

Thermal Conductivity Calculation of Complex (Dusty) Liquids

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Thermophysical properties play a fundamental role in system design and optimization. Thermal conductivity in semiconductor superlattices and nanoscale materials has recently attracted attention because of the applications in thermoelectronic and optoelectronic devices. The microscopic dynamical origin of heat transfer is a fundamental problem in statistical mechanics with the derivation of modified equations of motion and fully homogenous systems as the ultimate goal. The subject of a complex multicomponent plasma containing grains of solid matter (dust particles) typically of a micrometer size is now attracting much attention. A novel and extended method proposed by Evans-Gillan is used to investigate the behavior of a homogenous Yukawa liquid under the action of external perturbation strength using computer simulated nonequilibrium molecular (NEMD) dynamics. Yukawa liquids are frequently used as a model system of dusty plasmas. Thermal conductivity calculations with appropriate normalizations in the limit of low value perturbation strengths are reported over a wide range of Coulomb coupling ($\Gamma \geq 2$) and screening ($\kappa \geq 1$) strengths. Present simulations provide more reliable data for Yukawa thermal conductivity than the previously known NEMD and molecular dynamics (MD) results. In this present simulation, periodic boundary conditions geometry is used with derived Ewald sums expression for the Yukawa potentials and forces. An improved formula describing the thermal conductivity of the Yukawa systems is presented. The Ewald sums for the energy current which enter in this formula are implemented in our numerical scheme. A simple analytical temperature representation of Yukawa thermal conductivities with suitable reduced frequencies is performed. Yukawa thermal conductivity values obtained from current NEMD simulations are higher than those previously obtained from different numerical schemes. Present simulation data with appropriate normalizations indicate that the position of minimum of thermal conductivity moves towards higher Γ with increasing κ as expected. The minimum values of frequency decrease with increasing κ .