Fluctuation theory for rarefied gases and complex macromolecular systems

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In this talk, I will present three relevant contents concerning fluctuation theory study based on statistical mechanics, including hydrodynamic fluctuation in rarefied gases, anomalous diffusion in polymer solutions as well as dynamic disorder in complex biomolecular systems.

Firstly, I will talk about how to incorporate thermal fluctuation into hydrodynamics for rarefied gases. We developed a theory of fluctuating hydrodynamics based on extended thermodynamics through studying the 13-variable theory for a monatomic rarefied gas as a representative case. After analyzing the relationship between the present theory and the Landau-Lifshitz theory, we discussed the hierarchy structure of the hydrodynamic fluctuations.

Secondly, I will talk about diffusion of nanoparticles in semidilute polymer solutions. We proposed a theoretical formalism to study the diffusion coefficient of nanoparticles in polymer solutions by using mode-coupling theory. The deviation of diffusion coefficient from Stokes-Einstein relation due to the density fluctuation of polymer solutions was quantitatively demonstrated. We evaluated explicitly how the diffusion coefficient depends on the volume fraction of the polymer solution, the nanoparticle size as well as the degree of polymerization. Results show a very good agreement with experiments.

Thirdly, I will talk about the dynamic disorder effect associated to biomolecular conformational fluctuation. We proposed a theoretical framework based on a generalized Langevin equation with fractional Gaussian noise to study the kinetics of protein unfolding. The dynamic disorder theory for single-molecule pulling experiments was established and the discrepancies between the kinetics with and without dynamic disorder was clarified. Besides, we adopted a fluctuation bottleneck model to analyze the escape rate of DNA from α-hemolysin nanopores. The non-exponential kinetics resulting from the subdiffusive conformational fluctuations of the biomolecular nanopores was investigated.

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