[P22] Dynamics of diatomic molecular fluid: The Generalized Langevin Equation description

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The fluid of diatomic molecules in two-dimension is simulated by molecular dynamics approach†. Non-Markovian nature in dynamical properties is investigated in particular. The autocorrelation functions of translational and angular momentum are determined, together with the mean square displacement of position and angular variables. Then we confirm the equivalence between the Green-Kubo theory and the Einstein-Enskog theory for various fluid densities by comparing the diffusion coefficients calculated from the two formulas. We further study the anisotropy of the motion by examining the behavior of the diffusion coefficients parallel ($D_{\perp}$) and orthogonal ($D_{\parallel}$) to the molecular axis, and confirm the equivalence between the two theories.

Finally, the memory function and the fluctuating force in the generalized Langevin equation (GLE) of diatomic molecules are determined for both translational and rotational motion, and their dependence on density are investigated. The fluctuation-dissipation theorem, which states the relation between the characteristic of the spontaneous thermal fluctuation and the response of the system, are satisfied up to sufficiently accurate level for not only translational GLE but also rotational GLE. Deviation of the fluctuating force distributions from the Gaussian form is observed for low density regime. However, they approach to the Gaussian form as the density increases.

† D.C. Rapaport, *The art of molecular dynamics simulations*, Cambridge University Press, Cambridge, (2004).