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A Unifying Perspective: Solitary Traveling Waves As Discrete Breathers in Hamiltonian Lattices and Energy Criteria for Their Stability

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In this work, we provide two complementary perspectives for the (spectral) stability of solitary traveling waves in Hamiltonian nonlinear dynamical lattices, of which the Fermi-Pasta-Ulam and the Toda lattice are prototypical examples. One is as an eigenvalue problem for a stationary solution in a co-traveling frame, while the other is as a periodic orbit modulo shifts. We connect the eigenvalues of the former with the Floquet multipliers of the latter and based on this formulation derive an energy-based spectral stability criterion. It states that a sufficient (but not necessary) condition for a change in the wave stability occurs when the functional dependence of the energy (Hamiltonian) H of the model on the wave velocity c changes its monotonicity. Moreover, near the critical velocity where the change of stability occurs, we provide an explicit leading-order computation of the unstable eigenvalues, based on the second derivative of the Hamiltonian $H''(c_0)$ evaluated at the critical velocity c_0. We corroborate this conclusion with a series of analytically and numerically tractable examples and discuss its parallels with a recent energy-based criterion for the stability of discrete breathers.

I. INTRODUCTION

Solitary traveling waves (STWs) are ubiquitous in Hamiltonian lattice dynamical systems with intersite interactions. They arise in the model at the very foundation of nonlinear science, namely the Fermi-Pasta-Ulam (FPU) lattice [1], as well as in the Toda lattice [2], one of the key systems of interacting particles, and, arguably, the most significant integrable one. In addition to their theoretical relevance in the above models, they constitute the most generic, robust and often experimentally tractable excitation in nonlinear systems, in particular, in granular crystals [3–5] and other materials.

Given the relevance of STWs in theoretical, numerical [6–8] and experimental [3, 4] studies, it is natural to be concerned about their stability. This may be accessible in some special cases, such as the Toda lattice [9], or the FPU problem in the low-energy (near-sonic) regime [10, 11], where specialized techniques become available due to the system's integrability (or proximity to it). Nevertheless, from a physical perspective, it would be desirable to have a more general criterion that would be intuitive as well as straightforward to test. This is especially important given that in a number of studies [12–14], the possibility of unstable STWs has been demonstrated.

In the present work, we offer such a criterion (a sufficient yet not necessary condition) by establishing that a change in the monotonicity of the STW's energy (Hamiltonian H) dependence on the velocity c will result in a change in its (spectral) stability. In other words, we establish that when, for a critical velocity c_0, it happens that $H'(c_0) = 0$, a pair of eigenvalues associated with the traveling wave vanish, entailing the potential for instability. While this criterion first appeared in [10], where it was motivated by the study of the FPU problem in the near-sonic limit, here we provide both a concise proof, and also a definitive leading-order calculation for these two near-zero eigenvalues to explicitly show why (and when) instability appears. We also systematically test the criterion numerically in a broad array of physically relevant cases.

Equally important in our approach is the fact that we provide a generalized perspective of the problem of the stability of STWs in a Hamiltonian lattice. In the frame traveling with the solution, the stability leads to a standard eigenvalue problem. Yet, here, motivated by earlier works such as [15], we also propose a complementary approach, where the solution is viewed as a *periodic orbit* of the map involving (a) running the solution for a period of h/c, where h is the lattice spacing, rescaled to unity below and (b) shifting back by one lattice site. In light of this periodicity, Floquet analysis can be brought to bear and will turn out to yield *coincident* stability conclusions about instabilities produced by the criterion put forth. Furthermore, this perspective enables a unification of the lattice STWs in such Hamiltonian systems through their consideration as discrete breathers. Here the effective frequency ω is proportional to their velocity c according to $\omega = 2\pi c/h$. This, in turn, directly connects the criterion we analyze with a recently established criterion for the spectral stability of discrete breathers [16]. We emphasize here that the unifying connection of STWs with breathers does not impose any a-priori restrictions on the nature of their decay of at

infinity.

The paper is organized as follows. In Sec. II we formulate the problem, analyze the properties of the linear operator associated with a STW and prove the energy-based stability criterion. We also describe the behavior of the relevant eigenvalues near the critical velocity, based on the derivation presented in Appendix A. In Sec. III we discuss an alternative perspective for the spectral stability, which is associated with the Floquet analysis. Our results are corroborated by numerical examples in Sec. IV, with further details provided in Appendix B. We summarize our findings and discuss some open questions in Sec. V.

II. STABILITY ANALYSIS IN THE CO-TRAVELING FRAME AND THE ENERGY CRITERION

We consider a rescaled Hamiltonian system of the form

$$\frac{du}{dt} = p, \quad \frac{dp}{dt} = F(u) = -\frac{\partial \mathcal{H}}{\partial u}, \tag{1}$$

where $\mathcal{H}$ denotes the Hamiltonian energy density of the system, $u(t)$ and $p(t)$ are infinite-dimensional vectors denoting the displacement and particle velocity values on the lattice, with components u_n and p_n, respectively. In a more compact notation, Eq. (1) can be written as

$$\frac{dU}{dt} = J\nabla\mathcal{H}(U), \tag{2}$$

where

$$U = \begin{pmatrix} u \\ p \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

We assume the existence of STWs for a continuous interval of velocities. These are localized solutions of the form

$$u_n(t) = \hat{u}(\xi), \quad p_n(t) = \hat{p}(\xi), \quad \xi = n - ct,$$

where c denotes the velocity of the wave, and ξ is the co-traveling frame variable (note that $\hat{p}(\xi) = -c\hat{u}'(\xi)$), with finite energy (see Appendix A for more details). Linearization about the STW in the co-traveling frame, with $u(\xi,t) = \hat{u}(\xi) + \epsilon e^{\lambda t} W(\xi)$ and $p(\xi,t) = \hat{p}(\xi) + \epsilon e^{\lambda t} P(\xi)$ for small ϵ, then yields the eigenvalue problem

$$\lambda Z = \mathcal{L} Z \tag{3}$$

for the linear operator

$$\mathcal{L} = c\partial_\xi + J\nabla^2\mathcal{H}(\hat{U}), \tag{4}$$

where

$$Z = \begin{pmatrix} W \\ P \end{pmatrix}, \quad \hat{U} = \begin{pmatrix} \hat{u} \\ \hat{p} \end{pmatrix}, \quad J\nabla^2\mathcal{H}(\hat{U}) = \begin{pmatrix} 0 & I \\ F'(\hat{u}) & 0 \end{pmatrix}.$$

Solving the problem in Eq. (3) provides information about the stability of the STW, through the spectrum of the linearization operator $\mathcal{L}$, with adjoint

$$\mathcal{L}^* = (-\nabla^2\mathcal{H}(\hat{U})J - c\partial_\xi) = -J^{-1}\mathcal{L}J \tag{5}$$

(note that $J\mathcal{L}$ is self-adjoint). Given the time translation symmetry, an important feature of $\mathcal{L}$ is the existence of an eigenvector $e_0 = -\partial_\xi \hat{U}$ associated with eigenvalue $\lambda = 0$. The corresponding generalized eigenfunction is $e_1 = \partial_c \hat{U}$, i.e., $\mathcal{L}e_1 = e_0$. In other words, the spectrum of $\mathcal{L}$ always contains a double eigenvalue at zero. Moreover, by symmetry, the algebraic multiplicity of the zero eigenvalue can only be even.

