

Solitary waves in FPU-type lattices

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Abstract

Lattice solitary traveling waves are nonlinear coherent structures that describe fundamental mechanisms of energy transport and signal transmission in many physical settings. This article reviews the main developments in studies of solitary waves in a Fermi-Pasta-Ulam chain and its various extensions that include long-range interactions, periodic heterogeneity and higher dimensions. It emphasizes recent contributions and discusses potential directions for future investigations.

Keywords: lattice dynamics, solitary wave, long-range interactions, stability, heterogeneity

1. Introduction

The interplay of dispersion and nonlinearity in spatially discrete systems often leads to formation of traveling solitary waves, localized nontopological excitations that propagate with amplitude-dependent constant velocity. Due to their ability to provide coherent energy transport and mechanical signal transmission, such waves play a fundamental role in many physical phenomena [1] and have been actively used in designing engineering applications, e.g., [2, 3]. The waves have been experimentally observed in electrical transmission lines [4], granular chains [5] and other settings, including origami-based metamaterials [6].

Since the discovery of solitary waves in lattices due to the seminal contributions of Fermi, Pasta and Ulam [7] and Zabusky and Kruskal [8], a large body of literature has been devoted to understanding their properties, as well as the conditions for their existence and stability. This review article describes the main findings of these investigations, from the early work on solitary waves in the original Fermi-Pasta-Ulam (FPU) chain¹ to the more recent studies of its various extensions that include interactions beyond nearest neighbors, periodic heterogeneity and higher dimensions. While some aspects of the problem have been covered in the earlier reviews of solitary waves and other nonlinear coherent structures in granular materials [9, 10] and in a broader range of discrete systems [11], the present discussion is limited to FPU-type lattices but considers general interaction potentials. It also focuses exclusively on solitary waves and their nonlocal generalizations in lattices with a periodic heterogeneous structure, leaving out other extensively studied waveforms observed in this setting, in particular, periodic [12, 13, 14, 15, 16] and heteroclinic [17, 18, 19, 20, 21] traveling waves, dispersive shock waves [22, 23, 24, 25, 26] and discrete breathers [27, 28], as well as the large body of work on the near-recurrence phenomena in FPU lattices (see, for example, [29, 30, 31, 32, 33] and the references therein). This is done with a goal of presenting a more comprehensive overview of the literature on solitary waves, including very recent results on lattices with piecewise quadratic potentials, competing interactions, stability and nonlocal solitary waves, while also describing the key developments from the earlier work. It goes without saying that

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To acknowledge the contribution of M. Tsingou to [7], the model is called FPUT in some recent literature.

this review can only give a “snapshot in time” of this very active research area, and we include a discussion of some of the many interesting directions for future work.

The remainder of this review article is organized as follows. In Sec. 2 we introduce the basic FPU problem and discuss the existence results for solitary wave solutions. Sec. 3 focuses on near-sonic and high-energy asymptotic limits of such solutions. Quasicontinuum and numerical approximations of solitary waves and their basic properties are discussed in Sec. 4. Construction of solitary waves in lattices with piecewise quadratic interaction potentials is described in Sec. 5. In Sec. 6 we turn to the problem that includes long-range interactions and discuss their effect on existence and properties of solitary waves. Sec. 7 is dedicated to stability results. In Sec. 8 we introduce periodic heterogeneity into the lattice structures and discuss nonlocal and embedded solitary waves that arise in this setting. Scalar and vectorial two-dimensional lattice problems are considered in Sec. 9. We conclude the review with a discussion of some open problems in Sec. 10.

2. Existence of solitary waves solutions of the FPU problem

The dimensionless governing equations for the basic FPU problem are

$$\ddot{u}_n = V'(u_{n+1} - u_n) - V'(u_n - u_{n-1}), \quad (1)$$

where $u_n(t)$ is the displacement of n th particle at time t , dot denotes time derivative, the particle mass is rescaled to unity, and $V(w)$ is the potential governing the interactions between the nearest neighbors. In what follows, we consider these equations over an infinite lattice with the total energy (Hamiltonian) given by

$$H = \sum_{n=-\infty}^{\infty} \left[\frac{1}{2} \dot{u}_n^2 + V(u_n - u_{n-1}) \right] \quad (2)$$

and conserved by the solutions of (1) along with the total momentum $P = \sum_{n=-\infty}^{\infty} \dot{u}_n$. It is often convenient to rewrite the equations of motion in terms of the strain (relative displacement) variables $w_n = u_n - u_{n-1}$:

$$\ddot{w}_n = V'(w_{n+1}) - 2V'(w_n) + V'(w_{n-1}). \quad (3)$$

Traveling wave solutions of (3) have the form

$$w_n(t) = w(\xi), \quad \xi = n - ct, \quad (4)$$

where c is the nonzero velocity of the wave, and thus must satisfy the advance-delay differential equation

$$c^2 w'' = V'(w(\xi + 1)) - 2V'(w(\xi)) + V'(w(\xi - 1)). \quad (5)$$

Note that (4) implies that such solutions are periodic modulo lattice shift:

$$w_{n+1}(t + T) = w_n(t), \quad T = \frac{1}{c}. \quad (6)$$

Solitary waves are traveling waves that are localized in space:

$$w(\xi) \rightarrow 0 \quad \text{as} \quad |\xi| \rightarrow \infty. \quad (7)$$

Due to the translational invariance of (5), such solutions are only defined up to an arbitrary shift in ξ . Note that (5) can be rewritten in equivalent integral form [34]

$$c^2 w(\xi) = \int_{\xi-1}^{\xi+1} (1 - |\xi - s|) V'(w(s)) ds; \quad (8)$$

see also [12, 34, 35] for alternative formulations of this nonlinear eigenvalue problem.

The first existence result for solitary wave solutions of (3) has been established by Toda in [36] for what is now known as the *Toda lattice*, an integrable system with the interaction potential that in rescaled variables has the form

$$V(w) = e^{-w} + w - 1. \quad (9)$$

This problem has the exact solitary wave solution (up to an arbitrary translation in ξ) of the form

$$w(\xi) = -\ln[(\sinh^2 \kappa) \operatorname{sech}^2(\kappa \xi) + 1], \quad (10)$$

where $\kappa > 0$ is the parameter that defines the velocity $c = \sinh \kappa / \kappa$, which must exceed the sound speed $c_s = (V''(0))^{1/2} = 1$, thus yielding *supersonic* waves. Solutions (10) exhibit the quasiparticle behavior (elastic collisions) observed in the Korteweg-de Vries equation discussed below and other integrable systems and can thus be termed *solitons* [8]. Other consequences of integrability of the Toda lattice are discussed in [37].

Most FPU systems, however, are not integrable, and existence of solitary wave solutions for a general class of interaction potentials was first proved by Friesecke and Wattis in [38]. Specifically, they proved existence of supersonic solitary waves for $C^2(\mathbb{R})$ potentials $V(w)$ such that $V(0) = 0$, $V(w) \geq 0$ in some neighborhood $(-\delta, \delta)$ of zero, and $V(w)$ has a *superquadratic growth* on at least one side, i.e., $V(w)/w^2$ is strictly increasing with $|w|$ for all w in Γ , where either $\Gamma = (0, \infty)$ (yielding *rarefactive* waves satisfying $w(\xi) > 0$) or $\Gamma = (-\infty, 0)$ (resulting in *compressive* waves, $w(\xi) < 0$). The proof is based on minimizing the average kinetic energy of the system subject to the constraint that the average potential energy K is fixed, with the velocity c being the Lagrange multiplier. The existence of minimizers is established for K above a certain nonnegative threshold using Lions's concentration-compactness principle [39, 14]. The authors further showed that if either $V''(0) = 0$ or $V(w) = V''(0)w^2/2 + \varepsilon|w|^p + o(w^p)$ for some $\varepsilon > 0$ and $2 < p < 6$ as w in Γ tends to zero, such solutions exist for any $K > 0$. This result establishes the existence of solitary waves for the Toda potential (9), among a broad class of potentials that includes the α -FPU potential

$$V = \frac{w^2}{2} + \alpha \frac{w^3}{3} \quad (11)$$

with nonzero α , the β -FPU potential

$$V = \frac{w^2}{2} + \beta \frac{w^4}{4} \quad (12)$$

with $\beta > 0$, the Lennard-Jones potential $V(w) = a[(d+w)^{-6} - d^{-6}]^2$, with $w > -d$ and $a, d > 0$, and contact interactions of power-law type [40, 41].

Another existence proof, based on constrained maximization of potential energy [12] and exploiting the invariance properties of an improvement operator, was given in [35] by Herrmann. Although it is restricted to FPU lattices with convex potentials, it refines the earlier results by showing the existence of unimodal (monotone for both $\xi \geq 0$ and $\xi \leq 0$) and even ($w(-\xi) = w(\xi)$) solitary waves under superquadratic growth conditions.

Smets and Willem [42] used a different approach, based on a variant of the mountain pass theorem [43, 44, 14], to prove existence of supersonic solitary waves with prescribed velocity c in the FPU problem with a superquadratic potential. Schwetlick and Zimmer [45] improved these results by requiring the superquadratic growth to hold only asymptotically, a condition satisfied by some double-well potentials. Pankov and Pflüger [13] used the mountain pass theorem to prove the existence of supersonic periodic traveling waves with prescribed speed and obtain solitary

waves in the limit of infinite period using concentration compactness. Similar techniques were used by Pankov and Rothos [46] to prove existence of supersonic solitary waves in FPU lattices with saturable nonlinearities, where the interaction potential is asymptotically quadratic at infinity.

These global existence results are complemented by the work of Iooss [17], who used center manifold reduction techniques to establish existence of *small-amplitude* solitary waves. For generic potentials satisfying $V(0) = V'(0) = 0$ and $V''(0) > 0$, the author showed that for $V'''(0) < 0$ (> 0) there exist even unimodal compressive (rarefactive) solitary waves with velocities slightly above the sonic limit. If $V'''(0) = 0$, both types of such waves exist when $V^{(4)} > 0$ but the system has no small-amplitude solitary waves when $V^{(4)} < 0$. This local approach also yields Taylor expansion of the obtained solutions in terms of the bifurcation parameter that measures the difference between the wave's velocity and the sound speed. Friesecke and Pego [47] proved the existence of near-sonic solitary waves under the assumptions $V(0) = V'(0) = 0$, $V''(0) > 0$ and $V'''(0) \neq 0$ and derived their properties, as discussed in more detail in Sec. 3.

3. Asymptotic limits

Two asymptotic limits of solitary wave solutions of the FPU problem are now well understood. They concern waves with low and high energy, respectively.

The close connection between the FPU dynamics with low-energy initial data and the Korteweg-de Vries (KdV) equation was first pointed out by Zabusky and Kruskal [8] who derived the KdV equation in the form

$$\eta_\tau + \eta\eta_y + \delta^2\eta_{yyy} = 0, \quad (13)$$

where δ^2 measures the strength of the dispersion term, as a weakly nonlinear continuum limit of the FPU equations (1) with quadratic nonlinearity [48, 49, 50]. It has traveling wave solutions of the form

$$\eta(y, \tau) = \eta_\infty + A \operatorname{sech}^2[(y - c\tau - \zeta_0)/\Delta], \quad c = A/3 + \eta_\infty, \quad \Delta = \delta(12/A)^{1/2}, \quad (14)$$

where A , η_∞ and ζ_0 are arbitrary constants. These solutions were named “solitons” in [8] due to their quasiparticle behavior. Under the rescaling $\tau \rightarrow 6^{3/2}\delta\tau$, $y \rightarrow 6^{1/2}\delta y$, the KdV equation (13) takes another commonly used form $\eta_\tau + 6\eta\eta_y + \eta_{yyy} = 0$. Numerical simulations in [8] of the evolution dynamics governed by (13) with initial condition $\eta(y, 0) = \cos(\pi y)$ demonstrated that formation and interaction of the KdV solitons lead to periodic near-recurrence of the initial data similar to that observed in [7, 51] for the lattice problem. Beyond this major breakthrough in understanding the near-recurrence phenomenon, the work [8] has ushered in an entire new era in nonlinear science by leading to many important discoveries about the structure of the KdV equation and other integrable systems [36, 37, 52, 53, 54, 55, 56].

Rigorous results connecting the near-sonic solitary wave solutions of the FPU problem and the KdV solitons were obtained in [47] by Friesecke and Pego, who then exploited this connection to prove stability of such solutions [57, 58, 59]. Specifically, these authors showed that for velocities just above the sonic speed $c_s = (V''(0))^{1/2}$, small-amplitude solitary wave solutions of (3) with potential satisfying $V(0) = V'(0) = 0$ are given (up to a translation in ξ) by

$$w(\xi) = \frac{\varepsilon^2 a}{4b} \operatorname{sech}^2\left(\frac{\varepsilon\xi}{2}\right) + O(\varepsilon^4), \quad c = \left(1 + \frac{\varepsilon^2}{24}\right) c_s \quad (15)$$

where $\varepsilon > 0$ is a small parameter, $a = c_s^2 = V''(0) > 0$ and $b = V'''(0) \neq 0$. The first term equals $\varepsilon^2\phi(\varepsilon\xi)$, where $\phi(x)$ is the KdV soliton satisfying the traveling wave equation $\phi'' - \phi + 6(b/a)\phi^2 = 0$.

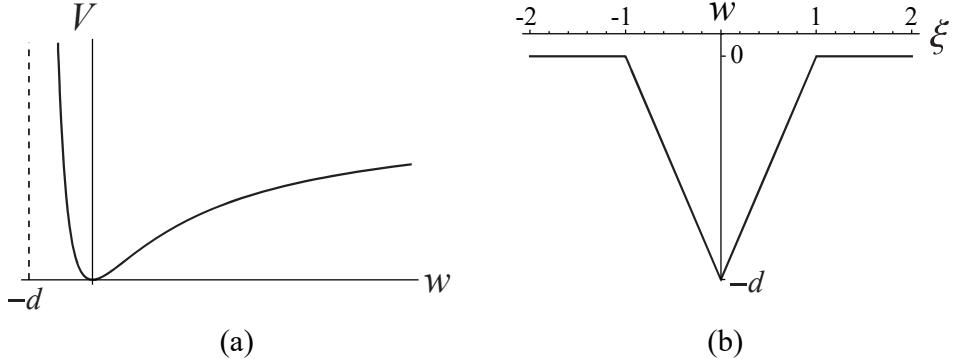


Figure 1: (a) Interaction potential $V(w)$ with a vertical asymptote. (b) Solitary wave solution $w(\xi)$ in the limit $c \rightarrow \infty$.

The energy of the solution (15) equals $H = \varepsilon^3 a^3 / (6b^2) + O(\varepsilon^5)$ and increases with velocity c . McMillan [60] obtained the leading order correction to (15) due to discreteness. The connection between the KdV and FPU dynamics was further investigated by Schneider and Wayne [61], who have shown that for small-amplitude long-wave initial data the evolution of the solutions of the FPU problem (3) can be approximated by a sum of solutions of the KdV equations corresponding to two counter-propagating waves up to $O(\varepsilon^{7/2})$ on time scales of $O(\varepsilon^{-3})$ (see also [62, 63, 64]).

