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Early time evolution of a localized nonlinear excitation in the β -FPUT chain^{*}

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We present the detailed dynamics of the particles in the β -Fermi–Pasta–Ulam–Tsingou (FPUT) chain after the initiation of a localized nonlinear excitation (LNE) by squeezing a central bond in the monodispersed chain at time t = 0 while all other particles remain in their original relaxed positions. In the absence of phonons in the system, the LNE appears to initiate its relaxation process by symmetrically emitting two very weak solitary waves. The next stage involves the spreading of the LNE and the formation of nonsolitary wave-like objects to broaden the excitation region until a stage is reached when many weak solitary wave-like objects can be emitted as the system begins its journey to quasi-equilibrium and then to equilibrium. In addition to being of fundamental interest, these systems may be realized using cantilever systems and could well hold the key to constructing the next generation of broadband energy harvesting systems.

*Calculations and analyses have been performed by Kashyap and Westley. Datta was involved in the code development and the theory work. Sen was involved in designing the study and in the analyses of the results. All four authors participated in writing the manuscript. [‡]Corresponding author.

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1. Introductory Remarks

Study of the dynamics of the monodispersed mass spring chain model with the springs represented by harmonic and nonlinear (e.g., quartic) nearest-neighbor interactions in the potential energy is given by

$$H = \sum_{i=1}^{N} p_i^2 / 2m + \sum_{i=1}^{N} [\alpha (x_{i+1} - x_i)^2 + \beta (x_{i+1} - x_i)^4], \qquad (1)$$

where *m* is the mass, α and β are constants, was initiated by Fermi, Pasta, Ulam and Tsingou (FPUT) in 1955.¹ We typically use N = 100 in our studies discussed here. Equation (1) uses nomenclature and terms slightly different from those in the original FPUT study where α and β are defined differently.²

Energy dispersion in this model can be slow or fast depending upon the initial conditions.^{3–8} The system accommodates phonons (for $\alpha > 0$).² For $\alpha = 0$ and $\beta > 0$, solitary waves and metastable localized nonlinear excitations (LNEs)^{9–13} are commonly encountered. In addition, a variety of excitations that are neither solitary waves nor LNEs, but are strongly nonlinear in nature may also appear for finite times. Additionally, phonons may also be present for $\beta > 0$ and $\alpha > 0$.^{2,14} The LNEs and related localized excitations are sometimes referred to as intrinsic localized modes (ILMs),⁹ breathers (for stable oscillations which do not break down see Refs. 15 and 16), etc. Though in existence for 60 plus years, it remains hard to understand how LNEs behave, even at early times, in the FPUT chain and this is the main focus of the paper.

It should be mentioned for the sake of putting the present work in perspective that there is a tremendous amount of literature on *breathers* that we refrain from here. The mathematics community has worked extensively on nonlinear equations obtained in the continuum approximation that can generate stable, localized, nonlinear oscillations (breathers) (see for example in Refs. 15 and 16). Likewise, there is a modest body of literature on how breathers and solitary waves/solitons actually break down in time and the system ends up in equilibrium at large enough times (see for example in Refs. 17–22).

The present paper builds on studies reported in Ref. 2 and has been influenced by the experimental works of Sievers *et al.*, and the simulational and theoretical studies of Vulpiani, Ruffo, Dauxois, Lindenberg, Lichtenberg and others.

LNEs can be regarded as regions with significant amounts of trapped energy for sufficiently long times. Hence, realization of mechanical systems that behave like FPUT systems or systems that are largely similar to FPUT systems can be useful for precipitating LNEs that could be useful for practical purposes such as for constructing novel sensors and for various energy harvesting applications. Cantilever systems have proven to be among those that can realize FPUT-like systems.^{23–29} Section 2 describes the time evolution of the system based upon simple arguments. Section 3 presents the details of numerical simulations with the results being described in Sec. 4. The summary and conclusions are presented in Sec. 4.

2. Time Evolution—Simple Arguments

Since $\alpha = 0$ in Eq. (1), our goal is to consider the following equation of motion:

$$m\ddot{x}_i = 4\beta[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3].$$
 (2)

In the simulational studies below, we will start with the initial condition that the central bond in the chain is squeezed by some amplitude 2A with each mass being moved towards each other by A. The rest of the particles would remain in their relaxed positions. However, this particular condition is not the most convenient one to work with for theoretical analyses for which we assume that particles i and i + 1 are given large symmetric velocity perturbations (i.e., either moving towards each other, or away from each other) at t = 0. This initial condition results in the vibration of the central bond. The central bond carries all the energy at initiation and the dynamics of particle i or i + 1 which sits at the extremities of the central bond can be readily described as follows³⁰:

$$\ddot{x}_i + 36\beta x_i^3 = 0, (3)$$

where we have assumed that $x_{i+1} = -x_i$ and that $x_i \gg x_{i-1}$.

Equation (3) can be solved in terms of Jacobi elliptic functions:

$$x_i(t) = A \operatorname{sn}(At \sqrt{18\beta}, -1), \qquad (4)$$

$$x_i(0) = 0, (5)$$

$$\dot{x}_i(0) = A^2 \sqrt{18\beta} \tag{6}$$

with initial conditions chosen such that the total energy in the system is $E = 9\beta A^4$ and where A is the amplitude of the motion. It is interesting to note that lowering β would stretch out the time evolution of the LNE whereas raising β would have the opposite effect.

