that they are constant all along the DNA.

The existence of twist-roll coupling indicates that there is indeed a difference between bending over major groove (positive roll) and bending over minor groove (negative roll): for positive values of D, the DNA has a tendency to untwist when roll is positive and to overtwist when roll is negative.

To account for the effect of asymmetry on the bending energy of DNA, we need a term in the energy density, which is an odd function of Ω_2, and does not depend on Ω_1 or Ω_3. There is no such term in the harmonic elastic energy, so we consider third-order terms in the expansion of energy density. The term proportional to Ω_2^3 has the desired property. On the basis of some theoretical analysis [21], as well as experimental evidences [22] and simulation studies [23], we assume that negative roll is more favorable than positive roll. Thus we write the third-order term in the form $+1/3!F^2\Omega_2^3$, where F is a real parameter. (It must be noted that the main conclusion of the paper remains valid if positive roll is easier than negative roll. To account for this case, one can write the third-order term in the form $-1/3!F^2\Omega_2^3$.) To keep the model as simple as possible, we neglect couplings in all orders, as well as higher-order corrections to the twist energy. So the only third-order term that enters in the model is $1/3!F^2\Omega_2^3$. Since the elastic energy must have a lower bound, we must keep the fourth-order correction to the roll energy, i.e., the term proportional to Ω_2^4, in the model. For consistency of the model, we also keep the corresponding fourth-order correction to the tilt energy. Since the anisotropy in bending energy is accounted for in the second order, to reduce the model free parameters, we write the fourth-order terms in the form $1/4!G^3(\Omega_1^4+\Omega_2^4)$, with G as real and positive. Adding third-order and fourth-order terms to the harmonic energy density, we obtain the asymmetric elastic rod model, which is given by

$$\mathcal{E}_{\text{asym}}=k_BT_r\left[\frac{1}{2}A_1\Omega_1^2+\frac{1}{2}A_2\Omega_2^2+\frac{1}{2}C(\Omega_3-\omega_0)^2+\frac{1}{3!}F^2\Omega_2^3 + \frac{1}{4!}G^3(\Omega_1^4+\Omega_2^4)\right]. \tag{5}$$

This model accounts for the asymmetry between positive and negative rolls, as well as the difference in the energies of roll and tilt. Since there is no coupling term in the model, roll, tilt, and twist can be regarded as independent deformations, and the energy density can be decomposed into three separate terms,

$$\mathcal{E}_{\text{asym}}[\Omega_1,\Omega_2,\Omega_3]=\mathcal{E}_1[\Omega_1]+\mathcal{E}_2[\Omega_2]+\mathcal{E}_3[\Omega_3], \tag{6}$$

where

$$\mathcal{E}_1=k_BT_r\left[\frac{1}{2}A_1\Omega_1^2+\frac{1}{4!}G^3\Omega_1^4\right], \tag{7}$$

$$\mathcal{E}_2=k_BT_r\left[\frac{1}{2}A_2\Omega_2^2+\frac{1}{3!}F^2\Omega_2^3+\frac{1}{4!}G^3\Omega_2^4\right], \tag{8}$$

$$\mathcal{E}_3=\frac{1}{2}k_BT_rC(\Omega_3-\omega_0)^2 \tag{9}$$

Depending on the values of A_2, F, and G, $\mathcal{E}_2$ can take three different forms (see Fig. 2). For small values of F, $\mathcal{E}_2$ has only one minimum at $\Omega_2=0$ and its curvature is always positive. For $F>(2A_2G^3)^{1/4}$ the curvature of $\mathcal{E}_2$ can change sign and there are two inflection points. For given A_2 and G there exists an upper bound $F_c=(8/3A_2G^3)^{1/4}$, beyond which $\mathcal{E}_2$ has two minima: one at $\Omega_2=0$ and the other one at a negative Ω_2. In this case DNA has two stable configurations, and there is always a barrier between them. However, one expects that the barrier is not large compared to k_BT_r for a real DNA.

