# Summary of the Thesis

Self-Interacting Polymer under Constant and Periodic Force

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## Abstract

In this work, I study the conformational and dynamical properties of a self-interacting polymer (SIP) under the influence of external mechanical forces. Using Monte Carlo simulations, Markov chains and the Metropolis algorithm, I investigate the response of the system to both constant and periodic pulling forces. The analysis provides insight into polymer phase transitions, such as the coil–globule transition, and reveals scaling behavior in the area of hysteresis loops consistent with theoretical predictions.

## Motivation and Background

Mechanical forces play a fundamental role in biological processes such as DNA unzipping, protein unfolding, and RNA transcription. Single-molecule experiments have shown that polymers exhibit non-trivial responses under stretching. Theoretical work by Mishra et al. (2013) motivated this thesis, aiming to bridge statistical mechanics models and biomolecular phenomena.

## Methods

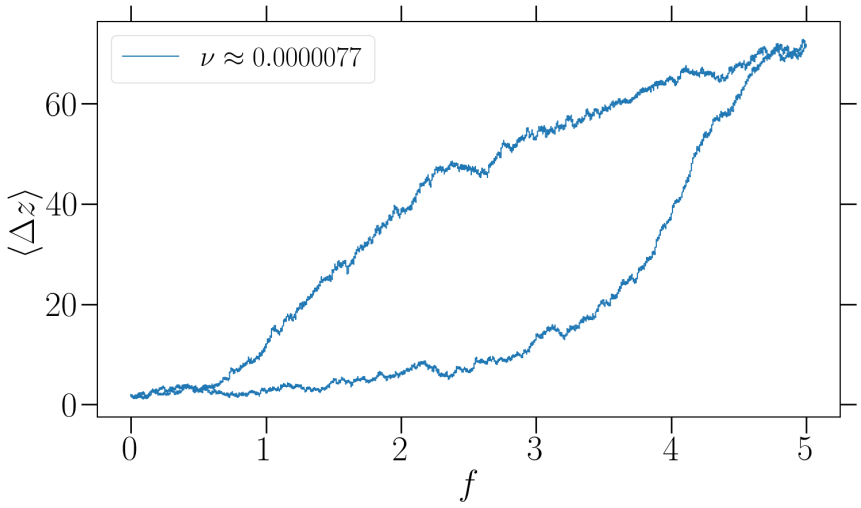
The simulations were performed with a coarse-grained polymer model of $N = 64$ monomers.

- **Constant force ensemble**: A Monte Carlo simulation with Metropolis updates, analyzing force–extension curves and phase diagrams.
- **Periodic force ensemble**: Cyclic variation of force to probe hysteresis effects and dynamical transitions.

C++17 was used for the simulations, and Python was employed for data analysis and visualization.

## Results

- Force–extension curves show clear evidence of the coil–globule transition.
- Under periodic driving, hysteresis loops appear whose area depends on the amplitude and frequency of the force.
- The scaling of loop area $A \sim F^{\alpha}\nu^{\beta}$ agrees with theoretical values known from spin systems.




Example of hysteresis loop obtained from the simulations.

## Conclusion and Outlook

The thesis demonstrates that simple coarse-grained polymer models can reproduce non-equilibrium phenomena relevant to biopolymers. Future extensions include longer chain lengths, explicit solvent interactions, and comparisons with experimental data.

## References

1. R. K. Mishra et al., *Scaling of hysteresis loop of interacting polymers under a periodic force*, J. Chem. Phys. 138, 244905 (2013).
2. J. Zierenberg et al., *Effect of grafting on the binding transition of two flexible polymers*, Eur. Phys. J. Spec. Top. 226, 683–692 (2017).