Pulse propagation in chains with nonlinear interactions

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Pulse propagation in nonlinear arrays continues to be of interest because it provides a possible mechanism for energy transfer with little dispersion. Here we show that common measures of pulse dispersion might be misleading; in strongly anharmonic systems they tend to reflect a succession of extremely narrow pulses traveling at decreasing velocities rather than the actual width of a single pulse. We present analytic estimates for the fraction of the initial energy that travels in the leading pulses. We also provide analytic predictions for the leading pulse velocity in a Fermi-Pasta-Ulam β chain.

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The stability of localized energy, e.g., in the form of breathers, in translationally invariant nonlinear arrays, and the way in which localized energy packets can be transported in these arrays, has been a topic of interest for several decades, and continues to be of great interest for a number of reasons. One is that many of the ideas on the subject have recently and increasingly been confirmed experimentally. Another is the possible importance of the subject in the transport of energy in biological systems. Third is the ever increasing numerical capability that allows simulations of larger systems over longer times. A recent focus issue of Ref. [1] contains some of the most current contributions and reviews of the subject, and covers the three topics just mentioned.

While the advances of the past few years are exciting and enormously instructive, the analytic understanding of these phenomena has been made difficult by the fact that the systems are nonlinear. Many of the available results (including those obtained in our group) are numerical, and it is sometimes difficult and even misleading to generalize from these results (for reviews of the subject preceding the special issue noted above, see Refs. [2,3], and references therein). Our contribution in this paper is an analytic understanding of results previously obtained only numerically.

A typical set of questions that one can pose is the following: Suppose that a single unit in a nonlinear array is given an initial velocity. How will this velocity/energy propagate through the array? Will some or all of the energy remain localized, or will it spread? If a localized moving pulse does develop, at what velocity will it propagate? These are some of the signal propagation issues that we address analytically.

We focus on the one-dimensional Fermi-Pasta-Ulam (FPU)-type problem for unit mass particles described by the Hamiltonian

$$H=\sum_i \frac{\dot{x}_i^2}{2}+\sum_i V_n(x_i-x_{i-1}), \tag{1}$$

where x_i is the displacement of particle i from its equilibrium position and $V(z)$ is the potential

$$V_n(z)=\frac{k'}{n}|z|^n+\frac{k}{2}z^2. \tag{2}$$

For the FPU β problem $n=4$, but we retain n as a general power because a number of theories and simulations deal with other values of n, and portions of our analysis do as well. The parameters k and k' are the harmonic and anharmonic force constants, respectively. The variables and the time can be scaled so that the only distinct cases of this problem are $k=0$ (purely anharmonic chain), $k'=0$ (purely harmonic chain), and $k,k'\neq 0$ ("mixed" chain; $k=k'=1$ is a convenient choice). The control parameter is then the initial velocity. The equation of motion for the ith particle in a mixed chain then is

$$\ddot{x}_i=|x_{i+1}-x_i|^{n-1}\mathrm{sgn}(x_{i+1}-x_i)+(x_{i+1}-x_i) -|x_i-x_{i-1}|^{n-1}\mathrm{sgn}(x_i-x_{i-1})-(x_i-x_{i-1}), \tag{3}$$

where $\mathrm{sgn}(x)=\pm 1$ for $x\gtrless 0$. Initially all particles are at rest in their equilibrium positions except for one particle (far from any boundaries) that has initial velocity v_0. We take the chain to be sufficiently long and the boundaries sufficiently far from the initial excitation that their precise nature does not matter for our analysis.