Another important asymptotic limit arises for realistic interaction potentials that have either a singularity at a certain strain value or a superpolynomial growth. Friescke and Matthies [65] considered nonnegative potentials $V \in C^3(-d, \infty)$ satisfying $V(0) = 0$, $V''(0) > 0$, the growth condition $V(w) \geq K(w + d)^{-1}$ for some $K > 0$ and all w near $-d$ and the hardening condition $V'''(w) < 0$ in $(-d, 0]$, $V(w) < V(-w)$ on $(0, d)$. An example of such potential is shown in Fig. 1(a), and prototypical ones are of Lennard-Jones type:

$$V(w) = a \left(\frac{1}{(w + d)^m} - \frac{1}{d^m} \right)^2, \quad a > 0, \quad m \in \mathbb{N}. \quad (16)$$

The authors of [65] used variational techniques to prove that under these assumptions, the solitary wave profile in the limit $c \rightarrow \infty$ has the tent-like shape $w(\xi) = d \min\{|\xi| - 1, 0\}$ depicted in Fig. 1(b). The limiting high-energy solitary wave corresponds to the hard-sphere collision dynamics, with one particle moving at a time. For the case of Toda lattice, this limit was also discussed in [37]. Treschev [34] used a fixed point argument to obtain more quantitative estimates about the hard-sphere limit under assumptions about the potential that are slightly different from those in [65]. The localization phenomenon was also discussed by Herrmann [35] for the case of potentials with a superpolynomial growth. Herrmann and Matthies [66] obtained improved asymptotic expressions for the high-energy solitary wave solutions and an explicit scaling law for their propagation speed for potentials with a singularity. The key ingredient in their approach is the derivation of an asymptotic ordinary differential equation for the appropriately rescaled strain profile. Herrmann [67] extended these results to the case of potentials with a superpolynomial growth.

4. Approximations and properties of solitary waves

In the crossover regime between the low-energy and high-energy limits, solitary wave solutions of the FPU problem with generic nonlinearities are typically approximated using quasicontinuum models, weak formulations, variational and numerical methods. In this section we describe the

basic ideas behind these approaches and summarize the properties of solitary waves obtained using these approximations for some commonly considered interaction potentials.

4.1. Quasicontinuum models and other approximations

Quasicontinuum models can be formally derived from lattice equations (1) or (3) in different ways. For example, one can set $u_n(t) = \varepsilon u(\varepsilon n, \varepsilon t)$ in (1), where ε is a small parameter, and $u(x, \tau)$ is a smooth function of $x = \varepsilon n$ and $\tau = \varepsilon t$ and expand the equation in Taylor series. For $V'(w) = w + \alpha w^2 + \beta w^3 + \dots$, this yields [68] the perturbed wave equation

$$u_{\tau\tau} = u_{xx} + \varepsilon^2 \left(2\alpha u_x u_{xx} + \frac{1}{12} u_{xxxx} \right)$$

up to $O(\varepsilon^4)$. Differentiating this with respect to x and setting $y = u_x$, one obtains

$$y_{\tau\tau} = y_{xx} + \varepsilon^2 \left(\alpha(y^2)_{xx} + \frac{1}{12} y_{xxxx} \right), \quad (17)$$

known as the “bad” Boussinesq equation since it leads to an ill-posed initial value problem [69, 70], with solutions blowing up in finite time [71]. Setting $\varepsilon = 1$ in (17), one can view it as a quasicontinuum description of the α -FPU lattice, with the dispersion term $\frac{1}{12} y_{xxxx}$ modeling some of the discreteness effects. More generally, rewriting (3) as

$$y_{tt} = L_D V'(y(x, t)), \quad L_D = 2(\cosh(\partial_x) - 1), \quad (18)$$

formally expanding L_D in truncated Taylor series and keeping only the linear part of $V'(y)$ in the second term yields what is known as the standard continuum approximation:

$$y_{tt} = (V'(y))_{xx} + \frac{1}{12} y_{xxxx}, \quad (19)$$

where we assume $V''(0) = 1$. Similar to (17), it leads to an ill-posed initial value problem and implicitly assumes weak nonlinearity.

Collins [72] proposed an improved approximation based on inverting the discrete operator L_D in (18) by using the Euler-Maclaurin summation formula, which leads to an integro-differential equation. Noting that this inversion may not be unique since the operator is of the form $L_D = \partial_x^2 L_A$ with $L_A = 1 + \frac{1}{12} \partial_x^2 + \dots$, and hence yields a double pole at zero, Rosenau [69] suggested to invert only L_A instead. Keeping just the first two terms in the Taylor expansion of the inverted operator results in the partial differential equation [69, 70]

$$y_{tt} = (V'(y))_{xx} + \frac{1}{12} y_{xxtt}, \quad (20)$$

which replaces the fourth spatial derivative in (19) by a mixed space-time one. Unlike (17) and (19), it leads to a well-posed initial value problem, and its linearized version is associated with a bounded dispersion relation. Seeking solutions of (20) in the form of a traveling wave $y(x, t) = w(\xi)$, $\xi = x - ct$, that tends to zero as $|\xi| \rightarrow \infty$ and integrating yields

$$V'(w(\xi)) = c^2 \left(w(\xi) - \frac{1}{12} w''(\xi) \right). \quad (21)$$

With $V(0) = 0$ this equation has the first integral

$$(w'(\xi))^2 = \frac{24}{c^2} \left(\frac{c^2}{2} w^2 - V(w) \right), \quad (22)$$

which also follows from the method of Collins [72, 73].

This and other quasicontinuum equations for solitary waves can be obtained systematically following the approach of Wattis [74] (see also [73]). The starting point is to rewrite (5) in the form

$$c^2 w'' = f(\xi + 1) - 2f(\xi) + f(\xi - 1), \quad f(\xi) = V'(w(\xi)), \quad (23)$$

and take the Fourier transform under the assumption that $w(\xi)$ and its derivatives vanish at infinity along with $f(\xi)$. This yields

$$c^2 W(k) = \Lambda(k) F(k), \quad \Lambda(k) = \frac{4 \sin^2(k/2)}{k^2}, \quad (24)$$

where k is the wave number, and $W(k)$ and $F(k)$ are the Fourier transforms of $w(\xi)$ and $f(\xi)$, respectively. Substituting rational Padé approximations of $\Lambda(k)$ at small k into (24) then leads to various quasicontinuum models. In particular, the $(0, 2)$ Padé approximation, $\Lambda(k) \approx (1 + k^2/12)^{-1}$, yields (21). Its first integral (22) then gives the relation $c^2 w^2(0) = 2V(w(0))$ between the velocity and the height of the solitary wave, as well as explicit solutions for α -FPU potential (11),

$$w(\xi) = \frac{3(c^2 - 1)}{2\alpha} \operatorname{sech}^2 \left(\frac{\xi \sqrt{3(c^2 - 1)}}{c} \right),$$

and β -FPU potential (12),

$$w(\xi) = \pm \sqrt{\frac{2(c^2 - 1)}{\beta}} \operatorname{sech} \left(\frac{2\xi \sqrt{3(c^2 - 1)}}{c} \right)$$

for $c > 1$ [73, 74]. The $(2, 0)$ Padé approximation, $\Lambda(k) \approx 1 - k^2/12$, yields the height-velocity relation $c^2(w(0)V'(w(0)) - V(w(0))) = V'(w(0))^2/2$ but does not provide simple explicit solutions for potentials (11) and (12) [74]. This is also true for the more accurate $(2, 2)$ Padé approximation $\Lambda(k) \approx (1 - k^2/20)/(1 + k^2/30)$ considered in [74].

These approximations are all based on expansions of $\Lambda(k)$ at small wave numbers k and thus provide local quasicontinuum models that are only valid for slowly varying solitary waves. To obtain a model that captures tall and narrow (and thus highly localized) waves, one needs to approximate $\Lambda(k)$ globally over the entire spectrum. Wattis [74] considered replacing $\Lambda(k)$ in (24) by $\tilde{\Lambda}(k) = 1/(1 + k^2/4)$, which satisfies $\tilde{\Lambda}(0) = \Lambda(0)$, minimizes the L^2 norm of $\Lambda(k) - \Lambda_\gamma(k)$ among the functions of the form $\Lambda_\gamma = (1 + \gamma k^2)^{-1}$ and, similar to $(0, 2)$ Padé expansion, provides explicit solutions for polynomial potentials such as (11) and (12). This choice sacrifices the accuracy of the approximation at smaller k but improves it at the higher values.

Another approach to capture highly localized solitary waves was proposed by Druzhinin and Ostrovsky [75]. Considering the α -FPU model (11) and assuming that only three particles participate in the motion, they derived an ordinary differential equation for the core part of the wave, which can be solved in terms of elliptic functions, and found the approximate height-velocity relation $c \approx (1 + \frac{2}{3}\alpha w(0))^{1/2}$.

Duncan and Wattis [76] considered two other methods that can provide explicit relations between velocity, height and width of solitary waves in the entire velocity range. In the first approach, they substituted a suitable test function with free parameters controlling the height, width and shape of the wave into the weak formulation of the advance-delay equation (5) and derived algebraic equations that relate the wave's parameters to its velocity. Their second method relies on the variational formulation of the problem. In it, a kink-type test solution $u(\xi) = g \tanh(h\xi)$

depending on two parameters g and h is substituted into the action functional $I(u)$ associated with the traveling wave equation for (1) obtained by setting $u_n(t) = u(\xi)$, $\xi = n - ct$, yielding a function $\hat{I}(g, h)$. The parameters are then found by solving $\partial\hat{I}/\partial g = \partial\hat{I}/\partial h = 0$.

It should be noted that most of these approaches are designed to approximate the form of a solitary wave solution and some of its characteristics, such as height-velocity and width-velocity relations and core structure. The obtained approximate profiles can then be used as initial seeds in an iterative numerical procedure, as described below. In particular, the quasicontinuum equations often play only an auxiliary role in the process of obtaining such approximations and may not provide a suitable description of the general lattice dynamics. Indeed, similar to (17) and (19), some of these equations result in ill-posed problems, and even the regularized equations with bounded dispersion relations, such as (20), may lead to unphysical short-wave instabilities of periodic traveling waves [77]. Expansions at the level of the equations of motion may significantly alter or even destroy the Hamiltonian structure of the lattice problem, an issue that Rosenau [78] addressed by approximating the lattice Hamiltonian.

4.2. Numerical methods

A common approach to obtain solitary waves is to use direct numerical simulations of either (1) or (3) on a finite lattice with fixed, free or periodic boundary conditions and an appropriately chosen initial profile, which can be obtained using one of the quasicontinuum approximations described above. Alternatively, in some cases one can generate a solitary wave by applying an impact at one end of the chain. Standard ODE solvers such as `ode45` in Matlab based on the Runge-Kutta (4,5) formula [79] are often used with tight enough tolerances to ensure approximate energy and momentum conservation. For simulations performed over long enough time periods, symplectic solvers are more appropriate for the Hamiltonian lattice problem at hand; see, e.g., [80, 81, 82, 83, 84].

While direct numerical simulations are easy to implement and provide a useful tool to assess stability and other properties of solitary waves, they can only capture some presumably stable solutions. To obtain all solitary waves (up to translation), one needs to either solve the advance-delay differential equation (5) or, equivalently, find time-periodic-modulo-shift (recall (6)) spatially localized solutions of (3).

Hochstrasse, Mertens and Büttner [73] proposed an iterative method for computing localized pulse solutions of (5) based on (24). The first approximation $w^{(1)}(\xi)$ for the iterative procedure, with corresponding $W^{(1)}(k)$ and $F^{(1)}(k)$ in Fourier space, is obtained from the quasicontinuum equation (22), which can be integrated in quadratures to yield closed-form solutions for some potentials $V(w)$ (e.g. polynomial and piecewise quadratic ones) and solved numerically for others. Note that (24) implies that $F(0)/W(0) = c^2$, so that the subsequent iterations can be obtained from [73]

$$W^{(i+1)}(k) = \Lambda(k)F^{(i)}(k) \frac{W^{(i)}(0)}{F^{(i)}(0)}, \quad (25)$$

with the control parameter $\chi = W^{(i)}(0)$, which is invariant under the iteration procedure, and velocity of the wave determined a posteriori from

$$c_\infty^2 = \lim_{i \rightarrow \infty} \frac{F^{(i)}(0)}{W^{(i)}(0)}.$$

Eilbeck and Flesch [85] extended this linearly convergent iterative scheme to a quadratically convergent procedure based on pseudospectral collocation methods and path-following continuation

technique. Specifically, they approximated exact solutions of (23) by a truncated cosine Fourier series over a finite interval L :

$$w(\xi) \approx \sum_{j=0}^{n-1} a_j \cos \frac{2\pi j \xi}{L}, \quad (26)$$

an L -periodic even function that yields a solitary wave in the limit $L \rightarrow \infty$. Substituting (26) into (23) and evaluating the result at the collocation points $\xi_i = iL/(2(n-1))$, $j = 0, \dots, n-2$, yields $n-1$ algebraic equations for n unknown coefficients a_j . An additional equation is obtained by using the trapezoidal approximation over ξ_i , $i = 0, \dots, n-1$ of the relation

$$c^2 \int_{-\infty}^{\infty} w(\xi) d\xi = \int_{-\infty}^{\infty} F(\xi) d\xi,$$

which can be derived from (23) under the assumption that $w(\xi)$ and $w'(\xi)$ decay sufficiently fast at infinity [85]. This last constraint ensures convergence to a localized strain profile. The resulting nonlinear algebraic system is solved using the Newton-Raphson iteration procedure, with an initial guess that can be obtained from an exact quasicontinuum approximation or numerical solutions obtained at the previous step in the continuation procedure with c as the parameter. One can modify this approach by using different basis functions or solving for the values of the unknown function at the collocation points instead of the coefficients [86], and the general approach can be easily extended to other lattice traveling waves, e.g., [87, 88]. An alternative approach is to use a finite difference approximation of (23) with ξ_i and $\xi_i \pm 1$ included among the collocation points [89, 90].