The presence of an additional instability presupposes the *increase* of the algebraic multiplicity of the 0 eigenvalue. Since the kernel of $\mathcal{L}$ is one-dimensional, an algebraic multiplicity higher than two (i.e., at least four) implies that there exists e_2 such that $\mathcal{L}e_2 = e_1 = \partial_c \hat{U}$. Since $J^{-1}e_0 = -J^{-1}\partial_\xi \hat{U}$ is in the kernel of $\mathcal{L}^*$, this yields the solvability condition

$$\begin{aligned} 0 = \langle J^{-1}e_0, e_1\rangle &= \int (-J^{-1}\partial_\xi \hat{U}) \cdot (\partial_c \hat{U}) d\xi \\ &= \int \frac{1}{c}\nabla\mathcal{H}(\hat{U}) \cdot \frac{\partial \hat{U}}{\partial c} d\xi = \frac{1}{c}\int \frac{\partial \mathcal{H}(\hat{U})}{\partial c} d\xi = \frac{1}{c}H'(c), \end{aligned}$$

where $H = \int \mathcal{H} d\xi$ is the conserved Hamiltonian of the system, and $\langle \cdot, \cdot \rangle$ denotes the relevant inner product.

As soon as c deviates from the critical velocity c_0 satisfying $H'(c_0) = 0$, the above solvability condition fails (e.g. assuming $H''(c_0) \neq 0$), and hence two eigenvalues start to move away from zero and can possibly emerge on the real axis. Thus the condition $H'(c_0) = 0$ constitutes a threshold for instability of STWs, as per the concise proof above and detailed numerical considerations below extending the formulation of [10]. In fact, by computing the leading-order approximation of these two near-zero eigenvalues near c_0 one can reveal the trend of their motion. Suppose, as will be typically the case when the stability changes (including examples in Sec. IV below), that the generalized kernel of $\mathcal{L}$ is exactly four-dimensional at c_0, with $\mathcal{L}^3 e_3 = \mathcal{L}^2 e_2 = \mathcal{L}e_1 = e_0 = -\partial_\xi \hat{U}$. Then, as shown in Appendix A, the pair of eigenvalues of $\mathcal{L}$ responsible for the change of stability will be given by

$$\lambda = \pm\sqrt{\frac{H''(c_0)}{\alpha_1 c_0}(c - c_0)} + O(|c - c_0|) \tag{6}$$

for c is near c_0, where nonzero α_1 is defined in (A2) in terms of generalized eigenvectors.

In Sec. IV we numerically verify the theoretical predictions (and test the validity of Eq. (6)), showing that a change of the monotonicity of $H(c)$ will constitute a sufficient (but not necessary) condition for the transition from stability to instability, or vice versa, depending on the sign of $H''(c_0)\alpha_1 c_0$.

III. A COMPLEMENTARY PERSPECTIVE: FLOQUET ANALYSIS OF THE TIME $T = h/c$ MAP

Let us now envision anew the case of a STW on a lattice. Over the period $T = h/c$ (below we again set $h = 1$), the STW $\hat{U}$ moves over by one lattice site. However, due to the integer shift invariance of the lattice, the configuration has to be identical to the one with which we started. This means that

upon running for a period and shifting back using the shift operator S such that $Su_n(t) = u_{n-1}(t)$, we generate a *periodic orbit* on the lattice [15]. Thus, a fixed point of this operation consisting of (a) run for $T = 1/c$ and (b) shift, is a discrete breather (DB) i.e., a localized time-periodic solution [17, 18] by construction with frequency $\omega = 2\pi c$. Yet, at the same time the resulting profile constitutes a lattice STW.

Two important consequences of this complementary perspective are as follows. (1) The fixed point operation discussed above has a corresponding monodromy matrix [17–19] whose eigenvalues are the Floquet multipliers (FMs) of the relevant periodic orbit. These FMs determine the stability of the periodic orbit (i.e., in this case of the STW), as do the eigenvalues of co-traveling problem computation. Hence, one should expect that an instability manifested through an eigenvalue crossing zero should be accompanied by a FM μ crossing unity, due to the well known relation $\mu = e^{\lambda T}$ between the multipliers and eigenvalues [20]. (2) Given the intimate connection of lattice STWs and DBs, an immediate correlation emerges between the criteria for stability change of discrete breathers, such as $H'(\omega) = 0$ that was recently established in [16] and the stability of lattice STWs discussed here (and also in [10]). Observing that for lattice STWs, $\omega = 2\pi c$, an alternative derivation of the latter from the former is, in fact, immediate.

IV. NUMERICAL CORROBORATION

We now test the above prediction in a set of numerical examples with the generalized Hamiltonian of the form

$$H = \sum_{n=-\infty}^{\infty} \left[\frac{p_n^2}{2} + V(u_{n+1} - u_n) + \sum_{m=-\infty}^{\infty} \frac{\Lambda(m)}{4} (u_n - u_{n+m})^2 \right]. \tag{7}$$

Here $V(u)$ is a generic potential governing the nonlinear interactions between nearest neighbors, and $\Lambda(m)$ are the coefficients of all-to-all linear long-range interactions, which decay as $|m| \to \infty$; in the absence of such interactions, $\Lambda(m) = 0$. For instance,

$$\Lambda(m) = \rho(\mathrm{e}^{\gamma} - 1)\mathrm{e}^{-\gamma|m|}(1 - \delta_{m,0}), \tag{8}$$

with $\rho > 0$ and $\gamma > 0$, corresponds to the Kac-Baker interactions, and $\Lambda(m) = \rho|m|^{-s}(1 - \delta_{m,0})$ with $s = 5$ ($s = 3$) corresponds to the dipole-dipole (Coulomb) interactions between charged particles on a lattice. In principle, the methodology can capture nonlinear long-range interactions, but here we consider linear ones for simplicity.