III. RESULTS AND DISCUSSION

To study the elastic behavior of DNA in the asymmetric elastic rod model, we calculate the distribution function $P(\theta)$, the probability that the DNA bends into an angle θ. The effective bending energy can be related to $\log P(\theta)$ as follows: for a two-dimensional (2D) DNA, the effective bending energy is defined as

$$E_{\text{eff}}^{\text{2D}}(\theta)=-k_BT_r\log P(\theta), \tag{10}$$

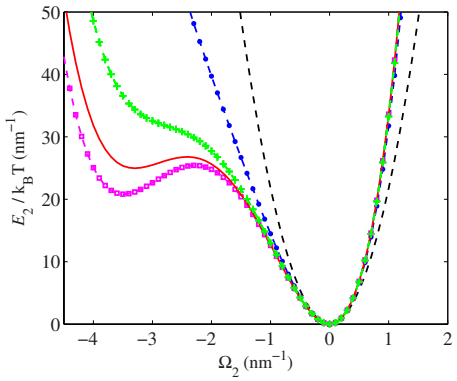

FIG. 2. (Color online) $\mathcal{E}_2$ as a function of Ω_2 for $A_2=43.50$ nm and different values of F and G. Dashed curve (black): $F=G=0$. Dash-dot curve: (blue) $G=3.20$ nm and $F=7.20$ nm; $\mathcal{E}_2$ has one minimum and its curvature is positive everywhere. Dash-cross curve (green): $G=3.20$ nm and $F=7.80$ nm; $\mathcal{E}_2$ has two inflection points and one minimum. Solid curve (red): $G=3.20$ nm and $F=7.90$ nm; $\mathcal{E}_2$ has two minima. Dash-square curve (magenta): $G=3.20$ nm and $F=7.94$ nm. Note that a change of 0.04 nm in F results in a change of about 1 $k_B T_r / l_0$ in $\mathcal{E}_2$ in the vicinity of the second minimum.

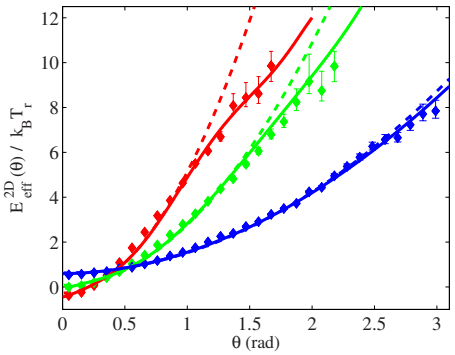

FIG. 3. (Color online) E^{2D}_{eff} as a function of θ for three different DNA lengths. Top (red): $L=5$ nm. Middle (green): $L=10$ nm. Bottom (blue): $L=30$ nm. Dots show the experimental data of Wiggins *et al.* [8]. Curves show the theoretical results. Dashed curves: isotropic-harmonic elastic rod model, with $A_1=A_2=54$ nm and $F=G=0$. Solid curves: $A_1=87.00$ nm, $A_2=43.50$ nm, $F=7.90$ nm, and $G=3.20$ nm.

while in three dimensions, the effective bending energy is given by [24]

$$E^{3D}_{eff}(\theta) = -k_B T_r \log \frac{P(\theta)}{\sin(\theta)}. \tag{11}$$

We use a Monte Carlo simulation to calculate $P(\theta)$. In this simulation we discretize each chain into separate segments of length $l_0=0.34$ nm, equal to the base-pair separation in DNA. The orientation of each segment is then determined by a vector $\vec{\Theta}$, where $|\vec{\Theta}|$ determines the rotation angle of the local coordinate system with respect to the laboratory coordinate system, and the direction of $\vec{\Theta}$ indicates the normal to the plane of rotation. The special angular velocity is related to $\vec{\Theta}$ as $\vec{\Omega}=\vec{\Theta}/l_0$. In each Monte Carlo move, we randomly choose a segment along the chain, and for that segment we change the vector $\vec{\Theta}$ by $\Delta\vec{\Theta}$. The direction of $\Delta\vec{\Theta}$ is random, and its magnitude is chosen randomly in the interval $[0, \Theta_0]$. Θ_0 is chosen so that the accept ratio is about 0.5. We do not include the self-avoiding in the simulation since the probability of self-crossing is small for the short simulated DNA molecules.

Recently, Wiggins *et al.* [8] used atomic force microscopy to measure distribution of the bending angle of short DNA molecules. Although the DNA molecules in the experiment of Wiggins *et al.* [8] has the characteristic properties of two-dimensional polymers [8], to simulate the experiment we do not confine the DNA completely in a plane. The reason is that the minimum-energy configuration of an anisotropic DNA is not planar, although the deviation from a planar configuration is negligible [25]. It is known in the anisotropic-harmonic elastic rod model that the effective bending constant of long DNA molecules in three dimensions is equal to the harmonic average of A_1 and A_2 [16,18,19], $A_{eff}=[1/2(1/A_1+1/A_2)]^{-1}$, while in the two dimensions the effective bending constant is given by $A^{2D}_{eff}=\sqrt{A_1 A_2}$ [26]. Since A^{2D}_{eff} is always greater than A_{eff}, confining the DNA in a plane costs energy. For this reason, we allow the DNA to come out of the plane by 0.3 nm, which is seven times smaller than DNA diameter and lies in the range of atomic length scales.

