

The Theta point of long flexible polymer chains: When does it exist?

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The standard description of the conformation of a long flexible polymer coil in dilute solution implies a swollen state under good solvent condition, while deterioration of solvent quality (by decrease of temperature) causes a (gradual) chain collapse below the Theta point. At the Theta point, the chain follows gaussian statistics, apart from logarithmic corrections.

Monte Carlo simulations of the bond fluctuation model will be discussed [1, 2] that provide evidence for a second scenario, where the chain experiences a first-order transition from the swollen state to a dense solid phase, provided the range of effective attractive interaction is sufficiently short. This scenario then implies that in solution at finite concentration no vapor-liquid like phase separation occurs. The analogy between this prediction and the behavior of some colloidal dispersions is discussed.

[1] W. Paul, T. Strauch, F. Rampf, K. Binder, Phys. Rev. E 75, 060801 (2007)

[2] W. Paul, F. Rampf, T. Strauch, K. Binder, Computer Physics Commun. (2008, in press)