As our first example, we consider the analytically tractable and well known case of the Toda lattice [2] where $V(u) = e^{-u} + u - 1$ while $\Lambda(m) = 0$, which has a one-soliton solution of the form $u_n(t) = \log\left[\cosh(\kappa(n - ct - 1))\mathrm{sech}(\kappa(n - ct))\right]$, where κ is the unique positive solution of $c\kappa = \sinh(\kappa)$. The resulting

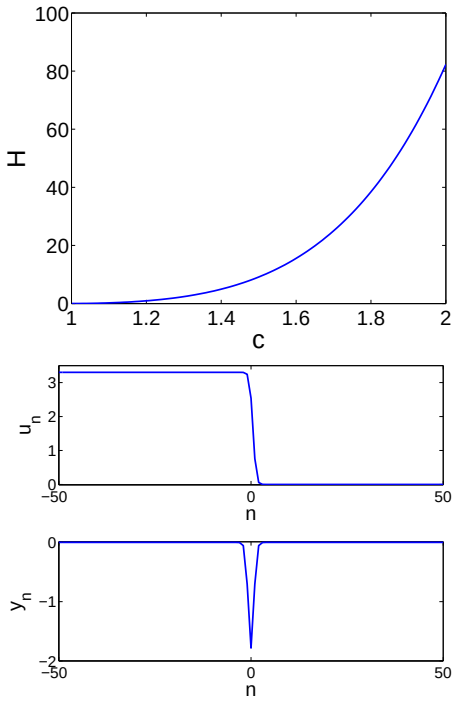

FIG. 1: Top panel: dependence of the energy H on the wave velocity c in the α-FPU model in Eq. (9) with $\Lambda(m) = 0$. Bottom panels: typical profile of the traveling wave with $c = 1.5$ in the displacement (u_n) and strain ($y_n = u_{n+1} - u_n$) variables.

Hamiltonian can be computed explicitly for the single soliton family: $H = \sinh(2\kappa) - 2\kappa$, leading to $H'(c) = 2(\cosh(2\kappa) - 1)\partial_c\kappa > 0$, resulting in generically (spectrally) stable solitary waves in the Toda lattice. This is also in tune with the nonlinear stability of the solitary waves in this case, which has been explored, e.g., in [21].

A second famous example consists of the α-FPU case [1], where

$$V(u) = \frac{u^2}{2} - \frac{u^3}{3}, \tag{9}$$

while $\Lambda(m) = 0$. In this case too, as identified via the methods of [6–8, 22] (see Appendix B, for details on numerical simulations) and shown in Fig. 1, the family of STWs numerically features $H'(c) > 0$, in full agreement with their identification as stable. Similar conclusions hold for the highly experimentally relevant solitary waves of granular crystals [3–5].

Arguably, these cases, while interesting from the prototypically nonlinear and experimental perspectives, are perhaps somewhat less exciting from the point of view of our criterion as they do not feature a stability change. Hence, we turn to some examples which, while more exotic from the point of view of practical applications, have been argued to be of interest and, additionally, feature a change of stability, which is especially relevant in the context of this work. The first such case that we will consider concerns the Kac-Baker interactions that have been argued to be of relevance for model-

ing Coulomb interactions in DNA molecules in [13]. In this case, we maintain the potential in Eq. (9) of the FPU case, but add long-range interactions with the kernel in Eq. (8). Fig. 2 showcases the power of the stability criterion and illustrates the complementary nature of the co-traveling steady state and the periodic orbit FM calculation approaches. It can be seen that $H'(c)$ becomes negative (the top panel of Fig. 2) for $1.6709 < c < 1.6937$, for our chosen values of $\gamma = 0.17$, $\rho = 0.0172$ selected in tune with [13]. For this very interval of velocities, an eigenvalue of the operator $\mathcal{L}$ crosses through $\lambda = 0$ and acquires a positive real part (dots in the bottom panel of Fig. 2). In fact, it can be shown [10] that the stability problem in the co-traveling frame also possesses eigenvalues $\lambda + i(2\pi jc)$, where $j \in \mathbb{Z}$. Finally, the solid curve in the bottom panel of the Fig. 2 showcases the FM calculation associated with the time $T = 1/c$ map of the corresponding periodic orbit, transformed (in order to compare with the steady state eigenvalue approach) according to the relation $\lambda = \log(\mu)/T$. Confirming the complementary picture put forth, we find that in this case a FM pair crosses through $(1, 0)$ and into the real axis for the exact same parametric interval.

To connect with the theoretical analysis of Eq. (6), the inset of Fig. 2 shows the dependence of λ^2 with respect to $c - c_0$, which, according to Eq. (6), must be linear in the vicinity of $c_0 \approx 1.6937$ with the slope $\beta = H''(c_0)/(\alpha_1 c_0) = -2.9794 \times 10^{-4}$. Our numerical calculations yield $\beta = -3.0383 \times 10^{-4}$; the mismatch of $\sim 2\%$ is likely due to the fact that α_1 in Eq. (6) cannot be computed at the precise value of c_0 in the numerical setup. A similar agreement was also found in the vicinity of the other critical point at $c_0 \approx 1.6709$.

As our final example, it is interesting to explore a case where the relevant theory does not directly apply due to limited regularity. As such an example, we consider an FPU model with the potential of the form

$$V(u) = \begin{cases} \frac{u^2}{2}, & |u| \le u_c \\ \frac{\chi}{2}(|u| - u_c)^2 + u_c|u| - \frac{u_c^2}{2}, & |u| > u_c, \end{cases} \quad (10)$$

which allows construction of explicit solitary waves [14], and $\Lambda(m) = 0$; here $\chi > 1$ and $u_c > 0$. In this case the potential possesses only one continuous derivative, and hence the calculation of eigenvalues λ and FMs μ is less straightforward to justify, given the relevant jump discontinuities. Nevertheless our detailed computations, in line with the numerical results and stability conjecture in [14], are in a clear agreement with the criterion put forth analytically in this work. Namely, $H'(c) > 0$ in this case too corresponds to dynamical stability, while $H'(c) < 0$ leads to the manifestation of instability.

In order to qualitatively measure the instability, we have defined two diagnostic quantities. The first of them is the energy dispersion, given by

$$\varepsilon(t) = 1 - \frac{\bar{H}(t)}{H},$$

where $\bar{H}(t)$ is the energy at the nine central sites of the STW. In the case of a stable propagating wave, $\varepsilon(t) \sim 10^{-4}$. The other quantity is the relative velocity change defined as