In Ref. [4], Sarmiento *et al.* analyze the pulse evolution in terms of the mean distance from the initial site ("pulse position") and its dispersion ("pulse width"),

$$\langle x\rangle=\frac{\sum_i |i|E_i}{\sum_i E_i}, \quad \sigma^2=\frac{\sum_i i^2E_i}{\sum_i E_i}-\langle x\rangle^2. \tag{4}$$

The local energy is defined as

$$E_i=\frac{\dot{x}_i^2}{2}+\frac{1}{2}V(x_{i+1},x_i)+\frac{1}{2}V(x_i,x_{i-1}). \tag{5}$$

We begin by considering the spreading of the initial pulse. The width of the pulse as time proceeds is often invoked as a measure of the ability of the nonlinearity to keep the energy localized. It is well known that in a harmonic lattice an initial pulse spreads even as it moves. In a mixed chain, one expects less spreading for a higher initial velocity v_0 since a more energetic pulse samples the more anharmonic portions

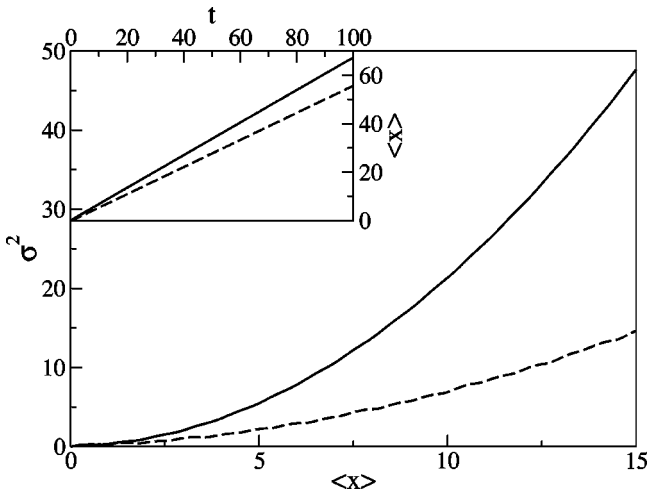

FIG. 1. Mean distance and dispersion of the pulse as defined in Eqs. 4 for a purely quartic potential (dashed line) and a mixed potential with $n=4$ and $v_0=1.0$ (solid line).

of the potential. Indeed, highly localized breathers have been shown to be exact solutions for the purely anharmonic chain in the limit $n\to\infty$ [5]. For a quartic anharmonicity ($n=4$) the contribution of the harmonic and anharmonic contributions to the potential energy are equal at the maximum displacement associated with kinetic energy $v_0^2/2=4$. Therefore when $v_0 \ll \sqrt{8}$ ($v_0 \gg \sqrt{8}$) the dominant contribution to the potential energy of the pulse is the harmonic (anharmonic) portion.

In Fig. 1 we show the pulse width as a function of pulse position for $n=4$ in two cases. In one, $v_0=1$ so that the harmonic portion of the potential is strongly sampled by the excitation. In the other, $v_0\to\infty$, i.e., the potential is essentially a purely quartic potential. The pulse in the purely anharmonic potential is more localized after traveling a given mean distance than is the pulse in the mixed system [4]. The inset shows the mean pulse position as a function of time (the pulses move at a constant speed).

We note that the lower energy pulse moves more rapidly than the higher energy pulse. This result may appear contradictory with those obtained earlier in Ref. [4] where, *for a given initial pulse energy*, pulse velocities in purely harmonic and purely anharmonic systems were compared. A pulse in a purely harmonic system moves at a speed that is independent of the initial velocity v_0, while the pulse speed in a purely quartic system increases with increasing v_0 [4]. Therefore, for sufficiently high initial pulse velocity, a pulse in a purely harmonic system moves *more slowly* than in a purely anharmonic chain [4]. In a mixed chain, on the other hand, the pulse speed as a function of v_0 is bounded *below* by the higher of the two (purely harmonic and purely quartic), approaching the purely harmonic behavior at low v_0 and the purely quartic behavior at large v_0.

Alternatively but equivalently, one can say that the velocity of a pulse in a purely harmonic chain is independent of its amplitude while in an anharmonic chain the pulse speed decreases with decreasing amplitude. This observation has important implications in the understanding of the way in

