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Statistical Analysis of Transitions in Finite Polymer Systems

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There has been an increased recent activity in studying polymer systems of finite size. This interest is mainly driven by the need for a better understanding of the structural behavior of such systems in applications on mesoscopic scales, but also by the apparent deficit in our knowledge about biological processes like protein folding. A complex structure formation process of this kind is not only accompanied but governed by surface effects. In order to address the structural transition behavior appropriately, consistent and systematic statistical analysis methods have to be introduced and examined. By means of microcanonical inflection-point analysis and conventional canonical investigations of fluctuation and response quantities, different applications to the thermodynamic behavior of coarse-grained polymer models will be presented in this talk. These models have turned out to be particularly successful in effectively addressing generic features of structural transitions for polymer systems. Major transition scenarios such as folding, aggregation, and substrate adsorption of flexible and semiflexible polymers and proteins will be discussed.

References:

1. S. Schnabel, D. T. Seaton, D. P. Landau, and M. Bachmann, *Phys. Rev. E*, **84**, 011127 (2011).
2. M. Bachmann, *Thermodynamics and Statistical Mechanics of Macromolecular Systems* (Cambridge University Press, Cambridge, 2014).
3. M. J. Williams and M. Bachmann, *Phys. Rev. Lett.*, **115**, 048301 (2015).