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Discrete breathers in Fermi–Pasta–Ulam lattices

S. Flach and A. Gorbach
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

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We study the properties of spatially localized and time-periodic excitations—discrete breathers—in Fermi–Pasta–Ulam (FPU) chains. We provide a detailed analysis of their spatial profiles and stability properties. We especially demonstrate that the Page mode is linearly stable for symmetric FPU potentials. A resonant interaction between a localized and delocalized perturbations causes weak but finite strength instabilities for asymmetric FPU potentials. This interaction induces Fano resonances for plane waves scattered by the breather. Finally we analyze the interplay between energy thresholds for breathers in the presence of strongly asymmetric FPU potentials and the corresponding profiles of the low-frequency limit of breather families. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1839151]

The Fermi–Pasta–Ulam (FPU) paradox was observed fifty years ago. The surprising finding was a localization of energy in the reciprocal *q*-space of a model with discrete translational invariance, despite the presence of interaction between extended normal modes. Thirty three years later Sievers, Takeno, and Kisoda reported on the observation of energy localization in real space for the same class of FPU models, which is as surprising since these excitations, called discrete breathers or intrinsic localized modes, violate the underlying discrete translational symmetry of the model. The past decade has witnessed a tremendous progress in the theory and applications of discrete breathers, which goes far beyond the scope of the original FPU frame. We use the modern theory of discrete breathers to investigate the properties of these solutions in FPU models, paying special attention to the issues of stability, resonances, wave scattering and energy thresholds.

INTRODUCTION

The celebrated Fermi–Pasta–Ulam (FPU) model was introduced fifty years ago in order to study the process of equilibration of energy among normal modes due to mode–mode interactions.[1] It can be viewed as a toy version of a model describing the dynamics of lattice vibrations of perfect crystals. The original FPU model reduced space dimension to one, and attributed one degree of freedom to each lattice site. It is worth mentioning that in the absence of mode–mode interactions, that model is often used in solid state physics textbooks to explain the basic features of phonons and is then called a *monoatomic chain*.[2] Some of these textbooks deal also with mode–mode interactions, coining them *anharmonic corrections* (since they appear as anharmonic terms in the Taylor expansion of the potential energy of the lattice with respect to atomic displacements). Notably these anharmonic terms are used to explain thermal expansion of crystals, among many other features. It is also worth stressing that solid state physicists did not seriously question the assumed fact that in thermal equilibrium the energy *is* equipartitioned among the normal modes—due to the bulk of accumulated experimental evidence for that fact. The more time-resolved spectroscopical methods advance, the more questions arise concerning these topics when studying lattice dynamics in the presence of strong nonlinearities (i.e., mode–mode interactions). Returning to the FPU model calculations, they revealed the surprising fact that at least for some cases (for some sets of initial conditions) the evolution of the FPU model showed *no* equipartioning among the normal modes.[1] In other words, the FPU *paradox* seems to consist primarily of the observation of *localization* of energy in a few normal modes, despite the presence of interaction between all modes, which would be capable of distributing the energy among all normal modes of the system.[3]

While the modern view on this FPU paradox observation is for sure discussed in other contributions to this Focus Issue, we will not dwell on that further. In what follows, we will discuss another interesting aspect of the dynamics in the FPU model and its various generalizations. This concerns localization in *real space*. In other words, we will show that FPU models allow for solutions of the corresponding equations where the energy is not equally shared among the *local* constituents (using the solid state physics language, among the different atoms). These solutions are coined *intrinsic localized modes* (ILM), or *discrete breathers* (DB). Whatever the nomenclature, ILMs/DBs turn out to be generic to a much larger class of *Hamiltonian lattices*, and FPU models together with their generalizations represent one of the subclasses of these lattices (see Fig. 1 for a schematic representation of various DBs). ILMs/DBs are time-periodic and spatially localized solutions, and exist thanks to the interplay between nonlinearity and discreteness.[4] Many studies of DBs have been successfully launched, on such topics as rigorous existence proofs, dynamical and structural stability and computational methods of obtaining DBs in classical models as well as their quantum aspects. In addition DBs have been detected and studied experimentally in such different systems as interacting Josephson junction systems,[5] coupled nonlinear optical waveguides,[6] lattice vibrations in crystals,[7]