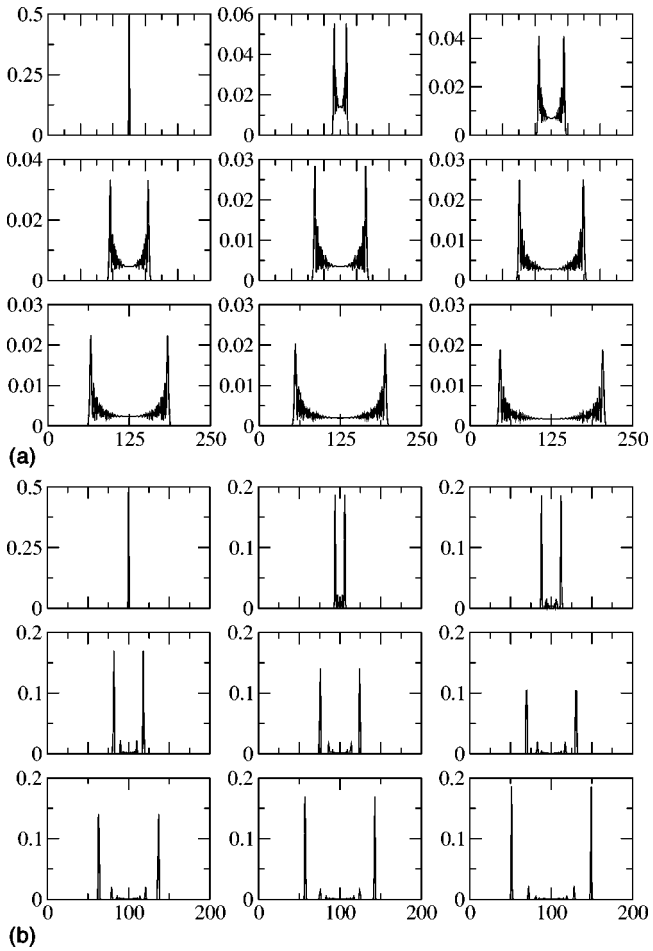

FIG. 2. Snapshots of the normalized local energy profile vs lattice site for the mixed potential with $n=4$ and initial pulse velocity $v_0=1$ (a) and $v_0\to\infty$ (b). From left to right and top to bottom, time runs from 0 to 80 in steps of ten (adimensional) units.

which the pulse width increases as the pulse travels away from the site of origin. To see this, consider a low-velocity pulse launched in a mixed chain. The harmonic portion of the potential here dominates the evolution of the pulse, as shown in Fig. 2(a). Two symmetric fronts travel away from the origin carrying part of the energy and spreading. The remaining energy is progressively distributed among the particles between the pulses. Altogether one observes a gradual broadening of the two pulses, exactly as one imagines a pulse broadening to occur.

However, for a mixed potential with high initial pulse velocity the situation is quite different, as can be seen in Fig. 2(b). Now a portion of the energy travels symmetrically away from the center in extremely localized pulses that in fact *remain highly localized*. The remaining energy is successively ''launched'' from the origin in the form of secondary pulses of smaller and smaller amplitude which travel more and more slowly (the low initial velocity or nearly harmonic case can be thought of in these terms as well, but the secondary pulses travel at essentially the same speed as the primary pulses). Hence, there is a series of narrow pulses of decreasing amplitude that are getting further apart from one another, giving rise to the apparent ''dispersion.'' Moreover,

the maxima of the pulses oscillate; when the energy is more concentrated in one particle the maximum is higher than when it is shared between two or more.

The extreme localization of the pulses suggests that a two- or three-particle approximation may capture the essence of the physics of the problem, and it is this feature that we use to arrive at analytic results. The point to stress here is that *the second moment σ^2 is in fact a deceptive measure of the dispersion of the pulse* except in an essentially harmonic system.

We begin by estimating the energy in the primary pulses and, from this, the pulse velocity as determined by the pulse energy. We assume that the only effects of the restoring forces are to split part of the energy into two pulses, and to keep the remainder of the energy at the origin, from where it will create the secondary pulses. Therefore we need to calculate how much energy is transmitted from the particle at $i=0$ to the particles at $i=\pm 1$, and how quickly it is transmitted.

The first step is achieved by considering a three-particle system and neglecting the rest of the chain. This approximation presupposes that the potential is sufficiently steep such that the particles at $i=\pm 2$ barely move before the particles at $i=\pm 1$ have acquired their full velocity. Obviously, this is not strictly true for finite n; however, we will show that it is a very good approximation, especially for high pulse velocities.

