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The quasi-equilibrium phase in nonlinear 1D systems

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Abstract

We consider 1D systems of masses, which can transfer energy via harmonic and/or anharmonic interactions of the form $V(x_{i,i+1}) \sim x_{i,i+1}^{\beta}$, where $\beta > 2$, and where the potential energy is physically meaningful. The systems are placed within boundaries or satisfy periodic boundary conditions. Any velocity perturbation in these (non-integrable) systems is found to travel as discrete solitary waves. These solitary waves *very nearly* preserve themselves and make tiny secondary solitary waves when they collide or reach a boundary. As time $t \to \infty$, these systems cascade to an equilibrium-like state, with Boltzmann-like velocity distributions, yet with no equipartitioning of energy, which we refer to and briefly describe as the "quasi-equilibrium" state.

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1. Introduction

The study of normal modes in 1D mass–spring systems (e.g., [1]) is central to our understanding of basic lattice dynamics starting from the initiation of a velocity perturbation imparted at a site to the distribution of the perturbation energy among the available modes of the system, i.e., of the *equipartitioning* of the available energy [2]. The study of the system evolution following a perturbation in real time is more challenging to solve exactly for harmonic chains [3]. This problem has remained a centerpiece of non-equilibrium statistical physics for nearly half a century. Chains with combined harmonic and anharmonic springs have attracted significant attention since

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1950s [4]. The study of the dynamics of such nonlinear chains has precipitated fundamental advances in our understanding of solitons and have led us to examine issues such as the equipartitioning of perturbation energy into available modes of the system and of the approach to equilibrium in systems with highly nonlinear interactions [5].

In this work, we focus on systems which have no harmonic term in the interaction potential at all—meaning systems in which the masses do not necessarily move back and forth in *rhythmic harmonic motion* to produce phonons or sound waves. Do such systems exist? The answer is yes. It turns out that the repulsion between two elastic grains upon compression is completely nonlinear [6]. Any perturbation, irrespective of its magnitude, in such systems travels as shock waves (typically as a single large shock wave followed by many tiny ones) [7]. It is conceivable that some long chain biological molecules (such as proteins) may exhibit strongly nonlinear interactions albeit with a weak harmonic part to the interaction [8]. In addition, we consider systems in which boundaries, periodic or otherwise, play a role. We consider systems placed between rigid (or for that matter soft) boundaries as well as systems with periodic boundary conditions. The presence of boundaries is best viewed as a way to alter the local conditions associated with the travel of some perturbation in the systems of interest and leads to significant modifications in the system dynamics.

Again, we keep our focus on perturbations initiated by setting some velocity or velocities to non-vanishing values at the initial instant. We do not consider perturbations initiated only by stretching bonds, which may give rise to long-lived localized modes. Our calculations suggest that the relative strengths of the linear and nonlinear pieces dictate the time scale associated with the emergence of equipartitioned behavior.

2. The model

We start by considering a Hamiltonian of the following form:

$$E = \sum_{i=1}^{N} \frac{p^2}{2m} + \alpha_1 \sum_{i=1}^{N} V_1(x_{i,i+1}^2) + \alpha_2 \sum_{i=1}^{N} V_2(x_{i,i+1}^{\beta}), \quad \beta > 2 , \tag{1}$$

where V_1 is the harmonic term and V_2 is the anharmonic term. Before we drop the V_1 term from further consideration, it is important to note the following physics associated with particle dynamics that is controlled by these terms. We consider our chain systems to be finite, typically with N between 20 and 100. The systems satisfy periodic boundary conditions or are placed between rigid walls.

3. Summary of system dynamics

The parabolic potential introduced by the V_1 term allows the particles in the 1D chain to move back and forth about their equilibrium positions with any of the *allowed harmonic frequencies* of the system and thus *share* their energies with other masses in the system. The V_2 term plays a markedly different role in the context of system dynamics. Given that $\beta > 2$, the anharmonic potential is *softer* than harmonic when the masses are slightly pushed into one another but *steeper* than harmonic when two adjacent particles get sufficiently close. Thus, when a particle starts closing in on a neighbor, initially the dynamics is slow, and then as the potential steepens, the rapidly developing repulsion gets the particles to abruptly recoil. The energy transfer during such processes is inevitably in a "bundled" form and unlike the harmonic case, there is less oscillation of the particles due to V_2. Bundled energy transfer is often associated with the presence of solitary waves and of solitary wave-like objects in systems [9,10].

When both V_1 and V_2 are present in a system, the harmonic term allows extended oscillations and thus facilitates the sharing of modes between particles, in addition to supporting the presence of solitary waves. The result is that the presence of V_1 tends to drive the system to a state with equipartitioned energy at asymptotically large times [2].