Let us now consider the particle adjacent to the center. To leading order, once again assuming $x_i \gg x_{i-1} \gg x_{i-2}$, Eq. (2) becomes

$$\ddot{x}_{i-1} = 4\beta x_i^3 = 4\beta \left(A \, \operatorname{sn}(At\sqrt{18\beta}, -1) \right)^3. \tag{7}$$

Once again, we may solve exactly by using appropriate energy-conserving initial conditions and the property of the Jacobic elliptic function,^{31,32}

$$\operatorname{sn}^{3}(t,-1) = \frac{1}{2} \left(\operatorname{sn}(t,-1) - \frac{d^{2}}{dt^{2}} \operatorname{sn}(t,-1) \right) , \qquad (8)$$

giving

$$x_{i-1}(t) = \frac{A}{9} \, \operatorname{sn}\left(At\sqrt{18\beta}, -1\right).$$
(9)

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Note that at some point, the assumption of $x_{i-j} \gg x_{i-j-1}$ no longer holds. However, it is instructive to examine the pattern for the next several neighbors. By the reasoning followed above, with $\operatorname{sn}(\cdot)$ representing $\operatorname{sn}(At \sqrt{18\beta}, -1)$, we obtain $x_{i-2} = \frac{A}{9^4} \operatorname{sn}(\cdot), x_{i-3} = \frac{A}{9^{13}} \operatorname{sn}(\cdot), x_{i-4} = \frac{A}{9^{40}} \operatorname{sn}(\cdot)$, etc. So, we could separate the solutions order-by-order in powers of $\epsilon = \frac{1}{9}$.

Based on the Duffing equation [see Eq. (3)], the dynamics of particle *i* is expected to be oscillatory with several dominant frequencies among an infinite set. Particles i - 1 and *i* are connected by a nonlinear spring in which *i* undergoes very rapid oscillations and with significant energy content whereas particle i - 1 is barely starting to move. The enormous energy difference between the two particles would prompt particle i - 1 to eventually catch up with particle *i* though this is not attainable in short time. Early time behavior of particle i - 1 hence is expected to be largely periodic, but with abrupt reversals in the direction of motion and with a smaller amplitude than that of *i*. The energy transfer that can happen to i - 2, i - 3, etc. is also expected to be interesting with expected abrupt reversals in the direction of motion.

We observe that the energy contained in the LNE would swing periodically between being purely potential and purely kinetic as in a harmonic oscillator. At this point, let us address in which direction the energy leaking out of the LNE would predominantly move in. We recall the virial theorem of classical mechanics,^{33,34} which states that $\langle K \rangle = 2 \langle U \rangle$, where K, U denote the kinetic and potential energies, respectively, and $\langle \cdots \rangle$ denotes time average. Then, for $\alpha = 0$ in Eq. (1), we get $\langle K \rangle = \frac{2}{3}E$, where E is the total energy. Thus, the energy in the LNE would predominantly become kinetic as the energy begins to leak out of it, which means that the structure of the LNE must break down in time as suggested by Fig. 1. For this to happen, energy flow when looked over long enough times must be outward from the LNE. We would hence expect that the predominant direction in which



Fig. 1. Plot of total potential (U) and kinetic (K) energies as function of time with total energy E being shown in black. Initially the K and U alternate in time. The complexity in the behavior of U is linked to the emission of the various structures between $t \sim 500$ and $t \sim 1000$. Observe that K always remains quite high.

particles i, i - 1, i - 2, etc., would move would be away from the LNE and toward the boundary. The same would be true for the particles on the opposite side of the LNE.

Thus, biased and small displacements experienced by particles farther away from the LNE at early times are to be expected. Given Eq. (2), we would expect symmetric emission of very weak solitary waves out of the smallest short lived perturbations in the direction away from the LNE. At later times, when the energy reaches the sites that are several sites away from i, we would initially expect the formation of irregular spatio-temporal clumps of energy. These clumps would break down farther away from the LNE into solitary waves. Since solitary waves move in velocities that are related to the energies carried, it is likely that the emissions will progressively carry higher energies and generate higher energy solitary waves as the LNE evolves in time. Interactions between the various solitary waves, the original LNE and the existing clumps are expected to generate more solitary waves, metastable but weaker LNEs and clumps as the entire system ultimately evolves to an equilibrium-like state (which we call the quasi-equilibrium state³⁵) at late enough times.

3. The Dynamical Simulations

For all the numerical studies reported here, we use the velocity Verlet algorithm³⁶ to integrate the equations of motion given by Eq. (2) above for each *i*. We set $\alpha = 0, \beta = 1$ and m = 1 for our calculations. The values that appear in the graphs are hence in system units. The parameter A will be used to define the amount by which a mass is shifted from its equilibrium position at time t = 0 and hence sets the energy scale of the perturbation in the study. We will use 0 < A < 1 with typical values being no more than 0.3 or so. A time step of 10^{-6} used throughout is found to conserve energy to about 1 part in 10^7 over the lengths of the runs. Lowering the energy below this point does not give us any more benefits. We set the boundaries to be perfectly reflecting.

