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Random phase approximation and renormalized Gaussian chain for charged hetero-biopolymers and their sequence-specific phase behavior

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The liquid-liquid phase separation in biological systems has recently attracted intense interest in molecular biology, biophysics, and polymer sciences. Intrinsically disordered proteins (IDPs), proteins that do not fold into a unique structure when isolation because of the depletion in hydrophobicity and the abundance of polar, charged, and aromatic residues, have been discovered to undergo liquid-liquid phase separation in the cell, constructing various intracellular membraneless organelles with distinct biomolecular compositions and biological functions. Based on the sequence-function principle in molecular and structural biology, the phase behavior of a charged IDP must be determined by its unique amino acid sequence, the charge distribution on which is not necessarily fixed but can also be modified by phosphorylation or change of pH value. To understand phase separation in biology, we develop a sequence-specific random phase approximation (RPA) theory for charged IDPs. In addition, we take into account the sequence-specific structure factor of charged polymers by utilizing a variation principle to approximate the IDP by a Gaussian chain with an effective Kuhn length. We apply the theory to both polyelectrolytic biopolymers with large net charges and nearly-neutral polyampholytic IDPs with almost equal number of opposite charges, and obtain theoretical predictions consistent with experimental observations. Phase behavior under the influence of salt and counter ions is also investigated. The augmented renormalized-Gaussian RPA theory, termed rG-RPA, is a general theory for polymers with arbitrary charge sequences, providing a concise theoretical framework for not only studying sequence specificity in individual biopolymer systems but also conducting high-throughput sequence analysis.

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