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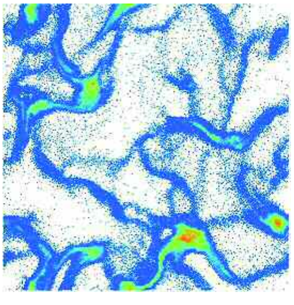
Transport coefficients for dense hard-disk systems

Abstract

A study of the transport coefficients of a system of elastic hard disks, based on the use of Helfand-Einstein expressions is reported. The pressure, the viscosity, and the heat conductivity are examined for different density and system-size. While most transport coefficients agree with Enskog theory below the disorder-order transition, a striking power law divergence of the viscosity with density is obtained at this density. The other transport coefficients show a drop in that density regime, relative to the Enskog theoretical prediction. The deviations are related to shear band instabilities and the contept of dilatancy.

Introduction

Transport coefficients characterize the different mechanisms in non-equilibrium fluid states. At the macroscopic level, they are introduced by phenomenological equations, like the Navier-Stokes equations for a simple fluid, which predict the time evolution of mass, momentum and energy [1]. Each transport coefficient is related to the propagation of one (or more) of these microscopic quantities, bridging therefore the hydrodynamic and the microscopic scale. In the case of low density gases, the macroscopic equations have been justified, their range of validity has been determined, and explicit expressions for the transport coefficients have been obtained using the Boltzmann kinetic equation as starting point [2-4]. At higher but moderate densities, the Enskog equation has also proved to give a quite accurate description of a gas of hard spheres or disks.



In the last years, there has been a revived interest in transport processes in systems composed by hard particles motivated by the study of granular media in general, and granular gases as a special case [5,6,7]. If dissipation is added to the hard disk system, one has a granular gas [3] and one typically observes density inhomogeneities, as displayed in the figure to the left: Low density (white) co-exists with extremely high densities. The color-code indicates the collision rate, being higher in the denser regions (red). The challenge of current research is to predict the transport coefficients for such systems, not only for low densities but also for the highest densities possible.

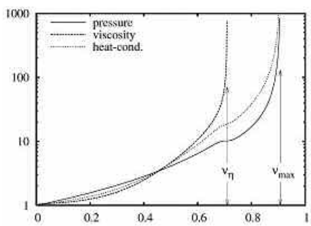
A remarkable and fundamental development in the statistical mechanics theory of transport processes was the derivation of expressions for the transport coefficients based on equilibrium time-correlation functions. These are the so-called Green-Kubo formulas, and they involve different microscopic fluxes [8]. These expressions are of general validity and have been extensively used for the analysis and modelling of transport in denser systems. In particular, they are applied to compute transport coefficients from molecular dynamics simulations. Alternative formal expressions for the transport coefficients are provided by the Einstein-Helfand formulas [8], the simplest of which being Einstein's formula for the self-diffusion coefficient in terms of the second moment of the displacements.

The Einstein-Helfand expressions for the other transport coefficients involve moments of corresponding dynamical variables, which are the time integrals of the microscopic fluxes appearing in the Green-Kubo relations. Considerations about long-time tails in the correlation functions have only recently been considered by Kumaran [9], who proposed a cut-off wavelenght, above which the correlation functions become integrable.

Results

Pressure and the heat conductivity drop at υ_c=0.70 due to the increased mean free path in an ordered configuration and, eventually, diverge at υ_{max}=0.9069. Most interestingly, the shear viscosity diverges at much smaller density, close to the crystallization density, at υ_η = 0.71. For higher densities, in the solid-like regime for $\upsilon>\upsilon_\eta$, shear seems impossible. This power-law divergence of viscosity at $\upsilon_\eta \sim \upsilon_c$, with values above Enskog theory already becoming visible at intermediate densities, $\upsilon>0.5$, renders viscosity different from all other transport properties studied. Note however, that the results presented here were obtained from "non-sheared" systems.

The divergence of viscosity can in fact be understood as the reason for shear-band formation [6,7]: A sheared system at high densities typically splits into sheared bands (with lower density) and compressed, denser, ordered bands. From a different point of view, our observations are also consistent with the concept of dilatancy: A dense packing, with $\upsilon>\upsilon_\eta$, can only be sheared by first experiencing dilatancy so that density drops.



Schematic plot of the non-dimensionalized transport coefficients pressure, viscosity, and heat conductivity, in an elastic hard disk system, as function of density (area fractionl). For small densities <<1, all coefficients accord with the predictions from kinetic theory for hard sphere gases. For higher densities around c=0.70, the system of disks shows a transition from a disordered to an ordered state.

References

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