Fully consistent and transferrable coarse-graining model for polymer solutions

Carlo Pierleoni Physics Department, University of L'Aquila, Italy

I review the basis of the coarse-graining strategy for polymers in solution which maps groups of "microscopic" monomers into effective monomers (blobs) with monomer-averaged effective interactions[1]. The level of coarse-graining, that is the number of blobs per chain, defines the length scale below which structural details are lost. At the highest level of coarse-graining, chains are mapped onto soft particles interacting by density dependent pair potentials [1]. The use of state dependent interactions, although essential to reproduce the thermodynamics, introduces some pathologies [2] and makes the extension of this model to more complex situations impractical.

Based on an original idea of J.P. Hansen [3], we have developed a systematic coarse-grained strategy which, by tuning the level of coarse-graining, exploits zero density potentials even at densities deep into the semidilute regime both in good solvent conditions and in the thermal crossover regime from good solvent to theta conditions for chains of finite length [4,5,6].

Extension of the same strategy to colloid-polymer solutions is also possible and I will present preliminary results on the phase diagram including the demixing transition.

References:

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