Figure 2 plots the kinetic energy (in gray scale) as functions of position and time for the study. At t = 0, the compression of the central bond and its subsequent release produces the LNE. It is important to note that the kinetic energy is shown on a logarithmic scale. On a linear scale, it would be difficult to see the details of how energy leaks out of the LNE. Indeed, as we noted in the discussions below Eq. (9), the energy carried by the individual particles falls rapidly at early times as one moves away from the perturbed bond.

At the earliest times, we see that the energy that is slowly leaking outward from particles 50 and 52 eventually leads to the formation of a solitary wave on each side of the LNE. Figure 3 shows the velocities of particles 50 through 43. The weak solitary wave forms at particle 46 and propagates forward in time as seen by looking at the velocities of particles 45, 44 and 43. This behavior is expected based upon the discussions in Sec. 2 above.



Fig. 2. We plot the kinetic energy per particle as a function of time where the energy plotted is shown on a logarithmic scale. With $\alpha = 0$, there are no phonons in the system. The system is not in equilibrium even at the latest times shown. The state beyond the dispersion of the LNE has been referred to as the quasi-equilibrium state which is populated by a large number of solitary waves and related transient entities.



Fig. 3. The velocity versus time data are shown for selected particles as one moves from the LNE (particle 50) toward the wall near particle 1. The magnitude of velocity shown along the y-axis suggests that the energy moving outward from the LNE is very, very small at early enough times. The formation of a solitary wave is clearly seen in the dynamics of particle 46 at $t \sim 50$.

Observing Figs. 2 and 3 in the time interval between t = 0 and 1800 reveals insights into the rich dynamics that we find in the FPUT system. This can be seen in the panels in Fig. 4. The dynamics of particle 50 is strongly oscillatory and carry a multitude of frequencies, as one may expect from Eq. (3). The energy leaks out of particle 50 very slowly though a fraction of the energy excites particle 49 as discussed above in Sec. 2. The frequencies accessible to particle 49 are lower and fewer, again consistent with the discussions in Sec. 2 (see Figs. 3 and 4). Further,



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Fig. 4. (Color online) Kinetic energy versus time for particles 50–46, 42, 40 and 39.

particle 49's oscillations are characterized by abrupt turns which can be seen in Fig. 3 and on a phase diagram for the same (not shown here). The dynamics of particles 48-42 are overall quite similar and hence to save space not all are shown here. What we find is that a lump of energy is slowly pushing away from the LNE, a part of this moves faster than the other (see 48 at t between 600 and 800, 47 at t

between 800 and 900 and 46 at t between 900 and 1200 or so) slowly merging into a formidable amount of energy which then slows down and gets essentially localized as one can see by examining particles 40 and 39 [Figs. 4(c)–4(h)]. The localization of the energy into a region around particles 39–40 can be thought of in terms of the formation of an LNE which lasts between t around 1000 and t around 1800. As before, our studies suggest that the regions of LNE carry a significant amount of potential energy relative to the kinetic energy, i.e., locally, the ratio of $\bar{K}/\bar{U} < 2$, where \bar{K} and \bar{U} denote local averages of K and U. The LNEs tend to disperse into mobile chunks of energy, be they in terms of solitary waves or disorganized energy bundles.

As shown in Fig. 2, the time evolution of the LNE continues well beyond the times discussed above. The slow energy leakage from the LNE leads to the emissions of lumps of energy that do not quite become solitary waves, that can slow down and form metastable LNE-like structures and also in turn emit weak solitary waves. Eventually, enough energy leaks out such that locally and all over $\langle K \rangle / \langle U \rangle \approx \bar{K} / \bar{U}$ ends up being close to 2, at which point the system reaches the quasi-equilibrium state and eventually a smoother version of the same, the equilibrium state (which we do not attain in the simulations shown in Fig. 2).³⁷

4. Summary and Conclusion

We have attempted to describe the very slow dispersion of the potential energy embedded in a squeezed central bond in an FPUT chain in the absence of harmonic interactions, i.e., when the system is in a sonic vacuum. Absence of phonons have a profound effect on the system's dynamics. Energy can only leak out of the LNE in terms of purely nonlinear excitations such as solitary waves and in terms of not-sowell-formed solitary waves, which we have called lumps of energy (for the lack of a better name for them). These solitary waves and lumps evolve to become highly metastable LNEs and so on. Eventually, the repeated interactions between these entities and the LNE result in the ultimate breakdown of the LNE. The system slowly proceeds to quasi-equilibrium and then to equilibrium.

As one would expect, the system size has an important role to play in influencing the lifetime of the LNE. If the boundaries are near enough, such that solitary wave formation can be severely suppressed, the LNEs may have significantly longer lifetimes than shown here. Further, the entry of phonons into the system could also suppress the tendency to form solitary waves and solitary wave-like structures and that too will increase LNE stability as discussed in earlier work by Mohan and Sen and others. These systems will be discussed separately in the near future.

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