As we shall show below, when $\alpha_1 = 0$, a system only transfers energy from one mass to the next via solitary waves. The solitary waves are always of fixed spatial width [10]. This spatial width is controlled by β. When $\beta \to \infty$, the width of the solitary wave shrinks to the minimum physically meaningful width. The solitary waves that end up running through a bounded system continuously collide with each other. The collision process is such that the waves end up leaving tiny residual solitary waves after a collision event and attenuates slightly in amplitude through the collision process [11]. Eventually, the system drives itself into a state in which a large set of small amplitude solitary waves of various amplitude distributions and speeds are found in the process of constant modification as they collide. The perturbation energy is never equipartitioned in these systems and the systems forever remain in the "quasi-equilibrium" state, which is necessarily characterized by large fluctuations against what would have been the fluctuations in a state with energy equipartitioning. Our simulations suggest that the final state of the system is independent of initial velocity perturbation conditions (e.g., whether the velocity perturbation was imparted to one particle at a desired position or to two chosen particles or more, etc.).

What happens when $\alpha_1/\alpha_2 \to 0$? What role do boundaries play in the long time dynamics of such systems? These remain outstanding issues to be addressed. Our preliminary work suggests that for finite α_1/α_2, the "quasi-equilibrium" state eventually gives way to a state where the system energy ends up being equipartitioned and thus, an equilibrium distribution is eventually achieved. Why would one be even interested in exploring the pure "quasi-equilibrium" limit (i.e., when $\alpha_1/\alpha_2 \to 0$)? At a fundamental level, the "quasi-equilibrium" state can be viewed as a *new* phase that has not been probed in the literature, where the dynamics of a system resembles the equilibrium state and yet the system remains out of equilibrium and shows large fluctuations. At a more applied level, one can see that physical systems such as granular systems, which are intrinsically dissipative, can exhibit a quasi-equilibrium like state across some appropriate time regime. In addition, long-chain molecules such as proteins are known to possess highly anharmonic molecular bonds and large fluctuations can allow them to modify their states and structures. Perhaps, these systems exploit the large fluctuations that are found in the "quasi-equilibrium" like state to initiate structural changes.

4. Specific results

We now consider two specific examples of 1D systems with nonlinear algebraic potentials and briefly discuss mechanical energy propagation in these systems. These systems are: (i) a horizontally placed alignment of elastic beads and (ii) a mass–spring chain with linear and nonlinear springs connecting each mass. The first system is addressed in some detail. The second system, which is significantly more complex, is briefly outlined.

(i) *A horizontally placed alignment of elastic beads:* When two spherical, elastic grains of radii R_i and R_{i+1} compress against one another, they repel. We assume that σ and E denote the Poisson ratio and the Young's modulus for the elastic spheres. The repulsive potential is described by Hertz potential [6], which states $V(\delta_{i,i+1})=a_{i,i+1}\delta_{i,i+1}^{5/2}$, where the overlap function $\delta \equiv (R_i + R_{i+1} - x_{i,i+1})$, $x_{i,i+1}$ gives the distance between the two spheres when they are compressed and $a_{i,i+1} = (2/5D)\sqrt{R_i R_{i+1}/(R_i + R_{i+1})}$, $D = 3/2((1-\sigma^2)/E)$. If one assumes that initially the grains are barely touching each other, i.e., they are not precompressed, the grains lose contact when they recoil from each other and hence feel no force between them. If instead, the grains are mutually compressed (i.e., the system is "loaded") at all times, they never lose contact. Thus, they can interact as they move back and forth. In loaded systems, a harmonic part arises in the potential and acoustic propagation becomes possible. We ignore consideration of the precompressed granular chain problem, which has been extensively discussed elsewhere [9]. The dynamics of each grain is described by the following equation, $m_i\ddot{x}_i = \frac{5}{2}\,[a_{i-1,i}\delta_{i-1,i}^{3/2} - a_{i,i+1}\delta_{i,i+1}^{3/2}]$, which can be solved iteratively to any desired accuracy for *monodisperse* chains when i is far from the boundaries [10]. Any perturbation travels through a monodisperse system as a solitary wave [12]. The width of this wave is about 3 grain diameters or $6R$ ($R_i = R$). What role do boundaries play? Let us assume that the chain is placed between two rigid walls. Such walls can be modeled by setting the radius of two edge spheres to be infinite, which alters the potential between the last mass and the boundaries. Any solitary wave must turn around as it reaches each boundary. During the process of turning around, the local interactions change and lead the solitary wave to break down and reconstruct itself. Collisions between two opposite propagating solitary waves and between solitary waves of different sizes also lead to the breakage of the solitary waves. In all cases that we have studied, the process of reconstruction is imperfect. The original solitary wave is replaced by a solitary wave of amplitude that is slightly less. The remaining energy is used to make one or more secondary solitary waves. The process of distributing available energy from the breakdown of an original solitary wave into many secondary solitary waves may itself take many decades in time as shown in Fig. 1 [11]. Such long times appear to be necessary because the system at least needs three body collisions to make each secondary solitary wave (which is $6R$ in width). Three-body collisions do not happen very often in these systems.