$$\eta(t) = \frac{X(t) - X(0)}{tc} - 1,$$

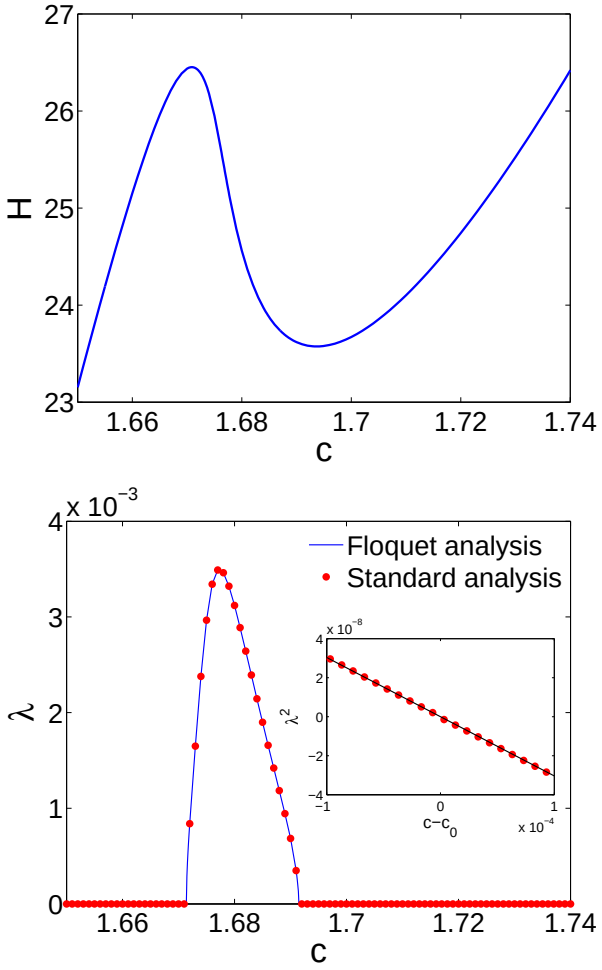

FIG. 2: Stability and instability of the lattice traveling waves in the α-FPU lattice with nearest neighbor interactions governed by the potential in Eq. (9) and Kac-Baker long-range interactions with the kernel in Eq. (8). Here $\gamma = 0.17$ and $\rho = 0.0172$. The top panel shows the energy dependence on the speed, with $H'(c) > 0$ implying (spectral) stability, and $H'(c) < 0$ implying instability. The bottom panel confirms this by showing the relevant eigenvalue obtained by diagonalizing the linearization operator $\mathcal{L}$ (dots) and transforming the relevant Floquet multiplier μ into a corresponding eigenvalue (for comparison) via the relation $\lambda = c\log(\mu)$ (solid curve). The inset of the bottom panel shows the dependence of λ^2 on $c - c_0$ for c near $c_0 = 1.6937$, the location of the second bifurcation; it fits a straight line $\lambda^2 = \beta(c - c_0)$, with $\beta = -3.0383 \times 10^{-4}$.

with $X(t)$ being the energy center of the STW.

The top panel of Fig. 3 shows the curve $H(c)$ for the FPU model with the potential of Eq. (10) and parameters $\chi = 4$ and $u_c = 1$; the bottom panels of this figure display the dependence of $\varepsilon_\infty \equiv \varepsilon(2000T)$ and $\eta_\infty \equiv \eta(2000T)$ with respect to c. In accordance with our stability criterion, $\varepsilon_\infty \sim 10^{-4}$ in the region for which $H'(c) > 0$, confirming a stable propagation. In the region with $H'(c) < 0$ there are three intervals of high dispersion, as measured by corresponding values of ε, and two intervals where the dispersion drops to low values. The region of low dispersion corresponds to STWs whose

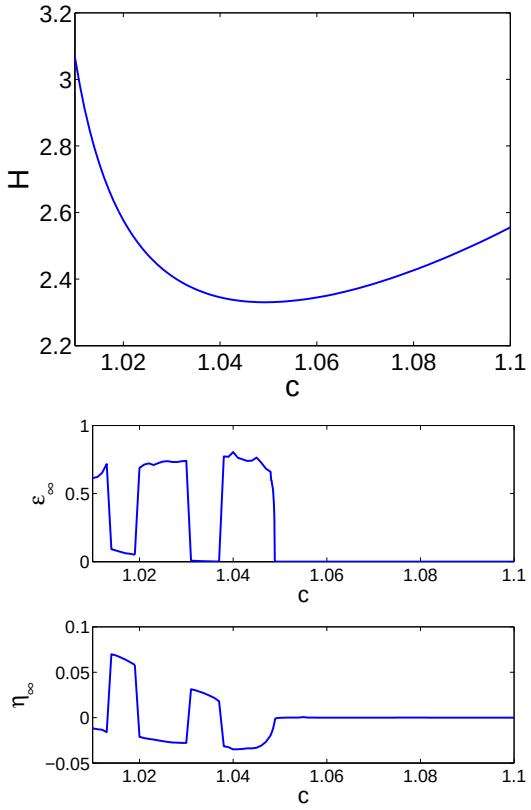

FIG. 3: Stability and instability of the lattice traveling waves of the model of [14] with the potential in Eq. (10). Here $\chi = 4$ and $u_c = 1$. The top panel displays the $H(c)$ dependence, which possesses a minimum at $c = c_0 = 1.0493$. The bottom panels show the dependence of the energy dispersion ε_∞ and relative velocity change η_∞ (see the text) with respect to the velocity c, which manifest the instability of solitary waves with $c < c_0$, where c_0 is such that $H'(c_0) = 0$.

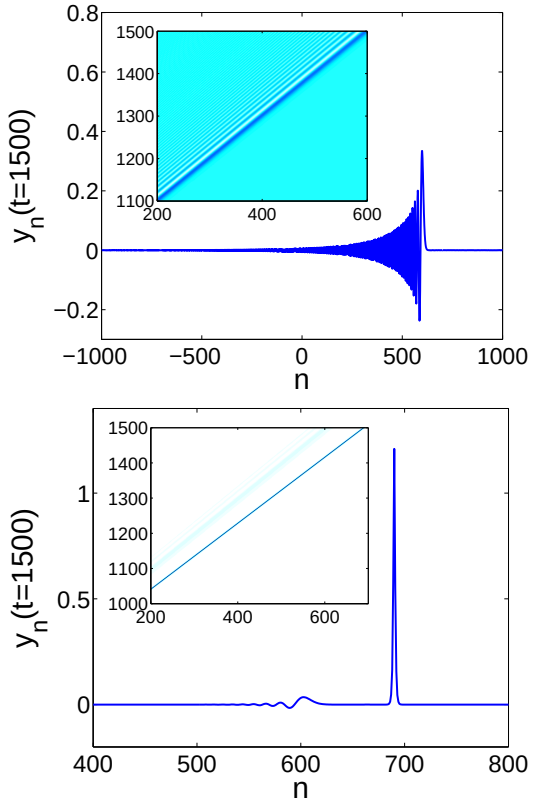

FIG. 4: Evolution of unstable travelling waves in the model of [14] with the potential in Eq. (10). Here $\chi = 4$ and $u_c = 1$. The panels show the profile of the strains $y_n(t) = u_{n+1}(t) - u_n(t)$ at $t = 1500$ and zooms in the space-time evolution dynamics of the strains are represented in the insets. Top and bottom panels correspond to $c = 1.025$ and $c = 1.034$, respectively. In the the example shown in the bottom panel, the velocity eventually oscillates in time around an average value of 1.0626.

velocity is higher than the initial one (indeed, higher than the critical one and hence reverting to the stable propagation regime). Fig. 4 shows the evolution of unstable STWs in two cases, corresponding to high ($c = 1.025$) and low ($c = 1.034$) dispersion. In the former, linear waves are continuously being created and the STW degrades with time; in the latter, a linear wave is expelled from the STW, which transforms into a wave with a different (now in the stable regime of $c > c_0$) velocity. Note that in addition to demonstrating instability of waves with $c < c_0$, these results suggest the potential bistability between dispersive waveforms and STWs with $c > c_0$.

