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Standing wave instabilities, breather formation and thermalization in a Hamiltonian anharmonic lattice

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Abstract. Modulational instability of travelling plane waves is often considered as the first step in the formation of intrinsically localized modes (discrete breathers) in anharmonic lattices. Here, we consider an alternative mechanism for breather formation, originating in oscillatory instabilities of spatially periodic or quasiperiodic nonlinear standing waves (SWs). These SWs are constructed for Klein-Gordon or Discrete Nonlinear Schrödinger lattices as exact time periodic and time reversible multibreather solutions from the limit of uncoupled oscillators, and merge into harmonic SWs in the small-amplitude limit. Approaching the linear limit, all SWs with nontrivial wave vectors ($0 < Q < \pi$) become unstable through oscillatory instabilities, persisting for arbitrarily small amplitudes in infinite lattices. The dynamics resulting from these instabilities is found to be qualitatively different for wave vectors smaller than or larger than $\pi/2$, respectively. In one regime persisting breathers are found, while in the other regime the system thermalizes.

PACS. 63.20.Ry Anharmonic lattice modes – 45.05.+x General theory of classical mechanics of discrete systems – 05.45.-a Nonlinear dynamics and nonlinear dynamical systems

We review some recent results concerning the role of a certain class of exact solutions, *Standing Waves (SWs)* in the dynamics of Hamiltonian anharmonic lattices. The SWs are time-periodic non-propagating solutions, which are periodic or quasiperiodic in space. We showed in [1] that such solutions are unstable through oscillatory instabilities under quite general conditions. Here, the main ideas from [1] will be recalled, and further we will describe the long-time dynamics resulting from the instabilities, identifying their role in the processes of breather formation and thermalization. Further details appear in [2,3].

We will here mainly focus on the model described by the discrete nonlinear Schrödinger (DNLS) equation:

$$i\dot{\psi}_n = \delta\psi_n - \sigma|\psi_n|^2\psi_n + C(\psi_{n+1} + \psi_{n-1} - 2\psi_n). \quad (1)$$

The DNLS equation describes generically the slow small-amplitude dynamics of Klein-Gordon (KG) chains of coupled anharmonic oscillators with weak intersite coupling [4,5,2]. In this context, ψ_n is proportional to the fundamental Fourier harmonic of the amplitude of the oscillator at site n, δ represents the nonlinear frequency shift, and $\sigma = -1$ ($\sigma = +1$) for soft (hard) anharmonicity. The DNLS equation also appears in many other contexts, *e.g.* in models for nonlinear optical waveguide arrays [6].

In the KG model, SWs are time-periodic solutions which can be chosen time reversible, reducing for small amplitudes to the harmonic form $\epsilon\cos(Qn + \phi)\cos(\omega t)$[1]. Thus, all Fourier components are real and time independent, so that the (generally complex) amplitude ψ_n representing a SW in the DNLS approximation (1) also can be chosen real and time independent. Consequently, the SWs can be identified as bounded trajectories of the 2D real symplectic cubic map $(\psi_{n-1}, \psi_n) \to (\psi_n, \psi_{n+1})$ defined by

$$\psi_{n+1} = (2 - \frac{\delta}{C})\psi_n + \frac{\sigma}{C}\psi_n^3 - \psi_{n-1}. \quad (2)$$

We can choose $\sigma = -1$ and $C > 0$ without loss of generality. Rescaling $\psi_n \to \sqrt{C}\psi_n$, it is clear that the qualitative properties of the map only depend on the parameter $\frac{\delta}{C}$.

An illustration of this map is given in Figure 1 (*cf.* [9]). Among all trajectories we consider those which, when

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[1] By contrast, *propagating waves* in the KG model are continuations of harmonic plane-waves $\epsilon\cos(Qn - \omega t)$ [7,8].

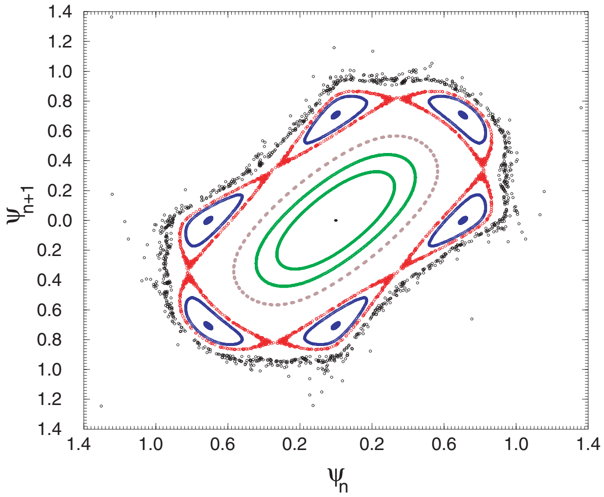

Fig. 1. The DNLS map (2) for $\sigma = -1$, $\delta = 0.5$, $C = 1$.

