Kinetic theory of a confined quasi-one-dimensional gas of hard disks

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In recent years, the study of transport phenomena in gases or liquids confined in spaces whose characteristic length is comparable to the molecular size, has attracted a lot of attention. This has been prompted and stimulated by the relevant new technological applications of nanofluidics. The experimental advances ask for a better understanding, at a conceptual level, of the effects that strong confinement has on the non-equilibrium behavior of fluids. Because under these conditions the particles do not explore a bulk-like environment, and because of the asymmetry generated by the confining boundaries, strongly confined systems exhibit inhomogeneity and anisotropy, that have both a great impact on their macroscopic properties.

Most of the studies carried out up to now on transport in confined fluids consider, more or less explicitly, that hydrodynamics holds in all the directions, i.e. it is supposed that the length characterizing the confinement is larger that the characteristic hydrodynamic length. Then, for instance, to study diffusion in a fluid that is confined between two parallel plates, the starting point is the three-dimensional diffusion equation, with the appropriate boundary conditions confining the system. In more general transport problems, some ad hoc extrapolation of the Navier-Stokes equations to confining geometries are employed. In these works, the theoretical problem is how to project the three-dimensional dynamics on a one-dimensional or two-dimensional space, depending on the specific geometry of the system at hand. Nevertheless, when dealing with strongly confined fluids, it is not clear that hydrodynamics hold in the direction perpendicular to the confining walls. Kinetic theory and non-equilibrium statistical mechanics provide the appropriate context to investigate which is the right macroscopic description of transport under strong confinement, providing also the expressions for the needed transport coefficient.

In this work we consider one of the simplest model to tackle the above mentioned general problem: A dilute gas of hard disks confined between two straight parallel lines. The distance between the two boundaries is in between one and two particle diameters, so that the system is quasi-one-dimensional. A Boltzmann-like kinetic equation, that takes into account the limitation in the possible scattering angles, is derived. It is shown that the equation verifies an H theorem implying a monotonic approach to equilibrium. The implications of this result are discussed, and the equilibrium properties are derived. Closed equations describing how the kinetic energy is transferred between the degrees of freedom parallel and perpendicular to the boundaries are derived for states that are homogeneous along the direction of the boundaries. The theoretical predictions agree with results obtained by means of molecular dynamics simulations.

References

[1] M. Mayo, J. Javier Brey, M. I. García de Soria, P. Maynar, Physica A 597, 12723 (2022).