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Kratky-Porod model

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February, 2013.

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1.Introduction:

The worm-like chain (WLC) model in polymer physics is used to describe the behavior of semi-flexible polyers; it is sometimes referred to as the Kratky-Porod model.

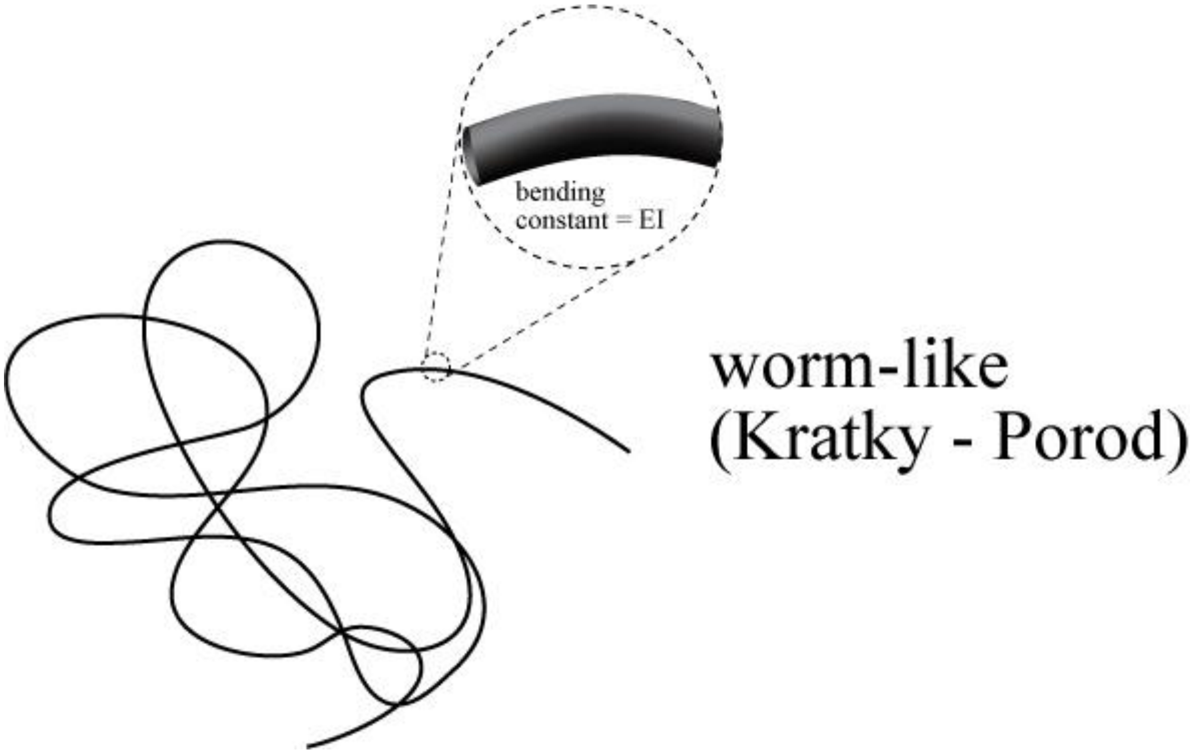

Figure 1. Worm-like

The worm-like chain model is particularly suited for describing stiffer polymers, with successive segments displaying a sort of cooperativity: all pointing in roughly the same direction. At room temperature, the polymer adopts a conformational ensemble that is smoothly curved; at T= 0K, the polymer adopts a rigid rod conformation.

The elastic properties of DNA are essential for its biological function. They control its bending and twisting as well as the induction of structural modifications in the molecule. These can affect its interaction with the cell machinery.

In the particular case of stretching DNA in physiological buffer (near neutral pH, ionic strength approximately 100 mM) at room temperature, the compliance of the DNA along the contour must be accounted for.

1. DNA:

DNA is one of the longest molecule in nature. A human chromosome for example is a few centimeters long. To squeeze such a lengthy molecule in a micron-size nucleus DNA is strongly bent and wrapped around histones, forming the bead on a string structure of chromatin, itself further compactified by extensive coiling. The bending and torsional properties of DNA (and chromatin) are therefore essential to an understanding of its compactification in the nucleus.

DNA is a polymer, i.e. a linear chain made of repeating structural units. These consist of a ribose-phosphate to which four different groups can be linked: adenine (A), guanine (G), cytosine (C) or thymine (T).

DNA differs from most polymers in that it is formed by the winding around each other of two ribose-phosphate polymer chains (a DNA strand) locked by hydrogen bonding between their complementary bases: adenine (guanine) on one strand with thymine (cytosine) on the other. This double helical structure prevents the relaxation of torsional stress by rotation about a single covalent bond as common with man-made polymers. Moreover, the stacking of the bases on top of each other confers unto DNA an unusually large fexional rigidity.