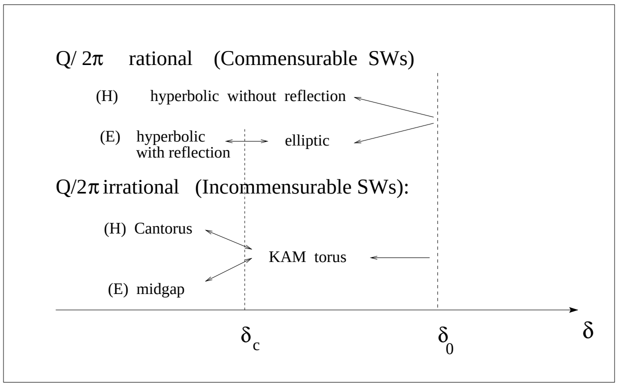

Fig. 2. Classification of SW map trajectories ($\sigma = -1$).

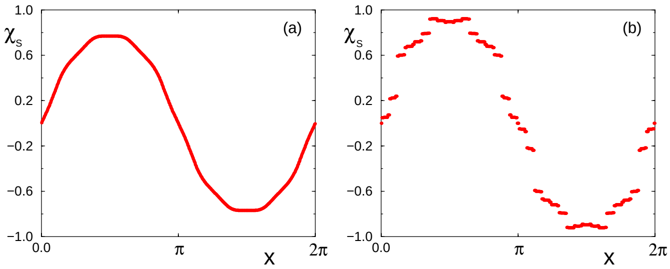

Fig. 3. SW hull functions $\psi_n = \chi_S(Qn + \phi)$ for $Q/2\pi = 233/610 \simeq (3 - \sqrt{5})/2$. (a) $\delta = 3.0$; (b) $\delta = 2.8$. $C = 1$.

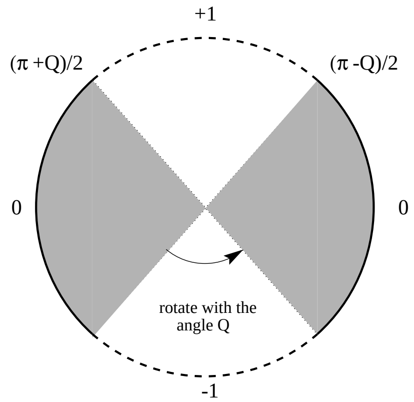

Fig. 4. Circle map generation of the SW coding sequences.

varying $\frac{\delta}{C}$ at fixed rotation number Q, are smoothly continued to the fixpoint (0,0) into a *linear* SW at $\delta = 4C\sin^2 Q/2 \equiv \delta_0(Q)$. These are either periodic cycles corresponding to SWs *commensurate* with the lattice, or quasiperiodic trajectories yielding *incommensurate* SWs. For any Q, SWs exist for *all* $\delta < \delta_0(Q)$ when $\sigma = -1$. Moreover, the large-amplitude limit $\delta \to -\infty$ is equivalent to the uncoupled (*anticontinuous* [10]) limit $C = 0$ for fixed $\delta < 0$.

The evolution of the trajectories corresponding to different types of SWs with fixed wave vector Q when varying $\frac{\delta}{C}$ is summarized in Figure 2. As for any rational $Q/2\pi$ there are always two distinct periodic cycles (hyperbolic resp. elliptic for δ close to $\delta_0(Q)$), there are two distinct classes of commensurate SWs. For (typical) irrational $Q/2\pi$, there is a unique KAM-torus for δ close to $\delta_0(Q)$ representing an incommensurate SW. At some critical value $\delta_c(Q)$ the elliptic cycle with rotation number Q ($Q/2\pi$ rational) becomes hyperbolic with reflection, while the smooth, analytic KAM torus with irrational $Q/2\pi$ breaks up into a trajectory with a Cantor set structure ('Cantorus') and another trajectory with the same Q consisting of isolated, nonrecurrent points in the gaps of the cantorus ('midgap trajectory') [11]. This break-up constitutes a Transition by Breaking of Analyticity (TBA) [11]. Defining the 2π-periodic *hull* (envelope) *function* $\chi_S(x)$ for a SW as $\psi_n = \chi_S(Qn + \phi)$ (*i.e.* the shape of the wave rescaled into one period 2π), the TBA at $\delta_c(Q)$ for this hull function for an incommensurate SW is manifested as shown in Figure 3.

