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Unified View on the Mean-Field Order of Coil-Globule Transition[1] DELIAN YANG, QIANG WANG, Colorado State University — It is well known that a polymer chain immersed in a small-molecule solvent undergoes the coil-globule transition (CGT) as the solvent quality changes. In the study of CGT, a mean-field theory, either of the Flory-type or the self-consistent field theory, has been commonly used; the transition order predicted by the mean-field theory, however, has been controversial. By examining the first- and second-order derivatives of the Helmholtz free energy with respect to the solvent equality, the continuity of which defines the transition order but has not been reported in the literature, we concluded that the mean-field CGT of a polymer chain of finite length N exhibits the type-I behavior; that is, it is either a first-order phase transition, a critical point, or a crossover depending on the location of the critical point. It becomes a second-order phase transition with respect to the solvent equality characterized by the Flory-Huggins parameter χ (or equivalently the second virial coefficient v or the temperature T) only in the limit of $N \to \infty$. Even in this limit, it still has the type-I behavior with respect to $vN^{1/2}$ (or equivalently $(1-2\chi)N^{1/2}$).

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