

Analytical extension/force curve of the freely jointed chain (FJC) and the discrete wormlike chain model (DWLC) with extensible bonds

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We calculate analytically the extension under a stretching force of a polymer modeled as a freely jointed chain (FJC) with extensible bonds, the latter modeled as harmonic springs. We obtain an approximated formula for the extension/force curve that can reproduce with high precision the chain elongation.

More complicated is the wormlike chain model, where a Transfer Matrix procedure allowed to calculate numerically the extension/force curve of the polymer in the presence of two elastic contributions: the longitudinal harmonic bonds giving the extensibility and the bending recoil between two consecutive bonds. Also, an analytical approximation has been calculated from the exact partition function, that results in the most accurate formulas for the semiflexible polymers at the date.

In both EFJC and EDWLC models, the curves obtained have been double checked by means of numerical experiments provided by Langevin simulations. The analytical expressions revealed an excellent agreement with the numerical outcomes, also at low values of the elastic parameters where previous phenomenological proposals differ substantially.

References

- [1] S.B. Smith, L. Finzi, C. Bustamante, Direct mechanical measurements of the elasticity of single DNA molecules by using magnetic beads. *Science* 258, 1122 (1992).
- [2] J.F. Marko, E.D. Siggia, Stretching DNA, *Macromolecules* 28, 8759 (1995).
- [3] A. Rosa, T.X. Hoang, D. Marenduzzo, A. Maritan, Elasticity of semiflexible polymers with and without self-interactions. *Macromolecules* 36, 10095 (2003).
- [4] A. Rosa, T.X. Hoang, D. Marenduzzo, A. Maritan, A new interpolation formula for semiflexible polymers. *Biophys. Chem.* 115, 251 (2005).
- [5] A. Fiasconaro, F. Falo, Analytical results of the extensible freely jointed chain model, *Physica A* 532, 121929 (2019).
- [6] A. Fiasconaro, F. Falo, Elastic traits of the extensible discrete wormlike chain model, *Phys. Rev. E* 107, 024501 (2023).