Kinetic Theory and Shear Viscosity of Dense Dipolar Hard Sphere Liquids

Faezeh Pousaneh and Astrid S. de Wijn ^{C, S}

Mechanical and Industrial Engineering, Norwegian University of Science and Technology, Trondheim, Norway astrid.dewijn@ntnu.no

Transport properties of dense fluids are fundamentally challenging, because the powerful approaches of equilibrium statistical physics cannot be applied. Polar fluids compound this problem, because the long-range interactions preclude the use of a simple effect-diameter approach based solely on hard spheres. Here, we develop a kinetic theory for dipolar hard-sphere fluids that is valid up to high density. We derive a mathematical approximation for the radial distribution function at contact directly from the equation of state and use it to obtain the shear viscosity. We also perform molecular-dynamics simulations of this system and extract the shear viscosity numerically. The theoretical results compare favorably to the simulations.

References:

Phys. Rev. Lett. 124, 218004 (2020)