When $C = 0$, a time-independent solution to equation (1) can only take three possible values: $\psi_n = \pm\sqrt{-\delta}$ or $\psi_n = 0$. This defines a *coding sequence* $\{\tilde{\sigma}_n\}$ as $\tilde{\sigma}_n = \pm 1$ when $\psi_n = \pm\sqrt{-\delta}$ and $\tilde{\sigma}_n = 0$ when $\psi_n = 0$. Time-periodic solutions defined *via* a coding sequence and continued from an anticontinuous limit are generally called *multibreathers* [10]. Continuing the SW map trajectories to $\frac{\delta}{C} \to -\infty$, their coding sequences are found as generated by a circle map $\tilde{\sigma}_n = \chi_0(Qn + \phi)$ (*cf.* Fig. 4), with a 2π-periodic odd function $\chi_0(x)$ defined for $x \in [0, \pi]$ as

$$\chi_0(x) = \begin{cases} 1 & \text{for } (\pi - Q)/2 \le x \le (\pi + Q)/2, \\ 0 & \text{elsewhere.} \end{cases} \tag{3}$$

(The function $\chi_0(x)$, rescaled with a factor $\sqrt{-\delta}$, is the limit for $C = 0$ of the hull function $\chi_S(x)$ defined above.) The two classes of SWs for each Q are distinguished by the phase ϕ (corresponding to the initial point of the iteration). For all $\phi \ne \phi_m \equiv \pm(\pi - Q)/2 - mQ$ (m integer) we obtain the SWs classified as '(H)' in Figure 2, while for $\phi = \phi_m$ we obtain SWs denoted as '(E)'. They differ by the property that, as $x = Qm + \phi$ is at a discontinuity of

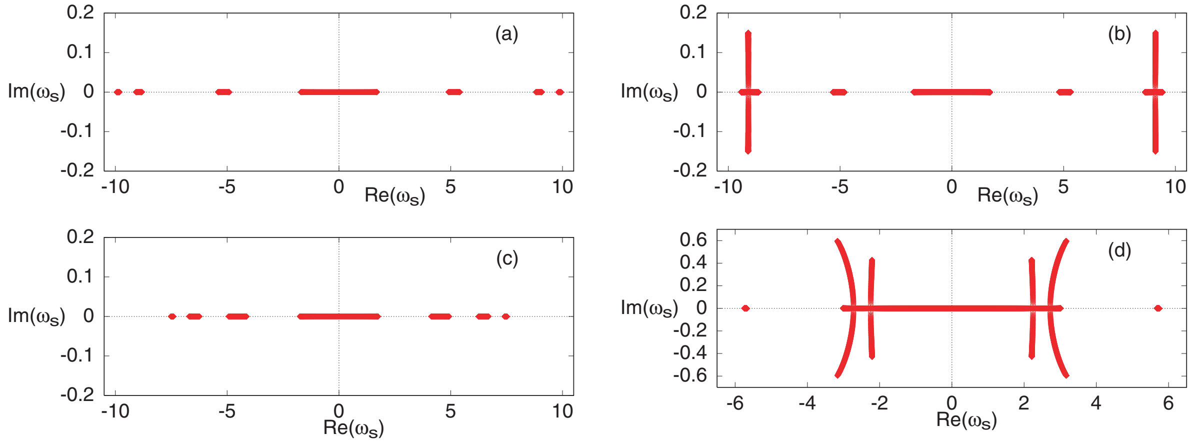

Fig. 5. Eigenvalues of (4) for H-SW with $Q = 3\pi/4$. (a) $\delta = -8.0$; (b) $\delta = -7.5$; (c) $\delta = -4.5$; (d) $\delta = -0.5$ ($C = 1$).

$\chi_0(x)$ when $\phi = \phi_m$, E-SWs necessarily contain two consecutive codes $+1$ or -1, while H-SWs contain no such consecutive codes. As a consequence, a result from [10] yields that, generically for small coupling, H-SWs are dynamically *linearly stable* while E-SWs are *unstable*.

