PRAMANA — journal of physics
© Indian Academy of Sciences
Vol. 64, No. 3
March 2005
pp. 423–431

The quasi-equilibrium phase of nonlinear chains

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Abstract. We show that time evolution initiated via kinetic energy perturbations in conservative, discrete, spring-mass chains with purely nonlinear, non-integrable, algebraic potentials of the form $V(x_i - x_{i+1}) \sim (x_i - x_{i+1})^{2n}$, $n \geq 2$ and an integer, occurs via discrete solitary waves (DSWs) and discrete antisolitary waves (DASWs). Presence of reflecting and periodic boundaries in the system leads to collisions between the DSWs and DASWs. Such collisions lead to the breakage and subsequent reformation of (different) DSWs and DASWs. Our calculations show that the system eventually reaches a stable 'quasi-equilibrium' phase that appears to be independent of initial conditions, possesses Gaussian velocity distribution, and has a higher mean kinetic energy and larger range of kinetic energy fluctuations as compared to the pure harmonic system with $n = 1$; the latter indicates possible violation of equipartition.

Keywords. Solitary waves; FPU chain; equipartition; quasi-equilibrium.

PACS Nos 05.45.-a; 43.25.+y; 52.25.Gj

1. Introduction

The study of normal modes in 1D mass-spring systems (see, for e.g., [1]) is central to our understanding of lattice dynamics. The problem of how a perturbation spreads through a harmonic system in real time has been solved exactly (see for instance [2,3]). Later the perturbation energy is, on average, equally distributed among the available degrees of freedom in harmonic chains. Chains with combined harmonic and anharmonic springs continue to garner significant attention in nonlinear dynamics and statistical physics ever since the pioneering work of Fermi, Pasta and Ulam (FPU) [4] in the 1950s. The FPU paper served as the starting point for the rediscovery of solitons [5], initiated several studies of the chaotic/ordered phase space structure of systems with large number of degrees of freedom [6], and has been the corner-stone of studies pertaining to the relation of classical mechanics with statistical mechanics (see, for a recent review, [7]).

In this work, we focus on mass-spring systems which have *no* harmonic term in the interaction potential at all. In these systems, the masses do not necessarily move

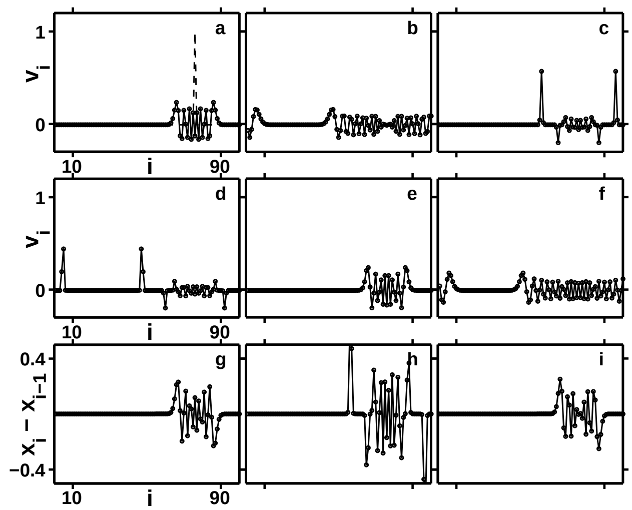

Figure 1. Dispersion vs. solitary waves in a 100 particle chain described by eqs (1) and (2). Axes have been labelled for each row in the leftmost panel with i being the position index of the particle in the chain, v_i its velocity and x_i its displacement from its equilibrium position. In figures 1a and 1b, the initial perturbation (shown in dashed lines) disperses in a harmonic chain, i.e. with $\beta = 0$ in eq. (2); the perturbation splits up into pairs of compression and dilation waves as shown in the displacement plot in figure 1g corresponding to figure 1a. If $\alpha = 0$ in eq. (2), we get solitary wave pulses which are shown in figures 1c and 1d, again in pairs of compression and dilation pulses as can be seen from the displacement plot of figure 1h corresponding to figure 1c; note how the primary pulses are well-separated from the subsequent rattling at the site of initial perturbation, from which can be seen emerging secondary solitary wave pulses. If both α, $\beta \neq 0$ in eq. (2) (see figures 1e and 1f), we have dispersion as the final result albeit controlled by the relative strengths of α and β. The displacement plot corresponding to figure 1e is shown in figure 1i.

