

Understanding Hydrodynamics from Molecular Dynamics



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Brownian motion has provided as a corner stone of the mathematical theory of stochastic process and diffusion process. In particular, the description of Brownian motion by Langevin equation in terms of Newtonian equation of motion including damping and random forces has provided powerful tool to model and to numerically simulate such processes. Mori suggested microscopic derivations of so-called 'generalized Langevin equation' that also allow for memory effects. The Mori formalism is based on the projection operator that can also be used to derive generalize nonlinear Langevin equations as well as generalized Master equations. On the other hand, molecular dynamics provides direct tool to determine the motion of a Brownian particle in a fluid by numerically solving the Hamiltonian equation of motions for Brownian and surrounding fluid particles.

In the present talk, I will discuss on the memory effect and the role of the fluctuating forces in the generalized Langevin equation in relation with the diffusional process. In two-dimensional fluid, self-consistent mode coupling theory predicts the self-diffusive motion of fluid particles to follow a logarithmic correction to the algebraic behavior. Such anomalous diffusive behavior will be discussed from the view point of both the memory function approach and hydrodynamic approach. Next, the hydrodynamic description to the transport phenomena based on the linear response theory will be discussed. We will further show that i) the generalized Langevin approach to the fluid dynamics can be extended to any conserved thermodynamic variables, and from them, ii) we can describe the dynamical behavior of fluid in intermediate time- and spatial-scale in relation with the fluctuating hydrodynamic approach.