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 [1, 2]. 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 bulklike 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. 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, a dilute gas of hard disks confined between two straight parallel lines is considered. 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 when particularized for the equilibrium situation, the result agrees, in the appropriate limit, with the entropy computed by means of equilibrium statistical mechanics methods [3, 4]. 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 of relaxation time of the System is:

$$\tau = \frac{3}{4\varepsilon^3}. \quad (1)$$

Equation (1) is agree with results obtained by means of Molecular Dynamics simulations (see Fig. 1).

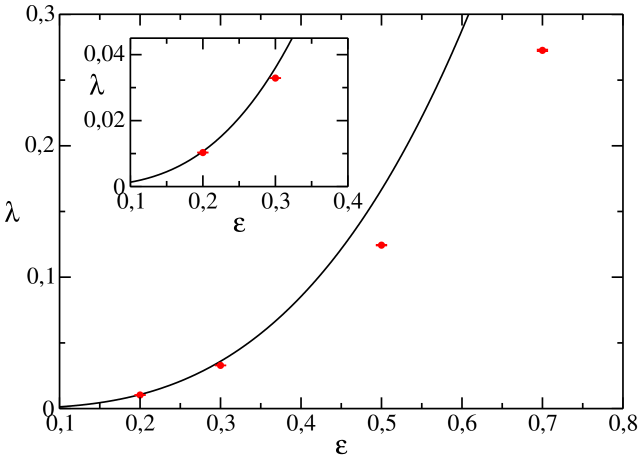

Fig. 1. Inverse of the characteristic relaxation time, λ , of the temperature parameters in a confined quasi-one-dimensional systems of hard disks, as a function of the dimensionless parameter $\varepsilon \equiv (h-\sigma)/\sigma$, that is a measure of the width of the system.

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