It is also possible to construct solitary wave solutions of (3) using an iterative procedure in physical space applied to the nonlinear integral equation (8) or its alternative formulations [12, 34, 35]. In particular, this approach was proposed by English and Pego [91] in the case of power-law potentials

$$V(w) = aw^{p+1}/(p+1), \quad p > 1, \quad (27)$$

which for $w \geq 0$ describe Hertzian interactions in granular materials without precompression [92, 93] (in the context of contact interactions one needs to redefine the strain variables as $w_n = u_{n-1} - u_n$ and set $V(w) = 0$ for $w < 0$). Existence of such solutions was proved by MacKay [40] and Ji and Hong [41] using the results of Friesecke and Wattis [38]. In this case it suffices to consider

$$r''(\xi) = r^p(\xi+1) - 2r^p(\xi) + r^p(\xi-1),$$

since then $w(\xi) = (a/c^2)^{1/(1-p)}r(\xi)$ is the solution of (23) with $V'(w) = aw^p$, and the integral equation (8) reduces to [91, 94]

$$r(\xi) = (\mathcal{K} * r^p)(\xi) := \int_{-\infty}^{\infty} \mathcal{K}(\xi - s) r^p(s) ds, \quad (28)$$

where the kernel

$$\mathcal{K} = (1 - |\xi|)_+ = \begin{cases} 1 - |\xi|, & |\xi| \leq 1, \\ 0, & |\xi| > 1, \end{cases}$$

is the Fourier transform of $\Lambda(k)$ defined in (24) divided by 2π . The iterative approach of [91] consists of using $r_0 = \mathcal{K}(\xi)$ as the starting point and computing the subsequent iterates via

$$\tilde{r}_m(\xi) = (\mathcal{K} * r_{m-1}^p)(\xi), \quad C_m = \frac{\int_{-\infty}^{\infty} r_{m-1}(\xi) d\xi}{\int_{-\infty}^{\infty} \tilde{r}_m(\xi) d\xi}, \quad r_m(\xi) = C_m \tilde{r}_m(\xi), \quad m = 1, 2, \dots$$

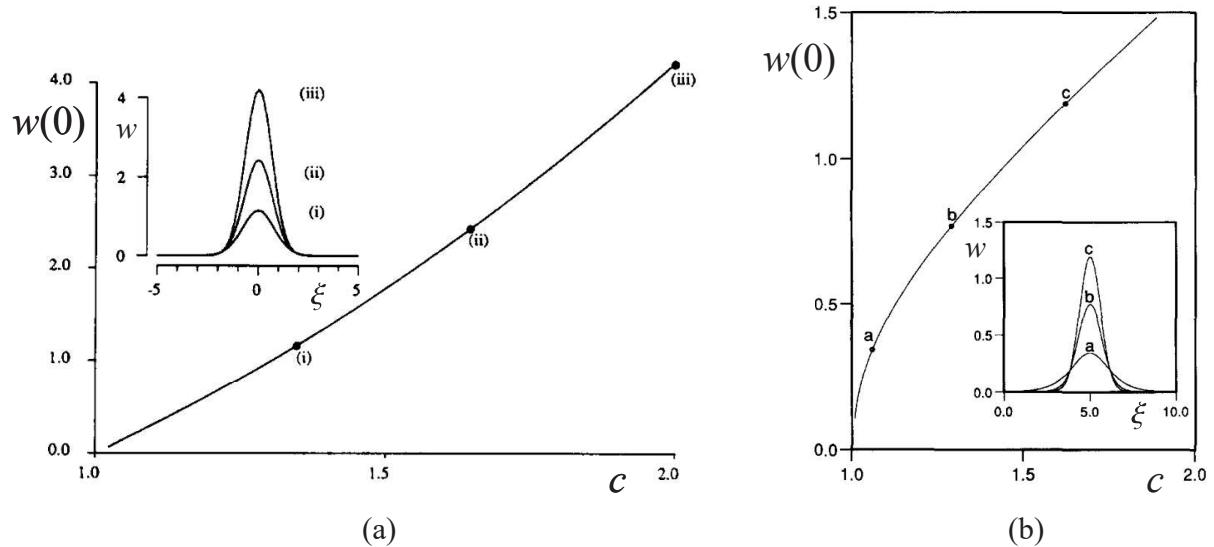


Figure 2: Height $w(0)$ of the solitary wave versus its velocity c for (a) α -FPU model (11) with $\alpha = 1$ (adapted with permission from Fig. 1 in [102], Copyright (1993) by Elsevier); (b) β -FPU model (12) with $\beta = 2$ (adapted with permission from Fig. 2 in [85], Copyright (1990) by Elsevier). Insets show solitary wave solutions at sample velocities.

Anhert and Pikovsky [94] pursued a similar iterative approach to compute solitary wave solutions in an FPU chain with homogeneous interaction potentials of the form $V(w) = |w|^{p+1}/(p+1)$ with nonnegative strains $w_n = u_n - u_{n-1}$. Stefanov and Kevrekidis [95] used the formulation (28) to provide an alternative proof of existence of solitary waves in generalized Hertzian chains and investigate their properties.

Recall that all traveling wave solutions (4) of (3), including solitary pulses, are periodic modulo lattice shift, as stated in (6), and thus are fixed points of the nonlinear map

$$\begin{bmatrix} \{w_{n+1}(T)\} \\ \{\dot{w}_{n+1}(T)\} \end{bmatrix} \rightarrow \begin{bmatrix} \{w_n(0)\} \\ \{\dot{w}_n(0)\} \end{bmatrix}, \quad T = 1/c, \quad (29)$$

where $w_n(t)$ satisfy (3). This suggests that such solutions can be computed for given c using Gauss-Newton or Newton-Raphson iterative methods on a finite lattice, with appropriate boundary conditions, a prescribed pinning condition to eliminate time-translational invariance and an initial guess obtained from either a quasicontinuum approximation or a solution from the previous step in a parameter continuation procedure. While this approach is not widely used to compute solitary waves in FPU chains, it is a common way to obtain moving breathers [96, 97, 98, 99] and has also been employed in computing some lattice traveling waves [100, 101].

4.3. Some properties of solitary waves

We now summarize some basic properties of solitary wave solutions of (1), starting with generic potentials that have nontrivial harmonic contribution ($V''(0) > 0$).

As the velocity of the solitary wave increases, its height $w(0)$ and energy grow, with specific functional relations depending on the interaction potential. Fig. 2 shows examples of the height-velocity relations for rarefactive solitary waves in α -FPU and β -FPU models computed using the pseudospectral method of Eilbeck and Flesch [85] in [102] and [85], respectively. One can see that the dependence of height on the velocity is convex for the cubic potential and concave for the purely

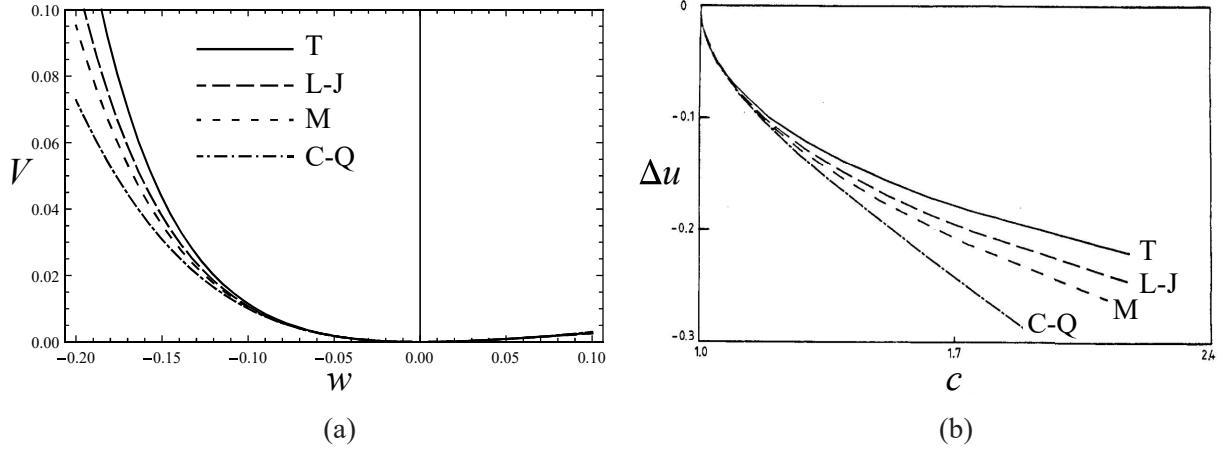


Figure 3: (a) Cubic-quartic (C-Q) potential $V(w) = \frac{1}{2}w^2 + \frac{1}{3}\alpha w^3 + \frac{1}{4}\beta w^4$ with $\alpha = -10.5$, $\beta = 62$, Morse (M) potential $V(w) = P(e^{-aw} - 1)^2$ with $P = 0.0102041$, $a = 7$, Lennard-Jones (L-J) potential (16) with $m = 6$, $d = 1$, $a = 1/72$ and Toda (T) potential $V(w) = ab^{-1}(e^{-bw} + bw - 1)$ with $a = 1/21$, $b = 21$. The potentials have the same Taylor expansion up to $O(w^4)$. (b) Amplitude $\Delta u = u(\infty) - u(-\infty)$ of the displacement $u(\xi)$ of the compressive solitary wave versus its velocity c for the potentials shown in (a). Panel (b) is adapted with permission from Fig. 6 in [103], Copyright (1989) by IOP Publishing.

quartic one. Sample solutions depicted in the insets show that in both cases the waves become more narrow as c grows.

Flytzanis, Pnevmatikos and Peyrard [103] investigated this relation for compressive solitary waves in lattices with cubic-quartic, Morse, Lennard-Jones and Toda potentials that were chosen to have the same asymptotic behavior near the bottom of the potential well at $w = 0$ (see Fig. 3(a)). Instead of the pulse height, they plotted the kink amplitude $\Delta u = u(\infty) - u(-\infty)$, where $u(\xi)$ is the traveling wave solution of (1). For the Toda potential $V(w) = ab^{-1}(e^{-bw} + bw - 1)$, the parametric dependence of Δu on c is known explicitly (one has $\Delta u = -2\kappa/b$ and $c = \sqrt{ab} \sinh(\kappa)/\kappa$), and direct numerical simulations were used in [103] to compute the relation for the other potentials. The results are shown in Fig. 3(b). One can see that as the result of matching the potentials near the well, the dependence of the amplitude on c is nearly the same for all four potentials near the sonic limit but the curves diverge at larger velocities, with $|\Delta u(c)|$ increasing slower for steeper potentials.

In all of the above examples, solitary waves delocalize to zero as c tends to the sound speed and are well approximated by the KdV solitons (15) near this limit. This is *not* the case for rarefactive waves in FPU chains with interaction forces that are *sublinear* near $w = 0$, with $V'''(0) < 0$. This includes bistable interactions that are governed by a nonconvex potential and are relevant in modeling phase transitions in mechanical and biological systems [104, 105, 106, 107, 108]. As shown in [109], in this setting the waves approach a nontrivial sonic limit, with nonzero energy and algebraic decay at infinity. This is illustrated in Fig. 4 for cubic-quartic potentials with $\alpha = V'''(0)/2 < 0$, where the solutions of (5) were computed in [109] using the pseudospectral method of [85] (see also the results of the direct numerical simulations shown in Fig. 4(a) in [103]). As $|\alpha|$ is increased, the limiting solution becomes more localized near $\xi = 0$, and its height and energy grow.

Given the widespread use of quasicontinuum models, it is important to know the regimes of their validity in approximating solitary waves in the discrete problem. For the FPU problem with cubic and purely quartic potentials, this issue was systematically investigated by Wattis [74], who

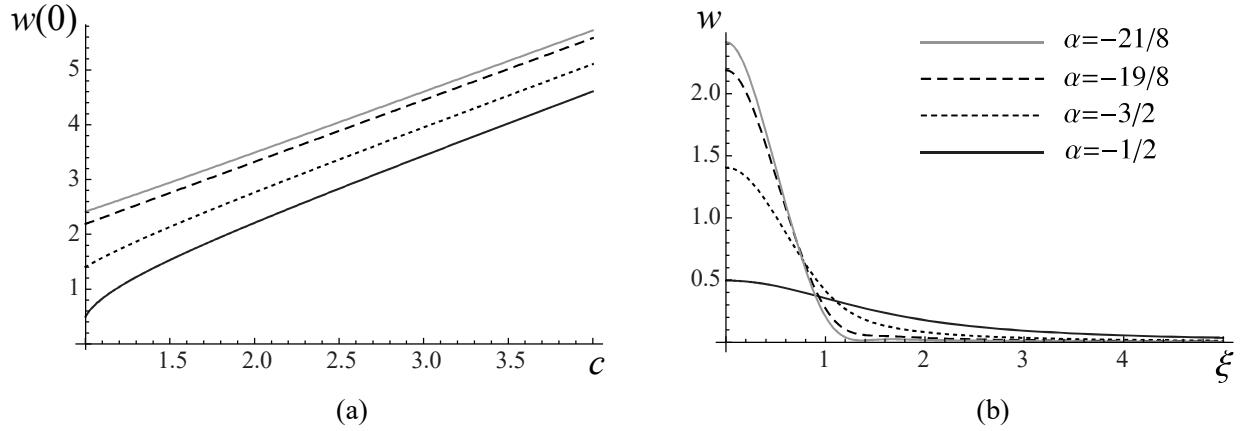


Figure 4: (a) Height $w(0)$ of the rarefactive solitary wave versus its velocity c for cubic-quartic potential $V(w) = \frac{1}{2}w^2 + \frac{1}{3}\alpha w^3 + \frac{1}{4}w^4$ with different negative values of α . (b) Solutions near the sonic limit ($c = 1.001$). Due to the even symmetry, only the part with $\xi \geq 0$ is shown. The figure is adapted with permission from Fig. 2 in [109], Copyright (2020) by the American Physical Society.

compared solitary wave solutions found using the models arising from $(0, 2)$, $(2, 0)$, $(2, 2)$ Padé and global approximations of $\Lambda(k)$ in (24), as well as the standard continuum model (19), to the numerically generated waves in the FPU lattice by monitoring the percentage of energy lost to radiation in simulations initiated by the quasicontinuum solution. As expected, all local approximations are quite accurate near the sonic limit, where solutions undergo KdV-type delocalization, but the models based on $(2, 0)$ and $(2, 2)$ Padé expansions work surprisingly well far away from this limit. For large enough velocities, the global approximation outperforms the most accurate local one, $(2, 2)$ Padé, but the latter works better at lower velocities. The situation is different in the case of rarefactive waves in chains with cubic-quartic potential with $\alpha < 0$ studied in [109]. At large enough $|\alpha|$ solitary waves become strongly localized in the entire velocity range and are not approximated well by any of the standard quasicontinuum models.

In non-integrable FPU lattices the interactions between solitary waves are inelastic. For example, numerical results in [103], shown in Fig. 5(a), illustrate that a head-on collision of compressive and rarefactive solitary waves propagating with the same speed in a β -FPU lattice leads to some energy loss in the form of radiation (see also [110] for an example of two rarefactive waves in an overtaking collision). As shown in [103], the amount of energy loss is maximal if the collision takes place on a particle and minimal if it occurs in the middle of the lattice spacing. The maximum percentage of radiated energy depends on the velocity but appears to be independent of the parameter β in (12); see Fig. 5(b). The collision is almost elastic near the sonic limit.