Initially, the three particles are in their equilibrium positions and all of the energy $E_0=v_0^2/2$ is concentrated in the middle particle, $i=0$. Some of the energy is transferred to the neighbors as the springs compress and stretch, and at some time later the energy of the three particles is once again all kinetic. The symmetry of the system requires that this occur when the particles at $i=\pm 1$ acquire their maximum velocity u (equal by symmetry), and the one at $i=0$ its minimum velocity u_0. The three-particle system oscillates back and forth between these two configurations, but we are only interested in this first portion of the cycle. Energy and momentum conservation lead to

$$u=\tfrac{2}{3}v_0, \quad u_0=-\tfrac{1}{3}v_0. \tag{6}$$

Each primary pulse therefore carries away an energy

$$E_p=\tfrac{1}{2}u^2=\tfrac{2}{9}v_0^2=\tfrac{4}{9}E_0. \tag{7}$$

Figure 3 shows simulation results for the primary pulse energy as a function of the power n of the potential for two cases. The circles correspond to an initial pulse velocity $v_0 \to \infty$ (or, alternatively, a purely quartic potential with any v_0). The squares correspond to an initial pulse velocity $v_0=10$. Both lie in the regime where the dynamics is dominated by the anharmonicity, $v_0 \gg \sqrt{8}$, but our theory is expected to improve with increasing v_0. The asymptotic value for the high v_0 case is $E_p/E_0=4/9$, exactly as predicted. The agreement is very good even for $n=4$, where our prediction is already within a few percent of the correct value. For the lower initial pulse velocity the energy ratio is asymptotically only about 7% smaller than predicted, a reflection of the fact

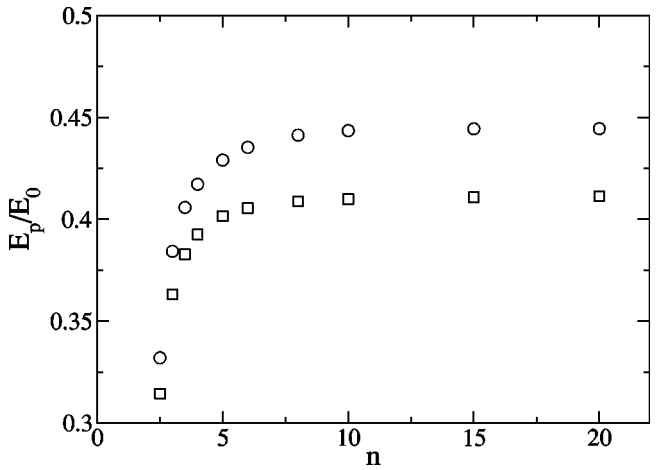

FIG. 3. Relative energy in the primary pulse as a function of the nonlinearity n in the potential. Circles: purely anharmonic potential. Squares: mixed potential with $v_0=10$.

that as the harmonic component becomes more important the pulse occupies more than three sites.

Next we turn our attention to the calculation of the velocity of the primary pulse when $n=4$ (the FPU case). For this calculation we simplify our model even further and consider only a two-particle system, one of which has the initial velocity $u=2v_0/3$. We then calculate the time $T(v_0)$ for the second particle to acquire the same velocity as the first, i.e., the time at which the velocities of the two particles are equal. We maintain that this is the time necessary for the primary pulse to travel from one particle to the next. To calculate this time it is not necessary to actually integrate the equations of motion. Defining $z=x_1-x_2$, we have for $n=4$, $\ddot{z}=-2z^3-2z$. This equation of motion is derived from a potential $V(z)=z^4/2+z^2$, and the initial conditions are $z(0)=0$ and $\dot{z}(0)=u$. From energy conservation we have that the final energy (kinetic plus potential) is equal to the initial energy (all kinetic),

$$\tfrac{1}{2}\dot{z}^2+V(z)=\tfrac{1}{2}u^2, \tag{8}$$

from which it follows that $\dot{z}=\sqrt{u^2-2z^2-z^4}$. Furthermore, the two particles have the same velocity when $\dot{z}=0$. It immediately follows that the relative displacement at that moment is given by $z_m=\sqrt{\sqrt{1+u^2}-1}$. Now we can integrate $\dot{z}$,

