Stretching an extensible discrete wormlike chain (EDWLC)

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Based on classical statistical mechanics, we calculate the exact partition function of the length extension of a discrete extensible wormlike polymer under a stretching force [1, 2, 3, 4]. The bonds extensibility is modeled with harmonic springs with elastic constant k, and the links present the transversal bending recoil typical (with bending constant k_b) of the wormlike chain (WLC) model.

The evaluation has followed two methods: From the one hand by using the Transfer Matrix procedure to calculate numerically the extension/force curve of the polymer, whose outcomes have been double checked with numerical experiments given by Langevin MD simulations [6]. On the other hand, by calculating some approximated analytical extension/force functions, the most accurate at the date, that can reproduce with high precision the numerical curves also at low values of the longitudinal elastic constant where the usual phenomenological proposals differ considerably.

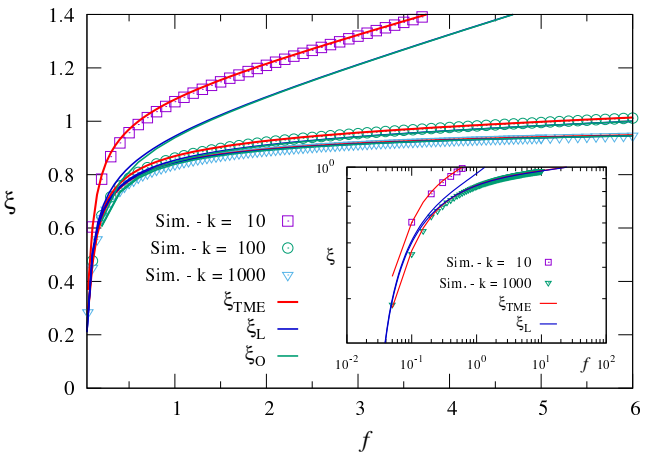

Fig. 1. Normalized end-to-end distance ξ as a function of the force f = the extensible discrete WLC model, for different elastic constant k, with the bending constant $k_b = 10$ and $l_0 = 1$. The symbols represents the Langevin simulations, the curves which superimpose with the symbols are the transfer matrix evaluation. ξ_L and ξ_O are the *naïve* extensible generalization (with f/kl_0) to the discrete inextensible and WLC formulas by Rosa *et al.* at high forces from references 3 and 4, respectively.

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