

Theory of Semiflexible Diblock Copolymer and Random Copolymers in Solvents: Supplemental Materials

Shifan Mao,[†] Quinn MacPherson,[‡] Chunzi Liu,[†] and Andrew J.

Spakowitz^{*,†,¶,§,||,⊥}

[†]Department of Chemical Engineering, Stanford University, Stanford, CA, 94305

[‡]Department of Physics, Stanford University, Stanford, CA, 94305

[¶]Department of Applied Physics, Stanford University, Stanford, CA, 94305

[§]Department of Materials Science and Engineering, Stanford University, Stanford, CA, 94305

^{||}Biophysics Program, Stanford University, Stanford, CA, 94305

[⊥]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025

E-mail: ajspakow@stanford.edu

Structure factors of diblock copolymer solutions

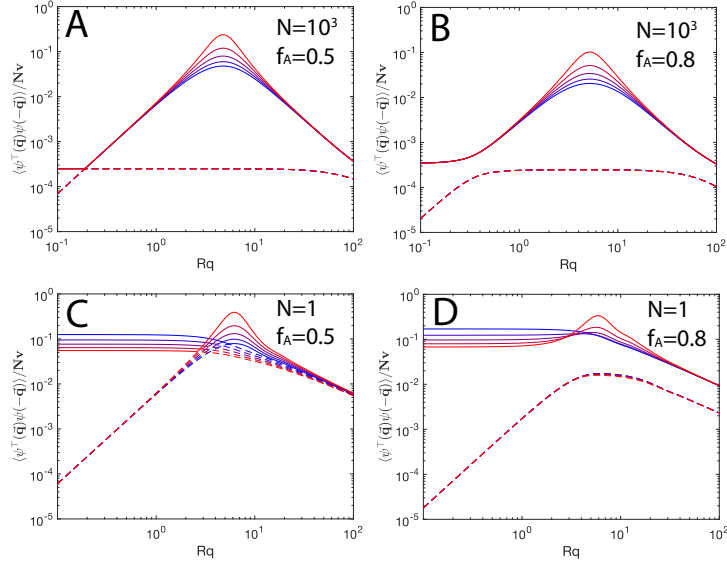


Figure 1: Dominant density correlations $\langle \mathbf{v}_1 \cdot \mathbf{v}_1 \rangle$ and sub-dominant density correlations $\langle \mathbf{v}_2 \cdot \mathbf{v}_2 \rangle$ of symmetric diblock copolymer solutions with $N = 1000$ (A) and $N = 1$ (C), and asymmetric diblock copolymer solutions with $f_A = 0.8$, and $N = 1000$ (B) and $N = 1$ (D). In all figures, total polymer concentration is $\bar{\phi}_P = 0.50$. Colors indicate increasing Flory Huggins parameter $\chi/\chi_{AB}^* = 0.0, 0.2, 0.4, 0.6, 0.8$ from blue to red.