Following other studies [4,27], we assume that $A_1=2A_2$, $C=100$ nm, and $\omega_0=1.8$ nm^{-1}. The values of A_2, F, and G are then determined by fitting the theoretical results to the experimental data of Wiggins *et al.* [8] for $L=5$ nm, with the constraint that the persistence length of the DNA is 54 nm. A good fit is shown in Fig. 3, which corresponds to $A_2=43.50$ nm, $G=3.20$ nm, and $F=7.90$ nm. It can be seen that, with this set of the parameters, the model can explain the experimental data for $L=5$ nm, as well as $L=10$ nm and $L=30$ nm.

We report the values of the fitting parameter with three significant digits. The reason is that $\mathcal{E}_2$ is very sensitive to the changes of the parameters, especially when it has two minima. In fact, a change in the order of 10^{-2} nm in these parameters may results in a change in $\mathcal{E}_2$ on the order of $1 k_B T_r / l_0$ (see Fig. 2) and therefore can significantly affect the elastic behavior of DNA. We must note here that the ratio A_1/A_2 is also relevant to the fitting procedure. However, one can obtain equally good fits for different values of A_1/A_2.

The predictions of isotropic-harmonic elastic rod model are shown in Fig. 3 for comparison. As can be seen, both in the experiment and our model, $E^{2D}_{eff}(\theta)$ deviates from the harmonic model at large bending angles.

The functional form of $\mathcal{E}_2$ for $A_2=43.50$ nm, $F=7.90$ nm, and $G=3.20$ nm is shown in Fig. 2, which has two minima. The second minimum occurs at $\Omega_2=-3.3$ nm^{-1}, which corresponds to a $-64°$ roll between adjacent base pairs. Thus, the existence of a second minimum can lead to the formation of kinks in the minor groove direction in a tightly bent DNA. Continuing the graphs in Fig. 3, they arrive to an approximately linear regime. This linear behavior is a signature of kink formation. Both the slope of the line and the crossover point are related to the values of F and G.

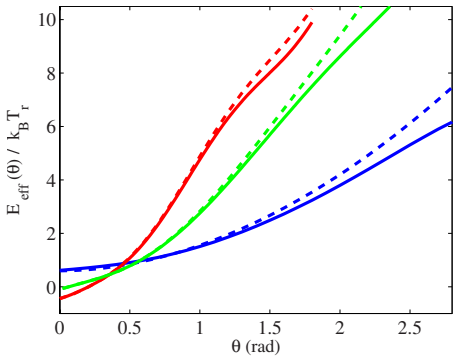

FIG. 4. (Color online) Effective bending energy as a function of θ for three-dimensional (solid curves) and two-dimensional (dashed curves) DNA molecules with different lengths. Top curves (red): $L=5$ nm. Middle curves (green): $L=10$ nm. Bottom curves (blue): $L=30$ nm. The values of the elastic constants are given in the caption of Fig. 3.

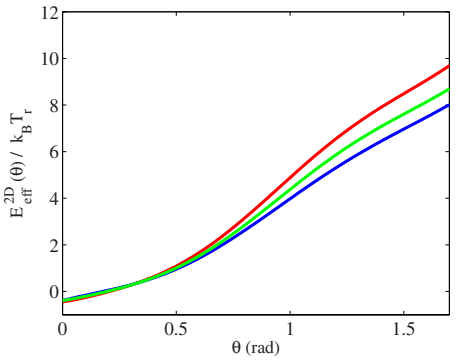

FIG. 5. (Color online) $E_{\mathrm{eff}}^{\mathrm{2D}}$ as a function of θ for $L=5$ nm and three different temperatures. From top to bottom: $T=T_r=300$ °K (red), $T=330$ °K (green), and $T=360$ °K (blue). The values of the elastic constants are given in the caption of Fig. 3.

