# Analytical solution of extensible freely jointed chain model

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Based on classical statistical mechanics, we calculate analytically the length extension under a pulling force of a polymer modeled as a freely jointed chain (FJC) with extensible bonds, the latter being considered as harmonic springs. We obtain an highly approximated formula for the extension curve, as well as an independent one for high force. These formulas can reproduce with high precision force-extension curves also at low values of the elastic constant of the spring, where previous proposals differ substantially. We successfully validate the analytical results together with the phenomenological expressions used in the literature by analysing the precision of their fit on data obtained from Langevin simulations.

Force-extension curve for rigid bond FJC model is given by the well known Langevin function $\xi = \mathcal{L}(\beta f l_0) = \coth(\beta f l_0) - 1/\beta f l_0$, where $\xi$ is the normalised extension. To take into account a bond finite elastic constant $k$, two different corrections have been proposed in literature. The first one [1] is $\xi_{\rm N} = \mathcal{L}(\beta f l_0) + f/k l_0$ and the second [2] $\xi_{\rm M} = \mathcal{L}(\beta f l_0)(1 + f/k l_0)$. Both are phenomenological and not based in any first principle statistical mechanics calculation.

In this work [3], we make use of the Weiestrass transform to obtain a very precise expression for the partition function of the extensible FJC model and thus derive an extension-force formula given by

$$\xi_{\rm E} = \mathcal{L}(\beta f l_0) + \frac{f}{k l_0} \times \left[1 + \frac{1 - \mathcal{L}(\beta f l_0)\coth(\beta f l_0)}{1 + \frac{f}{k l_0}\coth(\beta f l_0)}\right]. \tag{1}$$

The same expression was also obtained by a different method in [4].

Another approximation, only valid at high forces can be also derived as [3]

$$\xi_{HF} = \mathcal{L}(\beta f l_0) + \frac{f}{k l_0} + \frac{1}{\beta l_0 (k l_0 + f)} + 1 - \coth(\beta f l_0). \tag{2}$$

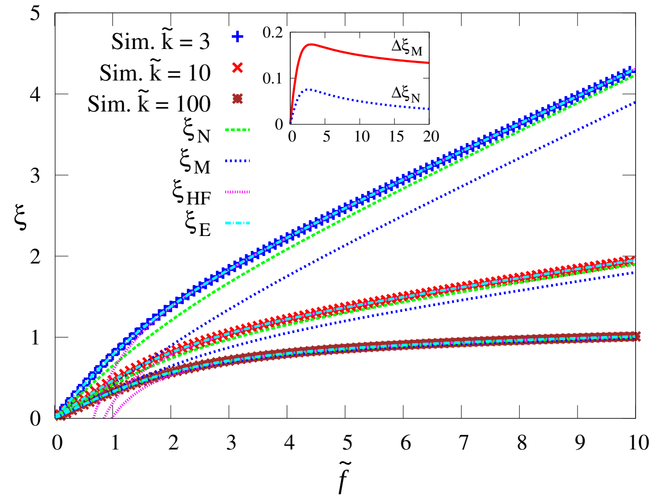


Fig. 1. Normalized extension $\xi$ as a function of the dimensionless force $\tilde{f} = \beta f l_0$ for three values of the dimensionless elastic constant $\tilde{k} = \beta l_0^2 k$ in the extensible FJC model. The symbols represent the data from the simulations, and the lines the analytical expressions defined in the text.

A comparison with Langevin molecular dynamics simulations of the model are shown in the figure. Expression from Eqs. (1) and (2) reproduce very accurately the simulations whereas phenomenological approximations clearly deviate.

We will also discuss the fit of simulations to different models as well other interesting effects as the contribution of the extensibility to model fluctuations.

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