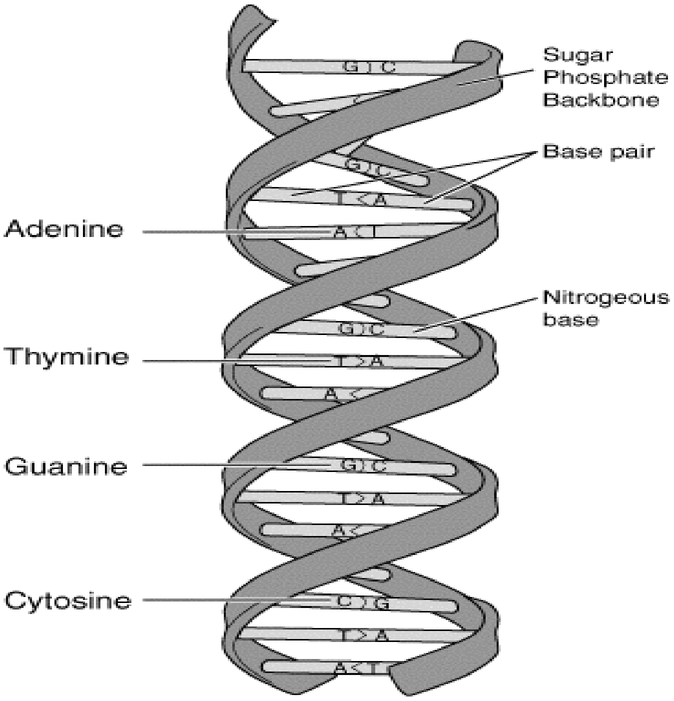

Figure 2. Scheme of DNA molecule

This structure also poses some formidable mechanical problems to the cellular machinery which has to read, transcribe and replicate the instructions of the genetic code buried inside the double helix.

2. Models of polymer elasticity:

Just like any polymer in solution, free DNA adopts a random coil conformation which maximizes its entropy. Pulling on the molecule reduces this entropy and costs energy. The associated entropic forces result from a reduction of the number of possible configurations of the system consisting of the molecule (be it a polymer, DNA or a protein) and its solvent (water, ions), so that at full extension there is but one configuration left: a straight polymer linking both ends. To reach that configuration work has to be done against entropy, a force has to be applied. The entropic forces are rather weak, typically 510 pN. Beyond this regime and up to about 70 pN DNA stretches like any spring: it is in an enthalpy dominated regime.

2.1. The Kratky-Porod model:

For simplicity, let us first consider a polymer chain with no torsional stress. Such a chain is often described by the Kratky-Porod model a succession of N segments of length b and orientation vector $\mathbf{t}_i$. The energy $\mathscr{E}_{\mathrm{KP}}$ of a given chain configuration (the ensemble of segment orientations $\{\mathbf{t}_i\}$) is the sum of the bending energies of successive segments:

$$\mathscr{E}_{\mathrm{KP}} = -\frac{B}{b}\sum_{i=2}^{N} \mathbf{t}_i \cdot \mathbf{t}_{i-1} = -\frac{B}{b}\sum_{i=2}^{N} \cos\theta_i \qquad (1)$$

where θ_i is the angle between successive orientation vectors and B is the bending modulus. There is analogy between the statistical mechanics of a Kratky-Porod chain and that of a classical one-dimensional magnetic (spin) system .This model has been solved exactly . The angular correlation decays exponentially with distance along the chain:

$$\langle \mathbf{t}_i \cdot \mathbf{t}_j \rangle = \mathrm{e}^{-b|i-j|/\xi_T} \tag{2}$$

Where $\xi_T = B/k_{\mathrm{B}}T$ is the decay length of the angular correlation. It reflects the stiffness of the chain and is known as *the persistence length*. The chain end-to-end mean square distance **R_g** satisfies.

$$R_g^2 \equiv \langle \mathbf{R}^2 \rangle = \left(b \sum_{i=1}^{N} \mathbf{t}_i \right)^2 \simeq 2Nb\xi_T = 2l_0\xi_T \tag{3}$$

where **l_0 =*Nb*** is the chain length. A DNA molecule in solution thus adopts a fluctuating random coil configuration of typical size Rg, known as the gyration radius. For many years, the measurement of **R_g** by various means (sedimentation, light scattering, etc.) was the only way to estimate the persistence length of DNA (or any polymer).

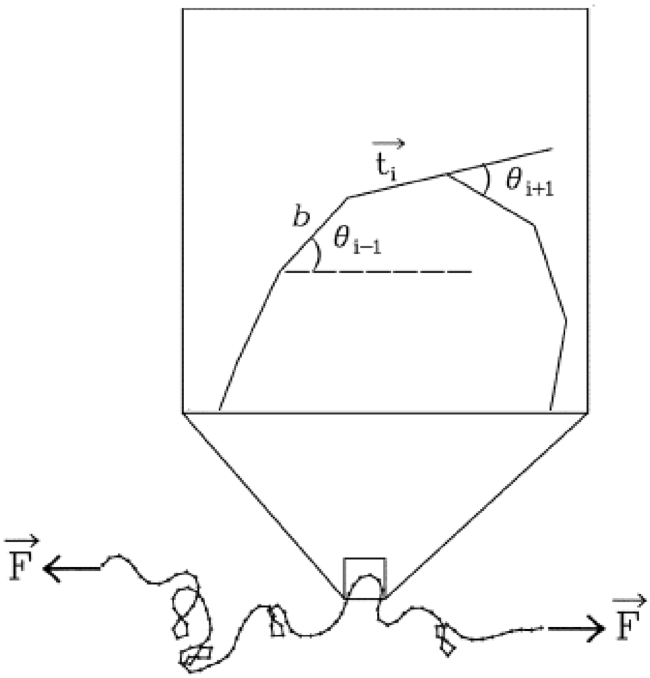

Figure 3. A continuous polymer chain can be simulated by a chain of freely rotating segments of size b and orientation vector **t***i . The direction of the stretching force F defines the z-axis.*

The stretching of a single DNA molecule now provides a much more precise way of measuring ξ_T.