The possibility of kink formation in the DNA structure has been considered previously by other authors. It was first mentioned by Crick and Klug [21], who proposed an atomistic structure for a kinked DNA. They suggested that DNA can be kinked most easily toward the minor groove. Nelson and co-workers [14] presented a simple model for kinkable elastic rods in which the kinks are completely flexible and can be formed in any direction with equal probability. Their model can explain the high cyclization probability of short DNA molecules [6,7]. The linear behavior is also observed in their model [14] but the slope of the line is always zero. In a recent experiment, Du *et al.* [28] proved the existence of kinks in DNA minicircles of 64–65 bp. Kinks in the direction of minor groove have been observed in the structure of nucleosomal DNA [22]. Molecular dynamics simulations on a 94 bp minicircle [23] also show that kinks are formed, with the same structure predicted by Crick and Klug [21] and with a $-80°$ roll angle at the kink location. This roll angle is somewhat higher than the value obtained from the data of Wiggins *et al.* [8], but since the DNA is not free in this simulation, the difference may be due to the existence of the external stress. This discrepancy can also be due to the difference in the values of the elastic constants. In the experiment of Wiggins *et al.* [8], DNA is absorbed electrostatically on a mica surface using magnesium ions, and the solvent is dried. It is expected that the elastic constants of DNA in these conditions differ from the elastic constant of DNA in solution [13].

Kinks are also observed in the crystal structures of nonhistone protein-DNA complexes [20,29]. In these complexes, DNA has a clear tendency to kink in the major groove direction. Du *et al.* [28] found the distribution function $P(\theta)$ for a base-pair step in these complexes [10]. Although it is contradictory to our primary assumption that kinks are formed toward the manor groove, our model can be fitted to the data of Du *et al.* [28] by writing the third-order term in the form $-1/3!F^2\Omega_2^3$, and choosing $F=8.86$ nm and $G=3.83$ nm. We found that the model with these values of F and G cannot explain the experimental data of Wiggins *et al.* [8]. This shows that the statistical property of DNA in the protein-DNA complexes certainly differs from the free DNA. This difference is probably due to the interaction of proteins with DNA, which can alter the DNA conformation dramatically, and leads to different effective elastic constants.

In the asymmetric elastic rod model, the bending energy depends on the bending direction. Thus, it is possible that confining the DNA in a plane affects the elastic properties of DNA, and the elastic behavior of DNA in 2D and 3D may be different. Figure 4 shows the effective energy in three dimensions for three different DNA length with the same elastic constants obtained from the data of Wiggins *et al.* [8]. The dashed curves in Fig. 4 are the same curves depicted in Fig. 3 and show the effective bending energy for a (nearly) two-dimensional DNA. A constant is added to the three-dimensional effective energy so that $E_{\mathrm{eff}}^{\mathrm{3D}}$ is equal to $E_{\mathrm{eff}}^{\mathrm{2D}}$ at $\theta=0$. It can be seen that, with the parameter used in Fig. 4, the anharmonic effects show up also in three dimensions. In addition, there is a significant difference between the two-dimensional and the three-dimensional effective bending energies, especially at large bending angles where the asymmetric term in the bending energy is dominant. The effective energy is lower in 3D, which is expected since in three dimensions there is more possible ways for DNA to bend in the easy directions. A similar behavior is observed for the anisotropic-harmonic DNA [26].

It is important to study the effect of temperature changing on the elastic behavior of DNA in our model. In principle, the elastic constants of DNA are temperature dependent. But even if they do not depend on temperature, it is expected that changing the temperature affects $P(\theta)$, especially when there exist two minima in the roll energy. Figure 5 shows $E_{\mathrm{eff}}^{\mathrm{2D}}(\theta)$ for $L=5$ nm and three different temperatures. It can be seen that the effective bending energy depends strongly on temperature, especially at large bending angles where the probability of the kink formation is high. The behavior shown in Fig. 5 is not specific to the asymmetric elastic rod model and is observed in all kinds of kinkable elastic rod models [13].

IV. CONCLUSION

In this paper, we presented a generalization of the anisotropic elastic rod model, assuming that the energies of posi-

tive and negative rolls are different as a result of the asymmetric structure of DNA. We showed that this model can explain the elastic behavior of short DNA molecules. We also showed that this model allows the formation of kinks in the DNA structure when the DNA is tightly bent. The kinks always form in one of the groove directions, as suggested by other studies. The elastic behavior of DNA in three dimensions and the dependence of the effective bending energy on the temperature were also studied.

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