back and forth about their equilibrium positions to produce phonons. Hence, these are systems that do not support the propagation of sound waves. Purely nonlinear systems are realized, for example, in the case of forces between two elastic grains upon compression [8]. Any perturbation, irrespective of its magnitude, travels as shock waves in such systems [9]. It is also conceivable that some long chain biological molecules may exhibit strongly nonlinear interactions albeit with a weak harmonic part to the interaction [10]. We are interested in the long-time behaviour of these purely nonlinear chains, and we will consider their behaviour with periodic boundaries and rigid, perfectly reflecting walls at the two ends.

2. Model and calculations

We consider the problem of propagation of a kinetic energy perturbation initiated via $v_i|_{t=0} \neq 0$ for some i, with $v_j|_{t=0} = 0$ for $j \neq i$, in an alignment of N equal masses connected via springs. We consider the Hamiltonian as

$$E = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + V(x_i - x_{i+1}) \right], \tag{1}$$

$$V(x_i - x_{i+1}) = \frac{\alpha}{2}(x_i - x_{i+1})^2 + \frac{\beta}{4}(x_i - x_{i+1})^4, \tag{2}$$

with $\alpha, \beta \geq 0$ in general; in the case of a purely nonlinear chain, $\alpha = 0$. We henceforth set $m = 1$ without any loss of generality and let x_j denote the displacement of mass j from its equilibrium position. It may be noted that our results remain qualitatively unchanged if potentials of the form $(x_i - x_{i+1})^{2n}$ with $n > 2$ are considered. Steeper potentials introduce challenges in maintaining computational accuracy when studying dynamics over many decades. Energy is conserved in our systems. Typically, $N = 100$ in the studies discussed below. We have considered systems as large as $N = 1000$. However, larger systems take significantly longer to run without adding significant new insights on the system dynamics. The integration time-step $\Delta t = 10^{-5}$ in most of our analyses, typical runs are up to $t = 10^5$ time-steps and a velocity-Verlet algorithm [11] was employed. In most of our studies, energy conservation was maintained up to 10 decimal places.

Before we consider the purely nonlinear problem, we recall the nature of the purely harmonic system with $\alpha > 0$, $\beta = 0$. We set $\alpha = 1$ without loss of generality. In figures 1a and 1b, we present snapshots of how a perturbation spreads in a $N = 100$ harmonic chain with periodic boundary conditions. The leading edges of the perturbation diminish in amplitude and spread in width as the excitation spreads symmetrically in both directions into the system. The perturbation energy gets distributed in the system through the 'rattling' of the masses. The effect of such 'rattling' is seen in the trailing tails of the propagating pulses in figures 1a and 1b. Each mass vibrates in all the available normal modes. The average total energy per mass very quickly approaches E_0/N where E_0 is the initial perturbation energy and equipartition is achieved. Note that the normal modes are non-interacting in this system and specially prepared initial conditions corresponding to any of the normal modes would see the system continuing to oscillate in the same mode.

The purely nonlinear case, with $\alpha = 0$ and $\beta = 1$, is shown in figures 1c and 1d. We note that a discrete solitary wave (DSW) and a discrete antisolitary wave (DASW) are initially formed. To identify that one of these is a DSW and the other is a DASW, it is instructive to look at the displacement graph in figure 1g corresponding to figure 1c. These waves travel away from the site of initial perturbation with equal velocity. This velocity is proportional to their amplitudes (which are equal). In this system, secondary DSW and DASW pairs of ever reducing amplitudes are formed at the site of initial perturbation and they break away and follow the earlier formed pairs at regular intervals of time; in figures 1c and 1d, we see the succeeding two generations of the solitary wave pairs. The key observation is that with $\alpha = 0$, $\beta = 1$, there is no tendency for the initial pulses to disperse. We have confirmed this with longer chains where interactions with boundaries are delayed and, to the limits of our accuracy, no loss in energy was detected.