To model the behavior of a polymer chain under tension, it suffices to add to Eq.(1).

A term representing the work

$$W = -\mathbf{F} \cdot \mathbf{R} = -Fb \sum t_{i,z} = -Fb \sum \cos \Theta_i$$

done by a force **F** acting on the chain along the z-axis (**θ**$_i$ is the angle between **t**i and the z-axis):

$$\mathscr{E}_{\mathrm{KP}} = -\frac{B}{b} \sum_{i=2}^{N} \mathbf{t}_i \cdot \mathbf{t}_{i-1} - Fb \sum_{i=1}^{N} t_{i,z} = -\frac{B}{b} \sum_{i=2}^{N} \cos \theta_i - Fb \sum_{i=1}^{N} \cos \Theta_i \qquad (4)$$

Unfortunately, this model can be solved only for small forces, where the mean extension of the chain $l \ll l_0$ is

$$l = \frac{2F\xi_T}{3k_\mathrm{B}T} l_0 = \frac{F}{3k_\mathrm{B}T} R_g^2 \qquad (5)$$

To compute the elastic response of a chain at higher forces one has to resort to numerical calculations (e.g. transfer matrix methods) or to various approximations of the Kratky-Porod model.

An interesting limit is the freely jointed chain (FJC) model, which consists in setting **B= 0** in Eq. (4).

It models a chain whose segments are unrestricted in their respective orientation and corresponds to a discretization of a polymer with segments of length $b = 2\xi_T$ ***(the so-called Kuhn length)***. In the FJC model the energy of a given chain configuration { **t**i }is thus

$$\mathscr{E}_{\mathrm{FJC}} = W = -Fb \sum \cos \Theta_i.$$

The partition function $\mathcal{Z}$ is

$$\mathscr{Z} = \sum_{\mathbf{t}_i} \mathrm{e}^{-\mathscr{E}_{\mathrm{FJC}}/k_{\mathrm{B}}T} = \sum_{\mathbf{t}_i} \prod_{i=1}^{N} \mathrm{e}^{Fb\cos\Theta_i/k_{\mathrm{B}}T}$$

$$= \left[\int \mathrm{d}\Omega\, \mathrm{e}^{Fb\cos\Theta/k_{\mathrm{B}}T}\right]^N = \left[\frac{2\pi k_{\mathrm{B}}T}{Fb}\sinh\frac{Fb}{k_{\mathrm{B}}T}\right]^N \tag{6}$$

From the free energy

$\mathscr{F} = -k_{\mathrm{B}}T \log \mathscr{Z}$ one can compute the mean extension of the chain ***l***.

$$l = -\frac{\partial \mathscr{F}}{\partial F} = l_0\left(\coth\frac{Fb}{k_{\mathrm{B}}T} - \frac{k_{\mathrm{B}}T}{Fb}\right) \tag{7}$$

Notice that at small forces one recovers our previous result, Eq. (5). However, as shown in Fig. 4, the FJC model is too crude and is not a good approximation of the elastic behavior of a DNA molecule at large extensions $(l > R_g)$.

2.2. The worm like chain model :

A much more precise description is afforded by the worm like chain (WLC) model, the continuous $(b \to 0)$ limit of Eq. (4):

$$\frac{\mathscr{E}_{\mathrm{WLC}}}{k_{\mathrm{B}}T} = \frac{\xi_T}{2}\int_0^{l_0}\left(\frac{\mathrm{d}\mathbf{t}}{\mathrm{d}s}\right)^2 \mathrm{d}s - \frac{F}{k_{\mathrm{B}}T}\int_0^{l_0}\cos\Theta(s)\,\mathrm{d}s \tag{8}$$

where *s* is the curvilinear coordinate along the chain. The calculation of the partition function Z and the free energy F of that model calls upon an analogy with the quantum mechanical problem of a dipole in an electric field.

Though there is no analytic formula equivalent to Eq. (8) for the force vs. extension behavior of a WLC, a simple and eficient numerical solution with an approximation better than 0.1%:

$$F = (k_B T/\xi_T)g(x)$$

where $x = l/l_0$ and

$$g(x) = x - \frac{1}{4} + \frac{1}{4(1-x)^2} + \sum_{i=2}^{7} a_i x^i$$

With

$a_2 = -0.5164228,\ a_3 = -2.737418,\ a_4 = 16.07497,\ a_5 = -38.87607,\ a_6 = 39.49944,\ a_7 = -14.17718$

However, when compared over the whole extension range, the WLC model is a much better description of the behavior of DNA than the FJC model. As shown in Fig. 4 the WLC model fits extremely well the measured data and allows a very precise estimation of the DNA's persistence length $\xi_T = 52 \pm 2$ nm in physiological conditions (10 mM phosphate buffer (pH .=7.5), 10 mM NaCl).

