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Monte Carlo Field-Theoretic Simulations for Melts of Symmetric Diblock Copolymer[1]

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Monte Carlo field-theoretic simulations (MC-FTS) are performed on melts of symmetric diblock copolymer for invariant polymerization indexes extending down to experimentally relevant values of $\bar{N} \sim 10^4$. The simulations are performed with a fluctuating composition field, $W_-(\mathbf{r})$, and a pressure field, $W_+(\mathbf{r})$, that follows the saddle-point approximation. Our study focuses on the disordered-state structure function, $S(k)$, and the order-disorder transition (ODT). Although short-wavelength fluctuations cause an ultraviolet (UV) divergence in three dimensions, this is readily compensated for with the use of an effective Flory-Huggins interaction parameter, χ_e. The resulting $S(k)$ matches the predictions of renormalized one-loop (ROL) calculations over the full range of $\chi_e N$ and $\bar{N}$ examined in our study, and agrees well with Fredrickson-Helfand (F-H) theory near the ODT. Consistent with the F-H theory, the ODT is discontinuous for finite $\bar{N}$ and the shift in $(\chi_e N)_{\mathrm{ODT}}$ follows the predicted $\bar{N}^{-1/3}$ scaling over our range of $\bar{N}$.

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