

## Correction to Critical Point of Symmetric Binary Homopolymer Blends

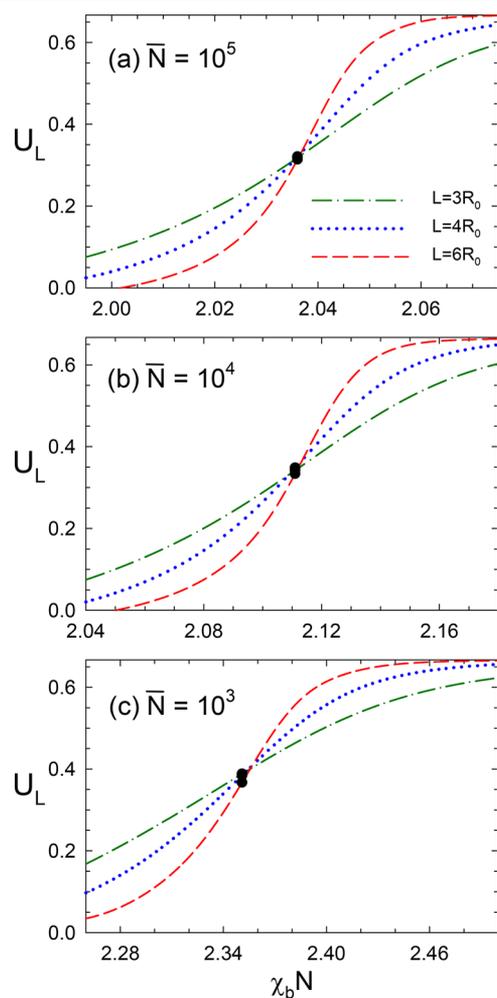
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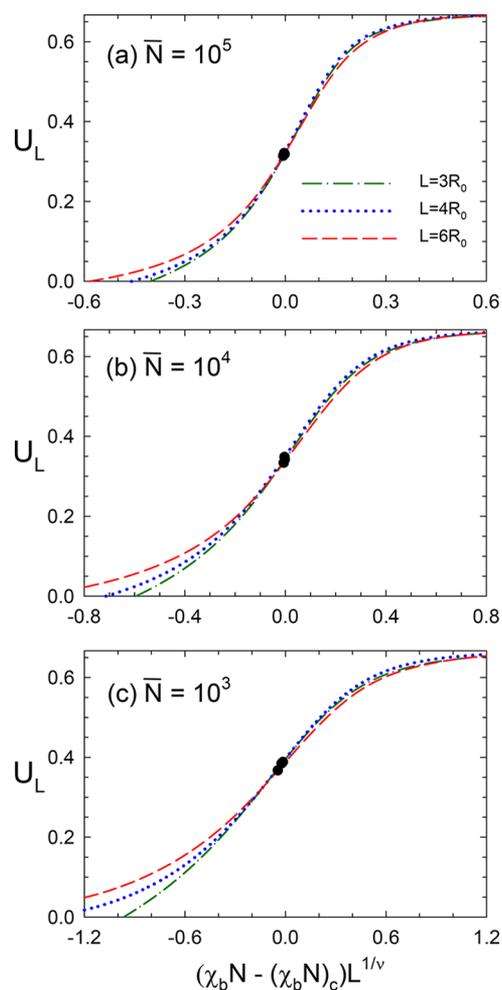
In some of the field-theoretic simulations (FTS) from our paper,<sup>1</sup> the Monte Carlo (MC) move that changes the average value of the  $W_{\mathbf{r}}$  field was accidentally disabled, leading to poor statistics. Only a few of the results are significantly affected, but one of the main conclusions of the paper has changed. Here the simulations are repeated with the MC move enabled and a new semi-grand canonical ensemble that helps increase the computational speed and accuracy.<sup>2</sup>

Figure 3 shows the corrected cumulant calculations. The data for  $\bar{N} = 10^5$  and  $10^4$  are close to those in the original

paper; however, there is a notable difference in the crossing point for  $\bar{N} = 10^3$ . The collapse of the scaled curves, shown in Figure 4, is somewhat better than in the original paper, as a result of the improved statistics.



**Figure 3.** Fourth-order cumulant,  $U_L$ , calculated using different system sizes,  $L$ , for (a)  $\bar{N} = 10^5$ , (b)  $\bar{N} = 10^4$ , and (c)  $\bar{N} = 10^3$ . Simulations were conducted with a grid spacing of  $\Delta = 0.5R_0$ , and MC reweighting was performed about the points indicated by solid dots.



**Figure 4.** Analogous to Figure 3 but with the horizontal axes scaled using the 3D-Ising critical exponent,  $\nu = 0.629\ 97$ .