In the context of weakly nonlinear (precompressed) granular chains, the accuracy of two integrable models, the KdV approximation and the Toda lattice, in capturing the collision dynamics of near-sonic solitary waves was examined by Shen, Kevrekidis, Sen and Hoffman [64]. They showed that the KdV model, which describes only unidirectional motion, accurately captures collisions of solitary waves propagating in the same direction. Meanwhile, the Toda lattice provides a very good approximation of both head-on and overtaking collisions of solitary waves in this limit.

Over the last few decades, much attention has been focused on solitary waves in purely anharmonic lattices, where $V''(0) = 0$ yields to the ‘sonic vacuum’ setting with zero sound speed. As mentioned above, such solutions are physically relevant in granular chains without precompression, which are governed by the Hertzian potential (27) for nonnegative relative displacements

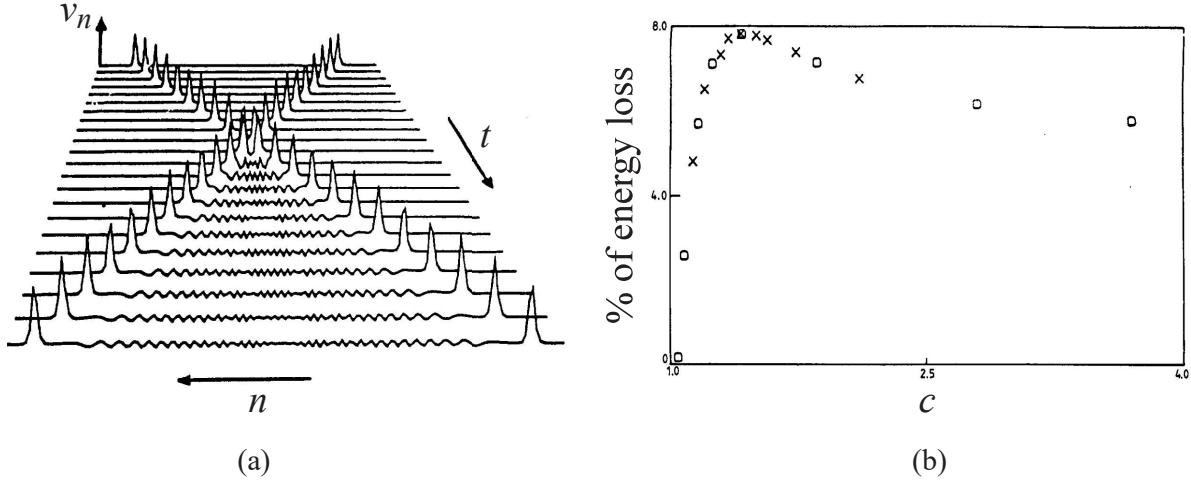


Figure 5: (a) Particle velocities $v_n(t) = u_n(t)$ in a kink-antikink collision of compressive and rarefactive solitary waves with opposite initial velocities of magnitude $c = 1.855$ in a β -FPU chain (1), (12) with $\beta = 62$. (b) Maximum percentage of energy loss due to radiation as a function of velocity in a β -FPU chain with $\beta=62$ (circles) and $\beta = 1$ (crosses). Panels (a) and (b) are adapted from Fig. 9 and Fig. 11, respectively, in [103], Copyright (1989) by IOP Publishing.

$w_n = u_{n-1} - u_n$. Instead of the exponential decay at infinity exhibited by solitary waves in FPU chains with generic potentials, the waves in such systems have *double exponential* decay. This was first argued by Chatterjee [111] and later rigorously proved by English and Pego [91] using the integral reformulation (28) of the problem. In the quasicontinuum descriptions of the type originally proposed by Nesterenko [112] such fast decay is approximated by solutions with compact support called *compactons* [5, 9, 94, 113, 10], with the traveling wave profile of the form

$$w(\xi) = \begin{cases} |c|^{\frac{2}{p-1}} A(p) \cos^{\frac{2}{p-1}}(B(p)\xi), & |\xi| < \pi/(2B(p)), \\ 0, & |\xi| \geq \pi/(2B(p)), \end{cases} \quad (30)$$

where $A(p)$ and $B(p)$ have different form depending on whether the model was obtained using Taylor expansion of u_n or w_n [94]. Note that (30) implies that the amplitude of the wave depends on its velocity as $w(0) \sim |c|^{\frac{2}{p-1}}$, a scaling that can also be deduced from the governing equation [9], and that its shape does not depend on its amplitude. More accurate series-based approximations of the solitary waves were developed in [114, 9, 115]. James and Pelinovsky [116] showed that in the limit $p \rightarrow 1^+$ both near-sonic solitary waves of the FPU problem and their compacton approximations approach the Gaussian solitary wave solutions of the log-KdV equation $\eta_\tau + \eta_{yyy} + (\eta \ln |\eta|)_y = 0$ that are linearly orbitally stable (see also [117], where the log-KdV equation is justified for granular chains with precompression). Similar to other non-integrable systems, interactions of the solitary waves in Hertzian chains involve inelastic collisions but in this case, in the absence of the linear spectrum, such collisions are accompanied by the formation of secondary waves [9]. For more on the remarkable properties of these solutions and other waveforms arising in granular chains, the reader is referred to the review papers [9, 10] and references therein.

Interaction of a solitary wave with lattice defects has been investigated by a number of authors. Such a defect may be introduced, for example, by replacing one of the masses in the FPU chain by a lighter or heavier mass or by changing the parameters of the interaction potentials for bonds connecting an intruder (an impurity particle) to its nearest neighbors. Early work in this direction

focused on the Toda lattice [118, 119, 120, 121, 122, 123] and the FPU chains with cubic, quartic and Morse potentials [124, 125, 126], exploiting the integrability of the homogeneous Toda lattice and the KdV approximation of the weakly nonlinear near-sonic regime to explain some results of the numerical simulations. These studies showed that a solitary wave interacting with an intruder loses energy due to the generation of a reflected wave and, in the case when the intruder that has either a light mass or strong nearest-neighbor bonds, excitation of a localized oscillation mode with amplitude-dependent frequency in the vicinity of the impurity site. Later investigations [127] for a variety of interaction potentials revealed that the dependence of the velocity amplitude of a mass defect on the mass ratio possesses a number of resonances. Revisiting the monatomic Toda lattice that has a local defect due to a change of the coupling constants a and b in the interaction force $V'(w) = a[1 - \exp(-bw)]$, Vergara and Malomed [128] showed that the generation of the defect mode may be suppressed under certain conditions on the coupling parameters for a given amplitude of the incident wave. In granular chains without precompression scattering of a solitary wave with an intruder bead was studied numerically [129, 130, 131], experimentally [130] and analytically [131]. In the case of a light intruder, it consists of two stages [130, 131]: fast oscillation of the intruder bead under heavy compression by its neighbors, followed by the separation of the intruder from its neighbors and excitation of a localized transient breather due to collisions of the intruder and the neighboring beads. Meanwhile, a solitary wave colliding with a heavy impurity fragments into a train of pulses with decreasing amplitude [129]. Interaction with a different type of defect, in the form of a harmonic oscillator attached to one of the beads, was studied in [132] (see also [133] for further numerical and experimental investigations). A fundamental difference of this system from the ones with mass defects is its ability to asymptotically trap some of the energy of the incident wave.

5. Piecewise quadratic potentials

As we have seen, one typically has to rely on numerical solutions and various approximations to study solitary waves in non-integrable FPU lattices away from the asymptotic low-energy and high-energy regimes. However, piecewise linear interactions, which, incidentally, were among the ones included in the FPU report [7], allow one to construct exact solitary wave solutions. Truskinovsky and Vainchtein [134] considered rarefactive solitary wave solutions of (3) with continuous bilinear interaction force

$$V'(w) = \begin{cases} w, & w \leq w_c \\ \alpha(w - w_c) + w_c, & w \geq w_c, \end{cases} \quad (31)$$

where $\alpha > 1$ is the ratio of the two linear slopes, and $w_c > 0$ is the critical strain separating the two linear regimes. For $1 < c < \sqrt{\alpha}$ one can then obtain solitary wave solutions of the form

$$w(\xi) = \begin{cases} a_0 + \sum_{j=1}^{\infty} a_j \cos(\gamma_j \xi), & |\xi| \leq z, \\ \sum_{j=1}^{\infty} b_j \exp(i\lambda_j^+ |\xi|), & |\xi| \geq z, \end{cases} \quad (32)$$

where λ_j^+ are the roots of the characteristic equation $L(k) = 4 \sin^2(k/2) - c^2 k^2 = 0$ for the first linear regime with positive imaginary part, and γ_j are the roots of the equation $G(k) = 4\alpha \sin^2(k/2) - c^2 k^2 = 0$ for the second linear regime with positive real part. In [134] such solutions were constructed as the limit of a series of approximations that include finitely many roots of the characteristic equations that are located within a strip of increasing width in the complex plane. The procedure involves finding $z > 0$ that ensures the existence of an odd function $h(\xi)$ that vanishes for $|\xi| > z$,

satisfies $\int_0^z h(s)ds = 1$ and solves the linear integral equation

$$(\alpha - 1) \int_{-z}^z q(\xi - s)h(s)ds + h(\xi) = 0, \quad |\xi| < z, \quad (33)$$

where

$$q(\xi) = \frac{1}{2\pi(\alpha - 1)} \int_{-\infty}^{\infty} \left(\frac{G(k)}{L(k)} - 1 \right) e^{ik\xi} dk.$$

This constitutes a nonlinear eigenvalue problem of the type recently studied by Herrmann and Matthies [135], who established the existence and uniqueness of such solutions. More generally, for

$$V'(w) = \begin{cases} w, & w < w_c \\ \alpha(w - b), & w > w_c \end{cases}, \quad \varepsilon = \alpha b - (\alpha - 1)w_c \geq 0, \quad (34)$$

which yields (31) at $\varepsilon = 0$ and a discontinuous bilinear interaction force corresponding to a non-convex two-parabola potential when $\varepsilon > 0$, the eigenvalue problem can be written in the following form [136]:

$$(\alpha - 1) \int_0^z \left(K(\xi, s) - \frac{\varepsilon K(\xi, z)R(z, s)}{w_c + \varepsilon R(z, z)} \right) h(s)ds = h(\xi), \quad 0 \leq \xi < z, \quad (35)$$

where $\int_0^z h(s)ds = 1$,

$$K(\xi, s) = q(\xi + s) - q(\xi - s) = -\frac{2}{\pi(\alpha - 1)} \int_0^{\infty} \left(\frac{G(k)}{L(k)} - 1 \right) \sin(ks) \sin(k\xi) dk,$$

and

$$R(\xi, s) = -\frac{2}{\pi(\alpha - 1)} \int_0^{\infty} \left(\frac{G(k)}{L(k)} - 1 \right) \frac{\sin(ks) \cos(k\xi)}{k} dk.$$

The solution is then obtained using

$$w(\xi) = \frac{\int_0^z R(\xi, s)h(s)ds}{\int_0^z R(z, s)h(s)ds} (w_c + \varepsilon R(z, z)) - \varepsilon R(\xi, z). \quad (36)$$

Numerical computations using (35) and (36) for the case $\varepsilon > 0$ suggest existence and uniqueness of solutions for c in $(1, \sqrt{\alpha})$ [136] but rigorous results along these lines have not yet been established.

The simplest approximation of (32) considered in [134] includes only the first four nonzero roots $\pm\gamma_1 = \pm r$, $\lambda_1^{\pm} = \pm ip$ of the characteristic equations, where $r > 0$ and $p > 0$ depend on c , and has the simple form

$$w(\xi) = \begin{cases} \frac{w_c}{\alpha - c^2} \left(\alpha - 1 + (c^2 - 1) \sqrt{1 + (r/p)^2} \cos(r\xi) \right), & |\xi| \leq z, \\ w_c \exp[-p(|\xi| - z)], & |\xi| \geq z, \end{cases} \quad (37)$$

with

$$z = \frac{1}{r} \left(\pi - \arctan \frac{r}{p} \right). \quad (38)$$

As noted in [134], quasicontinuum models based on $(2, 0)$ and $(0, 2)$ Padé expansions of $\Lambda(k)$ in (24) yield solutions that are also given by (37) and (38), but with $r = \sqrt{12(1 - c^2/\alpha)}$, $p = \sqrt{12(c^2 - 1)}$ in the case of $(2, 0)$ expansion and $r = \sqrt{12(\alpha c^{-2} - 1)}$, $p = \sqrt{12(1 - c^{-2})}$ for the $(0, 2)$ model. As

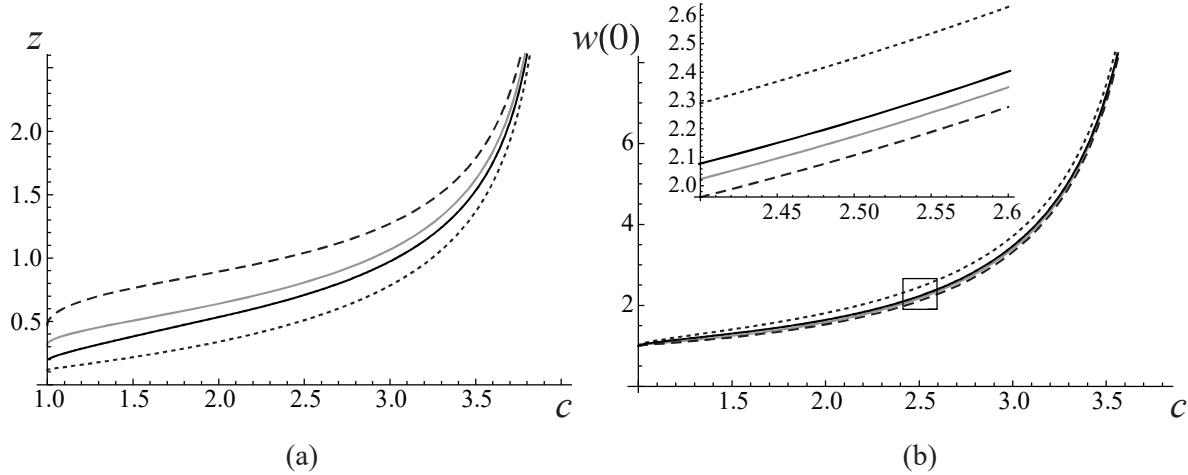


Figure 6: The dependence on c of (a) the parameter z and (b) the height $w(0)$ of the solitary wave obtained numerically (black curves) and using the first-root (gray curves), $(2, 0)$ Padé (dashed curves) and $(0, 2)$ Padé (dotted curves) approximations (37), (38). Inset zooms in on the region inside the rectangle in (b). Here $\alpha = 16$, $w_c = 1$. The figure is adapted with permission from Fig. 5 in [134], Copyright (2014) by the American Physical Society.

illustrated in Fig. 6, the two quasicontinuum models do not capture the solution of the discrete model as well as the truncated series solution. Note also that due to the degeneracy of the bilinear model, the solution delocalizes to $w(\xi) = w_c > 0$ in the lower sonic limit $c \rightarrow 1$, and as a result its energy (2) tends to infinity in this limit, instead of approaching zero, as it does for the generic potentials in the KdV limit. Nevertheless, both low-energy and high-energy asymptotic regimes can be captured in this setting by allowing w_c and α to depend on c and considering appropriate double limits [134].