For general $\frac{\delta}{C}$, the dynamical linear stability of SWs in the DNLS model (1) can be obtained by substituting $\psi_n \to \psi_n + \epsilon_n(t)$ into (1) and linearizing [12]. The general solution to the linearized equations can be written as a linear combination of solutions of the form $\epsilon_n(t) = \frac{1}{2}(U_n + W_n)\,\mathrm{e}^{\mathrm{i}\omega_s t} + \frac{1}{2}(U_n^* - W_n^*)\,\mathrm{e}^{-\mathrm{i}\omega_s^* t}$, with eigenfrequencies ω_s and eigenmodes $\{U_n, W_n\}$ determined by the (non-Hermitian) eigenvalue problem

$$
\begin{aligned}
(2C - \delta - \psi_n^2)W_n - C(W_{n+1} + W_{n-1}) &= \omega_s U_n \\
(2C - \delta - 3\psi_n^2)U_n - C(U_{n+1} + U_{n-1}) &= \omega_s W_n. \quad (4)
\end{aligned}
$$

The SW ψ_n is linearly stable if and only if all eigenvalues ω_s are real. Defining the *Krein signature* (see *e.g.* [10]) as $\mathcal{K}(\omega_s) = \mathrm{sign}\sum_n \mathrm{Re}\,[U_n W_n^*]$, where $\{U_n, W_n\}$ is the eigenvector with eigenvalue $\omega_s > 0$, instabilities may occur if eigenvalues with opposite $\mathcal{K}$ collide when varying $\frac{\delta}{C}$.

When $C = 0$ ($\frac{\delta}{C} \to -\infty$), equation (4) is easily solved. Eigenvalues are $\omega_s = 0$, with eigenmodes $\{U_n \equiv 0, W_n\}$ localized at sites where $|\tilde{\sigma}_n| = 1$, and $\omega_s = \pm\delta$, with eigenmodes $\{U_n, W_n = \mp U_n\}$ at sites with $\tilde{\sigma}_n = 0$. When $C > 0$, these degenerate eigenvalues spread into *bands*. For commensurate SWs the number of bands are finite, while a Cantor-like spectrum appears for incommensurate SWs. The instability of the E-SWs appears as eigenvalues move out on the imaginary axis, while for H-SWs the bands spread initially only along the real axis showing their linear stability for small C (Fig. 5a). Increasing $\frac{\delta}{C}$ the bands broaden, and the main gap separating the bands originating from $\omega_s = 0$ (with $\mathcal{K} = -1$) with those from $\omega_s = \pm\delta$ (with $\mathcal{K} = +1$) shrinks to zero. Then, eigenvalues *collide* and move out in the complex plane, generating *oscillatory instabilities for the SW* (Fig. 5b). For some Q, stability is temporarily regained for intervals of $\frac{\delta}{C}$ where no bands overlap (Fig. 5c). However, more instabilities

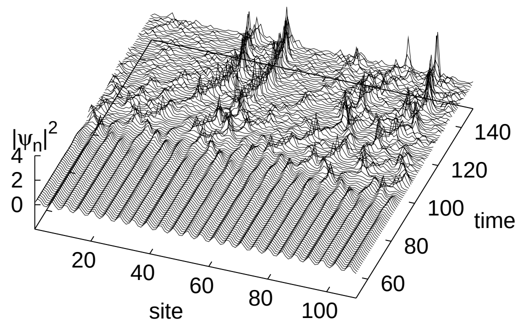

Fig. 6. Slightly perturbed H-SW with $Q = 12\pi/55 < \pi/2$, $\delta = 0.06$, $C = 1$ (rational approximant to analytic SW).

associated with band overlap appear as $\frac{\delta}{C}$ is further increased (Fig. 5d), and close to the linear limit *all* SWs with $0 < Q < \pi$ are linearly unstable for infinite systems.

In [1,2] the generic instability of SWs close to the linear limit was shown by perturbation theory; here we will recall an intuitive argument for the commensurate case. *At* the linear limit ($\delta = \delta_0(Q), \psi_n^2 = 0$), equation (4) has two sets of plane wave solutions $U_n = \pm W_n = \mathrm{e}^{\mathrm{i}qn}$ yielding the eigenvalue spectrum $\omega_s = \pm 2C(\cos Q - \cos q)$ with Krein signatures $\mathcal{K}(\omega_s) = \mathrm{sign}(\cos Q - \cos q)$. Thus, eigenvalues with opposite $\mathcal{K}$ overlap in an interval around $\omega_s = 0$. Going away from the linear limit, each band splits into a *finite* number of bands with *nonzero* width. Consequently, bands with opposite $\mathcal{K}$ still overlap, and resonant coupling causes oscillatory instabilities *as soon as* $\psi_n^2 \neq 0$.

