Calculation of viscosity using quantum molecular dynamics simulation and transverse current correlation function

Onegin A.S.[1,2,@], **Paramonov M.A.**[2], **Fokin V.B.**[1,2] **and Demyanov G.S.**[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia

[@] onegin.as@phystech.edu

This study investigates the viscosity of liquids using data obtained from molecular dynamics simulations. The viscosity was calculated via a method based on the transverse current correlation function [1–3], which captures the system's microscopic dynamics. Special attention was given to the convergence of results concerning the number of particles in the simulated system. We introduce a novel technique for integrating the correlation function, offering a robust method for analyzing transport properties. Classical molecular dynamics simulations were performed for liquid aluminum, while quantum molecular dynamics simulations were used for liquid lead to determine the viscosity as a function of temperature under isobaric conditions.

We compared our results with experimental data and validated our findings through extensive verification. The results highlight the impact of system size on the accuracy of viscosity measurements and confirm the efficacy of this approach for studying the transport properties of liquids and, in particular, liquid metals.

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