The solution procedure (35), (36) can be extended to a trilinear up-down-up $V'(w)$, which involves solving two coupled integral equations [137]. In this case the potential $V(w)$ is nonconvex, with two upward parabolas connected by a downward one. Katz and Givli [138, 139] studied this problem using direct numerical simulations of (3) and explicit quasicontinuum solutions. They showed that solitary wave solutions are independent of the energy barrier separating two convex regions of the potential and identify two dimensionless parameters that determine the shape of the wave for given c . Similar to the bilinear case and in contrast to the fully nonlinear up-down-up interactions [100], the energy of a solitary wave tends to infinity in the lower sonic limit $c \rightarrow 1$ in the trilinear model. In both bilinear and trilinear cases, as the velocity increases away from this limit, the energy decreases to a minimum value and then grows, tending to infinity as the upper sonic limit $\sqrt{\alpha}$ is approached [134, 136, 139].

6. Long-range interactions

While the original FPU problem (1) includes only nearest-neighbor bonds, long-range interactions often play an important role in realistic systems, such as DNA molecules [140]. With this in mind, we now consider the more general problem

$$\ddot{u}_n = \sum_{m=1}^M \left[V'_m(u_{n+m} - u_n) - V'_m(u_n - u_{n-m}) \right], \quad (39)$$

where $M \geq 1$ and $V_m(w)$ is the potential describing the interaction between particles separated by m lattice spaces. Clearly, the nearest-neighbor problem (1) is recovered when $M = 1$, while $M = \infty$ corresponds to all-to-all interactions. The undeformed (zero-strain) configuration is stable when $\omega^2 > 0$ for k in $(0, \pi]$, where

$$\omega^2 = 4 \sum_{m=1}^M V_m''(0) \sin^2 \frac{mk}{2} \quad (40)$$

is the dispersion relation for the associated linearized problem. For this it is necessary that $d^2\omega^2(0)/dk^2 > 0$, implying that

$$c_s^2 = \sum_{m=1}^M m^2 V_m''(0) > 0, \quad (41)$$

where c_s is the sound speed. Another necessary stability condition is $\omega^2(\pi) > 0$, which yields

$$\sum_{m=1, m \text{ odd}}^M V_m''(0) > 0.$$

Violation of this condition corresponds to the microscopic unstable eigenmode $(-1)^n$ (see, e.g., [141]). Note that it is not necessary for all $V_m''(0)$ to be nonnegative: for example, in the $M = 2$ case $V_1''(0) > 0$ and $V_1''(0) + 4V_2''(0) > 0$ are both necessary and sufficient (see, e.g., [142]) for the undeformed chain to be stable, which allows negative $V_2''(0)$ of sufficiently small magnitude.

Existence of supersonic solitary wave solutions of (39) was recently proved by Pankov [16] under the assumptions that all moduli $V_m''(0)$ are nonnegative, which implies (41), and $V_m(w)$ have certain monotonicity properties needed to use variational techniques. Herrmann and Mikikits-Leitner [143] used asymptotic analysis to prove existence of KdV-type solitary waves propagating with velocities just above the sonic limit. They also assumed positive moduli for all interaction potentials, while noting that it is feasible to generalize their argument to the case when some moduli are negative, provided that (41) holds, along with some additional requirements ensuring that the leading-order problem is not degenerate. Generalization of this result to the case $M = \infty$ is possible under sufficiently fast decay of the coefficients in $V_m(w)$ with respect to m .

Herrmann and Matthies [144] considered the lattice with long-range interactions as a special case of a one-dimensional peridynamic elastic solid [145, 146] with scalar displacement field $u(x, t)$ governed by the nonlocal integro-differential equation

$$u_{tt} = \int_{-\infty}^{\infty} f(u(x + \zeta, t) - u(x, t), \zeta) d\zeta, \quad (42)$$

where ζ is the bond variable, and the elastic force f satisfies $f(w, \zeta) = -f(-w, -\zeta)$ and is related to the micropotential $\Psi(w, \zeta)$ via $f = \partial\Psi/\partial w$. The lattice equations (39) are then recovered in the discrete case $\Psi(w, \zeta) = \sum_{m=1}^M V_m(w) \delta_m(\zeta)$, where $\delta_m(\zeta)$ is the Dirac delta function centered at m . In the continuum setting micropotentials of the form $\Psi(w, \zeta) = \alpha(\zeta) V(\beta(\zeta) w)$ were considered in [144], the case also studied by Pego and Van [147]. Existence of solitary wave solutions in both discrete and continuum cases was established in [144] under the assumptions that potentials V_m and V are C^3 , increasing, convex and grow at least quadratically on $[0, \infty)$, while $\alpha(\zeta)$ and $\beta(\zeta)$ are nonnegative and satisfy a certain integrability condition. The proof generalizes the variational approach in [35]. Another proof for the continuum case, which follows the variational framework of [38], was given in [147].

6.1. Second-neighbor interactions

In the case $M = 2$ the problem (40) with quartic and cubic potentials was studied in a series of papers by Flytzanis, Peyrard, Pneumatisos and Remoissenet [148, 149, 150] using direct numerical simulations and quasicontinuum approximations. Along with a variety of other waveforms [149], they observed the existence of *subsonic* traveling waves, $c < c_s$, in the regime when the interactions are sufficiently competitive, i.e., $V_2''(0)/V_1''(0) \in (-1/4, -1/16)$, while $V_1''(0) > 0$. Such solutions are not true solitary waves because they are accompanied by radiation of small-amplitude oscillations [148] and thus do not satisfy (7). Interestingly, however, low-order quasicontinuum theories, such as the standard continuum approximation examined in these works, predict the existence of genuine subsonic solitary waves. To see this, it suffices to consider the case when the second-neighbor potential is quadratic, $V_2(w) = (\gamma/8)w^2$, and the traveling wave problem for the strain variables can be written as

$$c^2 w''(\xi) = V'(w(\xi + 1)) - 2V'(w(\xi)) + V'(w(\xi - 1)) + \frac{\gamma}{4}(w(\xi + 2) - 2w(\xi) + w(\xi - 1)), \quad (43)$$

where $V(w) = V_1(w)$ satisfies $V''(0) = 1$, and $\gamma > -1$ must hold to ensure stability of the undeformed configuration. In this case we have $c_s = \sqrt{1 + \gamma}$. Various approximations of (43) were studied by Wattis [151]. In particular, the standard continuum approximation results in the traveling wave equation

$$\frac{1 + 4\gamma}{12} w'' + (\gamma - c^2)w + V'(w) = 0, \quad (44)$$

which can be solved explicitly for an α -FPU nearest-neighbor potential (11), yielding

$$w(\xi) = \frac{3}{2\alpha} (c^2 - c_s^2) \operatorname{sech}^2 \left(\xi \sqrt{\frac{3(c^2 - c_s^2)}{1 + 4\gamma}} \right), \quad (45)$$

and the β -FPU case (12):

$$w(\xi) = \pm \sqrt{\frac{2(c^2 - c_s^2)}{\beta}} \operatorname{sech} \left(2\xi \sqrt{\frac{3(c^2 - c_s^2)}{1 + 4\gamma}} \right). \quad (46)$$

The solutions are subsonic when $-1 < \gamma < -1/4$ and supersonic for $\gamma > -1/4$, with subsonic solutions existing for sublinear $V'(w)$ ($\alpha < 0$ in (45) and $\beta < 0$ in (46)) and supersonic for superlinear $V'(w)$ [151]. More generally, the characteristic equation for the linearization of (44) about $w = 0$,

$$c^2 = c_s^2 - \frac{1 + 4\gamma}{12} k^2, \quad (47)$$

where k is the wave number, implies that a decay at infinity, which must hold for a solitary wave, is possible only in the subsonic regime if $-1 < \gamma < -1/4$ and only at supersonic velocities if $\gamma > -1/4$.

Recently, the problem (43) was revisited by Truskinovsky and Vainchtein [152] who argued that solitary waves for the discrete problem are in fact *strictly supersonic* when $-1 < \gamma < -1/4$, meaning that their velocity satisfies

$$c > c_m > c_s, \quad -1 < \gamma < -1/4, \quad (48)$$

where the lower bound c_m is the largest phase velocity of plane waves in this regime, which is strictly above the (conventionally defined) sound speed; see Fig. 7(a). The argument is based on considering the characteristic equation

$$c^2 = \frac{\omega^2(k)}{k^2}, \quad \omega^2(k) = 4 \sin^2 \frac{k}{2} + \gamma \sin^2 k, \quad (49)$$

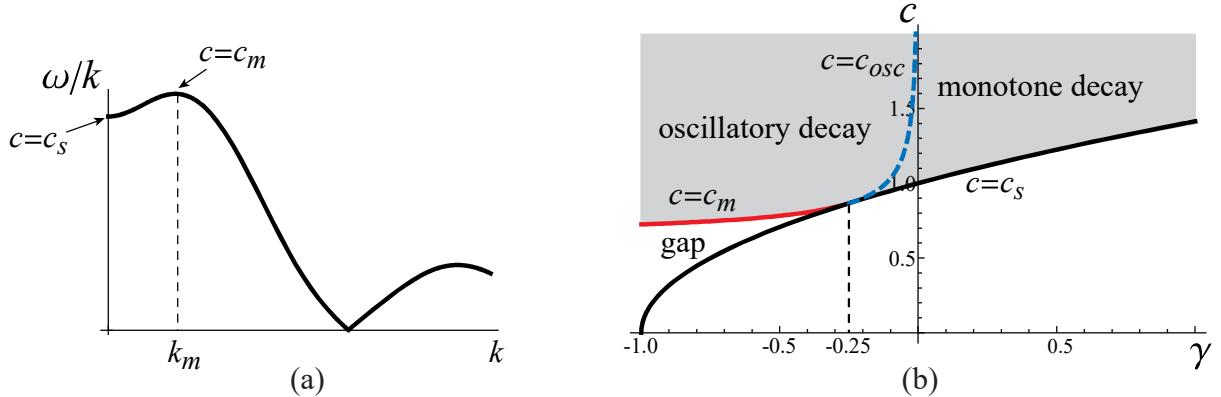


Figure 7: (a) Typical dispersion curve for the phase velocity at $-1 < \gamma < -1/4$, with a maximum $c_m > c$ at $k = k_m$. Solitary waves bifurcate from the maximum point and have velocities $c > c_m$. (b) The domain (shaded region) in (γ, c) plane where solitary waves may exist according to the structure of the nonzero roots of (49). The figure is adapted with permission from Fig. 2 in [152], Copyright (2018) by Elsevier.

where $\omega(k)$ is the dispersion relation, and determining the regions in the (γ, c) plane where a solitary wave, when it exists, has an exponential decay according to the structure of the nonzero roots of (49). The results are shown in Fig. 7(b). Note that the standard continuum approximation (44) replaces the strictly supersonic waves at $-1 < \gamma < -1/4$ by subsonic ones because its characteristic equation (47) misses the peak of ω/k at $c = c_m$ and only approximates the phase velocity near the minimum at $k = 0$. The root structure of (49) also shows that if a solitary wave solution exists, its decay at infinity is *oscillatory* rather than monotone when the wave's velocity exceeds a certain threshold $c_{osc} > c_s$ for $-1/4 < \gamma < 0$ (as noted earlier by Wattis [151]) and for $c > c_m$ at $-1 < \gamma \leq -1/4$ (at $\gamma = -1/4$, $c_m = c_{osc} = c_s$).

While in the case $\gamma > -1/4$ one expects the delocalization of small-amplitude solitary waves as they approach the sonic limit to be described by the KdV equation, strictly supersonic waves at $-1 < \gamma < -1/4$ bifurcate instead from the linear wave with the wave number k_m that corresponds to c_m , as shown in Fig. 7(a). This bifurcation is analogous to the one observed for capillary-gravity water waves [153, 154, 155, 156] and can be similarly described by a nonlinear Schrödinger (NLS) equation with higher-order corrections [155, 156] for small modulation amplitude of the steady envelope wave. For the discrete problem (43) this equation and the corresponding approximation of the solitary waves near the bifurcation point are formally derived and numerically tested in [152]. Recently, Hilder, de Rijk and Schneider [157] used the center-manifold reduction procedure to prove the existence of such strictly supersonic solutions in the more general case of competing interactions where $V_2(w)$ may contain anharmonic terms.

To capture this bifurcation on a quasicontinuum level, it is necessary for the model's characteristic equation to include enough terms in order to approximate the peak in the phase velocity seen in Fig. 7(a). To construct such higher-order quasicontinuum model, one can follow the approach in [151] and consider the Fourier transform of (43) in the form

$$\Omega(k)W(k) = F(k), \quad \Omega(k) = \frac{c^2 k^2 - \gamma \sin^2 k}{4 \sin^2(k/2)}, \quad (50)$$

where, as in (24), $W(k)$ and $F(k)$ are the Fourier transforms of $w(\xi)$ and $f(\xi) = V'(w(\xi))$, respectively. Taylor expansion of $\Omega(k)$ in (50) up to $O(k^6)$ then yields a quasicontinuum model with the

following fourth-order traveling wave equation [152]:

$$\frac{1}{240}(c^2 - 5\gamma)w''' - \frac{1}{12}(3\gamma + c^2)w'' + (c^2 - \gamma)w = V'(w). \quad (51)$$

Its linearization about $w = 0$ has the characteristic equation

$$c^2 = \frac{c_s^2 - (\gamma/4)k^2 + (\gamma/48)k^4}{1 + (1/12)k^2 + (1/240)k^4}, \quad (52)$$

which was shown in [152] to provide a good approximation of (49) in the regime $-1 < \gamma < 0$, including the transition from monotone to oscillatory decay when $-1/4 < \gamma < 0$ marked by the dashed line in Fig. 7(b). For a bilinear $V'(w)$ given by (31), the model (51) adequately captures the solutions of the discrete problem at $-1 < \gamma < 0$, which were constructed in [152] by extending the approach described in Sec. 5 to include second-neighbor interactions.

