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The Quasi-Equilibrium State: A Tale of Certain Soundless Systems

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We consider a $1D$ system with *purely* non-linear interactions such that no acoustic propagation is possible. We show that our system can attain an equilibrium-like state, which we call the "quasi-equilibrium" state. The quasi-equilibrium state is found to be independent of the initial conditions with the particle velocities satisfying a Gaussian velocity distribution. However, in the absence of sound propagation in the system, no energy equi-partitioning is achieved. Our system shows huge temperature fluctuations. Linear response theory seems inapplicable in describing the propagation of a perturbation in the quasi-equilibrium state.

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I. INTRODUCTION

Solids, liquids, and gases can often be found in the equilibrium state. Consider water in a bottle, for instance. If we slightly perturb the bottle, the water quickly settles at its original level, no clue of the perturbation can be seen after the water level has settled and the temperature of the system can be easily measured to great accuracy by using an ordinary thermometer. An equilibrium state is one that does not depend upon the initial conditions, in which the particles show a gaussian distribution of velocities and in which the energy of the system is approximately equally partitioned among the constituent molecules [1].

What allows the equipartitioning of energy? Typically, a perturbation spreads throughout the system. This spreading happens in a way such that energy exchange is readily possible between the particles in the system. More importantly, the exchange of energy can happen between individual particles. Thus, eventually, all particles end up sharing the systems energy more or less equally over time [2].

What if the interactions in a system are such that the exchange of energy between individual particles is somehow not possible? What if the energy exchange must happen between small groups of particles. Each particle will then not end up having more or less the same energy over time. Thus, the temperature of such a system may not be well defined, yet conceivably, the particles may still have a Gaussian distribution of velocities and reach a state that is independent of initial conditions. Such a system would then exhibit an equilibrium-like state, that would have large temperature fluctuations and that would be different from the equilibrium state that we typically encounter in conventional solids, liquids, and gases.

Indeed, there are systems in which energy exchange happens between groups of particles. A small impulse propagating through an alignment of elastic spheres is one such system [3, 4]. There may be other examples, such as chains with algebraically nonlinear inter-particle interactions, such as chains with purely quartic interactions. There may even be biologically relevant systems that realize such nonlinear chains [5]. In what follows, we briefly discuss one of these systems.

II. SYSTEMS WITH UNUSUAL ENERGY EXCHANGE BETWEEN PARTICLES

Let us consider two adjacent elastic spheres i and $i+1$ made of the same material (not a necessary assumption) in mutual contact. When these spheres with radii R_i and R_{i+1} are squeezed against each other such that they are $x_{i,i+1}$ apart, they obviously repel. This repulsive potential $V(\delta_{i,i+1})$, where $\delta_{i,i+1} \equiv R_i + R_{i+1} - x_{i,i+1}$, is described by the Hertz law [6], which states that

$$V(\delta_{i,i+1}) = \frac{2}{5D}\sqrt{\frac{R_i R_{i+1}}{R_i + R_{i+1}}}\,\delta_{i,i+1}^{n}, \qquad (1)$$

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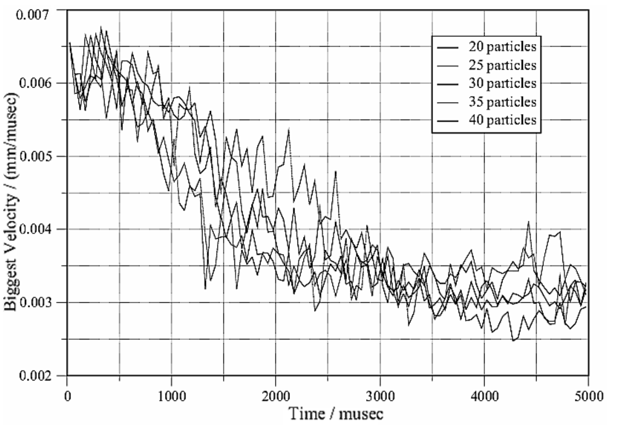

Fig. 1. The vertical axis plots the biggest absolute velocity recorded in a granular alignment of silicon-carbide spheres across short time intervals against time. The pattern shows that the biggest velocity shows a Gaussian (or Maxwellian) decay in time.

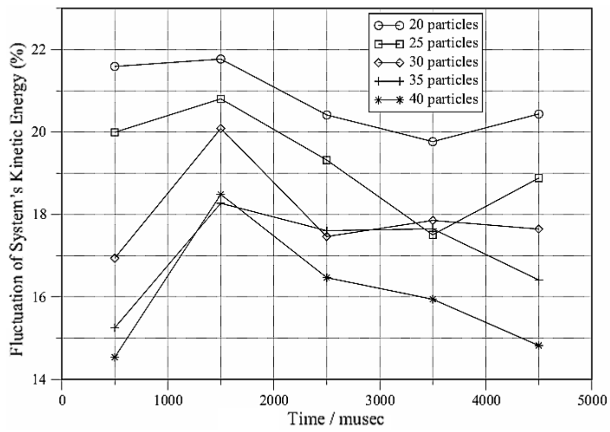

Fig. 2. The fluctuation in the kinetic energy of the system, $\delta K(t)$, is plotted as a function of time for a granular alignment for various system sizes. Large fluctuations persist for all system sizes for well over four decades in time. The magnitudes of the fluctuations seem to decay more slowly as N increases.

