



After Bustamante et al., *Current Opinion in Structural Biology*, 2001

Snapshots of a T4 Double Stranded DNA in an Aqueous Solution

Image removed due to copyright considerations.

P. Doyle 2003



Contour length = $64 \mu\text{m}$

ELASTICITY OF FJC AT ARBITRARY FORCES

- Ensemble: constant T, V, N, \underline{f} or force

- Boltzmann Distribution:

$$P_j = \frac{1}{Q'} \exp\left(\frac{-U_j}{kT}\right) \exp\left(\frac{\underline{f} \cdot \underline{r}_j}{kT}\right)$$

- Useful Relationship:

$$Q' = \int_{\text{phase space}} \exp\left(\frac{-U_j}{kT}\right) \exp\left(\frac{\underline{f} \cdot \underline{r}_j}{kT}\right)$$

$$\frac{\partial Q'}{\partial \underline{f}} = \int_{\text{phase space}} \frac{\underline{r}_j}{kT} \exp\left(\frac{-U_j}{kT}\right) \exp\left(\frac{\underline{f} \cdot \underline{r}_j}{kT}\right)$$

$$\therefore \boxed{\langle \underline{r} \rangle = \frac{kT}{Q'} \frac{\partial Q'}{\partial \underline{f}} = kT \frac{\partial}{\partial \underline{f}} \ln Q'}$$

- FJC : $Q' = \int_{\text{phase space } \{b_i\}} \exp\left(\frac{\underline{f} \cdot \underline{r}_i}{kT}\right)$

$$\underline{r} = \sum_{i=1}^N \underline{b}_i$$

$$\underline{f} \cdot \underline{b}_i = f b \cos \theta_i$$

$$Q' = \int_{\text{p.s.}} \exp\left[\frac{f b \cos \theta_1}{kT}\right] \exp\left[\frac{f b \cos \theta_2}{kT}\right] \dots \exp\left[\frac{f b \cos \theta_N}{kT}\right]$$

decoupled

$$Q' = \left[\int_0^{2\pi} \int_0^{\pi} \exp\left[\frac{f b \cos \theta}{kT}\right] \sin \theta d\theta d\phi \right]^N$$

$$Q' = \left[\frac{2\pi \sinh\left(\frac{fb}{kT}\right)}{fb/kT} \right]^N$$

$$\langle r \rangle = kT \frac{\partial}{\partial F} \ln Q' = NkT \frac{\partial}{\partial F} \ln \left[\frac{2\pi \sinh\left(\frac{fb}{kT}\right)}{fb/kT} \right]$$

$$\langle r \rangle = \underbrace{Nb}_{\text{chain length}} \underbrace{\left[\coth\left(\frac{fb}{kT}\right) - \frac{kT}{fb} \right]}_{\substack{\text{Langevin function} \\ \mathcal{L}\left(\frac{fb}{kT}\right)}} \underbrace{\frac{f}{F}}_{\substack{\text{unit vector in} \\ \text{direction of } \underline{f}}}$$

$$\coth(x) = \frac{e^x + e^{-x}}{e^x - e^{-x}}$$

Limits

* Small fb/kT

$$\langle r \rangle \approx \frac{1}{3} \frac{fb}{kT} Nb \left(\frac{f}{F} \right) \quad \checkmark \Leftrightarrow$$

recall Gaussian chain:
 $\underline{r} = \frac{1}{3} Nb \frac{\langle \underline{f} \rangle b}{kT}$

* large fb/kT

$$\langle r \rangle \approx Nb \left[1 - \frac{kT}{fb} \right] \left(\frac{f}{F} \right)$$