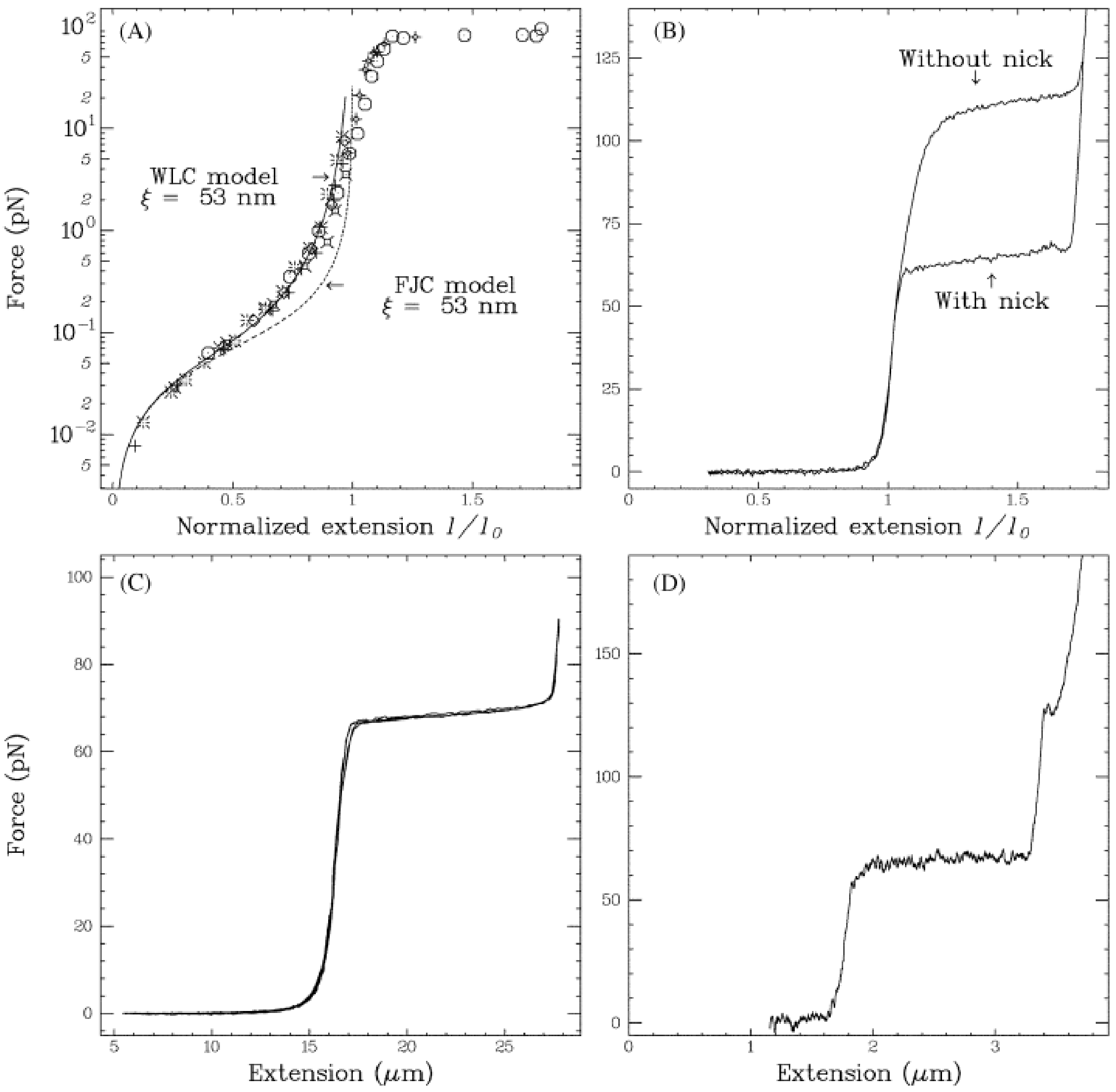

Figure 4.Force versus extension curves of single DNA molecules obtained by different groups. (A) The dots correspond to several experiments performed over a wide range of forces. The force was measured using the Brownian fluctuation technique . The full line curve is a best fit to the WLC model for forces smaller than 5 pN. The dashed curve is the result of the FJC model with the same persistence length (it is clearly a worse description of the behavior of DNA under stress than the WLC model). At high forces, the molecule first elongates slightly, as would any material in its elastic regime. Above 70 pN, the length abruptly increases, corresponding to the appearance of a new structure called S-DNA. (B) The same transition observed using a glass needle deflection on a nicked molecule and an unnicked molecule (the transition occurs for a higher force). (C) The transition is also observed using optical tweezers. (D) Finally, also the transition using an AFM.