V. CONCLUSIONS AND FUTURE CHALLENGES

In summary, in this work we have presented a unified perspective connecting the stability of lattice solitary traveling waves with that of discrete breathers of an appropriate map involving running for the time associated with moving by one lattice site and shifting back. We have also concisely established a (sufficient but not necessary) criterion for the change in spectral stability of the Hamiltonian lattice STWs that seems to be in very good agreement with numerical observations and to constitute a natural extension of a criterion recently put forth for the spectral stability of discrete breathers. The specific eigenvalue responsible for the instability was theoretically identified and favorably compared to detailed numerical computations.

Nevertheless, there are numerous problems that remain open for future consideration. One relevant issue concerns the fact that the FM computation leads to as many multipliers as lattice points, while the computation of eigenvalues for a STW involves a partial differential equation (PDE). While the latter will capture the lattice instabilities, it may also feature instabilities *absent* on the lattice, which are a by-product of this PDE's ability to resolve scales smaller than h. Hence, a more systematic connection between the spectra of the two problems (and of the instabilities that each may feature) is of paramount importance. Observe also that while this work dealt with families of STWs parameterized by velocity, in some cases such entities occur for isolated velocity values [23, 24], potentially being members of a wider family

encompassing waveforms with non-vanishing tails. It would be interesting to explore whether our considerations can be extended to such cases. Another question is that of going to the continuum limit: our proof did not directly use the underlying lattice nature of the system (only its time reversal invariance). On the other hand, in the continuum limit, symmetries (like Galilean or Lorentz invariance) may arise. Future work will involve reconciling these two features in a consistent continuum limit picture, as well as connecting our criterion with well-established existing stability criteria, such as [25–27], in continuum systems. Finally, analysis of the stability of lattice STWs in systems with limited regularity, such as our last example, also merits future consideration.

Acknowledgments

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Appendix A: Proof of the leading-order approximation of the near-zero eigenvalues

In this Appendix we prove Eq. (6) in Sec. II, which provides the leading-order approximation of the eigenvalues splitting away from zero at velocities near the critical value c_0.

First, we observe that while we consider a lattice Hamiltonian system in the displacement form (2), the problem can be alternatively formulated in terms of strain variables $y_n(t) = (S^{-1} - I)u_n(t) = u_{n+1}(t) - u_n(t)$, where we recall from Sec. III that S denotes the shift operator such that $Su_n(t) = u_{n-1}(t)$. If the Hamiltonian energy density can be written as $\mathcal{H}(y, p, t)$, we have, for $Y = (y, p)^T$,

$$\frac{dY}{dt} = J_1 \nabla \mathcal{H}(Y), \quad J_1 = \begin{pmatrix} 0 & S^{-1} - I \\ I - S & 0 \end{pmatrix}. \tag{A1}$$

In what follows, we focus on the formulation (2), but our arguments also work for Eq. (A1).

Suppose Eq. (2) has a family of solitary traveling-wave solutions $U(t; c)$ parametrized by the velocity c taking values in some continuous interval. Then

$$U(t; c) = \hat{U}(\xi; c) = \begin{pmatrix} \hat{u}(\xi) \\ \hat{p}(\xi) \end{pmatrix}, \quad \xi = n - ct,$$

where ξ is the co-traveling frame variable and $\hat{p}(\xi; c) = -c\partial_\xi \hat{u}(\xi; c)$. Considering the ansatz

$$U(\xi, t) = \begin{pmatrix} \hat{u}(\xi) \\ \hat{p}(\xi) \end{pmatrix} + \epsilon e^{\lambda t} \begin{pmatrix} W(\xi) \\ P(\xi) \end{pmatrix} = \hat{U}(\xi) + \epsilon e^{\lambda t} Z(\xi)$$

with small ϵ and linearizing around the traveling wave $\hat{U}$, we obtain Eq. (3), where the operator $\mathcal{L}$ and its adjoint $\mathcal{L}^*$ are given by Eq. (4) and Eq. (5), respectively.

Suppose $\hat{U} \in H^1(\mathbb{R}^2)$, so that its partial derivatives in ξ and c are in $L^2(\mathbb{R}^2)$. While this assumption implies that the displacements are localized, for problems with kink-type traveling waves in terms of displacement that tend to nonzero constant limits at infinity, we can use the strain formulation (A1), in which case we assume that the traveling wave solution $\hat{Y} \in H^1(\mathbb{R}^2)$, i.e., the strains are localized. One can show that the operator $\mathcal{L}$ is densely defined on $L^2(\mathbb{R}^2)$. By differentiating Eq. (2) in ξ and c, respectively, we find that $\mathcal{L}e_0 = 0$ and $\mathcal{L}e_1 = e_0$, where $e_0 = -\partial_\xi \hat{U}$ and $e_1 = \partial_c \hat{U}$ (or, more generally, $e_1 = \partial_c \hat{U} + d_{10}e_0$, where d_{10} is any constant), implying that the algebraic multiplicity of the eigenvalue $\lambda = 0$ for $\mathcal{L}$ is at least two. Let c_0 denote the critical velocity such that $H'(c_0) = 0$. Then $\langle e_1, J^{-1}e_0\rangle = 0$ at this critical value, and there exists e_2 such that $\mathcal{L}e_2 = e_1$. Since

$$\begin{aligned} \langle e_2, J^{-1}e_0\rangle &= \langle e_2, J^{-1}\mathcal{L}e_1\rangle = \langle J^{-1}\mathcal{L}e_2, e_1\rangle \\ &= \langle J^{-1}e_1, e_1\rangle = 0, \end{aligned}$$

we have $e_2 \in (\ker(\mathcal{L}^*))^\perp = \mathrm{im}(\mathcal{L})$, so e_2 belongs to the range of $\mathcal{L}$, and hence there exists e_3 such that $\mathcal{L}e_3 = e_2$. Assuming that the zero eigenvalue of $\mathcal{L}$ at c_0 is exactly quadruple, which is the generic case for traveling waves in Hamiltonian lattices due to symmetry, we have

$$\alpha_1 = \langle e_0, J^{-1}e_3\rangle = -\langle e_1, J^{-1}e_2\rangle \neq 0. \tag{A2}$$

