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Electrostatic Correlations and the Polyelectrolyte Self Energy[1]
KEVIN SHEN, ZHEN-GANG WANG, Caltech — We address the effects of chain connectivity on electrostatic fluctuations in polyelectrolyte (PE) solutions using a field-theoretic, renormalized Gaussian fluctuation (RGF) theory. As in simple electrolyte solutions (Z.-G. Wang, Phys. Rev. E. **81**, 021501 (2010)), the RGF provides a unified theory for electrostatic fluctuations, accounting for both dielectric and charge correlation effects in terms of the self-energy. Unlike simple ions, the PE self energy depends intimately on the chain conformation, and our theory naturally provides a self-consistent determination of the response of intramolecular chain structure to PE and salt concentrations. The theory captures the expected scaling behavior of chain size from the dilute to semi-dilute regimes; by properly accounting for chain structure the theory provides improved estimates of the self energy in dilute solution and correctly predicts the eventual N-insensitivity of the critical temperature and concentration of salt-free solutions of flexible PE. We show that the self energy can be interpreted in terms of an infinite-dilution energy $\mu^{el}_{m,0}$ and a finite concentration correlation correction μ^{corr} which tends to cancel out the former with increasing concentration.

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