

Characterization of Strain Rate Exponents for the Pressure and Energy of Shearing Fluids

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Recent simulation work has established that the widely accepted mode-coupling theory for the strain rate dependence of the pressure and energy of simple fluids under shear (i.e., energy and pressure are functions of strain rate to the power $3/2$ [1]) is only observed in the vicinity of the triple point [2-4]. Away from the triple point the exponent of the strain rate was seen to be closer to 2 than $3/2$, suggesting a possible analytic behaviour [4]. In this paper we conduct nonequilibrium molecular dynamics simulations to accurately determine the exponent behaviour for a Lennard-Jones fluid in the dense fluid region and find that it varies continuously between ~ 1.2 to ~ 2 as a function of density and temperature, thus confirming its non-analyticity. We furthermore find that the behaviour of the exponent is characterized by a simple linear function of density and temperature, and represents a planar surface in thermodynamic state-space. The coefficients of this planar equation are either universal (i.e., true for all simple fluids) or else can only be a property of intermolecular potential.

Keywords: Nonequilibrium molecular dynamics, shear flow, classical fluids.

References

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