where $D = \frac{3}{2}(\frac{1-\sigma^2}{Y})$. σ and Y are the Poisson ratio and Young's modulus of the material, respectively. The potential vanishes when the spheres are not in contact. For spheres, $n = 5/2$. The Hertz potential is softer than the harmonic potential for sufficiently small $\delta_{i,i+1}$ and is steeper than the harmonic potential for sufficiently large $\delta_{i,i+1}$. The nature of this potential is such that energy transport from one grain to another inevitably starts off slowly (due to the softness at short range) in time, then speeds up (due to the steepening of the potential), and ends abruptly. Detailed simulations for all $n > 2$ reveal that energy transport is in bundled form in these systems [7]. In other words, these systems transport energy via solitary waves. The width of the solitary waves depend upon the magnitude of n. For $n = 5/2$, the width is about 5 grain diameters wide [3, 4, 7]. As $n \to 2$, the width diverges. As $n \to \infty$, the width tends to one grain diameter. The widths of the waves is independent of the energy carried by these solitary waves. Further, solitary waves that carry more energy move faster [3, 4]. If the grains are initially barely in touch, they lose contact when they recoil from each other. This means that sound propagation is not possible in these systems.

It is easy to see that energy transport in a granular chain happens with the energy being carried by solitary waves of different amplitudes. The solitary waves formed in the system as a result of some initial perturbation do not preserve themselves when they hit a boundary, e.g., an infinitely massive wall or a soft wall. Instead, they break and produce secondary solitary waves, which are many orders of magnitude smaller than the original waves but possess the same spatial extent [8]. Thus, the presence of boundaries leads to the formation of solitary waves with various energies and moving at a distribution of velocities. Not only that collisions between solitary waves and the walls break the solitary waves, but solitary waves of different sizes can also break apart upon collision. Eventually, a steady state is reached in the system, where at any given instant, one finds a large number of solitary waves, with a large variety of sizes, propagating in one or the other direction in the chain [9].

When a "large" solitary wave collides with a "small" solitary wave traveling in the same direction, the momenta are simply exchanged. There is no further breakdown of the individual waves [10]. The break down continues until an approximately uniform Gaussian distribution of grain velocities in reached. At larger times, there is only marginal change in the tails of the velocity distributions. The quasi-equilibrium phase is reached at this stage [11].

It is instructive to look at the kinetic energy fluctuations in the system against what would be the system temperature (defined say by the average kinetic energy of the system) when the quasi-equilibrium phase has been reached. One quantity to probe is

$$\delta K(t) \equiv \frac{1}{\langle \sum_{i=1}^{N} K_i(t) \rangle_{time}} \times \sqrt{[\frac{1}{\tau}\sum_{t}^{t+\tau}\sum_{i=1}^{N} K_i(t) - \langle \sum_{i=1}^{N} K_i(t) \rangle_{time}]^2}, \quad (2)$$

where $K_i(t)$ is the kinetic energy of grain i at time t, τ is an appropriately small block of time across which the time-averaged average kinetic energy of the system can be probed. Our studies reveal that $\delta K(t)$ typically exhibits large fluctuations (between 10 % and 30 % or so) about the mean kinetic energy per particle, *i.e.*, about the mean temperature of the system, for N between 20 and 40. We have also probed $\delta K(t)$ for systems with up to 10^3 grains. Our results reveal that large energy, persistent fluctuations are reduced, but do not disappear, when N is raised, an expected result in view of the fact that the fluctuations are due to the existence of solitary waves rather than random fluctuations that are strongly sensitive to the system size [9]. Our results remain valid as n is varied [8].

We have studied the dynamics of perturbations in $1D$ systems with purely quartic (spring-like) interactions between the particles. Both compression and dilation pulses, and hence solitary and antisolitary waves, are created by a velocity perturbation in these systems. These waves break upon collisions with each other. However, the nature of wall collisions in these systems can be different from that discussed above. One finds a Gaussian distribution of velocities in this system as well, and the final steady-state (quasi-equilibrium state) appears to be independent of the initial conditions and to be characterized by large fluctuations. More details about this system are discussed elsewhere [9,12].

Breakdown of the equipartition theorem does not allow one to define an equilibrium temperature in these purely anharmonic systems in which no sound propagation is possible. Hence, one can no longer readily define the effect of a perturbation on a many-body system against a background where each particle in the system undergoes random motion due to temperature. Rather, in these systems, collections of particles undergo some kind of random motion. The kinetic-energy fluctuations are, therefore, much larger than what one would expect in systems where acoustic propagation is possible and where the equipartition theorem is satisfied.

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