

Mechanical unzipping of biomolecules: a simple model

A. Prados,¹ A. Carpio,² and L.L. Bonilla³

¹*Física Teórica, Facultad de Física, Universidad de Sevilla,
Apartado de Correos 1065, E-41080 Sevilla*

²*Departamento de Matemática Aplicada,
Universidad Complutense, Madrid 28040*

³*Universidad Carlos III Madrid, Av. Universidad 30, 28911, Leganés, Madrid*

We propose a simple model for the mechanical unzipping of biomolecules. It comprises a macroscopic (elastic) degree of freedom, modelled by a one-dimensional oscillator, and some internal degrees of freedom, modelled by Glauber spins with nearest-neighbour interaction and a coupling constant proportional to the oscillator position. This spin-oscillator coupling gives rise to a first-order phase transition when a mechanical force F is applied to the system: there is a critical force F_c at which the equilibrium oscillator rest position abruptly changes. If the system is pulled (increasing F), the oscillator position increases discontinuously at a certain value of the force $F_+ > F_c$, which depends on the pulling rate. Afterwards, in the pushing back experiment (decreasing F) with the same rate, the oscillator position decreases discontinuously at a value of the force $F_- < F_c$, and hysteresis shows up. Processes at constant load F close to the critical value F_c are also discussed, in which the system stochastically jumps between the two (stable and metastable) possible rest positions of the oscillator.

The system behaviour is analogous to that of biomolecules in real experiments, and it stems from the existence of the first order phase transition and its associated region of metastability. This phase transition is a consequence of the spin-oscillator coupling, which introduces an effectively long-range interaction among the spins. Similar hidden 1d long range effective correlations are present in real biomolecules.

[1] A. Prados, A. Carpio, and L. L. Bonilla, Phys. Rev. E **86**, 021919 (2012).