2.3. Chains of leinght P are not rigid:

To develop an intuitive grasp of P, it is instructive to consider the properties of an ensemble of molecules, each of length P. Kratky - Porod derived the expression

$$\langle R^2 \rangle = 2P^2[L/P - 1 + \exp(-L/P)]$$

for the mean-squared, end-to-end separation, $<R^2>$, of an ensemblewormlike chains of contour length L and persistence length P. If L = P and the end-to-end separation is expressed as a fraction, f, of the contour length, then $<f^2>=2e^{-1}$.
Eight computer-generated chains, each of contour length L = P, are displayed in Figure 5. It is clear that such chains are not rigid rods.

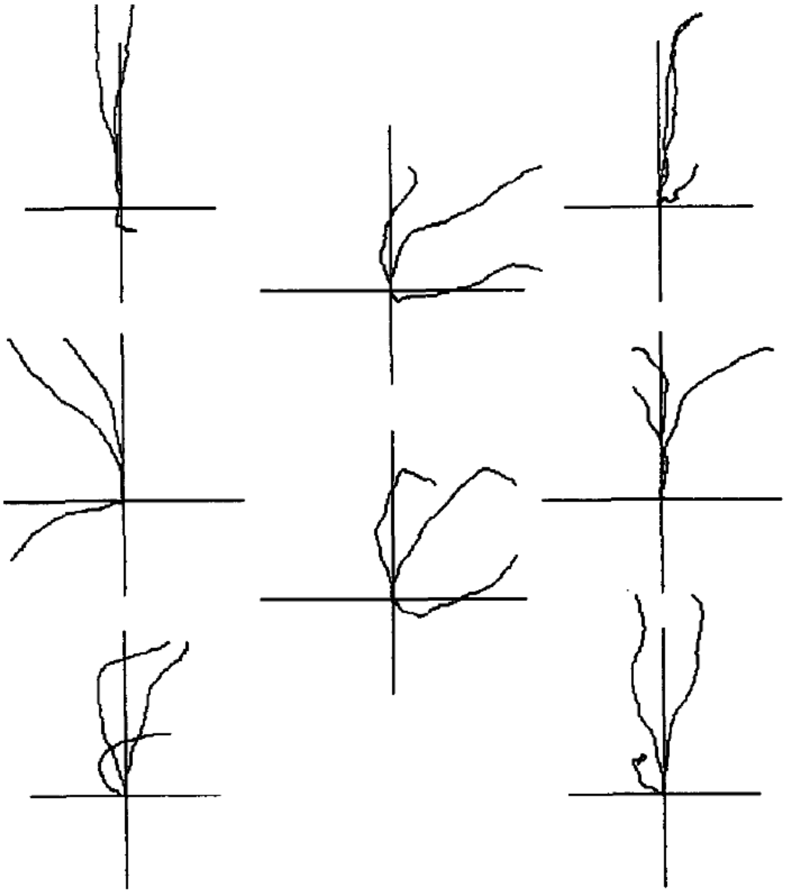

Figure 5. Collection of wormlike chains, each of length P. For each coordinate frame three contour projections (x-y, x-z, y-z) are represented. For x-z and y-z projections, the z axis is vertical.

4.Torsional stiffness of DNA:

The torsional stiffness of DNA is defined as the resistance of the helix to changes in helix twist. Like the preceding discussion of bending stiffness, the current discussion is couched in terms of an isotropic, elastic rod. That is, the free energy associated with a torsional fluctuation is a quadratic function of the torsional strain.

4.1.Relation between torsional stiffnes and chain conture:

If a population of nicked, circular molecules is subjected to ligase-catalyzed closure of the nick, the resulting covalently closed DNA circles will display a distribution with respect to the number of times the two strands of the helix are interwound. This distribution reflects the Brownian fluctuations in helical contour and twist at the time of closure. Since both strands are continuous, the number of times the strands are interwound must be an integer; this value is referred to as the linking number, *Lk,* of the molecule. *Lk* is related to the total helical twist, *Tw,* of the molecule through the defining relation **Lk = *Tw* + *Wr*,** where the remaining quantity, the writhe *(Wr),* is a function of the configuration of the closed contour in space [rigorous definitions and descriptions of Lk, Tw, and *Wr* are given elsewhere]. The deviations (fluctuations) of Lk about its equilibrium value can be expressed as △Lk; a corresponding value, △*Tw,* represents deviations in total helical twist. The defining relation can be recast as

$$\Delta Lk = \Delta Tw + Wr$$

For a system unconstrained at the time of closure, all three average quantities, (△Lk), *(△Tw),* and (Wr), will be zero; however, the averages of the squared quantities, $<(\triangle \mathrm{Lk})^2>$, $<(\triangle \mathrm{Tw})^2>$, and $<(\mathrm{Wr})^2>$, will in geral not be zero.

Thus $<(\triangle \mathrm{Lk})^2>$ is the variance over the distribution of△Lk and can be determined by experiment. In relating the observed linking number distribution to $<(\triangle \mathrm{Tw})^2>$ two additional assumptions are made:

(a) that the free energy of twisting is proportional to the square of the torsional displacementa, and (b) that fluctuations in twist and writhe occur independently of each other.

All experimental evidence to date supports these two assumptions. With the abovea ssumptionsin place, the defining relation for fluctuations becomes

$$\langle(\Delta Lk)^2\rangle = \langle(\Delta Tw)^2\rangle + \langle(Wr)^2\rangle \tag{9}$$

Since <(△Lk)^2> is an experimental observable, the torsional elastic constant, C (in erg-cm), can be obtained from the

$$\langle(\Delta Tw)^2\rangle = (L/4\pi^2)(k_B T/C)$$

for a molecule of length L once <(Wr)^2> is known.