We now consider a neighborhood of the critical speed $c = c_0$ where the derivative $H'(c)$ changes its sign. Assuming that $\hat{U}(\xi; c)$ is sufficiently smooth in c near $c = c_0$, we have the expansion $\hat{U}(\xi; c_0 + \epsilon) = U_0 + \epsilon U_1 + \epsilon^2 U_2 + \dots$ for small enough ϵ, where $U_0 = \hat{U}(\xi; c_0)$, $U_1 = (\partial_c \hat{U}(\xi; c))|_{c=c_0}$ and $U_2 = \frac{1}{2}(\partial_{cc}\hat{U}(\xi; c))|_{c=c_0}$. Accordingly, the operator $\mathcal{L}$ at $c = c_0 + \epsilon$ can be written as $\mathcal{L} = \mathcal{L}_0 + \epsilon\mathcal{L}_1 + \epsilon^2\mathcal{L}_2 + \dots$. Let $\{e_0, e_1, e_2, e_3\}$ be the eigenfunction and generalized eigenfunctions of $\mathcal{L}_0$ for $\lambda = 0$ such that

$$\mathcal{L}_0^3 e_3 = \mathcal{L}_0^2 e_2 = \mathcal{L}_0 e_1 = e_0 = -\partial_\xi \hat{U}(\xi; c_0).$$

We then define the following constants:

$$K_{jk} = \langle J^{-1}e_j, \mathcal{L}_1 e_k\rangle, \quad L_{jk} = \langle J^{-1}e_j, \mathcal{L}_2 e_k\rangle. \tag{A3}$$

Remark 1 *If the generalized kernel of $\mathcal{L}_0$ is exactly four-dimensional, then only the cases $\lambda \sim \epsilon^{1/2}$ and $\lambda \sim \epsilon$ are possible.*

Indeed, this follows from the fact that two of the four eigenvalues of $\mathcal{L}$ are always zero. It suffices to calculate the leading-order terms of the eigenvalues for the perturbed operator $\mathcal{L}$ at $c = c_0 + \epsilon$. By restricting the operator in the invariant subspace $G_4 = \mathrm{cl}(\mathrm{span}\{e_0, e_1, e_2, e_3\})$, the question reduces to the perturbation of the matrix

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

with two constraints that hold for any c,

$$\mathcal{L}(\partial_\xi \hat{U}(\xi;c)) = 0 \tag{A4}$$

and

$$\mathcal{L}(\partial_c \hat{U}(\xi;c)) = -(\partial_\xi \hat{U}(\xi;c)). \tag{A5}$$

Note that the characteristic polynomial of the unperturbed matrix A is $\lambda^4 = 0$. For the matrix A with $O(\epsilon)$ perturbation, the characteristic polynomial is $\lambda^4 + a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 = 0$ where the coefficients a_j are at most $O(\epsilon)$. Moreover, due to two existing constraints in Eq. (A4) and Eq. (A5), two of the eigenvalues are always zero, so we have $\lambda^2(\lambda^2 + a_3\lambda + a_2) = 0$. Thus, either $\lambda \sim \epsilon^{1/2}$ (if $a_2 \neq 0$) or $\lambda \sim \epsilon$ (if $a_2 = 0$).

Here we focus on the case $\lambda \sim \epsilon^{1/2}$ and show below that it requires $H''(c_0) \neq 0$. Since Eq. (A4) holds for any c, direct calculation shows that

$$\begin{aligned} 0 &= \mathcal{L}_0(\partial_\xi U_0), && \text{(A6)}\\ 0 &= \mathcal{L}_0(\partial_\xi U_1) + \mathcal{L}_1(\partial_\xi U_0), && \text{(A7)}\\ 0 &= \mathcal{L}_0(\partial_\xi U_2) + \mathcal{L}_1(\partial_\xi U_1) + \mathcal{L}_2(\partial_\xi U_0). && \text{(A8)} \end{aligned}$$

Moreover, utilizing the fact that (A5) is true for any c, one can expand both sides in ϵ and obtain

$$\begin{aligned} \mathcal{L}_0 U_1 &= -\partial_\xi U_0, && \text{(A9)}\\ 2\mathcal{L}_0 U_2 + \mathcal{L}_1 U_1 &= -\partial_\xi U_1. && \text{(A10)} \end{aligned}$$

Since $H'(c_0) = 0$, we can write $H(c) = H(c_0) + \frac{\epsilon^2}{2} H''(c_0) + o(\epsilon^2)$, where

$$\begin{aligned} &H''(c_0) = \nabla H \cdot 2U_2 + U_1 \cdot \nabla^2 H U_1 \\ &= \int [c_0 J^{-1}(e_0) \cdot 2U_2 + U_1 \cdot J^{-1}(\mathcal{L}_0 - c_0\partial_\xi) U_1] d\xi \\ &= \int [c_0 J^{-1}\mathcal{L}_0 U_1 \cdot 2U_2 + U_1 \cdot (J^{-1}\mathcal{L}_0 U_1 - c_0 J^{-1}\partial_\xi U_1)] d\xi \\ &= \int U_1 \cdot (J^{-1}e_0) d\xi + c_0 \int U_1 \cdot J^{-1}(\mathcal{L}_0 2U_2 - \partial_\xi U_1) d\xi \\ &= c_0 \int U_1 \cdot J^{-1}(-2\partial_\xi U_1 - \mathcal{L}_1 U_1) d\xi \\ &= -c_0 \int \mathcal{L}_0 e_2 \cdot J^{-1} 2\partial_\xi U_1 d\xi - c_0 \int e_1 \cdot J^{-1}\mathcal{L}_1 e_1 d\xi \\ &= -c_0 \int e_2 \cdot (-1) J^{-1}\mathcal{L}_0 2\partial_\xi U_1 d\xi - c_0 \int e_1 \cdot J^{-1}\mathcal{L}_1 e_1 d\xi \\ &= c_0 \int e_2 \cdot J^{-1}\mathcal{L}_1 2e_0 d\xi - c_0 \int e_1 \cdot J^{-1}\mathcal{L}_1 e_1 d\xi \\ &= -c_0(2K_{20} - K_{11}). \end{aligned} \tag{A11}$$

Assuming $\lambda = \epsilon^{1/2}\lambda_1 + \epsilon\lambda_2 + \epsilon^{3/2}\lambda_3 + \dots$ and $Z = Z_0 + \epsilon^{1/2}Z_1 + \epsilon Z_2 + \epsilon^{3/2}Z_3 + \dots$ and substituting these into Eq. (3), we obtain

$$0 = \mathcal{L}_0 Z_0, \tag{A12}$$

$$\lambda_1 Z_0 = \mathcal{L}_0 Z_1, \tag{A13}$$

$$\lambda_1 Z_1 + \lambda_2 Z_0 = \mathcal{L}_0 Z_2 + \mathcal{L}_1 Z_0, \tag{A14}$$

$$\lambda_1 Z_2 + \lambda_2 Z_1 + \lambda_3 Z_0 = \mathcal{L}_0 Z_3 + \mathcal{L}_1 Z_1, \tag{A15}$$

$$\begin{aligned} \lambda_1 Z_3 + \lambda_2 Z_2 + \lambda_3 Z_1 + \lambda_4 Z_0 = \mathcal{L}_0 Z_4 + \mathcal{L}_1 Z_2 \\ + \mathcal{L}_2 Z_0. \end{aligned} \tag{A16}$$

