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Monte Carlo field-theoretic simulations of a homopolymer blend[1]

RUSSELL SPENCER, MARK MATSEN, University of Waterloo — Fluctuation corrections to the macrophase segregation transition (MST) in a symmetric homopolymer blend are examined using Monte Carlo field-theoretic simulations (MC-FTS). This technique involves treating interactions between unlike monomers using standard Monte-Carlo techniques, while enforcing incompressibility as is done in mean-field theory. When using MC-FTS, we need to account for a UV divergence. This is done by renormalizing the FloryHuggins interaction parameter to incorporate the divergent part of the Hamiltonian. We compare different ways of calculating this effective interaction parameter. Near the MST, the length scale of compositional fluctuations becomes large, however, the high computational requirements of MC-FTS restrict us to small system sizes. We account for these finite size effects using the method of Binder cumulants, allowing us to locate the MST with high precision. We examine fluctuation corrections to the mean field MST, $\chi N = 2$, as they vary with the invariant degree of polymerization, $\bar{N} = \rho^2 a^6 N$. These results are compared with particle-based simulations as well as analytical calculations using the renormalized one loop theory.

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Russell Spencer
University of Waterloo

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