The significance of Equation 9 can be appreciated more readily by noting the relationships between the variances in twist and writhe and the corresponding eLastic constants C and P.

The larger C is, the smaller the variance in twist; i.e. torsional fluctuations are less favorable. Similarly, the larger P is, the less extensive are bendinge excursionst that contributet to writhe.

If <(Wr)^2> were overestimated, the interpretation of the experimental value for <(△Lk)^2> would lead to underestimation of <(△Tw)^2>, and hence overestimation of C.

5. Twist-stretch coupling:

Loop formation depends on thermal fluctuations. In an unconstrained environment, DNA forms an entropically favorable Gaussian coil . The conformation of the coil and with it the spatial location of the operators fluctuate thermally. This fluidity allows the operators to align for looping. However, as the DNA is stretched, it transitions from an isotropic coil to an extended form. Because tension restricts the ability of DNA operator sites to diffuse randomly, it decreases looping probability. If DNA is stretched with enough tension, looping will be prevented. Given that thermal energy can bend DNA that is a persistence length long, the force scale over which DNA is extended is

$$k_B T/l_p = 80\,\text{fN}.$$

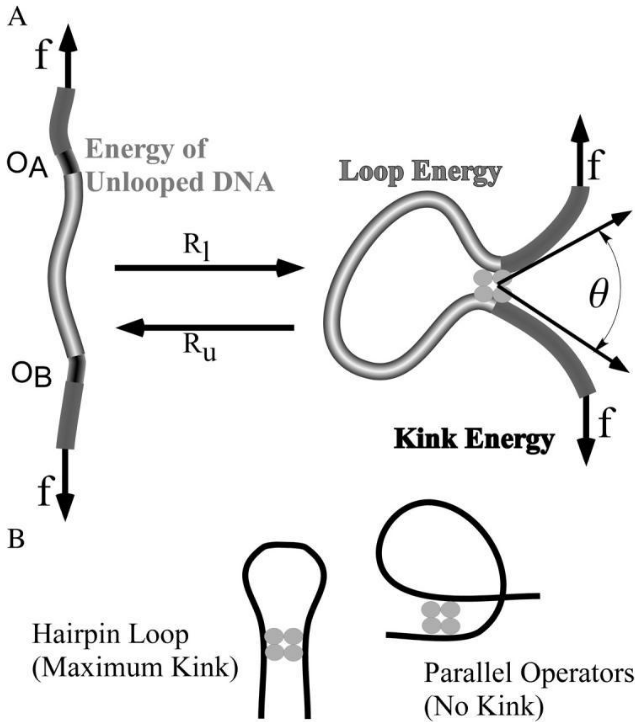

*Figure 6. Statistical mechanics of protein-mediated DNA looping. (*A*) DNA looping as a two-state system. Three free energies determine the lifetimes of the looped and unlooped states: the energy of unlooped DNA, the loop energy, and the kink energy.*

To determine how much tension is necessary to prevent the formation of protein-mediated DNA loops, we treat the interaction of linker protein and DNA as a two-state "looped" or "unlooped" system. In this representation, "looped" DNA refers to the instance in which one linker protein (or protein complex) forms a bridge between two specific sites on the same DNA molecule. Meanwhile, "unlooped" DNA refers to the case in which some protein may be bound to DNA (possibly at multiple sites), but no protein bridges exist . Analysis rests on computing the difference in free energy, ΔF, between looped and unlooped DNA, whereby we can account for the thermal fluctuations of the substrate DNA. The relationship between looped lifetime τ_l and unlooped lifetime τ is given by the thermodynamic expression for detailed balance, detailed balance,

$$\tau_l = \tau \exp\left[-\frac{\Delta F}{k_B T}\right] .$$

(10)

As sketched in Figure 6, there are three contributions to ΔF:

$$\Delta F = F_{\text{loop}} - F_{\text{DNA}}(l, f) + F_{\text{kink}}(f, \theta).$$

(11)

F_{loop} represents the intrinsic energy of the DNA loop. It includes the free energy of protein-DNA interactions and the energetic cost of bending DNA into a loop. As explained below, the specific value of F_{loop} is not relevant for our analysis of the effect of tension. Meanwhile, F_{DNA} represents the intrinsic free energy of DNA that has no mechanical constraints other than tension. This energy is subtracted from ΔF because loop formation effectively reduces the length of DNA exposed to tension. F_{DNA} is a function of the loop length, l, and the applied tension, f. Lastly, the need for the protein-binding operators to orient themselves in a manner compatible with loop formation imposes internal and external geometrical constraints on the DNA. Whereas the interior geometric constraint affects the overall topology of the loop structure it is not included in our analysis because it is uncoupled to external tension. In contrast, the exterior angular orientation is coupled to externally applied tension. F_{kink} is the energy associated with this external coupling constraint. In addition to tension, F_{kink} is a function of the angle, ϑ, that is created between the two pieces of DNA entering the loop .If the loop causes an antiparallel "hairpin" orientation between the two operators, then ϑ will be 0°. Conversely, if there is a parallel relationship between the operators, then ϑ will be 180°.