6.2. All-to-all long-range interactions

Another interesting problem concerns the case of all-to-all interactions ($M = \infty$), with harmonic interactions beyond nearest neighbors. In terms of strain variables this problem takes the form

$$\ddot{w}_n = V'(w_{n+1}) - 2V'(w_n) + V'(w_{n-1}) + \sum_{m=1}^{\infty} G_m(w_{n+m} - 2w_n + w_{n-m}) = 0, \quad (53)$$

where $V(w)$ is a nonlinear part of the potential governing the interaction between the nearest neighbors and G_m are the moduli of the harmonic long-range contribution that must decay sufficiently fast at infinity to ensure a finite sound speed (41). The case of Kac-Baker interactions [158, 159]

$$G_m = J(e^\alpha - 1)e^{-\alpha m}, \quad (54)$$

with the inverse radius $\alpha > 0$ and intensity measured by $J > 0$, and $V'(w) = w - w^2$ was investigated in a series of papers by Gaididei, Flytzanis, Mingaleev, Neuper and Mertens [160, 140, 161, 162]. In particular, they derived and analyzed a quasicontinuum approximation of (53) in this case, which yields the equation [140, 161]

$$(\partial_\xi^2 - s_+^2)(\partial_\xi^2 - s_-^2)w(\xi) = \frac{12}{c^2}(\partial_\xi^2 - \kappa^2)w^2(\xi), \quad (55)$$

where $\kappa = 2 \sinh(\alpha/2)$,

$$s_\pm^2 = \frac{1}{2} \left\{ \kappa^2 + 12 \frac{c^2 - 1}{c^2} \pm \sqrt{\left(\kappa^2 - 12 \frac{c^2 - 1}{c^2} \right)^2 + 48\kappa^2 \frac{c_s^2 - 1}{c^2}} \right\}, \quad (56)$$

and $w(\xi)$ is a supersonic solitary wave, with velocity $c > c_s = (1 + J(1 + e^{-\alpha})/(1 - e^{-\alpha})^2)^{1/2}$. The parameters s_\pm in (56) define two characteristic length scales, s_-^{-1} and s_+^{-1} [161]. At low velocities, only the first of these, s_-^{-1} , plays an important role, and waves have a sech^2 form, which changes to a crest-type form as a certain critical velocity is approached. At high velocities, both scales are important, and solutions can be represented as a sum of a sech^2 -form short-range component dominant in the core, and a long-range exponentially decaying component dominant in the tails [162].

Using a numerical approach that combines the methods in [73] and [85] appropriately extended to include long-range interactions, Mingaleev, Gaididei and Mertens [162] computed solitary wave

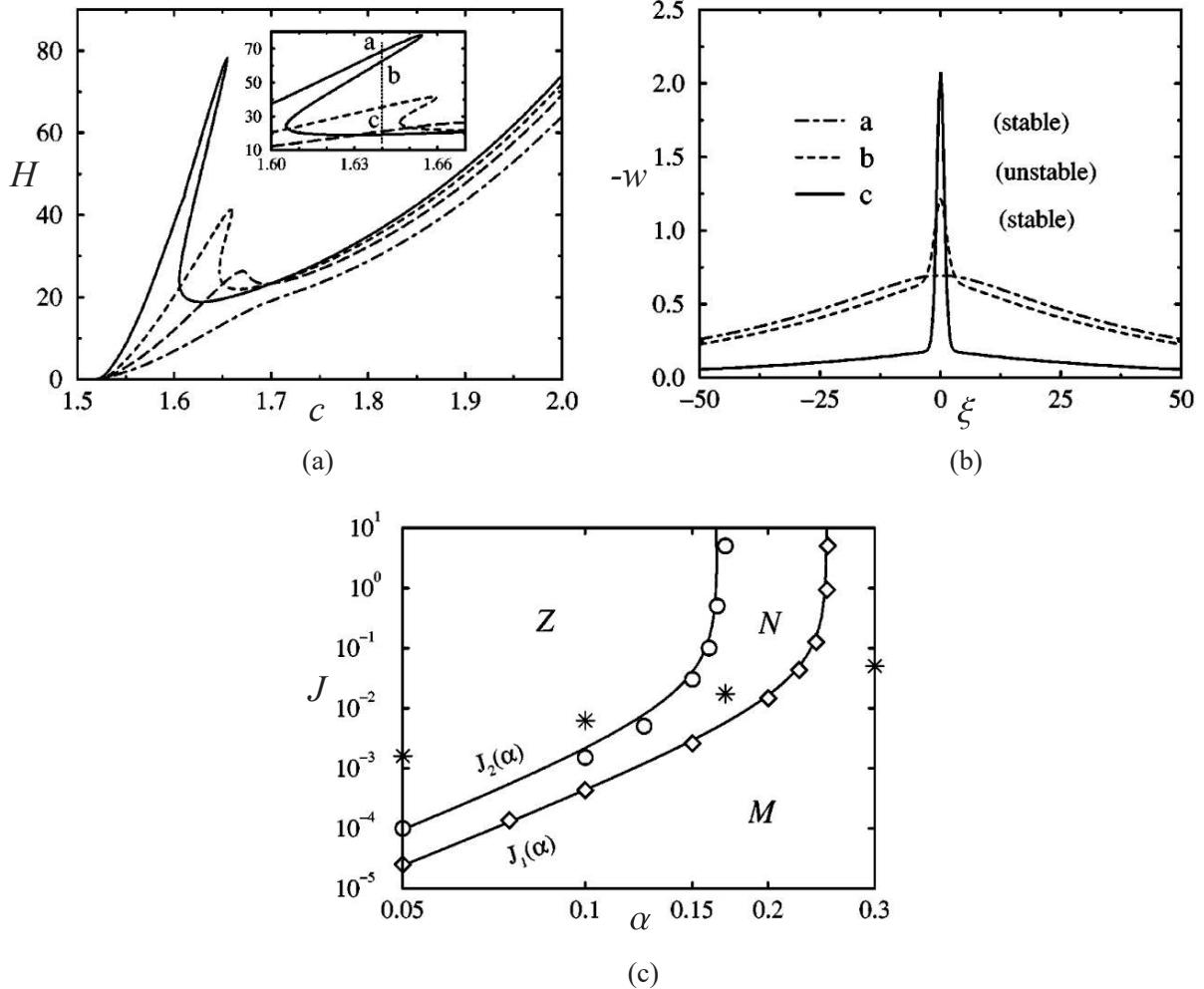


Figure 8: (a) Energy H of the solitary wave solutions of (53) with $V(w) = w - w^2$ and G_m given by (54) at $\alpha = 0.3$, $J = 0.05$ (dot-dashed curve), $\alpha = 0.17$, $J = 0.0172$ (long-dashed curve), $\alpha = 0.1$, $J = 0.0062$ (dashed curve) and $\alpha = 0.05$, $J = 0.0016$ (solid curve). In all cases $c_s = 1.515$. (b) Coexisting solutions at $c = 1.64$ at $\alpha = 0.05$, $J = 0.0016$ (points a, b and c in the inset in (a)). (c) Parameter region with monotone (M), non-monotone (N) and Z -shaped energy-velocity dependence. Stars mark the parameters used in (a). Panels (a), (b) and (c) are adapted with permission from Fig. 1, Fig. 4 and Fig. 3, respectively, in [162], Copyright (2000) by the American Physical Society.

solutions of (53) for different values of J and α in (54) and found that depending on the parameters, the functional relation of the wave's energy H on its velocity c can be monotone, *non-monotone* and even a Z -shaped curve (see Fig. 8(a)). In the last scenario, the function becomes *multivalued* for a certain velocity interval, so that three different solutions coexist at the same velocity (see Fig. 8(b)). Accordingly, three different parameter regions are identified in [162], as shown in Fig. 8(c): the M -region (monotone $H(c)$), the N -region (non-monotone), and the Z -region (Z -shaped). Non-monotone energy-velocity curves were also obtained for some parameters in the problem with power-law long-range interactions with $G_m = J/m^s$, $s > 3$ [163].

The possibility of non-monotone and even multivalued $H(c)$ dependence arises due to the scale competition in the presence of the long-range interactions and was also predicted in [160] using a variational approach. Direct numerical simulations in the N and Z regions [162] suggest that only

solutions from the upper and lower branches, where H increases with c , are stable. This will be further discussed in Sec. 7.

7. Stability

The general framework for proving stability of solitary wave solutions of (3) was established by Friesecke and Pego [57]. They introduced the notion of nonlinear ‘orbital plus asymptotic stability’, which means that a localized perturbation of a supersonic solitary wave results, asymptotically in time, in small changes of the wave’s velocity and phase, as well as a radiated part propagating slower than the wave and decaying locally near it. The main result in [57] is that such nonlinear stability follows from the corresponding property of the evolution equations

$$\ddot{\eta}_n = V''(\hat{w}_{n+1})\eta_{n+1} - 2V''(\hat{w}_n)\eta_n + V''(\hat{w}_{n-1})\eta_{n-1}, \quad (57)$$

obtained by linearizing (3) about a solitary wave $\hat{w}_n(t) = w(n - ct)$, under the assumptions of local convexity of the interaction potential, sufficient smoothness and decay of the solitary waves and the *energy-velocity transversality* condition

$$H'(c) \neq 0. \quad (58)$$

The approach involves working with exponentially weighted spaces that penalize perturbations in front of the moving pulse and shift the continuous spectrum of (57) into the left half-plane, so that only the the point spectrum needs to be investigated.

The problem thus reduces to establishing the required linear stability result. Proving it is complicated by the lack of translational symmetry in lattices. In the analogous continuum setting such symmetry provides an additional Noether invariant and has contributed to a well established stability theory for solitary waves [164, 165]. For the FPU problem (3) stability results have only been obtained so far in some special cases. Friesecke and Pego [47, 57, 58, 59] proved stability of near-sonic small-amplitude solitary waves by exploiting the fact that in this near-integrable regime the waves are well approximated by the KdV equation. Stability of solitons in the integrable Toda lattice was established by Mizumachi and Pego [166]. Mizumachi [167] improved these results by proving orbital and asymptotic stability of Toda solitons and small-amplitude FPU solitary waves in the energy space, which allows perturbations in the form of small-amplitude near-sonic solitary waves with arbitrarily small exponential decay rate. Hoffman and Wayne [168] used the result in [166] and proximity of the small-amplitude near-sonic solitary waves to those of the Toda lattice to provide a simplified proof of stability in this regime. They also proved global-in-time existence and stability of counter-propagating near-KdV solitary wave solutions of the FPU problem [62] and established the existence of the asymptotic two-soliton state [63], while multi-soliton states in the FPU problem were studied by Mizumachi [169, 170]. Benes, Hoffman and Wayne [171] proved stability of multi-soliton solutions in the Toda lattice. Khan and Pelinovsky [172] considered small-amplitude solitary waves in the FPU problem with weakly anharmonic interaction potential $V(w) = w^2/2 + \varepsilon w^{p+1}/(p+1)$ and showed that the time scales on which such waves are well approximated by the generalized KdV equation can be extended. The obtained bounds allow to deduce nonlinear metastability of small-amplitude FPU solitary waves from the orbital stability of the KdV solitary waves for $p = 2, 3, 4$. All of these results have focused on either the integrable (Toda) or near-integrable (low-energy) cases. However, recently Herrmann and Matthies [173] established stability of solitary waves in the high-energy asymptotic limit.

While there are no general rigorous stability results outside these special limits, it is known that the transversality condition (58) plays a key role [57]. In fact, it was proved in [59] that

when this condition fails, i.e. $H'(c) = 0$, the algebraic multiplicity of the zero eigenvalue of the linearization operator increases from two to at least three, suggesting a change of stability. The proof uses Fredholm alternative to show the Jordan chain associated with the zero eigenvalue is extended when $H'(c) = 0$ holds. Following the approach used in [174] to establish an analogous stability criterion for discrete breathers, Xu, Cuevas-Maraver, Kevrekidis and Vainchtein [175, 176] proved that $H'(c) = 0$ is *sufficient* for a stability change in a more general Hamiltonian problem that allows for long-range interactions and derived the leading-order expression for the near-zero eigenvalues associated with the onset of instability. The proof assumes that the displacements are localized and the contribution of the essential spectrum to the motion of the zero eigenvalue can be neglected to a leading order.

Direct numerical simulations [134, 139, 152, 162, 175] and computation of Floquet multipliers associated with the linearization of the nonlinear map (29) [175, 176, 177] further suggest that $H'(c) < 0$ is associated with instability. Interestingly, such non-monotonicity of the energy is known to take place in only a few cases. These include the problem (53) with Kac-Baker [162] and power-law [163] interactions in certain parameter regimes (see Fig. 8) and in the problem (3) with piecewise quadratic potentials, as described in Sec. 5. Another example, considered in [176], concerns a smooth approximation of the piecewise quadratic potential with $V'(w)$ given by (31) for $w \geq 0$ and its odd extension for $w < 0$. In this case one has $V(0) = V'(0) = 0$ and

$$V''(w) = 1 + \frac{\alpha - 1}{\pi} \left(\arctan \frac{w^2 - w_c^2}{\varepsilon^2} + \arctan \frac{w_c^2}{\varepsilon^2} \right), \quad (59)$$

where $\varepsilon > 0$ is a parameter that smoothens the corners of $V'(w)$ in the piecewise quadratic case obtained in the limit $\varepsilon \rightarrow 0$. As shown in Fig. 9(a), at small enough $\varepsilon > 0$ the energy $H(c)$ increases from zero value at $c_s = 1$, reaches a local maximum at $c = c_{max} > 1$, decreases to a local minimum at $c = c_{min} > c_{max}$ and then increases again. In the limit $\varepsilon \rightarrow 0$, c_{max} approaches the sound speed, and $H(c_{max})$ tends to infinity. The example in Fig. 9(b) shows that the velocity interval (c_{max}, c_{min}) , where $H'(c) < 0$, is associated with an emergence of a positive real eigenvalue for the linearized problem, manifesting an instability.