From Eq. (A12), we find that $Z_0 = -\partial_\xi \hat{U}(\xi; c_0) = e_0$. Then Eq. (A13) suggests that $Z_1 = \lambda_1 e_1 + d_{10} e_0$, where d_{10} is a constant. Note that Z_2 and Z_3 can be written as

$$Z_2 = \sum_{j=0}^{3} (d_{2j} e_j) + Z_2^\perp, \quad Z_3 = \sum_{j=0}^{3} (d_{3j} e_j) + Z_3^\perp,$$

where $Z_2^\perp$ and $Z_3^\perp$ are in $G_4^\perp$, and d_{2j}, d_{3j}, $j = 0, \dots, 3$ are constants. Projecting Eq. (A14) onto $J^{-1}e_0$ yields $\lambda_1\langle J^{-1}e_0, Z_1\rangle + \lambda_2\langle J^{-1}e_0, Z_0\rangle = K_{00}$. The left hand side is zero since $H'(c_0) = 0$, and one can show that the right hand side vanishes ($K_{00} = 0$) upon considering Eq. (A7). Projecting Eq. (A14) onto $J^{-1}e_1$ and recalling Eq. (A2), we obtain $d_{23}\langle J^{-1}e_1, e_2\rangle + K_{10} = d_{23}\alpha_1 + K_{10} = 0$, so

$$d_{23} = -\frac{K_{10}}{\alpha_1}. \tag{A17}$$

Projecting Eq. (A14) onto $J^{-1}e_2$ and using (A2), we find that $d_{22}\langle J^{-1}e_2, e_1\rangle + K_{20} = -d_{22}\alpha_1 + K_{20} = -\lambda_1^2\alpha_1$, and thus

$$d_{22} = \lambda_1^2 + \frac{K_{20}}{\alpha_1}. \tag{A18}$$

Projecting Eq. (A14) onto $J^{-1}e_3$, we have

$$d_{21}\alpha_1 + d_{23}\alpha_2 + K_{30} = (d_{10}\lambda_1 + \lambda_2)\alpha_1, \tag{A19}$$

where we used Eq. (A2) and set $\alpha_2 = \langle J^{-1}e_3, e_2\rangle$. Projecting Eq. (A15) onto $J^{-1}e_0$ yields $\lambda_1 d_{23}\langle J^{-1}e_0, e_3\rangle = -\lambda_1 d_{23}\alpha_1 = \lambda_1 K_{01}$, which again yields Eq. (A17) since $K_{01} = K_{10}$. Projecting Eq. (A15) onto $J^{-1}e_1$, we obtain

$$d_{33}\alpha_1 + \lambda_1 K_{11} + d_{10}K_{10} = \lambda_1 d_{22}\alpha_1. \tag{A20}$$

Finally, projection of Eq. (A16) onto $J^{-1}e_0$ yields

$$\begin{aligned} d_{21}K_{01} + d_{22}K_{02} + d_{23}K_{03} + L_{00} \\ = -\alpha_1(\lambda_1 d_{33} + \lambda_2 d_{23}). \end{aligned} \tag{A21}$$

Using the equations (A17), (A18), (A19), (A20), (A21) along with the fact that K is symmetric, we obtain

$$\begin{aligned} &\alpha_1\lambda_1^4 + (2K_{20} - K_{11})\lambda_1^2 \\ &\quad + (L_{00} + \frac{K_{20}^2}{\alpha_1} + \frac{\alpha_2 K_{10}^2}{\alpha_1^2} - \frac{2K_{10}K_{30}}{\alpha_1}) = 0. \end{aligned}$$

Since two eigenvalues are always zero, this equation should have two zero roots. This implies

$$L_{00} + \frac{K_{20}^2}{\alpha_1} + \frac{\alpha_2 K_{10}^2}{\alpha_1^2} - \frac{2K_{10}K_{30}}{\alpha_1} = 0,$$

which can also be shown directly using projections of Eq. (A7) onto $J^{-1}e_j$, $j = 0, \ldots, 3$, and projection of Eq. (A8) onto $J^{-1}e_0$. We then obtain

$$\lambda_1^2 = -\frac{2K_{20} - K_{11}}{\alpha_1} = \frac{H''(c_0)}{\alpha_1 c_0}.$$

Thus, for $\lambda \sim \epsilon^{1/2}$ it is necessary to have $H''(c_0) \neq 0$, and the behavior of the two eigenvalues splitting away from zero at $c \neq c_0$ is described by Eq. (6) in Sec. II.

Appendix B: Numerical methods for computing solitary traveling waves

In this Appendix, we describe the numerical procedures we used to compute solitary waves in a lattice with the Hamiltonian in Eq. (7) and analyze their stability. The governing equations corresponding to Eq. (7) are

$$\begin{aligned}\ddot{u}_n - V'(u_{n+1} - u_n) + V'(u_n - u_{n-1}) \\ + \sum_{m=1}^{\infty} \Lambda(m)(2u_n - u_{n+m} - u_{n-m}) = 0,\end{aligned} \tag{B1}$$

where the overdots here and in what follows denote the time derivatives. Since the solitary solutions we consider are kink-like in terms of displacement, it is more convenient to rewrite Eq. (B1) in terms of the strain variables $y_n = u_{n+1} - u_n$, obtaining

$$\begin{aligned}\ddot{y}_n + 2V'(y_n) - V'(y_{n+1}) - V'(y_{n-1}) \\ + \sum_{m=1}^{\infty} \Lambda(m)(2y_n - y_{n+m} - y_{n-m}) = 0.\end{aligned} \tag{B2}$$

To find solitary traveling wave solutions, we use the procedure followed in [28]. To this end, we seek solutions of Eq. (B2) in the co-traveling frame corresponding to velocity c:

$$y_n(t) = \Phi(\xi, t), \quad \xi = n - ct,$$

obtaining the advance-delay partial differential equation

$$\begin{aligned}&\Phi_{tt} + c^2\Phi_{\xi\xi} - 2c\Phi_{\xi t} \\ &= V'(\Phi(\xi+1,t)) + V'(\Phi(\xi-1,t)) - 2V'(\Phi(\xi,t)) \\ &- \sum_{m=1}^{\infty} \Lambda(m)(2\Phi(\xi,t) - \Phi(\xi+m,t) - \Phi(\xi-m,t)).\end{aligned} \tag{B3}$$

Traveling waves $\phi(\xi)$ are stationary solutions of Eq. (B3). They satisfy the advance-delay differential equation

$$\begin{aligned}&c^2\phi''(\xi) + 2V'(\phi(\xi)) - V'(\phi(\xi+1)) - V'(\phi(\xi-1)) \\ &+ \sum_{m=1}^{\infty} \Lambda(m)(2\phi(\xi) - \phi(\xi+m) - \phi(\xi-m)) = 0.\end{aligned} \tag{B4}$$

Solitary traveling waves are solutions that in addition satisfy

$$\lim_{\xi \to \pm\infty} \phi(\xi) = 0. \tag{B5}$$

Following the approach in [7], we assume that $\phi(\xi) = o(1/\xi)$ and $\phi'(\xi) = o(1/\xi^2)$ as $|\xi| \to \infty$, multiply Eq. (B4) by ξ^2 and integrate by parts to derive the identity

$$\left[c^2 - \sum_{m=1}^{\infty} m^2\Lambda(m)\right] \int_{-\infty}^{\infty} \phi(\xi)\mathrm{d}\xi - \int_{-\infty}^{\infty} V'(\phi(\xi))\mathrm{d}\xi = 0, \tag{B6}$$

which imposes the constraint (B5) on the traveling wave solutions. Here we assume that $\Lambda(m)$ decays faster than $1/m^3$ at infinity, so that the series on the left hand side converges.

