Extracting Structural information from Force-Extension Curves

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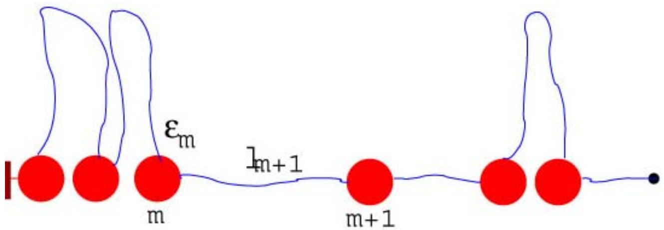
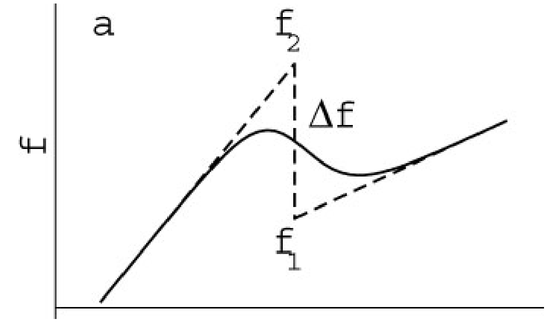
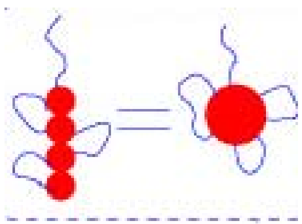
- Force-Extension curves
- Simple model
- Simple Equations
- Thermal Smoothening
- Matching Noise Pattern
- Why only few jumps
- Away from Thermal Equilibrium

Simple Model





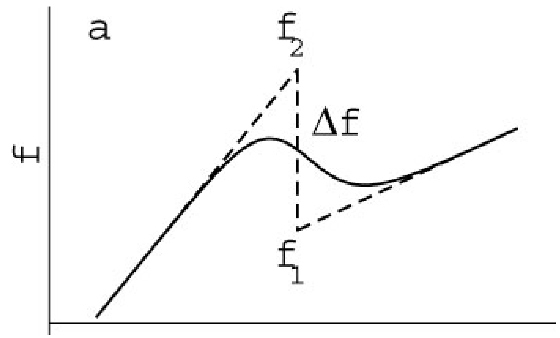


$$\frac{(z-2a_1^{n_h})^2}{L_m} = \frac{(z-2(a_1^m + a_{m+1}^{n_h}))^2}{L_m + l_{m+1}} + \varepsilon_{m+1}$$

$$\Delta f = f_m - f_{m+1} = \partial E_m/\partial z - \partial E_{m+1}/\partial z = [2z/L_m - 2z/(L_m + l_{m+1})](k_B T/b)$$

$$l_{m+1} = \frac{2\Delta f z}{f_{m+1} f_m} \frac{k_B T}{b} \qquad \varepsilon_{m+1} = \frac{\Delta f z}{2}$$

Thermal Smoothening



$$f(z) = f_m(z)\,\theta(z^* - z) + f_{m+1}(z)\,\theta(z - z^*),$$

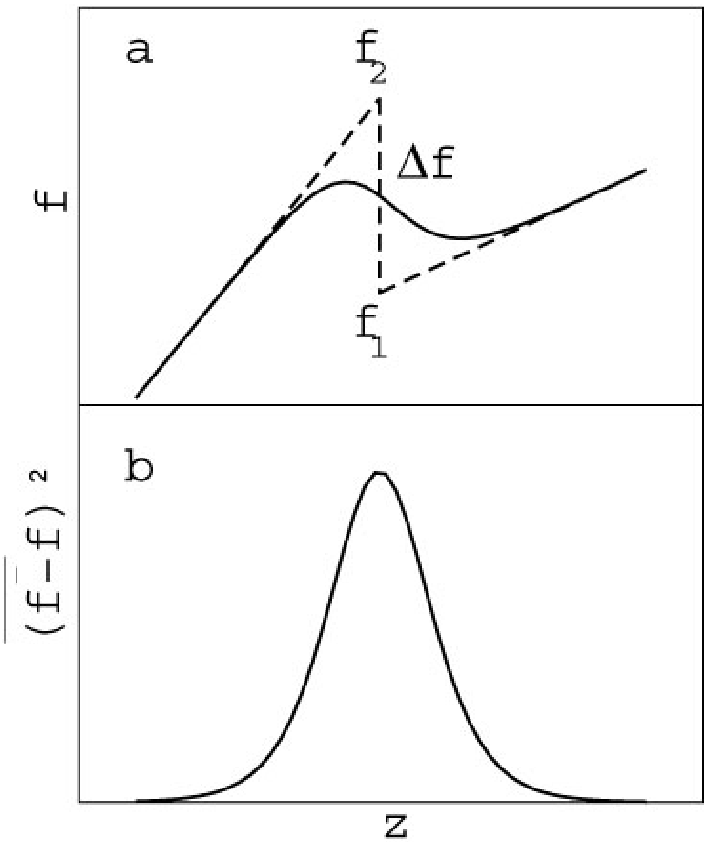
$$\bar{\theta}(z^* - z) = \frac{e^{-E_m(z)/k_B T}}{e^{-E_m(z)/k_B T} + e^{-E_{m+1}(z)/k_B T}} = \frac{1}{1 + e^{-(E_{m+1}(z) - E_m(z))/k_B T}}$$

$$\bar{\theta}(z^* - z) = \frac{1}{1 + e^{-\frac{z^* - z}{z^*}\frac{2\varepsilon_{m+1}}{k_B T}}}$$