8. Periodic heterogeneous lattices: nonlocal and embedded solitary waves

So far, we have considered homogeneous FPU-type lattices. However, realistic discrete systems often have a periodic heterogeneous structure in terms of mass or interaction potentials or both. FPU lattices with periodic heterogeneities include chains with varying masses (diatomic or dimer lattices [178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192]) or bond potentials [193, 194, 195, 196] and lattices with internal resonators [197, 198, 199, 200, 201, 202, 203, 204]. In such systems solitary wave solutions are no longer generic, and instead a traveling pulse radiates energy through non-decaying oscillations. These oscillations are associated with the presence of additional optical branches in the dispersion relation that exist for all phase velocities, including the supersonic range where solitary waves of homogeneous FPU lattices are known to exist. As discussed in more detail below, generic traveling waves in this case have symmetric non-decaying oscillatory wings. When the amplitude of their wings is small beyond all algebraic orders of the system's parameter (e.g., mass ratio in a diatomic lattice), these *nonlocal* solitary waves are called *nanoptera*, by analogy with capillary-gravity water waves of similar structure [205]; waves with wing amplitude that scales as a power of the parameter are called *microptera* [206, 190]. Numerical and asymptotic results suggest that the wing amplitude vanishes at certain *antiresonance* values of the system's parameter, yielding genuine solitary waves. Similar to the embedded solitons discovered

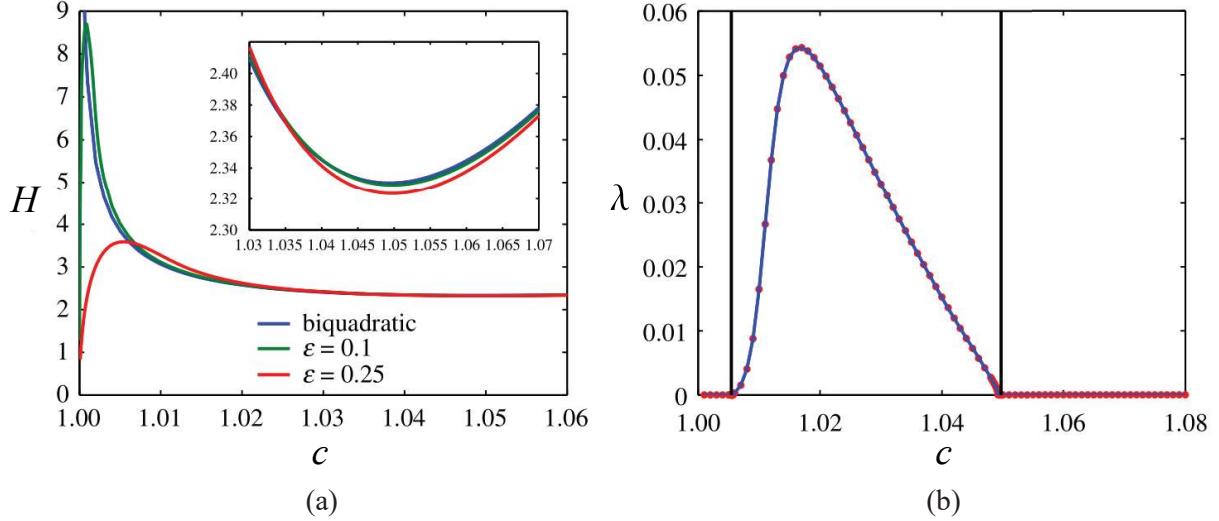


Figure 9: (a) Non-monotone energy-velocity dependence $H(c)$ for the potential $V(w)$ with $V(0) = V'(0) = 0$ and $V''(w)$ given by (59) at different ε . (b) Maximum real eigenvalue λ as a function of velocity c at $\varepsilon = 0.35$ obtained by diagonalizing the linearization operator (dots) and using $\lambda = \ln \mu$, where μ is the corresponding Floquet multiplier (solid curve). The vertical lines mark the values of c where $H(c) = 0$. Here $\alpha = 4$ and $w_c = 1$. Adapted with permission from Fig. 3 in [176], Copyright (2018) by the authors, published by the Royal Society.

in the earlier literature on nonlinear dispersive systems (e.g. [207, 208, 209, 210]), these waves have *isolated* velocity values.

As the first example of a system of this type, we consider a diatomic FPU lattice. After a rescaling, the governing equations become

$$m_n \ddot{u}_n = V'(u_{n+1} - u_n) - V'(u_n - u_{n-1}), \quad (60)$$

where $m_{2p-1} = 1$ and $m_{2p} = \mu$, and μ is the ratio of the two alternating masses in the original (unrescaled) system. Clearly, $\mu = 1$ corresponds to the monatomic FPU chain, while $\mu = 0$ constitutes another important monomer limit of the chain of only unit masses. The sound speed is given by

$$c_s = \sqrt{\frac{2V''(0)}{1 + \mu}}, \quad (61)$$

so that $c_s = (V''(0))^{1/2}$ at $\mu = 1$ and $c_s = (2V''(0))^{1/2}$ at $\mu = 0$. It is convenient to introduce the variables

$$y_p = \frac{u_{2p+1} - u_{2p-1}}{2}, \quad z_p = u_{2p} - \frac{u_{2p-1} + u_{2p+1}}{2}, \quad (62)$$

which measure the strain in the chain of the unit masses and the deviation of the displacement of the mass μ from the average of the displacements of the unit ones, respectively, and seek traveling wave solutions $y_p(t) = y(\xi)$, $z_p(t) = z(\xi)$, where $\xi = 2p - ct$ is the traveling wave coordinate. Due to the symmetry of the resulting equations, the problem then reduces to seeking an even $y(\xi)$, and an odd $z(\xi)$.

In the monatomic case $\mu = 1$, we have $y(\xi) = (w(\xi) + w(\xi + 1))/2$, $z(\xi) = (w(\xi) - w(\xi + 1))/2$, where $w(\xi)$ is a solitary wave solution of (3). Under the conditions of the Friesecke-Wattis theorem [38] such solution exists for $c > (V''(0))^{1/2}$. Similarly, in the case $\mu = 0$, when we have the chain of

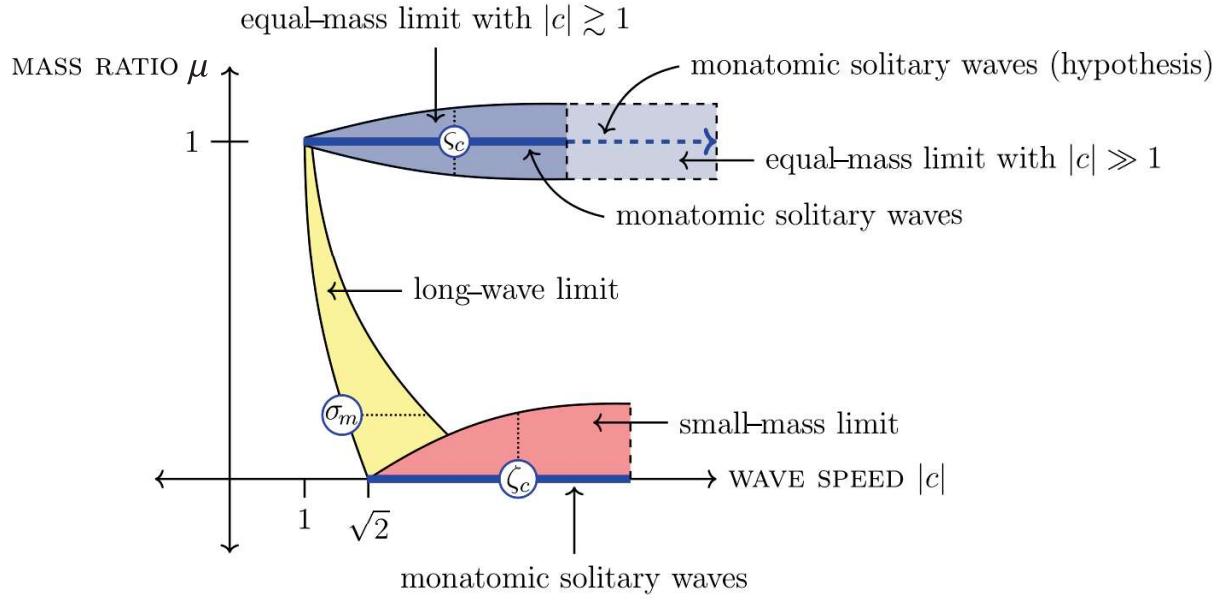


Figure 10: Existence results for traveling waves in a diatomic FPU lattice: small-mass limit (pink region) [187], long-wave limit (yellow region) [188] and equal-mass limit (blue region) [190]. The thick blue lines at $\mu = 1$, $|c| > 1$ and $\mu = 0$, $|c| > \sqrt{2}$ correspond to solitary waves in the corresponding monatomic chains. The left boundary σ_m of the yellow region corresponds to the sonic limit. Here $V''(0) = 1$ is assumed. The figure is adapted with permission from Fig. 2 in [190], Copyright (2020) by the authors, published by Elsevier.

unit masses only, the same conditions ensure existence of a solitary wave for $c > (2V''(0))^{1/2}$, with $y(\xi)$ given by an even profile, and $z(\xi) \equiv 0$. Near their corresponding sonic limits, these solutions are well approximated by the KdV solitons [47]. Known rigorous results about existence of nonlocal solitary waves away from these two limiting cases are summarized in Fig. 10 adapted from [190].

Hoffman and Wright [187] proved the existence of nanoptera in the limit of small mass ratio μ

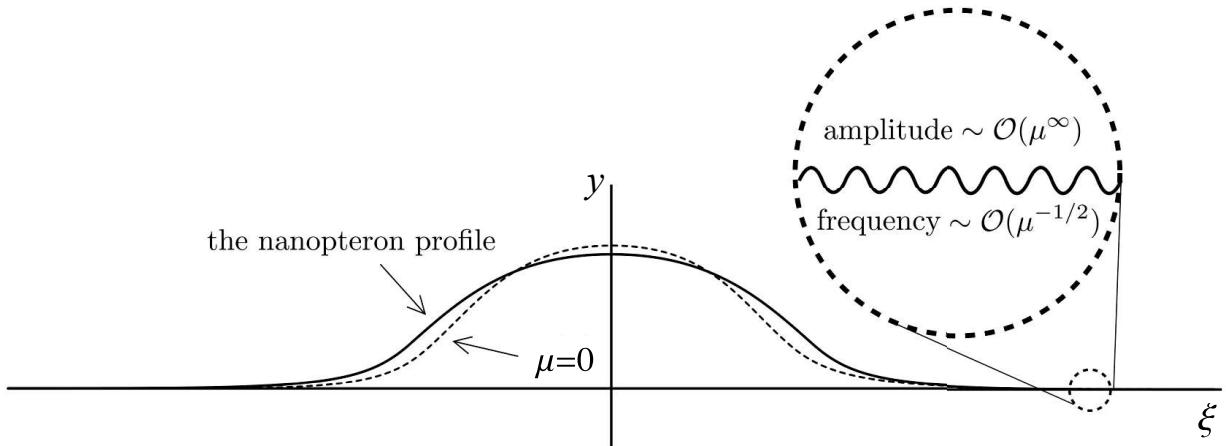


Figure 11: A schematic representation of $y(\xi)$ component of a nanoperturbation solution (solid curve) at $\mu = 0$ and the solitary wave solution (dotted line) at $\mu = 0$. The notation $\mathcal{O}(\mu^\infty)$ means ‘small beyond all orders of μ ’. The figure is adapted with permission from Fig. 3 in [187], Copyright (2017) by Elsevier.

on an open set that excludes a countable sequence of μ values converging to zero. Fig. 11 shows a

schematic representation of such solutions. Each traveling wave of this type possesses symmetric oscillatory wings of amplitude that is small beyond all algebraic orders of μ and frequency of order $\mu^{-1/2}$. In the context of the initial-value problem, error estimates for approximating the dynamics of the diatomic chain with small μ by the monatomic limit $\mu = 0$ were obtained by Pelinovsky and Schneider [211]. Faver and Wright [188] proved the existence of nanoptera in the long-wave limit just above the sound speed c_s defined in (61). These solutions are represented by an exponentially localized small perturbation of a KdV soliton and a periodic function whose frequency is $\mathcal{O}(1)$ and amplitude is small beyond all orders of $c - c_s$. In a more general setting that allows for periodic variations of both mass and bond potentials, approximation of heterogeneous FPU dynamics by KdV equations was studied by Chirilus-Bruckner, Chong, Prill and Schneider [212] and Gaison, Moscow, Wright and Zhang [213]. Wattis [214] derived higher-order corrections to this approximation for a diatomic lattice. Faver and Hupkes [190] proved the existence of microptera for $\mu \approx 1$; their result extends to arbitrarily large supersonic velocities under the hypotheses that include the existence of an exponentially localized and spectrally stable solitary wave solution for the monatomic problem at $\mu = 1$. The existence proofs in [187, 188, 190] are based on the modification of the method developed by Beale [215] for a capillary-gravity water wave problem.

While these works focus on nonlocal solitary waves, which possess non-decaying oscillations at infinity, earlier numerical and asymptotic results suggest that the amplitude of these oscillations vanishes at certain (c, μ) pairs, yielding genuine (localized) solitary waves. Tabata [180] found such a pair numerically for a diatomic Toda lattice governed by (60) with $V(r)$ given by (9). This observation has motivated the work of Ishiwata, Matsutani and Ônishi [216], where the formation of the discrete set of such pulses excited in a diatomic Toda chain was analytically predicted for the hard-core limit. Jayaprakash, Starosvetsky and Vakakis [183] considered a diatomic granular chain without precompression, where the sound speed (61) is zero, in the limit of small mass ratio μ . Using multiple-scale asymptotic analysis and Wentzel-Kramers-Brillouin (WKB) approximation [217] of the equation governing the fast dynamics of the light masses, they found a sequence $\{\mu_j\}$ of *antiresonance* mass ratio values that yield genuine solitary wave solutions within the asymptotic approximation and are in good agreement with numerical simulation results at large enough j . It is conjectured that this sequence is infinite and accumulates at zero. For the largest non-unit mass ratio value in the sequence, these results were corroborated numerically and experimentally in [185]. In [184] the authors considered a $1 : N$ granular dimer chain without precompression, with each heavy mass followed by N light ones, and showed that a sequence of antiresonance mass ratios can also be constructed for $N = 2$, but genuine solitary waves do not exist when $N > 2$. Following the asymptotic approach of [183], Vainchtein, Starosvetsky, Wright and Perline [186] considered a general diatomic FPU chain with nonzero sound speed (61) and used separation of slow and fast time scales in the limit of small μ to derive the Fredholm orthogonality condition for the antiresonance sequence $\{\mu_j\}$. Under this condition, the slow motion of the center of mass of the two neighboring heavy masses does not excite any fast oscillations of the light mass in between at large time. For a diatomic Toda lattice the antiresonance condition was made explicit in [186] by exploiting the integrability of the monatomic Toda lattice (which is, however, destroyed in the diatomic setting). Lustri and Porter [189] used exponential asymptotic techniques instead of scale separation to obtain the orthogonality condition for the diatomic Toda lattice. The same approach was used by Lustri [192] for an α -FPU lattice near the long-wave $\mu = 0$ limit approximated by a KdV soliton and by Deng, Lustri and Porter [203] for a diatomic granular chain without precompression.

Recently, Faver and Hupkes [191] used a collocation method developed in [89] and parameter continuation to find nonlocal traveling waves in a diatomic α -FPU lattice numerically, clarifying the relationship between the branches of microptera and nanoptera constructed in [187, 188, 190]. In particular, they uncovered several branches of genuine solitary waves.

A closely related problem is that of spring dimers, where instead of masses the bond potentials alternate. Faver [196] considered a monatomic chain with alternating cubic potentials with different coefficients and proved the existence of nanoptera in the long-wave near-sonic limit. Chaunsali, Toles, Yang and Kim [194] used asymptotic analysis to obtain localized waves in a granular chain with alternating soft and stiff contact interactions and zero precompression. They also provided numerical and experimental verifications of these results. Starosvetsky and Vainchtein [195] derived an antiresonance condition for a general FPU chain with alternating stiff and soft bonds and nonzero sound speed, which becomes explicit in the case of alternating Toda potentials.