To solve Eq. (B4) numerically, we introduce a discrete mesh with step $\Delta\xi$, where $1/\Delta\xi$ is an integer, so that the advance and delay terms $\phi(\xi \pm m)$ are well defined on the mesh. We then use a Fourier spectral collocation method for the resulting system with periodic boundary conditions [29] with large period L. Implementation of this method requires an even number $\mathcal{N}$ of collocation points $\xi_j \equiv j\Delta\xi$, with $j = -\mathcal{N}/2 + 1, \ldots, \mathcal{N}/2$, yielding a system for ξ in the domain $(L/2, L/2]$, with $L = \mathcal{N}\Delta\xi$ being an even number, and the long-range interactions are appropriately truncated. To ensure that the solutions satisfy Eq. (B5), we additionally impose a trapezoidal approximation of Eq. (B6) on the truncated interval at the collocation points. This procedure is independent of the potential and the interaction range. However, the choices of $\Delta\xi$ and L depend on the nature of the problem. In the particular cases considered in the paper, we used $\Delta\xi = 0.1$, $L = 800$ for the α-FPU lattice with nearest-neighbor potential in Eq. (9) and Kac-Baker long-range interactions with coefficients in Eq. (8) and $\Delta\xi = 0.025$, $L = 200$ for the FPU lattice with piecewise quadratic short-range interaction potential in Eq. (10) and no long-range interactions.

To investigate spectral stability of an obtained traveling wave $\phi(\xi)$, we substitute

$$\Phi(\xi, t) = \phi(\xi) + \epsilon a(\xi)\exp(\lambda t),$$

into Eq. (B3) and consider $O(\epsilon)$ terms resulting from this perturbation. This yields the following quadratic eigenvalue problem:

$$\begin{aligned}\lambda^2 a(\xi) = &-c^2 a''(\xi) + 2\lambda c a'(\xi) - 2V''(\phi(\xi))a(\xi) \\ &+ V''(\phi(\xi+1))a(\xi+1) + V''(\phi(\xi-1))a(\xi-1) \\ &- \sum_{m=1}^{\infty} \Lambda(m)(2a(\xi) - a(\xi+m) - a(\xi-m)).\end{aligned} \tag{B7}$$

By defining $b(\xi) = \lambda a(\xi)$, we transform this equation into the regular eigenvalue problem

$$\lambda \begin{pmatrix} a(\xi) \\ b(\xi) \end{pmatrix} = \mathcal{M} \begin{pmatrix} a(\xi) \\ b(\xi) \end{pmatrix} \tag{B8}$$

for the corresponding linear advance-delay differential operator $\mathcal{M}$. Note that this problem is equivalent to the eigenvalue problem (3) via the transformation $(a(\xi), b(\xi)) =$

$(W(\xi), P(\xi) + cW'(\xi))$. Spectral stability can be determined by analyzing the spectrum of the operator $\mathcal{M}$ after discretizing the eigenvalue problem the same way as the nonlinear Eq. (B4) and again using periodic boundary conditions. A solution is stable when the spectrum contains no real eigenvalues.

An alternative method for determining the stability of the traveling waves is to use Floquet analysis. To this end, we cast traveling waves $\phi(\xi)$ as fixed points of the map

$$\begin{bmatrix} \{y_{n+1}(T)\} \\ \{\dot{y}_{n+1}(T)\} \end{bmatrix} \to \begin{bmatrix} \{y_n(0)\} \\ \{\dot{y}_n(0)\} \end{bmatrix}, \tag{B9}$$

which is periodic modulo shift by one lattice point, with period $T = 1/c$. Indeed, one easily checks that $\hat{y}_n(t) = \phi(n - ct) = \phi(n - t/T)$ satisfies $\hat{y}_{n+1}(T) = \hat{y}_n(0) = \phi(n)$ and $\dot{\hat{y}}_{n+1}(T) = \dot{\hat{y}}_n(0) = -c\phi'(n)$. To apply the Floquet analysis, we trace time evolution of a small perturbation $\epsilon w_n(t)$ of the periodic-modulo-shift (traveling wave) solution $\hat{r}_n(t)$. This perturbation is introduced in Eq. (B2) via $y_n(t) = \hat{y}_n(t) + \epsilon w_n(t)$. The resulting $O(\epsilon)$ equation reads

$$\ddot{w}_n + 2V''(\hat{y}_n)w_n - V''(\hat{y}_{n+1})w_{n+1} - V''(\hat{y}_{n-1})w_{n-1} + \sum_{m=1}^{\infty} \Lambda(m)(2w_n - w_{n+m} - w_{n-m}) = 0. \tag{B10}$$

Then, in the framework of Floquet analysis, the stability properties of periodic orbits are resolved by diagonalizing the monodromy matrix $\mathcal{F}$ (representation of the Floquet operator for finite systems), which is defined as:

$$\begin{bmatrix} \{w_{n+1}(T)\} \\ \{\dot{w}_{n+1}(T)\} \end{bmatrix} = \mathcal{F} \begin{bmatrix} \{w_n(0)\} \\ \{\dot{w}_n(0)\} \end{bmatrix}. \tag{B11}$$

For the symplectic Hamiltonian systems considered in this work, the linear stability of the solutions requires that the monodromy eigenvalues μ (also called Floquet multipliers) lie on the unit circle. The Floquet multipliers can thus be written as $\mu = \exp(i\theta)$, with Floquet exponent θ.

Note that the two procedures for analyzing spectral stability described above require the potential $V(u)$ to be twice differentiable, as in the case of the α-FPU problem considered in Sec. IV. Due to the absence of such regularity in the case of the piecewise quadratic potential in Eq. (10), the examination of stability was performed solely on the basis of direct numerical simulations. Specifically, it was analyzed by means of tracking the dynamics of a slightly perturbed solution $[\{\hat{y}_n(0)\}, \{\dot{\hat{y}}_n(0)\}]$. To this aim, the fourth order explicit and symplectic Runge-Kutta-Nyström method developed in [30], with time step equal to 10^{-3}, was used.

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