And the fitting function for a transition is:

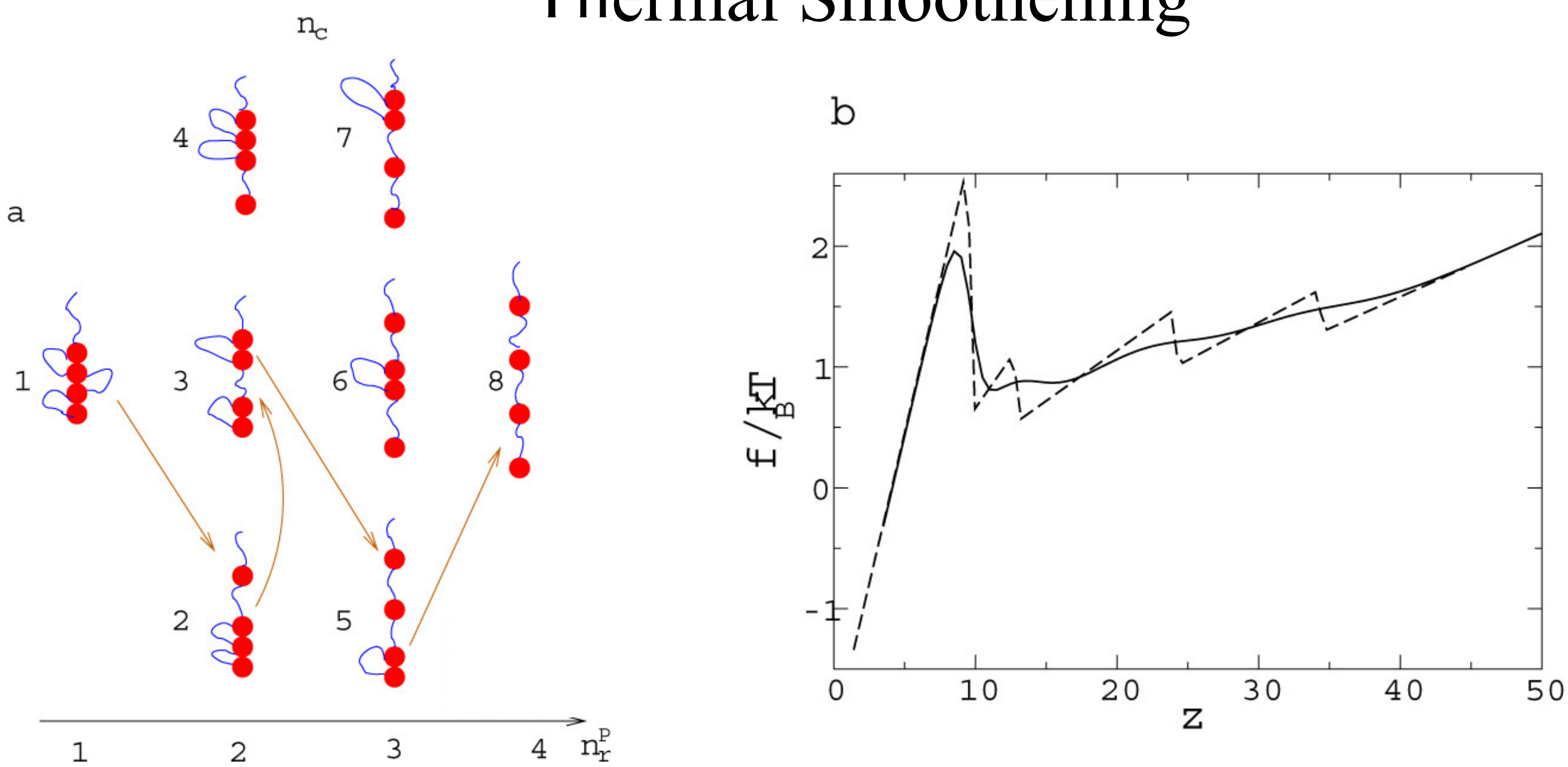
$$\overline{f(z)} = f_m(z)\,\bar{\theta}(z^* - z) + f_{m+1}(z_m)\,\bar{\theta}(z - z^*)$$

Matching Noise Pattern



$$\overline{(f(z) - \overline{f(z)})^2} = \bar{\theta}(z^* - z) \cdot \bar{\theta}(z - z^*) \frac{4{\varepsilon_{m+1}}^2}{z^{*2}}$$

Thermal Smoothening



$$\overline{f(z)} = f_m(z)\,\bar{\theta}\left(z_m^* - z\right) + f_{m+1}(z)\,\overline{\theta\left(z - z_m^*\right)\theta\left(z_{m+1}^* - z\right)} + f_{m+2}(z)\,\bar{\theta}\left(z - z_{m+1}^*\right)$$

$$\overline{\theta\left(z - z_m^*\right)\theta\left(z_{m+1}^* - z\right)} = \frac{e^{-E_{m+1}/k_\mathrm{B}T}}{e^{-E_m/k_\mathrm{B}T} + e^{-E_{m+1}/k_\mathrm{B}T} + e^{-E_{m+2}/k_\mathrm{B}T}}$$

$$(z_m^* - z_{m+1}^*)/z < k_\mathrm{B}T/2\varepsilon_m$$

Thermal Smoothening