An accurate determination of the intrinsic free energy of the protein-mediated loop, F_{loop} is the subject of much recent research. Because the WLC model assumes isotropic flexibility of DNA and ignores the possibility of sequence-dependent curvature, it cannot be used to accurately determine the bending energy within a loop. In addition, the specific contribution attributable to the protein-DNA interactions can vary substantially depending on the operator sequence and linker protein(s). Instead, we assume that tension in the external DNA does not alter the DNA-protein contacts associated with the linker protein. Under this assumption, F_{loop} is independent of tension.

To compute the free energy of stretched DNA, F_{DNA}, we use the wormlike chain model, which is characterized by isotropic elasticity and smooth transitions in the chain's curvature. For a WLC, the only intrinsic parameter that needs to be specified is the persistence length, l_{p}. This length is the characteristic length over which a WLC bends in response to thermal forces. For DNA in typical ionic conditions, l_{p} is ~53 nm or 156 bp. If x denotes the end-to-end extension of a DNA strand relative to its contour length, then the force-extension relationship for a WLC is

$$f = \frac{k_{\mathrm{B}}T}{l_{\mathrm{p}}}\left(\frac{1}{4}\left[\frac{1}{(1-x)^2}-1\right]+x\right). \tag{12}$$

F_{DNA} is the difference between the potential energy of a WLC and the work done by the tension, f, to stretch the chain. Thus,

$$F_{\mathrm{DNA}} = l\int_0^{\mathrm{x}} f(x')\mathrm{d}x' - flx = -\frac{k_{\mathrm{B}}Tlx^2}{4l_{\mathrm{p}}}\left[\frac{1}{(1-x)^2}+2\right].$$

(13)

It is important to recognize that F_{DNA} represents the relative change of free energy of the substrate DNA when it is shortened by looping. So in the context of DNA looping, Eq. 13 is valid for loop sizes that are both larger and smaller than the persistence length. The only constraint is that a small loop must exist in the context of a larger DNA strand so that tension is applied over a region that is longer than the persistence length.

It is harder to construct an exact expression for F_{kink}, the free energy associated with the orientational localization of the operator sites around the protein. Therefore, we construct an interpolated formula that matches the high and low force asymptotic solutions. The relevant force scale for deciding whether a given tension is small or large is $f_{\mathrm{c}} = k_{\mathrm{B}}T/l_{\mathrm{p}} = 80\,\mathrm{fN}.$

At this critical tension, a wormlike chain extends 45% of its contour length. As explained below, for applied tensions much smaller than f_{c}, entropic effects dominate and the kink energy can be calculated by a second-order expansion of force-free equations. Meanwhile, for tensions much larger than f_{c}, the kink energy is primarily determined by the enthalpic cost of bending a wormlike chain into its kinked shape.

In the low force limit, DNA is an entropic spring and F_{kink} is equal to the loss of entropy created by the kink. Specifically, let $\vec{R}$ denote the end-to-end vector of a wormlike chain and L denote its overall contour length. (Note that L is not the same as intraoperator distance and will drop out of the final expression for F_{kink}.) There are three degrees of freedom for the end-to-end vector of the chain, corresponding to a free energy of 3/2 $k_{\mathrm{B}}T$ in the thermodynamic limit. To second order, the free energy of an extended state is then

$$F_{\mathrm{WLC}} = \frac{3\vec{R}^2}{2\langle\vec{R}^2\rangle}k_{\mathrm{B}}T.$$

(14)

The entropic relationship between tension and free energy gives

$$\vec{f} = \frac{\partial F_{\mathrm{WLC}}}{\partial\vec{R}} = \frac{3\vec{R}}{\langle\vec{R}^2\rangle}k_{\mathrm{B}}T \Rightarrow F_{\mathrm{WLC}} = \frac{\langle\vec{R}^2\rangle}{6k_{\mathrm{B}}T}f^2.$$

(15)

The kink energy at low force, $F_{\mathrm{kink}}^{\mathrm{l}}$,is the difference in F_{WLC} for a nonkinked and kinked chain. Therefore,

$$F^{\mathrm{l}}_{\mathbf{kink}} = \frac{\delta\langle\vec{R}^2\rangle}{6k_{\mathrm{B}}T}f^2,$$

(16)

where $\delta\langle\vec{R}^2\rangle$ represents the correction to the mean square end-to-end distance that is attributable to the kink.