We have also shown the mixed case with $\alpha, \beta = 1$ in figures 1e and 1f, from where we see that the presence of harmonic term tends to wash out the effect of nonlinearity. Clearly, then, the comparative strengths of the linear and nonlinear terms become an important factor that decides the time taken to achieve equipartition.

To summarize, it is clear that, in the absence of boundaries of any sort, i.e. in an infinite system (to be interpreted as 'sufficiently long' for the boundaries to be far away and not involved in the dynamics), the perturbation energy gets equally distributed among the masses in the pure harmonic and mixed cases while, in the pure nonlinear case, solitary waves propagate undispersed with no equidistribution of energy among the masses. We now investigate how the boundaries act to break up the DSWs and DASWs and bring about a 'quasi-equilibrium'.

The nonlinear system evolves in such a way that the original DSWs and DASWs break and reform every time they meet and/or when they collide with system boundaries. The process of breakage and reformation leads to the formation of many DSWs and DASWs of very small amplitudes. This is shown in figure 2 where we have shown both the periodic boundary case (labelled PB) and the fixed boundary case (labelled FB). In each panel we have indicated the time after the initial perturbation in terms of time-steps through which the system has been time evolved. Figures 2a–2c show the 'breathing' nature as the solitary wave 'steps' over the particles. The DSWs and DASWs in our system are rather 'fragile' in the sense that they can break and reform upon certain kinds of collisions such as when waves collide against each other. The reformed waves are slightly reduced in amplitude (speed) and some energy left behind at the site of collision in the form of some 'rattling' (see figures 2d–2h). From the latter, successive generations of tinier DSWs and DASWs get generated. The detailed dynamics associated with the breakage of the DSWs and DASWs is presently under investigation. In figures 2i–2l, it can be seen that collisions of the DSWs and DASWs with the fixed boundary do not lead to loss of energy. Nevertheless, our extensive studies show that the original DSWs and DASWs disintegrate through mutual collisions and give rise to an equilibrium-like state where the system carries a large number of DSWs and DASWs with a Maxwellian distribution of particle kinetic energies (or absolute velocities). The system, finite as it is, appears to be in a state of 'quasi-equilibrium' with a higher mean kinetic energy and larger kinetic energy fluctuations, compared to the harmonic and mixed cases, characterizing the dynamics of each mass. We see typical snapshots of this state in figures 2m–2p.

The solitary waves are always of fixed width. We find that this width is purely a function of the nonlinearity of the potential [9]. In the case of the quartic potential, this width is approximately two bond lengths wide. As the potential steepens, eventually, the width approaches a single bond length. The width of the solitary waves is independent of the energy carried by them, and the latter only decides the velocity of the waves [9]. Our studies suggest that the interactions in the system are such that exchange of energy between individual particles, like in the case of the harmonic potential [12], is no longer possible. Energy is always bundled into packets in the form of two-bond excitations (in the case of quartic potential) [13] and the fluctuations in the system are consistently higher than what is seen with the harmonic potential (see below); these point to possible violation of equipartitioning of energy.

