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Abstract

Kullback-Leibler Divergence of a Freely Cooling Granular Gas of Inelastic Hard Disks and Spheres †

Alberto Megías and Andrés Santos

Department of Physics, University of Extremadura, Badajoz, Spain

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The velocity distribution function (f_{HCS}) of a granular gas modeled by inelastic hard d-spheres in the Homogenous Cooling State (HCS) is still unknown. Deviations from a Maxwellian distribution (f_{M}) at the system temperature by means of an infinite expansion in terms of Sonine polynomials is the typical approach. In the quest of finding the Lyapunov functional related to this system, the Kullback-Leibler divergences $D_{\mathrm{KL}}[f||f_{\mathrm{HCS}}]$ and $D_{\mathrm{KL}}[f||f_{\mathrm{M}}]$ of the time-dependent velocity distribution function (f) with respect to the HCS and Maxwellian distributions, respectively, are proposed and studied. Kinetic theory results for inelastic hard disks and spheres [1] are supported by Molecular Dynamics (MD) simulations. Whereas $D_{\mathrm{KL}}[f||f_{\mathrm{M}}]$ may present a non-monotonic behavior with time, it is observed that $D_{\mathrm{KL}}[f||f_{\mathrm{HCS}}]$ seems to be a valid candidate for a Lyapunov functional, as proposed in [2]. Interestingly, $D_{\mathrm{KL}}[f_{\mathrm{HCS}}||f_{\mathrm{M}}]$ exhibits a non-monotonic dependence on the coefficient of restitution. Moreover, for a more complete description of the problem, fourth- and sixth-order cumulants are revisited, MD simulation results being compared with kinetic-theory predictions for a wide range of values of the coefficient of restitution. Finally, in some simulations, and after a first freely cooling period, a sort of Maxwell's demon acts by reversing the instantaneous velocity of each particle in an attempt to return to the initial configuration. Although an initial ordering is apparently reached by the elastic system (Loschmidt's paradox), the complete reverted evolution is flatly rejected in the inelastic case since time reversal symmetry and detailed balance are broken down in that case, both results being in accordance with [3].

References

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