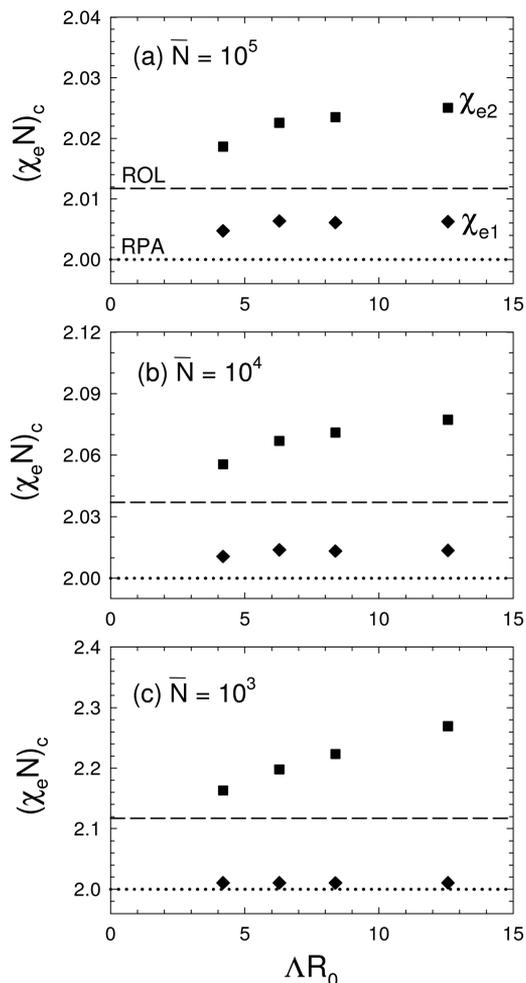
Table 1 lists the critical points for different grid resolutions,  $\Delta$ , in terms of the bare  $\chi_b$ , and Figure 5 plots the data using two different effective  $\chi_c$ 's. Comparing to the original data, there is little change for  $\bar{N} = 10^5$  and  $10^4$ ; however, there is a noticeable difference for  $\bar{N} = 10^3$ . As before,  $\chi_{e1}$  removes the UV divergence for  $\Delta \rightarrow 0$ . Note that we did not repeat the

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**Table 1.** Critical points,  $(\chi_b N)_c$ , in Terms of the Bare  $\chi_b$ , Calculated Using Different Grid Spacings,  $\Delta$ , and Invariant Polymerization Indexes,  $\bar{N}$

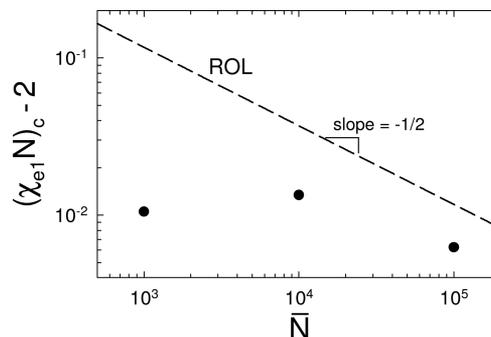
$\Delta/R_0$	$(\chi_b N)_c$		
	$\bar{N} = 10^5$	$\bar{N} = 10^4$	$\bar{N} = 10^3$
0.75	2.025	2.075	2.230
0.5	2.036	2.112	2.359
0.375	2.046	2.147	2.503
0.25	2.067	2.221	2.852



**Figure 5.** Critical point,  $(\chi_e N)_c$ , in terms of the effective  $\chi_{e1}$  (diamonds) and  $\chi_{e2}$  (squares) as a function of the wavevector cutoff,  $\Lambda = \pi/\Delta$ , calculated for (a)  $\bar{N} = 10^5$ , (b)  $\bar{N} = 10^4$ , and (c)  $\bar{N} = 10^3$ . The mean-field prediction of 2 and the renormalized one loop (ROL) prediction are denoted by the dotted and dashed lines, respectively.

highly computational calculation for  $\Delta = 0.1875R_0$  because the asymptotic behavior is already established by  $\Delta = 0.25R_0$ .

Figure 6 compares the critical points with renormalized one loop theory (ROL), which predicts  $(\chi N)_c \propto \bar{N}^{-1/2}$ . The critical point for  $\bar{N} = 10^3$  is below where it was in the original publication, now showing a substantial deviation from the  $\bar{N}^{-1/2}$  scaling. This, in fact, happened in particle-based simulations<sup>3</sup> when a linear definition of the effective  $\chi_e$  was employed. We are currently exploring a definition of  $\chi_e$  that is nonlinear in  $\chi_b$ , following the approach of ref 4.



**Figure 6.** Logarithmic plot showing the fluctuation correction to the mean-field critical point for the three values of  $\bar{N}$  simulated in this study. The dashed line denotes the ROL prediction.

## REFERENCES

- (1) Spencer, R. K. W.; Matsen, M. W. Critical Point of Symmetric Binary Homopolymer Blends. *Macromolecules* **2016**, *49*, 6116–6125.
- (2) Spencer, R. K. W.; Matsen, M. W. Fluctuation effects in blends of A+B homopolymers with AB diblock copolymer. *J. Chem. Phys.* **2018**, *148*, 204907.
- (3) Beardsley, T. M.; Matsen, M. W. Fluctuation correction for the critical transition of symmetric homopolymer blends. *J. Chem. Phys.* **2017**, *147*, 044905.
- (4) Glaser, J.; Medapuram, P.; Beardsley, T. M.; Matsen, M. W.; Morse, D. C. Universality of Block Copolymer Melts. *Phys. Rev. Lett.* **2014**, *113*, 068302.