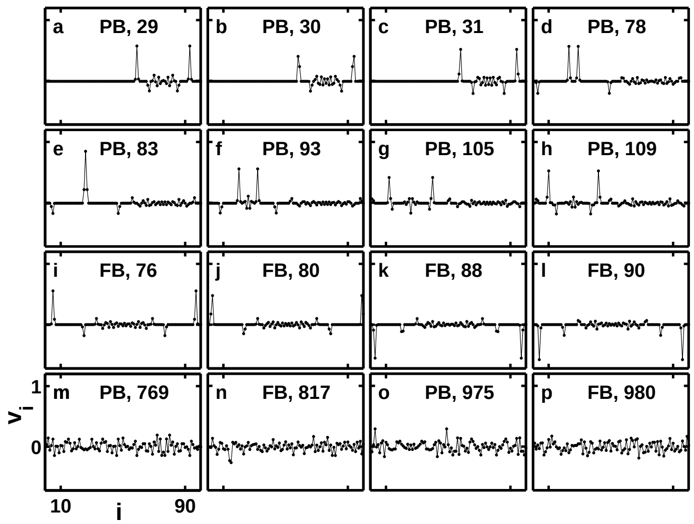

Figure 2. Collisions of solitary waves between themselves as also with walls. Axes have been labelled in panel m, and remains the same for all others; i is an index to the position of the particle in the 100 particle chain, and v_i its velocity. PB/FB indicates periodic/fixed boundary conditions, and the numbers next to them give the time after initial perturbation. Figures 2a–2c show the 'breathing' feature of the discrete chain as the solitary wave steps over the adjacent particles in its motion along the chain. The two primary pulses from the site of initial perturbation, in a chain with periodic boundaries, 'pass through' each other in figures 2d–2f leaving behind some energy at the site of the collision (figure 2f) in the form of prolonged rattling from which will emerge, subsequently, secondary solitary wave pairs, similar to the ones from the site of initial perturbation seen in earlier panels. The primary solitary waves meet up with the secondary ones from the site of initial perturbation and pass through each other in figures 2g and 2h. In figures 2i–2l, we show the collision of primary solitary waves from the site of initial perturbation, in a chain with fixed boundaries, with the walls at either ends, and their reflection with hardly any loss of energy. The panels in figures 2m–2p show the qualitatively similar, noisy, state of the chain, in both periodic and fixed boundary cases, in the asymptotic state after numerous collisions.

In figure 3, we focus on the features of the quasi-equilibrium phase in our system. Figures 3a–3c show 3000 successive samples each of $\langle v^2 \rangle$, where

$$\langle v^2 \rangle = \frac{1}{T} \sum_{t'=t}^{t+T} \frac{1}{N} \sum_{i=1}^{N} v_i^2(t').$$

Unit offset is given to t for each successive sample. In figure 3a, average has been taken over $T = 400$, in figure 3b, the average is over $T = 2000$ and, in figure 3c, the average is over $T = 3000$ (it may be noted that the y-axis has been scaled by 10^4). All the averages have been taken after $t = 75{,}000$. Clearly, the oscillations in kinetic

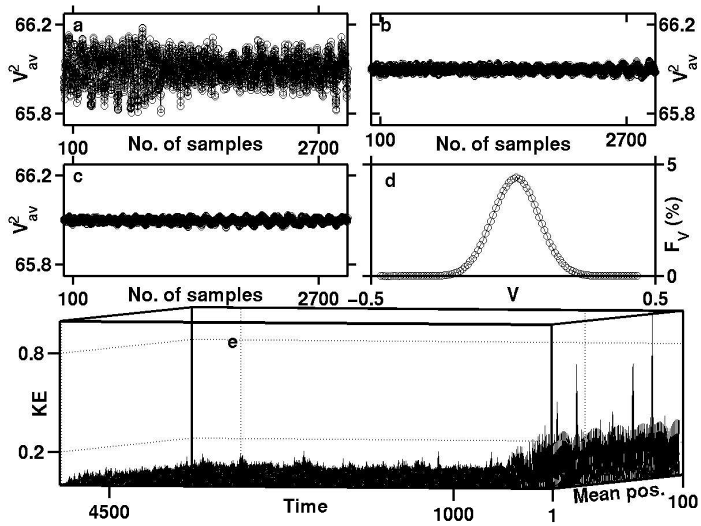

Figure 3. Nature of asymptotic state. The first three panels (figures 3a–3c) show the spatial average of the square of the velocity of the particles, averaged over three different time periods, $T = 400$, $T = 2000$ and $T = 3000$, respectively. Three thousand samples each are shown, which have been taken from consecutive starting points, after 75,000 time-steps of integration; y-axis has been scaled by 10^4. Note that, although the fluctuations in the average are quietened down with increasing T, no further smoothing is possible with larger T's. Figure 3d shows that the velocity distribution over the chain is Gaussian in this state. Figure 3e shows a plot of the kinetic energy of each particle against time, from $t = 0$ to $t = 5000$; note that the system reaches quasi-equilibrium very fast.

