

Coarse-graining strategy for polymers in solution

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I will discuss the basis of the coarse-graining strategy for polymers in solutions, which maps groups of monomers onto effective monomers, interacting through monomer-averaged state-dependent effective interactions. The level of coarse-graining, that is the number of effective monomer per chain, defines the length scale below which structural details are lost. I will present a recently developed model which allows to transfer effective interactions obtained at zero density, to any finite density by a suitable tuning of the level of coarse-graining, i.e. the number of effective monomers per chain [1]. This model, a refinement of previous unsatisfactory attempts [2,3,4], is able to provide accurate predictions for both the chain structure and the thermodynamics at any finite density, a feature, which is often missing in coarse-grained models. Extension to other thermodynamic conditions and to block copolymer chains will be discussed.

References:

- [1] G. D'Adamo, A. Pelissetto and C. Pierleoni: "Consistent and transferable coarse-graining model for semidilute polymer solution in good solvent", <http://arxiv.org/abs/1201.4275>
- [2] C. Pierleoni, B. Capone, and J. P. Hansen, *J. Chem. Phys.* 127, 171102 (2007).
- [3] A. Pelissetto, *J. Phys.: Condens. Matter* 21, 115108 (2009).
- [4] G. D'Adamo, A. Pelissetto and C. Pierleoni: "Coarse-graining strategy in polymer solutions", *Soft Matter* (in print), <http://arxiv.org/abs/1201.1193>