Structure factors of random copolymer solutions

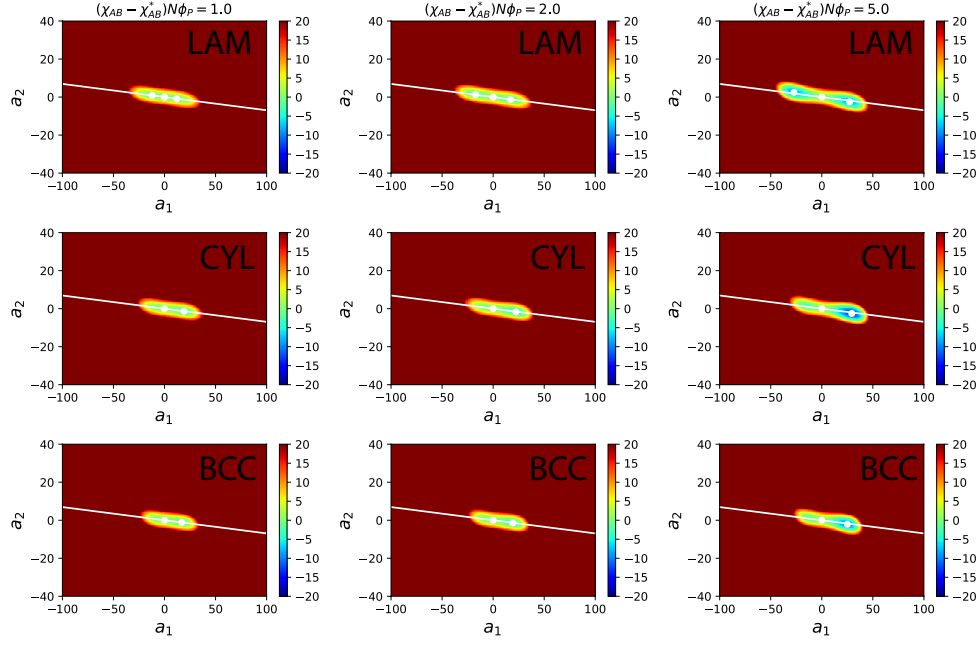


Figure 2: Dominant density correlations $\langle \mathbf{v}_1 \cdot \mathbf{v}_1 \rangle$ and sub-dominant density correlations $\langle \mathbf{v}_2 \cdot \mathbf{v}_2 \rangle$ of anticorrelated random copolymer solutions with $\lambda = -0.75$, $N_m = 100$ (A) and $N_m = 0.01$ (C), and ideal random copolymer solutions with $N_m = 100$ (B) and $N_m = 0.01$ (D). Colors indicate increasing Flory Huggins parameter $\chi/\chi_{AB}^* = 0.0, 0.2, 0.4, 0.6, 0.8$ from blue to red.

Free energies of diblock copolymer solutions

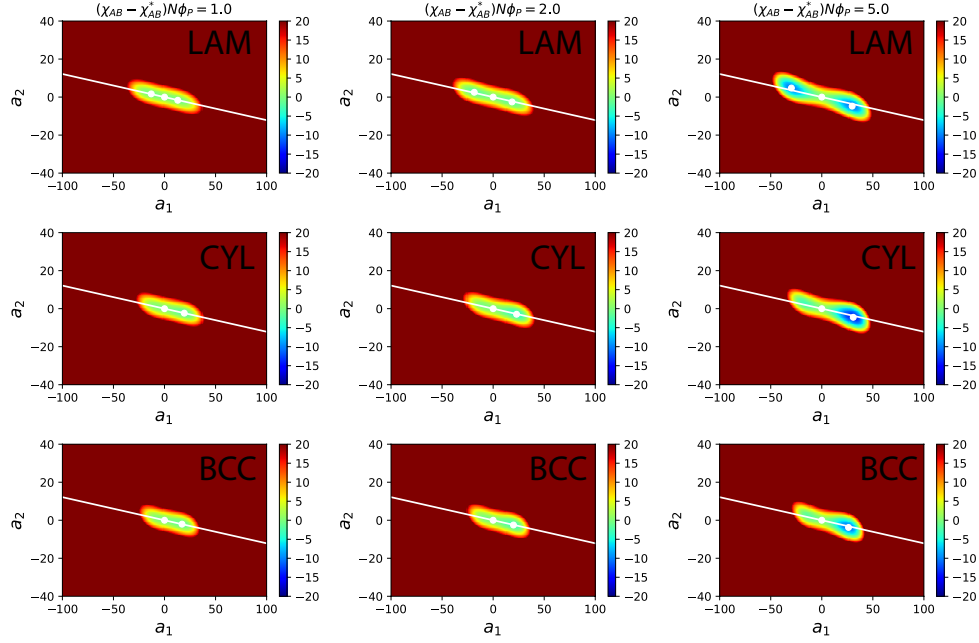


Figure 3: Free energy surfaces of lamellar (LAM), cylindrical (CYL), and body-centered-cubic (BCC) phases of diblock copolymer solutions with polymer length $N=100$, and Flory-Huggins parameter above the spinodal $(\chi_{AB} - \chi_{AB}^*)N\phi_P = 1.0, 2.0$, and 5.0 .

References

- [1] Jiang, Y.; Chen, J. Z. Influence of Chain Rigidity on the Phase Behavior of Wormlike Diblock Copolymers. *Physical review letters* **2013**, *110*, 138305.