energy reduce considerably if the average is over a larger T. Nevertheless, we have not been able to reduce the fluctuations any further by averaging over $T > 3000$. A comparison with the harmonic case (not shown here) revealed that the fluctuations are 3–4 times higher; in both cases, the initial perturbation was 0.5 in arbitrary units of energy. Furthermore, the mean value is also significantly higher (the mean in the harmonic case was only 49.5). In figure 3d, we present the velocity distribution in the asymptotic state, where the binning of the velocities has been carried out over a period of $T = 25{,}000$ steps of integration time. It is seen that the modulus of the velocity distribution is Gaussian in nature, as in the case of a thermalized system. We have shown elsewhere [14] that the velocity power spectrum of a typical particle decays logarithmically in frequency in contrast to it remaining roughly flat in harmonic systems. It can also be seen from figure 3e, where we have plotted the kinetic energies of each particle against time from $t = 0$ to $t = 5000$, that the perturbation energy gets quickly divided among the particles. However, let us remember that, as seen earlier in figures 3a–3c, the averages take longer to stabilize compared to the harmonic case. We have investigated the asymptotic limit for a variety of initial conditions and find that the quasi-equilibrium state is independent of initial conditions, as one would expect of a typical equilibrium phase.

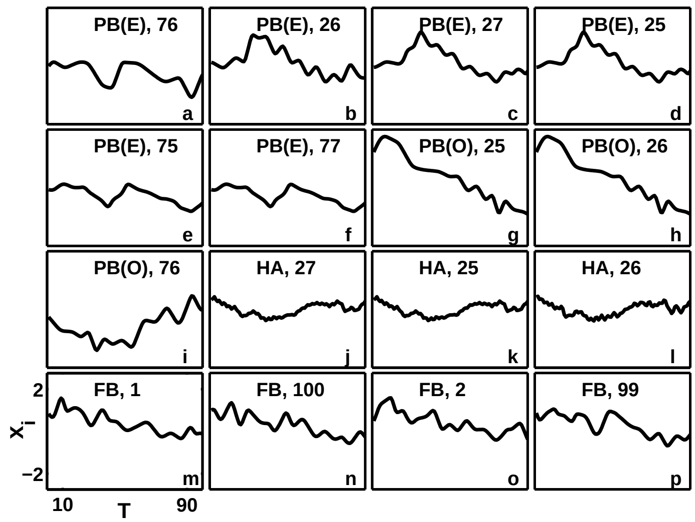

Figure 4. The figure shows correlations induced by boundary conditions. PB and FB refer to periodic and fixed boundary conditions, respectively. E and O further distinguish between chain with even number of particles (=100) and odd number (=101) of particles, respectively. HA refers to chain with only harmonic potential, even number of particles (=100) and periodic boundary conditions. The particle numbers are indicated next to these labels. Oscillations of selected particles over a time period of $T = 100$ arbitrary units, in the steady state are shown. Axes in all panels are as in figure 4m; x_i is the displacement of the ith particle from equilibrium position. Figures 4a and 4b show the two particles at the equatorial points diagonally across (see eq. (3)), both of which have their own unique dynamics. Particles on either side of these equatorial particles are (separately) synchronized as shown in figures 4c–4f. In the case of odd number of particles in a chain with periodic boundaries, only N_{eq} has its unique dynamics, while its diagonally opposite particle at the equator is now paired off with another in synchronized dynamics (figures 4g–4h); rhythms of N_{eq} are shown in figure 4i. The next three panels (figures 4j–4l) show that a similar situation to that with quartic potentials is obtained in a harmonic chain with periodic boundaries; synchronized rhythms of particles sitting across one of the equatorial particles are shown in figures 4j and 4k and the unique rhythm of the corresponding equatorial particle is shown in figure 4l. In the case of the chain with fixed boundaries, one does not see such synchronizations, as shown with the particles next to the walls and adjacent to those (figures 4m–4p) in a 100 particle chain.

