Generalized extended Navier-Stokes theory: Correlations in molecular fluids with intrinsic angular momentum

The extended Navier-Stokes theory accounts for the coupling between the translational and rotational molecular degrees of freedom. In this paper, we generalize this theory to non-zero frequencies and wavevectors, which enables a new study of spatio-temporal correlation phenomena present in molecular fluids. To discuss these phenomena in detail, molecular dynamics simulations of molecular chlorine are performed for three different state points. In general, the theory captures the behavior for small wavevector and frequencies as expected. For example, in the hydrodynamic regime and for molecular fluids with small moment of inertia like chlorine, the theory predicts that the longitudinal and transverse intrinsic angular velocity correlation functions are almost identical, which is also seen in the molecular dynamics simulations. However, the theory fails at large wavevector and frequencies. To account for the correlations at these scales, we derive a phenomenological expression for the frequency dependent rotational viscosity and wavevector and frequency dependent longitudinal spin viscosity. From this we observe a significant coupling enhancement between the molecular angular velocity and translational velocity for large frequencies in the gas phase; this is not observed for the supercritical fluid and liquid state points.

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