Title: Linear semiflexible polyelectrolytes in solutions
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Abstract:

In this thesis I used the Molecular dynamics simulations for study of charged polymers (polyelectrolytes) and their behaviour in solutions. Wide range of polyelectrolytes are semiflexible and in contrast to neutral polymers it is possible to influence their stiffness by changing the properties of solution as for example ionic strength. The chain flexibility may be characterized by the persistence length. Thesis explains how to express the persistence length from orientational correlation function which shows the double exponential decay. Two contributions to chain stiffness are discussed and the interest is concentrated around electrostatic persistence length which seems to be scale dependent. An effect of added salt on the chain conformation is studied. Salt is treated implicitly within the Debye-Hückel approximation. The results are confronted with OSF theory and the conclusions of variational calculations of Maghi and Netz. The presented thesis describes the conformational behaviour of polyelectrolytes in salty solutions, helps to understand the concept of persistence length and its relation to stiffness of macromolecules.

Keywords: polyelectrolytes, persistence length, simulations, salty solutions