

## Text S2. Method of Lagrange multipliers.

Olga Kononova<sup>1,2</sup>, Joost Snijder<sup>3</sup>, Yaroslav Kholodov<sup>2,4</sup>, Kenneth A. Marx<sup>1</sup>, Gijs J. L. Wuite<sup>3</sup>, Wouter H. Roos<sup>3,\*</sup>, Valeri Barsegov<sup>1,2,\*</sup>.

**1 Department of Chemistry, University of Massachusetts, Lowell, MA 01854, USA**

**2 Moscow Institute of Physics and Technology, Moscow Region, 141700, Russia**

**3 Natuur- en Sterrenkunde and LaserLab, Vrije Universiteit, 1081 HV Amsterdam, The Netherlands**

**4 Institute of Computer Aided Design Russian Academy of Science, Moscow, 123056, Russia**

To study the dynamical changes in  $x_H$  (Hertzian deformation) and  $x_b$  (beam-bending deformation) and their contribution to the total deformation  $X=x_H + x_b$  (see Fig. 4 in the main text), we employed the method of Lagrange multipliers [1]. This method allows us to find the values of  $x_H$  and  $x_b$  that minimize the total deformation force,  $F(x_H, x_b)=k_H x_H^{3/2} + K_b x_b s(x_b)$  (see *the inset* Fig. 4 in main text), subject to the constraint:  $X=x_H+x_b$ . To that end, we constructed the Lagrange function

$$\Lambda(x_H, x_b, \lambda) = F(x_H, x_b) + \lambda g(x_H, x_b), \quad (\text{S1})$$

where

$$g(x_H, x_b) = x_H + x_b - X \quad (\text{S2})$$

Here  $\lambda$  is the Lagrange multiplier. By calculating the partial derivatives of  $\Lambda(x_H, x_b, \lambda)$  with respect to each of the two variables  $x_H$  and  $x_b$ , we obtained equations of the form

$$\nabla_{x_H, x_b} F(x_H, x_b) = -\lambda \nabla_{x_H, x_b} g(x_H, x_b) \quad (\text{S3})$$

Next, by eliminating  $\lambda$  we arrived at the system of two equations:

$$3/2k_H x_H^{1/2} = K_b s(x_b) + K_b x_b s'(x_b) \quad (\text{S4})$$

$$X = x_H + x_b \quad (\text{S5})$$

For small deformations  $x_b$ , we expand the Weibull survival probability  $s(x_b)=\exp[-(K_b x_b/F_b^*)^m]$  in powers of the exponent  $z=K_b x_b/F_b^*$ , and retain the terms up to the first order in  $z$ . Then, Eq. (S4) becomes:

$$3/2k_H x_H^{1/2} - K_b \left(1 - \left(\frac{K_b x_b}{F_b^*}\right)^m\right) \left(1 - m \left(\frac{K_b x_b}{F_b^*}\right)^m\right) = 0 \quad (\text{S6})$$

Eq. (S5) allows us to eliminate  $x_H$  by substituting  $x_H=X-x_b$  into Eq. (S6) above:

$$3/2k_H (X - x_b)^{1/2} - K_b \left(1 - \left(\frac{K_b x_b}{F_b^*}\right)^m\right) \left(1 - m \left(\frac{K_b x_b}{F_b^*}\right)^m\right) = 0 \quad (\text{S7})$$

Simplifying Eq. (S7) and grouping terms of the same power in  $x_b$ , we arrive at the following polynomial equation:

$$a_1 x_b^{4m} + a_2 x_b^{3m} + a_3 x_b^{2m} + a_4 x_b^m + a_5 x_b + a_6 = 0 \quad (\text{S8})$$

with the following constant coefficients:

$$\begin{aligned}
a_1 &= m^2 K_b^2 \left( \frac{K_b}{F_b^*} \right)^{4m} \\
a_2 &= -2m(1+m) K_b^2 \left( \frac{K_b}{F_b^*} \right)^{3m} \\
a_3 &= (1+4m+m^2) K_b^2 \left( \frac{K_b}{F_b^*} \right)^{2m} \\
a_4 &= -2(1+m) K_b^2 \left( \frac{K_b}{F_b^*} \right)^m \\
a_5 &= \frac{9}{4} k_H^2 \\
a_6 &= K_b^2 - \frac{9}{4} k_H^2 X
\end{aligned} \tag{S9}$$

Eq. (S8) can be solved numerically (for example, using Mathematica software) for a given set of parameters  $k_H$ ,  $K_b$ ,  $F_b^*$ , and  $m$ , and for each specified value of the total deformation  $X$ . The obtained numerical solution for  $x_H$  and  $x_b$  can then be substituted into the expression for  $F(x_H, x_b)$  (Eq. (14) in the main text).

## References

- [1] McQuarrie DA. Statistical Mechanics. University Science Books; 2000.