$$T(v_0)=\frac{1}{z_m}\int_0^1 \frac{d\eta}{\sqrt{(1-\eta^2)[\coth^2(\phi/2)+\eta^2]}}, \tag{9}$$

where we have introduced the variables $\eta \equiv z/z_m$ and $\phi=\sinh^{-1}(u)$. This integral can be done analytically [6]:

$$T(v_0)=\frac{1}{\sqrt{2}\cosh^{1/2}(\phi)}K\left(\frac{[\cosh(\phi)-1]^{1/2}}{\sqrt{2}\cosh^{1/2}(\phi)}\right), \tag{10}$$

where $K(x)$ is the complete elliptic integral of the first kind [6]. The pulse velocity is just the inverse of this time:

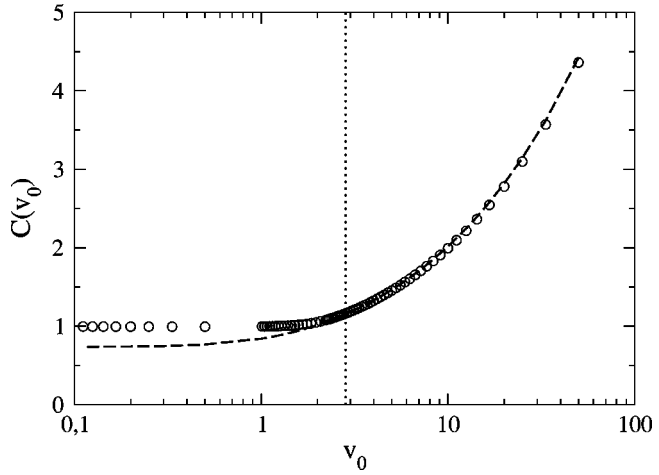

FIG. 4. Pulse velocity vs initial pulse velocity. The circles are the simulation results for a full chain and the broken line is Eq. (11). The dotted line corresponds to $v_0=\sqrt{8}$.

$$C(v_0)=T^{-1}(v_0). \tag{11}$$

For $v_0 \gg 1$ (strongly anharmonic potential) one finds from dimensional analysis [7] that $C(v_0)\sim v_0^{1/2}$.

In Fig. 4, we compare the results of our approximation with the numerical simulation of the full chain as a function of v_0. The circles are the simulation results and the broken line is our two-particle approximation, Eq. (11). The agreement is clearly excellent for initial pulse velocities above $v_0>\sqrt{8}$, the value that we offered as a limit for the validity of this approach.

In this paper we have shown that traditional measures of pulse propagation in arrays with nonlinear interactions may be misleading. We discussed systems with interactions that have both harmonic and anharmonic contributions, and argued that the behavior of a pulse launched by imparting an initial velocity v_0 to a particle at one site in such a system depends strongly on v_0. For low velocities the harmonic portions of the potential are primarily sampled, and the pulse behaves as it would in a harmonic system. For high velocities the anharmonic portions of the potential dominate the behavior, and the pulse propagates as it would in a purely anharmonic chain. It is in the anharmonic regime where one must view traditional measures of pulse propagation with some caution. In particular, we have shown that in the anharmonic regime the usual second moment ''pulse width'' is not a measure of the way a single pulse spreads, but rather of the span covered by a series of very narrow pulses of decreasing velocity. In a statistical measure this appears as a growing second moment. We have also presented analytic estimates for the energy and velocity of the leading pulse, and have shown by comparison with numerical simulations that our estimates are extremely accurate in the anharmonic regime.

A number of extensions of our approach are possible, albeit with some analytic complications. For example, the approach can be extended to the FPU α model that includes cubic as well as quartic interactions. Some of the polynomial solutions and integrations that we have carried out analytically might then have to be done numerically. The same would be true were one to include dissipation. The model can be extended to include a local harmonic potential, and also to higher dimensions. We are currently exploring these generalizations.

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