We now discuss the dynamics resulting from the oscillatory SW instabilities, which, generally, exhibits *three main regimes* (see Figs. 6–7). The initial oscillatory dynamics with exponentially increasing amplitude is well described by the most unstable eigenvector of equation (4), and typically yields modulations along the chain. When the oscillation amplitudes exceed some threshold the linearized description is no longer valid, and we observe an intermediate regime characterized by *inhomogeneous translational motion*, where the wave remains locally coherent

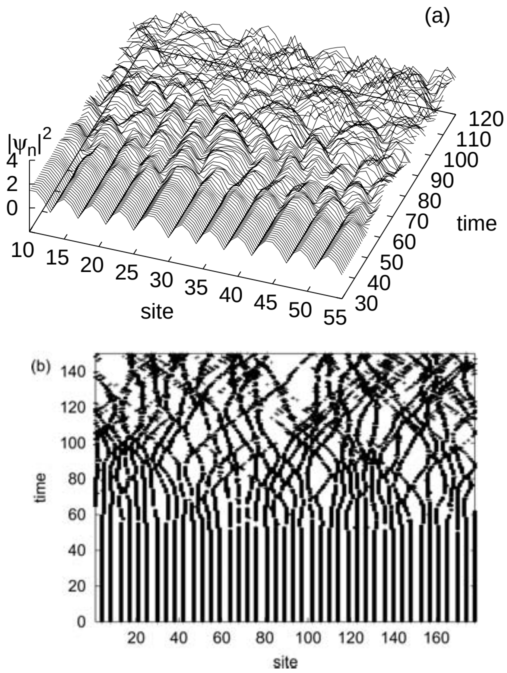

Fig. 7. (a) Slightly perturbed nonanalytic H-SW with $Q = 68\pi/89 > \pi/2$, $\delta = 2.3$, $C = 1$; (b) dynamics of 'discommensurations', defined as sites in (a) with $|\psi_n| < 0.6$.

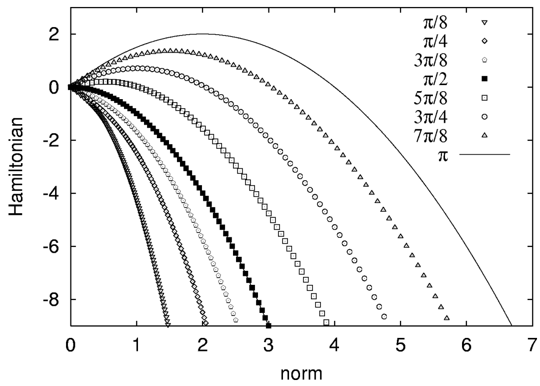

Fig. 8. $\mathcal{H}'/N$ *vs.* $\mathcal{N}/N$ for H-SWs with different Q increasing from left to right ($\sigma = -1, C = 1$).

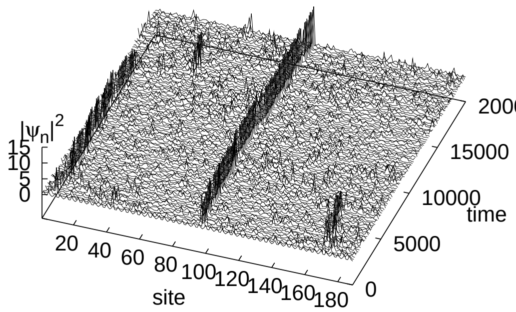

Fig. 9. Unstable H-SW in a chain of $N = 189$ sites with $Q = 2\pi/7 < \pi/2$ and $\delta = -0.2$ ($C = 1$).

but with its different parts moving with respect to each other. Gradually, the wave loses coherence and a final space-time chaotic regime appears, the statistical properties of which depend on Q as discussed below.