The process of breakdown of the solitary waves continues indefinitely, eventually leading to the formation of a state where a very large number of secondary solitary waves get continuously formed and destroyed. We describe this state as the "quasi-equilibrium state." The absolute value of the maximum velocity versus time

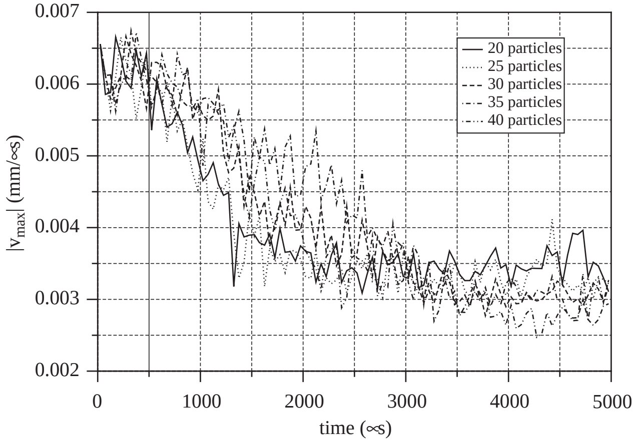

Fig. 1. The absolute value of maximum velocity recorded in the system of elastic grains is shown as a function of time. Quasi-equilibrium phase is reached at $t > 3000$ μs.

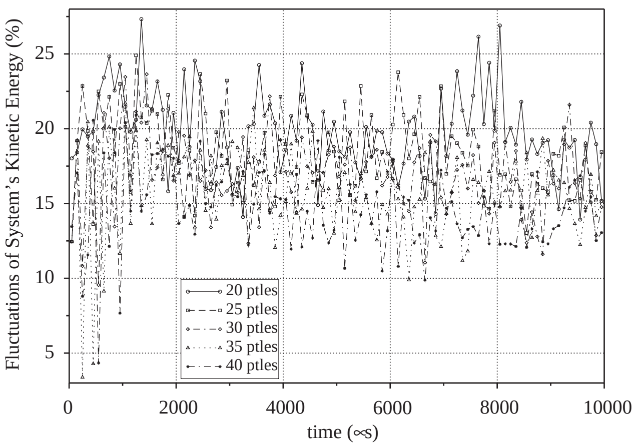

Fig. 2. Total kinetic energy fluctuations (between approximately 12% and 27%) against the time-averaged kinetic energy is shown.

for various system sizes is shown in Fig. 1. The velocity distribution of the grains remains roughly Maxwellian. Our calculations using different initial conditions (but still using velocity perturbations) suggest that the quasi-equilibrium state is independent of the details of the initial conditions. In Fig. 2, we present the kinetic energy fluctuations in the system by plotting the following quantity:

$$F_{E_{kinetic}}(t) = \frac{1}{\langle E_{kinetic}(\tau)\rangle} \sqrt{\left(\frac{1}{\{t\}}\right) \sum_{t}^{t+\tau} (E_{kinetic}(t) - \langle E_{kinetic}(\tau)\rangle)^2} \ ,$$

where $\{t\}$ is the number of points in the time interval τ and $\langle E_{kinetic}(\tau)\rangle$ is the effective temperature of the system defined as the total kinetic energy across a large enough time interval τ. As discussed above, the data suggests large fluctuations in instantaneous total kinetic energy against the effective temperature across four decades in time. As shown in Fig. 2, system size dependence is not very significant in reducing these fluctuations.