Another way to introduce periodic heterogeneity into an FPU setting is by introducing internal resonators. In such systems, each (primary) particle in the nonlinear chain is connected by a linear spring to a secondary particle, which has a different mass. The dimensionless equations are

$$\ddot{u}_n = V'(u_{n+1} - u_n) - V'(u_n - u_{n-1}) - \kappa(u_n - v_n), \quad \mu\ddot{v}_n = \kappa(u_n - v_n), \quad (63)$$

where $u_n(t)$ and $v_n(t)$ are the displacements of the n th primary and secondary particles, respectively, κ measures the stiffness of the linear coupling, and μ is the mass ratio. This model was originally used to describe granular chain configurations, with the local resonators being either inside [218] or outside [219] the primary spherical beads. It also describes the woodpile granular chain [198] consisting of orthogonally stacked rods, where every second rod is aligned. In this case, each resonator represents the primary internal vibrational mode of the woodpile rod. As the rod length increases, additional bending vibration modes need to be taken into account by augmenting (63) with the corresponding linear oscillators [220].

Numerical evidence [197, 199, 200] suggests that generic solitary wave solutions in a granular chain with internal resonators and zero precompression are nonlocal. Kevrekidis, Stefanov and Xu [199] proved that in this case the system (63) has genuine solitary wave solutions with velocity c when the antiresonance condition

$$\sqrt{\frac{\kappa(1+\mu)}{c^2\mu}} = 2\pi j \quad (64)$$

holds for any integer j . In particular, for a given c , there exists a countable infinity of mass ratios μ_j for which the wing amplitude is identically zero. Faver, Goodman and Wright [202] proved that for smooth enough potentials $V(r)$, solitary wave solutions of (63) persist under the condition (64) in the limits of small μ and large κ . Error estimates for approximating the lattice dynamics at small μ by the $\mu = 0$ FPU limit were obtained by Hadadifard and Wright [221]. Faver [201] considered cubic potentials and used Beale's ansatz [215] to prove the existence of nanoptera in an open set of small μ that excludes the antiresonance values. Deng, Lustri and Porter used exponential asymptotic analysis to approximate the wing amplitude in the nanoptera that arise in a woodpile chain with [203] and without [204] precompression.

9. Two-dimensional lattices

The simplest two-dimensional (2D) extensions of the FPU problem involve a scalar unknown variable. For example, one may consider

$$\ddot{w}_{l,m} = V'(w_{l+1,m}) + V'(w_{l-1,m}) + V'(w_{l,m+1}) + V'(w_{l,m-1}) - 4V'(w_{l,m}) \quad (65)$$

as a 2D scalar analog of (3) that can be derived from an electrical transmission network, where the variable $w_{l,m}(t)$ is the charge on a capacitor located at the (l, m) th node of the square lattice at

time t , and the nonlinear function $V'(w_{l,m})$ represents the voltage at the lattice site [222, 75, 223]. Seeking planar traveling wave solutions

$$w_{l,m}(t) = w(\xi), \quad \xi = l \cos \phi + m \sin \phi - ct$$

propagating with velocity c at the angle ϕ with respect to the horizontal (l) direction, one obtains the advance-delay differential equation

$$c^2 w''(\xi) = V'(w(\xi + \cos \phi)) + V'(w(\xi - \cos \phi)) + V'(w(\xi + \sin \phi)) + V'(w(\xi - \sin \phi)) - 4V'(w(\xi)). \quad (66)$$

A solitary wave solution satisfies (66) and (7). Due to the $\pi/2$ -periodicity of (66) and its symmetry about $\pi/4$, it suffices to consider ϕ in the interval $[0, \pi/4]$. At $\phi = 0$ and $\phi = \pi/4$ the problem reduces to the traveling wave equation (5) for the one-dimensional FPU problem, in the latter case after the change of variables $\xi \rightarrow \xi/\sqrt{2}$. Eilbeck [110] studied this problem numerically for $V(w) = (w^2 + w^4)/2$ and observed the anisotropic dependence of the height $w(0)$ of the solution on the angle ϕ , reaching its maximum at an angle larger than $\pi/8$. The anisotropy of solitary waves was also noted by Druzhinin and Ostrovsky [75]. Wattis [224] investigated various quasicontinuum models for this problem obtained by considering (66) in the Fourier space,

$$c^2 W(k) = \Lambda(k) F(k), \quad \Lambda(k) = \frac{4}{k^2} \left[\sin^2 \frac{k \sin \phi}{2} + \sin^2 \frac{k \cos \phi}{2} \right], \quad (67)$$

where $W(k)$ and $F(k)$ are Fourier images of $w(\xi)$ and $V'(w(\xi))$, respectively, and approximating $\Lambda(k)$. Among the models analyzed in [224], only the (2, 2) Padé approximation captures the anisotropy of the model. However, as shown in [225], where an exact planar traveling wave for the bilinear $V'(w)$ given by (31) was constructed and directly compared to quasicontinuum models, the (2, 2) approximation still misses the fact that the angle at which the height reaches its maximum depends on c .

Another scalar 2D problem that has been considered in the literature is a strongly anisotropic mechanical lattice governed by

$$\ddot{u}_{i,j} = u_{i+1,j} - 2u_{i,j} + u_{i-1,j} + \varepsilon^2(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) + a\varepsilon[(u_{i,j} - u_{i-1,j})^2 - (u_{i+1,j} - u_{i,j})^2], \quad (68)$$

where $u_{i,j}(t)$ is the displacement of (i, j) th particle at time t , $\varepsilon \ll 1$ is a small parameter, and a is an $\mathcal{O}(1)$ parameter. The model, studied by Duncan, Eilbeck, Walshaw and Zakharov [226], represents weakly coupled nonlinear one-dimensional chains. As shown in [226], it reduces to the Kadomtsev-Petviashvili equation of type II (KP-II) [227]

$$(24w_{\mathcal{T}} - 24aww_Z + w_{ZZZ})_Z + 12w_{YY} = 0 \quad (69)$$

in the continuum limit obtained by expanding the terms in (68) in terms of $u(x, y)$, setting $Z = \varepsilon(x - t)$, $Y = \varepsilon y$, $\mathcal{T} = \varepsilon^3 t$ and differentiating with respect to Z , with $w = u_Z$. More generally, Kadomtsev-Petviashvili equations can be brought to the form $(w_t + 6ww_x + w_{xxx})_x = \pm w_{yy}$, with plus and minus signs corresponding to type I (KP-I) and type II (KP-II) equations, respectively. Planar traveling wave solutions of (68) with small propagation angles were obtained numerically in [226, 110], along with a heuristic angle-dependent height-speed relation, which was shown to be in a good agreement with the numerical results. Wattis [74] investigated quasicontinuum descriptions of the problem based on the Padé expansions, with (2, 2) model giving the most accurate description of the height-speed relation, comparable to the one in [226].

More general scalar models that include nonlinear interactions between first neighbors and harmonic three-body interactions between the first and second nearest neighbors was considered by

Ioannidou, Pouget and Aifantis [228] and Astakhova and Vinogradov [229]. In the weakly nonlinear asymptotic limit the lattice dynamics is described by a KP-I equation. This connection was also established in the earlier work of Potapov, Pavlov, Gorshkov and Maugin [230] for a model that only takes into account nearest-neighbor interactions. In [228, 229] the authors investigated numerically the lattice dynamics initiated by a lump (i.e., localized in all directions) 2D soliton solution of the KP-I equation and identified the parameter region where the wave propagates through the lattice with little radiation. Numerical simulations of two such waves colliding in the lattice showed the scattering behavior similar to that of KP-I solitons. In [229] a pseudospectral method was used to compute the solitary wave solutions of the discrete problem.

While a number of authors studied vectorial 2D extensions of the FPU problem, few general results are known. Friesecke and Matthies [231] considered a 2D mechanical lattice with interactions along the diagonals and sides of a square unit cell (see Fig. 12(a)) governed by two different generic potentials depending on the two-component in-plane displacement vectors. They proved the existence of small-amplitude supersonic longitudinal solitary waves propagating in the horizontal direction and determined their asymptotic profile. Interestingly, the results hold even when the interaction potentials are quadratic due to the geometric nonlinearity of the lattice. The authors also proved non-existence of non-longitudinal (in particular, transversal) small-amplitude solitary waves that propagate in the horizontal direction. Chen and Herrmann [232] considered a general 2D framework that allows for different lattice geometries and arbitrary propagation directions. They proved the existence of KdV-like small-amplitude supersonic solitary waves under certain assumptions on the coupling constants in the advance-delay differential equation governing the traveling wave solution (these constants depend on the lattice geometry and the direction of propagation) and the parameters of the nonlinear interaction potentials. The validity of these assumptions was verified in [232] for square, triangle and diamond lattices (see Fig. 12). In particular, this analysis recovers the results proved in [231] in the special case of horizontal propagation direction in a square lattice.

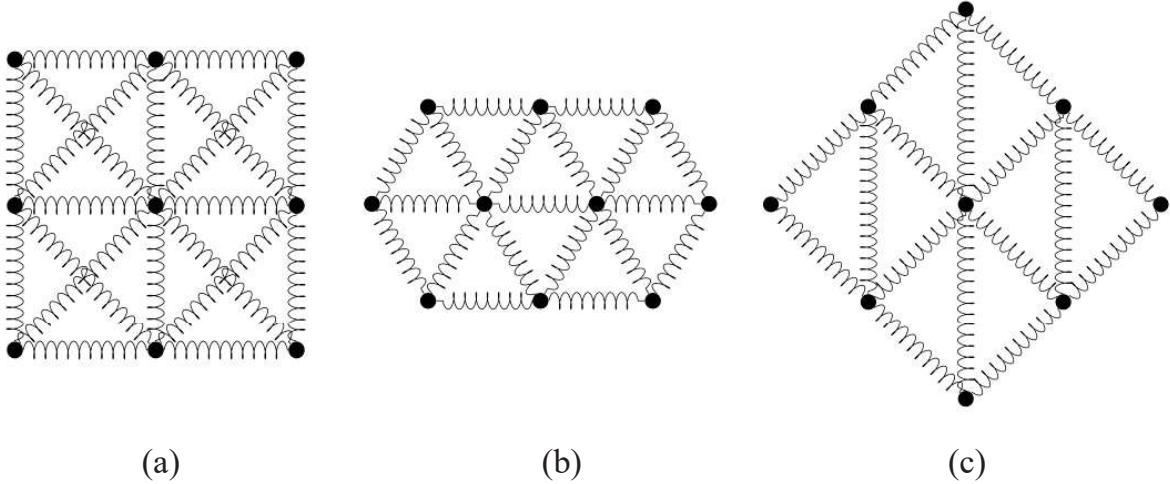


Figure 12: Some geometries of 2D lattices: (a) square, (b) triangle and (c) diamond lattices. the figure is adapted with permission from Fig. 1 in [232], Copyright (2018) by the American Institute of Mathematical Sciences.

Leonard, Fraternali and Daraio [233] conducted experimental and numerical investigations of a 2D square-packed granular array that reveal a quasi-1D solitary wave propagation. Leonard, Chong, Kevrekidis and Daraio [234] showed that such motion is impossible in the case of a hexagonal

packing, where the energy of an initial impact gradually spreads over an increasing number of neighbors, and the amplitude of the pulse has a power-law decay.

Zolotaryuk, Savin and Christiansen [235] numerically obtained planar solitary wave solutions in an isotropic hexagonal lattice governed by a Lennard-Jones interaction potential. They investigated the dependence of the solutions on the angle ϕ of propagation and showed that when $0 < \phi \leq \pi/6$, the solutions exist for only a finite interval of supersonic velocities.

Porubov and Osokina [236] considered a 2D lattice model of graphene with translational and angular interactions between two sublattices. They developed an asymptotic procedure to describe weakly transversely perturbed longitudinal plane waves. The procedure gives rise to a nonlinear equation for the longitudinal strain that generalizes the KP equation by allowing two-directional wave propagation and has planar solitary wave solutions.

10. Open problems

Despite a lot of progress in understanding solitary wave propagation in the original FPU lattice and its various extensions, a number of issues remain unresolved. Some of these are summarized below.

As discussed in Sec. 7, in the generic non-integrable case stability results have been proved only for the special asymptotic limits of near-sonic and high-energy waves. While there is plenty of numerical evidence that $H'(c) > 0$ is at least necessary for stability of lattice solitary waves, this has not been rigorously established. As noted in [57], such result would show that the sign of $H'(c)$ is the more fundamental diagnostic of orbital stability of solitary waves than the derivative of the time-invariant generalized momentum functional $I(c)$ associated with translational invariance in continuum theories [237, 238] (for example, for the generalized KdV equation $u_t + u^p u_x + u_{xxx} = 0$, $p \geq 1$, $I(c) = \frac{1}{2} \int_{-\infty}^{\infty} u_c^2 dx$, where $u(x, t) = u_c(x - ct)$ is the solitary wave solution with $c > 0$). While it has been established that the change of sign of $H'(c)$ is associated with the change in the multiplicity of the zero eigenvalue of the linearization operator [57, 175, 176], solitary waves in lattices could also become unstable through other mechanisms, including Hopf and period-doubling bifurcations. Determining the conditions that lead to these other scenarios of stability loss in FPU-type lattices is another open problem.

When the lattice is periodically heterogeneous, generic solitary waves are expected to be non-local, as discussed in Sec. 8. However, existence of such solutions has been proved only for certain asymptotic limits, summarized in Fig. 10 for the case of diatomic lattices. In addition, existence of genuinely localized solitary waves embedded in this class of solutions has not been rigorously established. Stability of both embedded and nonlocal solitary waves in such lattices is another unresolved and delicate issue. In particular, it is unclear what is the appropriate generalization of the stability threshold $H'(c) = 0$ is in this case, given that nonlocal waves do not have a finite energy (and thus one needs to work with renormalized energies instead), while for the embedded waves the energy is finite but only defined at isolated velocity values.

While it is already clear that long-range interactions may have a significant effect on the domain of existence, properties and stability of solitary waves (see Sec. 6), more work is needed to understand their role in a general framework. This includes proving existence of strictly supersonic solitary waves in lattices with competing first and second-neighbor interactions [152, 157] beyond small-amplitude limit and generalizing these results to the cases with longer-range interactions. Another open problem is determining the general conditions under which long-range interactions lead to non-monotone and multivalued energy-velocity relations as in [162, 163].

As discussed in Sec. 9, in the case of scalar and vectorial 2D lattices, few rigorous results have been established about existence, stability and asymptotic limits of lump and planar solitary waves.

The higher-dimensional setting and more complex lattice structure offer possibilities that have been barely explored, including more types of instability modes that lead to a variety of bifurcating waveforms, as well as new phenomena associated with long-range interactions, heterogeneity and disorder. The connection between lattice and KP dynamics needs to be further investigated building upon recent work in this direction [239].

Studies along these lines will lead to further development of mathematical tools that can also be used in studying traveling waves in other discrete systems, including emerging mechanical meta-material structures designed for impact mitigation and wave manipulation [6, 240].

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