The qualitatively different dynamics for small and large Q can be understood from the properties of the anticontinuous coding sequence (*cf.* Fig. 4). For small Q, the windows giving codes $\tilde{\sigma}_n = \pm 1$ are narrow, and thus the SW can be regarded as an array of interacting breathers with opposite phases, where each breather corresponds to a site with code ± 1, and the distance between the breathers increases as Q decreases. Thus, the intermediate regime can be interpreted as moving breathers colliding inelastically with each other (Fig. 6). On the other hand, for Q close to π the windows of codes $\tilde{\sigma}_n = \pm 1$ are wide, and we can regard each site with code 0 as a *discommensuration* (*cf. e.g.* [13]) in the stable wave with $Q = \pi$. As shown in [14], a single discommensuration ('discrete dark soliton') is oscillatorily unstable resulting in discommensuration motion. The intermediate regime can then be regarded as *moving discommensurations* colliding inelastically (Fig. 7).

Concerning the asymptotic dynamics, it was shown [15] for typical initial conditions to depend critically on the values of the two conserved quantities: Hamiltonian $\mathcal{H} = \sum_{n=1}^{N} \left(-\delta|\psi_n|^2 + \frac{\sigma}{2}|\psi_n|^4 + C|\psi_{n+1} - \psi_n|^2\right)$ and norm $\mathcal{N} = \sum_{n=1}^{N} |\psi_n|^2$. Redefining $\mathcal{H}$ into $\mathcal{H}' = \mathcal{H} + (\delta - 2C)\mathcal{N}$, a *phase transition* was found at the curve

$$\frac{\mathcal{H}'}{N} = \sigma \left(\frac{\mathcal{N}}{N}\right)^2 \tag{5}$$

in the thermodynamic limit when the number of sites $N \to \infty$. On one side of this line (below for $\sigma > 0$ and above for $\sigma < 0$), the system *thermalizes* in a Gibbsian sense with well-defined temperature and chemical potential. On the other side, the system shows a negative-temperature type behaviour, and *persistent localized high-amplitude standing breathers are created*. Equation (5) corresponds to the *limit of infinite temperature* in the Gibbsian regime, where each site is assumed to thermalize independently, *i.e.* the coupling term in $\mathcal{H}'$ is neglected. Noting that a H-SW with $Q = \pi/2$ has the form $\psi_{2m+1} = (-1)^m \sqrt{\frac{\delta}{\sigma}}$, $\psi_{2m} = 0$, the coupling term in $\mathcal{H}'$ is *exactly zero*, and thus this SW lies *exactly on the phase transition line*. Consequently, H-SWs with a given Q always belong to the same phase regardless on the value of δ/C, and *SWs with $Q < \pi/2$ and those with $Q > \pi/2$ always belong to different phases* (Fig. 8).

For $\sigma = -1$ we confirmed that unstable H-SWs in large DNLS systems approach thermalized states when $Q > \pi/2$ (*e.g.* the long-time limit of the simulation in Fig. 7), while persistent breathers appear when $Q < \pi/2$ (Fig. 9) (although for Q close to $\pi/2$ the system size required for breather formation is large). A similar behaviour was also observed for KG lattices with small coupling [2], but it is questionable whether a true transition exists also in the absence of a second conserved quantity. Likely, the 'breather phase' in KG lattices only describes the dynamics over long but finite times, with asymptotic equipartition similarly as for FPU systems [16].

We conclude by comparing some properties of nonlinear SWs with those of nonlinear propagating waves (PWs): (i) SWs are *time-reversible* continuations of harmonic solutions $\cos(Qn)\mathrm{e}^{-\mathrm{i}\omega t}$ (in the DNLS model time-independent in a rotating-wave frame), while PWs are continuations of harmonic *plane-waves* $\mathrm{e}^{\mathrm{i}(Qn-\omega t)}$ [7]; (ii) SWs are *multibreathers* with (quasi-)periodically repeated codes 1,0,-1, while PWs are continuations of anticontinuous solutions $\{\tilde{\sigma}_n\} \equiv 1$ with *phase torsion* [8]; (iii) small-amplitude SWs have *oscillatory* instabilities for *all* $0 < Q < \pi$, while PWs have *non-oscillatory* modulational instabilities *only* for $0 \leq Q < \pi/2$ ($\sigma = -1$) *or* $\pi/2 < Q \leq \pi$ ($\sigma = +1$); (iv) unstable SWs with $Q < \pi/2$ and $Q > \pi/2$ belong to different phases yielding *qualitatively different* asymptotic dynamics (breather formation or equipartition), while PWs with given Q may *cross* the phase transition line as the amplitude is varied [15].

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