(ii) *Nonlinear mass–spring chain*: Unlike in the Hertz problem, in a system where $\alpha_1 = 0$, $V_2 = \frac{1}{4}(x_i - x_{i+1})^{\beta}$, say $\beta = 4$, any perturbation generates a dominant set of compression and dilation pulses along with secondary waves. The compression pulses travel as solitary waves while the dilation pulses travel as antisolitary waves. These discrete waves meet whether the boundary conditions are periodic or fixed. Fixed *perfectly reflective* boundaries, not surprisingly, reveal the same dynamics as in the periodic boundary case. In all instances, this system eventually drives itself to a state where a large number of small amplitude solitary and antisolitary waves are found propagating through the system. These waves are formed and destroyed essentially continuously in time. As one would expect, system size makes a difference with regard to how these energy bundles are made and broken. In Fig. 3, we present a description of the emergence of this equilibrium-like phase. In Fig. 3(a), the data suggest that the average velocity of the particles remain time dependent at all times, in (b) we show that the velocity distribution of the particles is Gaussian, in (c) we show that the velocity power spectrum of a typical particle decays logarithmically in frequency in the nonlinear system, in contrast to remaining roughly flat in harmonic systems. The power spectrum of the maximum velocity of the particles also follows the behaviors shown in Fig. 3(c) and (d). It may be noted that as system size diverges, progressively small amplitude solitary waves are readily allowed in the system. Hence, one would expect that the logarithmic slope of the velocity power spectrum will become progressively flat. Indeed, this is what is found in preliminary studies to be reported elsewhere. In the limit of particle number going to ∞, the differences between the quasi-equilibrium state and the equipartitioned state become essentially indistinguishable. The detailed differentiation between this phase and the equipartitioned phase is presented elsewhere [13].

5. Summary

In this work, we have shown that purely anharmonic finite systems with algebraic nearest-neighbor interactions of the form discussed, support the existence of solitary waves. In the presence of boundaries, these solitary waves break and reform, in the process making smaller amplitude secondary solitary waves. At large times, the system dynamics is comprised of the constant construction and deconstruction of tiny solitary waves. The system possesses a Maxwellian distribution of velocities, but the energy is never equipartitioned. Kinetic energy fluctuations about the equipartitioned state, appear to remain significant in these systems at all times and the fluctuation size is controlled by the system size. The velocity power spectrum of these systems decay logarithmically in frequency as opposed to the same being roughly flat in harmonic systems.

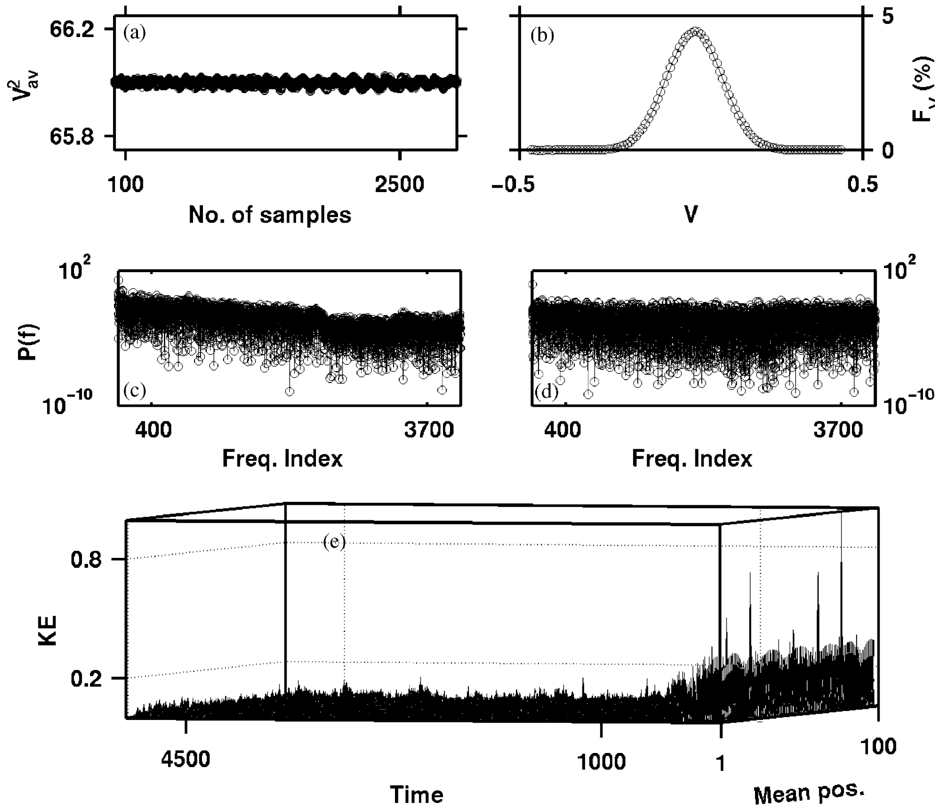

Fig. 3. (a) Spatial average of v^2 vs. t across 3,000 points in t. One finds bigger fluctuations for averages over $T < 3000$. (b) The velocity distribution of the particles is Gaussian in the quasi-equilibrium state. (c) and (d) Present the velocity power spectrum of the 25th particle in the system for the purely quartic and the purely harmonic systems, respectively. Both panels are for periodic boundary conditions. The FFT is similar if it is taken over the maximum velocity in the chains at successive instants. (e) Kinetic energy of each particle against time. The data conveys the rapidity with which the quasi-equilibrium phase is reached.

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