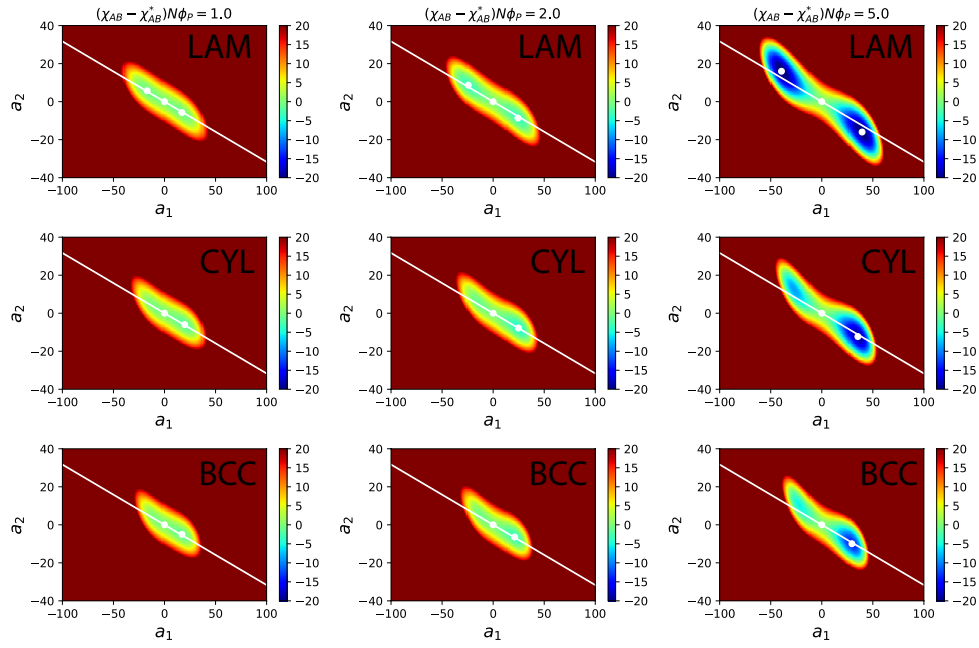


Figure 4: Free energy surfaces of lamellar (LAM), cylindrical (CYL), and body-centered-cubic (BCC) phases of diblock copolymer solutions with polymer length $N=50$, and Flory-Huggins parameter above the spinodal $(\chi_{AB} - \chi_{AB}^*)N\phi_P = 1.0, 2.0$, and 5.0 .

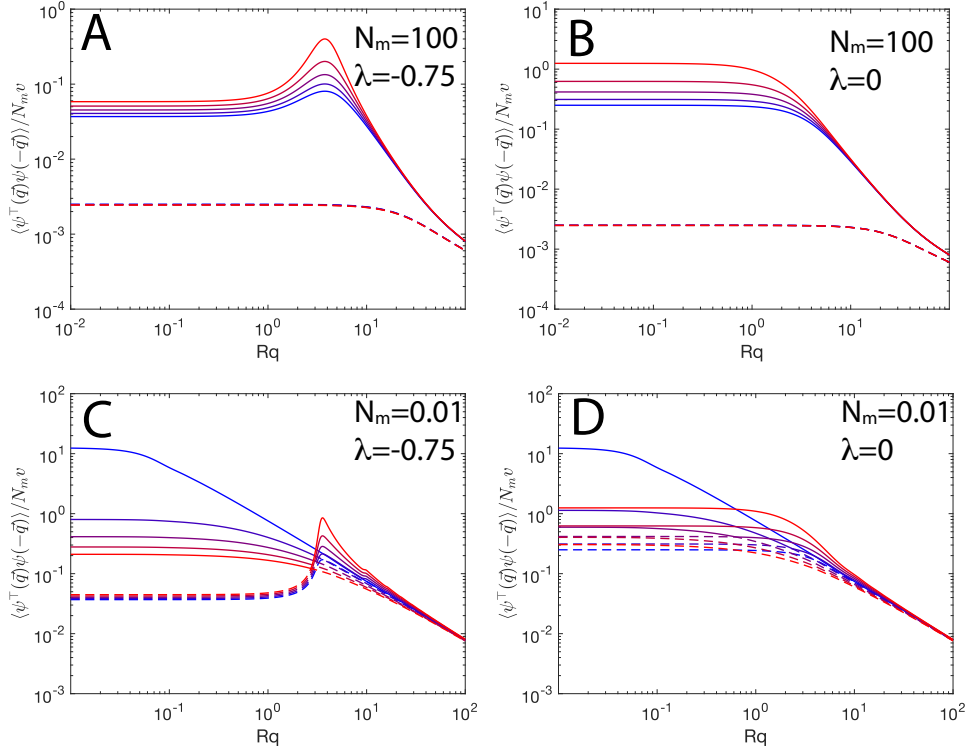


Figure 5: Free energy surfaces of lamellar (LAM), cylindrical (CYL), and body-centered-cubic (BCC) phases of diblock copolymer solutions with polymer length $N=10$, and Flory-Huggins parameter above the spinodal $(\chi_{AB} - \chi_{AB}^*)N\bar{\phi}_P = 1.0, 2.0, \text{ and } 5.0$.

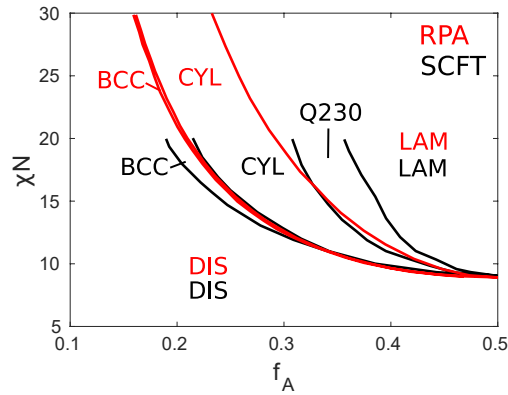


Figure 6: Here we compare the χN versus f phase diagram in the $\bar{\phi}_P \rightarrow 1$ limit (red) with that obtained by Jiang and Chen using self-consistent field theory (black)¹ We did not consider the Q230 phase, which Jiang and Chen show falling between the CYL and LAM phases.