Name of the Scholar: Rameez Farooq Shah
Name of the Supervisor: Dr. Syed Rashid Ahmad
Name of the Department: Physics

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Title of the Research: Dynamical Properties of Driven Granular Systems

Abstract

Granular materials, composed of macroscopic particles interacting through dissipative collisions, represent a fundamental class of nonequilibrium systems exhibiting complex dynamical behavior that markedly differs from that of conventional molecular fluids. Unlike molecular gases, granular gases lose energy continuously through inelastic collisions and therefore require external driving to sustain motion. This intrinsic dissipation gives rise to a wide range of nontrivial phenomena such as clustering, non-Gaussian velocity distributions, anomalous transport, aging, and breakdown of energy equipartition. The present thesis is devoted to a systematic numerical investigation of the dynamical properties of driven granular systems, with particular emphasis on diffusion, velocity statistics, aging behavior, and energy decay laws in both single-component and binary granular gases.

The study is carried out using large-scale Molecular Dynamics simulations, primarily employing the Event-Driven Molecular Dynamics (EDMD) technique, which is especially efficient for simulating dilute granular gases composed of inelastic hard spheres. To compensate for energy dissipation due to inelastic collisions, the systems are driven using a stochastic thermostat in the form of Gaussian white noise, allowing the granular gas to reach a nonequilibrium steady state. The role of dissipation is characterized by varying the coefficient of restitution over a wide range, and detailed simulations are performed in two and three dimensions. This approach enables a controlled investigation of how dissipation and external driving jointly influence the macroscopic and microscopic properties of granular gases.

A major part of this thesis focuses on the diffusion properties of a uniformly heated hard-sphere granular gas in three dimensions. The diffusion coefficient is determined from the long-time behavior of the mean square displacement of particles. The system initially exhibits a cooling regime due to inelastic collisions before reaching a steady state where the energy injected by the thermostat balances dissipation. The results reveal a nontrivial dependence of dif-

fusion on the coefficient of restitution. Although higher restitution coefficients lead to increased particle mobility and larger mean square displacement, the diffusion coefficient is found to decrease with increasing restitution. This counterintuitive behavior highlights the subtle interplay between collision dynamics, velocity correlations, and stochastic driving in nonequilibrium granular systems, providing new insight into transport processes in driven granular gases.

The velocity distribution function of a uniformly heated granular gas is examined in detail in three dimensions. The temporal evolution of the granular temperature shows that, irrespective of the restitution coefficient, the system relaxes to a steady-state temperature. In the steady state, the velocity distribution deviates significantly from the Maxwell–Boltzmann form due to inelasticity. These deviations are quantified using a Sonine polynomial expansion of the velocity distribution function. Numerical evaluation of the Sonine coefficients demonstrates that the second and higher-order coefficients attain finite non-zero values, indicating persistent non-Gaussian behavior. Furthermore, the magnitude of these coefficients increases with increasing dissipation, while higher-order coefficients decrease systematically, suggesting convergence of the expansion. This analysis provides a quantitative characterization of velocity statistics in driven granular gases.

The thesis further investigates aging phenomena in velocity autocorrelation functions of a uniformly heated granular gas. The normalized velocity autocorrelation function is analyzed as a function of both observation time and waiting time for different values of the coefficient of restitution. The results reveal explicit aging behavior, manifested through the dependence of the autocorrelation function on the waiting time, indicating a breakdown of time-translation invariance. The autocorrelation function exhibits an initial exponential decay followed by a slower relaxation at longer times due to the development of velocity correlations. Stronger dissipation leads to more persistent velocity memory at long waiting times, emphasizing the important role of inelastic collisions in governing slow relaxation and memory effects in driven granular systems.

In addition, the validity of Haff's law is examined in binary granular gases composed of particles with different masses. Large-scale molecular dynamics simulations are performed in two and three dimensions to study the cooling behavior of such systems in the absence of external driving. The results show significant deviations from the classical Haff's law observed in single-component granular gases. The two species cool at different rates, leading to energy non-equipartition and the emergence of inhomogeneous density structures. Heavier particles exhibit a stronger tendency to cluster compared to lighter ones, highlighting the influence of mass disparity on the dynamical evolution of binary granular gases. In conclusion, this thesis presents a comprehensive numerical study of the dynamical properties of driven granular systems. By systematically investigating diffusion, velocity distributions, aging behavior, and energy decay in both single-component and binary granular gases, the work advances the understanding of nonequilibrium phenomena in dissipative particle systems. The results provide valuable insights into granular gas dynamics and open avenues for future research on velocity-dependent restitution, dense granular flows, and multicomponent driven systems, thereby contributing significantly to the broader field of nonequilibrium statistical mechanics.