

Abstract Submitted
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Effective Coordination Number and Interaction Parameter In Simple Models of Polymer Blends DAVID MORSE, University of Minnesota
— One challenge faced when trying to quantify corrections to the RPA in either simulations or experimental measurements of correlations in polymer blends is the need to estimate the temperature or parameter dependence of a self-consistent field interaction parameter $\chi(T)$. In simulations of simple models, a useful independent definition of $\chi(T)$ may be obtained from a thermodynamic perturbation theory in which the difference between AB and AA interactions is treated as a perturbation of a one-component melt. For lattice models, this yields a value that, in the limit of long chains, is related to the Flory-Huggins value by replacing the coordination number z by an effective coordination number given by the average number of inter-molecular contacts per monomer, as proposed previously by M. Mueller. Generalizations of the idea are provided for continuum models, and for shorter chains. An analytic theory is presented that quantitatively predicts the N-dependence of the effective coordination number found in lattice simulations. The approach provides a clean to way to separate RPA from non-RPA effects in the analysis of simulations.

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