To evaluate $\delta\langle\vec{R}^2\rangle$, note that $\langle\vec{R}^2\rangle$ can be written as

$$\langle\vec{R}^2\rangle = \left\langle \int_0^L \int_0^L \vec{t}(s)\cdot\vec{t}(s')ds\,ds' \right\rangle,$$

(17)

where $\vec{t}(s)$ represents the tangent vector as a function of contour length. In the absence of externally applied tension, wormlike chains are characterized by an exponential decay in the correlation of tangent vectors as a function of intervening contour length. Thus, in the presence of a single kink of angle ϑ (see Fig. 1), the correlation is described by

$$\langle\vec{t}(s)\cdot\vec{t}(s')\rangle = \varsigma(s,s')e^{-|\mathrm{s}-\mathrm{s}'|/\mathrm{l}_{\mathrm{P}}},$$

(18)

where $\varsigma(s,s') = -\cos(\theta)$ if the segment between *s* and *s′* contains the kink and *1* otherwise. If the kink is located at $s = s_0$,

$$\begin{aligned}\delta\langle\vec{R}^2\rangle &= \langle\vec{R}^2\rangle_{\mathbf{no\_kink}} - \langle\vec{R}^2\rangle_{\theta}\\ &= 2\int_0^{s_0}\int_{s_0}^{L}[\langle\vec{t}(s)\cdot\vec{t}(s')\rangle_{\theta=\pi} - \langle\vec{t}(s)\cdot\vec{t}(s')\rangle_{\theta}]ds\,ds'\\ &= 2\int_0^{s_0}\int_{s_0}^{L}(1+\cos\theta)e^{-|s-s'|/l_{\mathrm{P}}}ds\,ds'\\ &\simeq 2l_{\mathrm{p}}^2(1+\cos\theta).\end{aligned}$$

(19)

In the last step, the approximation $L \gg l_{\mathrm{P}}$ is made, which is justified provided that tension on the DNA is applied at a point >53 nm from the protein binding sites. Substitution of Eq. 19 into Eq. 16 yields

$$F^{\mathrm{l}}_{\mathbf{kink}} = \frac{l_{\mathrm{P}}^2(\cos\theta+1)}{3k_{\mathrm{B}}T}f^2.$$

(20)

Meanwhile, in the high force limit, we can ignore the effects of thermal fluctuations. (An unpublished variational approach confirms that the entropic contribution is not important for our analysis, because it is essentially independent of tension.) Thus in the high force limit, F_{kink} is simply the bending energy of two rigid rods that are anchored at the origin, make an angle of $\vartheta/2$ with respect to the *y* axis and are pulled apart by tension that is directed along the *x* axis. With this model, equilibrium rod theory can be used to calculate the energy for each half of the kink. Specifically, for a curved rod, the bending energy per unit length is inversely proportional to the square of the radius of curvature. For a rigid rod to have the same bending modulus as a WLC, the constant of proportionality is such that a section of length l_{p} will contribute 1/2 $k_{\text{B}}T$ to the bending energy if its radius of curvature is also l_{p}. Thus the infinitesimal kink energy is

$$dF^{\text{h}}_{\text{kink}} = \frac{1}{2}\frac{k_{\text{B}}Tl_{\text{p}}}{\kappa^2}\,ds,$$

(21)

where the radius of curvature, κ, is a function of the arc length. Conservation of energy requires that the capacity of tension to do work on the rod must equal the actual amount of work done plus the energy of bending the rod. Thus

$$dF^{\text{h}}_{\text{kink}} + f\cos\phi\,ds = f\,ds,$$

(22)

where $\varphi$is the angle the tangent vector makes with respect to the *x* axis. Since κ is $(d\phi/ds)^{-1}$,Eqs. 21 and 22 yield

$$\frac{ds}{d\phi} = \sqrt{\frac{k_{\text{B}}Tl_{\text{p}}}{2f(1-\cos\phi)}}.$$

(23)

Integrating Eq. 21 for the two sides of the kink and substituting Eq. 22 and then Eq. 23 gives

$$\begin{aligned} F^{\text{h}}_{\text{kink}} &= 2\int dF_{\text{kink}} = 2f\int(1-\cos\phi)ds \\ &= 2\sqrt{\frac{k_{\text{B}}Tl_{\text{p}}f}{2}}\int_0^{(\pi-\theta)/2}\sqrt{1-\cos\phi}\,d\phi. \end{aligned}$$

(24)

Evaluation of the integral yields

$$F_{\mathbf{kink}}^{\mathrm{h}} = 4\sqrt{k_{\mathrm{B}}Tl_{\mathrm{p}}f}[1 - \cos((\pi - \theta)/4)].$$

(25)

Equation 25 shows that in the high force limit, the kink energy is proportional to the square root of tension. This relation arises because of a balance between two conflicting constraints associated with bending a rod. On the one hand, a gradual bend is preferable because the energy of bending is inversely proportional to the bending radius. On the other hand, a smaller bending radius is favorable, because it allows the external DNA to be stretched farther and thus increases the work that is done by the applied tension.

A standard interpolative formula that maintains the asymptotic limits is

$$\frac{1}{F_{\mathbf{kink}}} = \frac{1}{F_{\mathbf{kink}}^{\mathrm{l}}} + \frac{1}{F_{\mathbf{kink}}^{\mathrm{h}}}.$$

(26)

By defining a dimensionless force, $\tilde{f} = f/f_{\mathrm{c}}$, and setting $\alpha = \cos[(\pi - \theta)/4]$, trigonometric manipulations allows us to write our closed-form expression for F_{kink},

$$F_{\mathbf{kink}} = 4k_{\mathrm{B}}T\sqrt{\tilde{f}}\left(1 + \frac{3}{2\alpha^2(1+\alpha)\tilde{f}^{3/2}}\right)^1(1-\alpha).$$

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