It is interesting to observe that the consequences of the boundary conditions are, nevertheless, reflected in this equilibrium phase, and this is so even for the harmonic system. This is illustrated in figure 4 we have plotted the displacements of selected particles against time, for a time period of $T = 70$, and in the steady state (which we identify in the nonlinear system as the quasi-equilibrium phase). In the case of periodic boundary conditions, most of the particles pair off with another with which they oscillate in a synchronized fashion and the pairing can be given as

$$N_i \leftrightarrow \begin{cases} (N_{\rm eq} + N_{\rm de}) \bmod N & \text{if } N_i \le N_{\rm eq} \\ (N_{\rm eq} - N_{\rm de}) \bmod N & \text{if } N_i \ge N_{\rm eq}, \end{cases} \tag{3}$$

where $N_{\rm eq} = N_p + 1$ and $N_{\rm de} = |N_i - N_{\rm eq}|$; N_p is the site at which the initial perturbation was introduced. In the case of even number of particles in the chain, the only exceptions are $N_{\rm eq}$ and its diagonally opposite member, $N_{\rm eq} - N/2$. Both these particles oscillate in their own unique rhythms, i.e., they are not synchronized with each other. In the case of odd number of particles in the chain, only one particle, $N_{\rm eq}$, has a unique rhythm, and all others are paired off with a corresponding member given by eq. (3). This is shown in figures 4a–4f for the nonlinear chain with even number of particles and, in figures 4g–4i, for the chain with odd number of particles. This correlation pattern can be seen in the case of harmonic (figures 4j–4l) and mixed chains (not shown here) as well. The key point is that while the paired particles show correlated vibrations in the system in both linear and nonlinear chains and hence retain memory, the system does sink into an equilibrium-like phase. In this phase, it shows a higher mean kinetic energy and larger fluctuations around it in the nonlinear case as opposed to the linear case. On the other hand, we have a similar quasi-equilibrium in the chain with fixed boundaries but no synchronized vibrations between particles are obtained. However, there are indications that the dynamics changes in character uniformly with distance from the boundaries (see figures 4m–4p), and this is currently under further investigation.

3. Conclusions

Velocity perturbations in chains with purely nonlinear interactions have been probed and compared against the same in pure harmonic and mixed (harmonic + nonlinear) chains. We consider systems of finite number of particles with periodic and fixed boundaries. Our results reveal that, in purely nonlinear chains, the perturbations travel as discrete solitary and discrete anti-solitary waves which would travel undispersed in the absence of boundaries. Boundaries force them to meet and interact which leads to the generation of families of discrete, secondary solitary and anti-solitary waves of decreasing sizes. The distribution of kinetic energies and absolute velocities of the particles show Gaussian behavior and independence from the details of initial conditions. Nevertheless, the mean kinetic energy and fluctuations around it are significantly higher compared to the pure harmonic and mixed cases suggesting a ‘quasi-equilibrium’ phase with possibly no equipartitioning of energy. The particles in both the nonlinear and harmonic chains, with periodic boundary conditions, show oscillatory dynamics in such a way that the particles preserve their memory and no relaxation behavior is observed. In mixed systems, i.e., systems where both harmonic and nonlinear interactions are present, the effects of nonlinearity are eventually washed away by the harmonic term and equipartitioning is achieved in times that depend on the relative strengths of nonlinear and linear terms. We believe our results suggest that nonlinear chains that support discrete solitary and discrete antisolitary waves exhibit qualitatively different dynamics compared to systems that possess harmonic interactions.

Acknowledgements

The research has been partially supported by US National Science Foundation through grant number NSF CMS 0070055.

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