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Origins of Deviations from the RPA in Polymer Blends: Simulations and Theory JUN KYUNG CHUNG, School of Physics and Astronomy, University of Minnesota, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — We performed continuum Monte Carlo simulations of symmetric binary polymer blends to precisely quantify deviations from RPA predictions for composition fluctuations, including critical phenomena. This comparison is made possible by an unambiguous procedure for determining the self-consistent field (SCF) χ parameter by extrapolating thermodynamic perturbation theory to the limit of infinite chain length N. Corrections to the RPA are shown to be proportional to $N^{-1/2}$, and to be accurately predicted outside of the critical region by a renormalized one-loop theory. The difference between the apparent (i.e., measured) interaction parameter and the SCF value is positive (destabilizing) far from the spinodal ($\chi N \ll 1$) as the result of an N-dependence of the depth of the correlation hole in a melt. Near the critical point, this effect is almost exactly cancelled by the stabilizing effect of long-wavelength composition fluctuations, yielding a critical value of χN quite close to the RPA prediction of $(\chi N) \simeq 2$.

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