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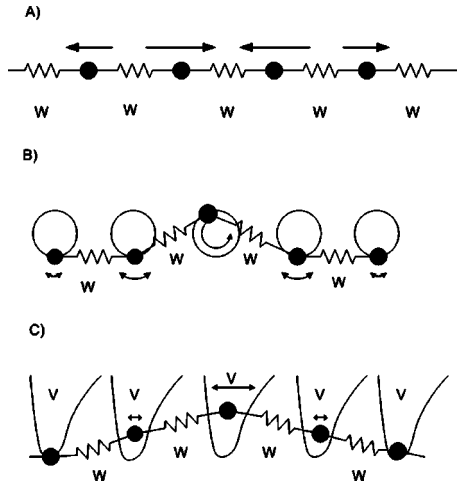

FIG. 1. A schematic representation of different types of discrete breathers: (a) Acoustic FPU breather; (b) acoustic rotobreather; (c) optical breather (for details see, e.g., Ref. 4).

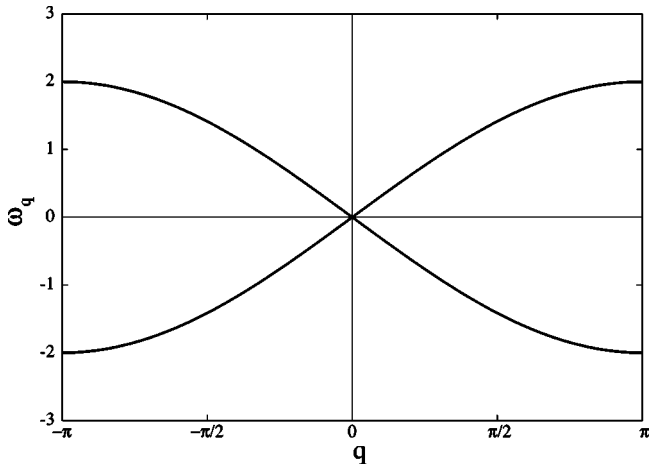

FIG. 2. Dependence of ω_q on q for $\phi_2=1$. Vertical and horizontal lines mark the values $q=0$ and $\omega_q=0$.

antiferromagnetic structures,[8] micromechanical cantilever arrays,[9] Bose–Einstein condensates loaded on optical lattices,[10] layered high-T_c superconductors.[11] DBs are predicted also to exist in the dynamics of dusty plasma crystals.[12] It is an equally interesting question of why ILMs/DBs have not been properly discussed when studying the lattice dynamics of crystals until very recently. We leave the answer to this question to the experienced and educated experts of that field.

SETTING THE STAGE AND EARLY RESULTS

We will consider the following class of one-dimensional Hamiltonian chains

$$H=\sum_l \left[\tfrac{1}{2}p_l^2 + W(x_l - x_{l-1})\right], \tag{1}$$

where x_l describes the scalar displacement of a particle (atom) from its equilibrium position, $p_l=\dot{x}_l \equiv dx_l/dt$ is its conjugated momentum (velocity), l denotes the number of the particle, and $W(x)$ is the interaction potential between nearest neighbors. The Hamiltonian H is assumed to take only nonnegative values for small values of the displacements and velocities, i.e., the potential W and its first derivative W' vanish for zero displacements $W(0)=W'(0)=0$ and the second derivative W'' is positive for small displacements $W''(0)>0$. The Hamiltonian equations of motions $\dot{x}_l = \partial H/\partial p_l$, $\dot{p}_l=-\partial H/\partial x_l$ lead to the following set of coupled differential equations:

$$\ddot{x}_l = -W'(x_l - x_{l-1}) + W'(x_{l+1} - x_l). \tag{2}$$

Let us expand the function W in the following series:

$$W(x)=\sum_{m=2}^{\infty} \frac{\phi_m}{m} x^m. \tag{3}$$

If the potential $W(x)$ is symmetric $W(x)=W(-x)$ it follows $\phi_{2m+1}=0$ for all positive integers m.

The celebrated FPU models[1] are obtained by choosing nonzero values for $\phi_{2,3,4}$ and zeroing all the others $\phi_{m>4}=0$. Thus we may consider the FPU models as low amplitude expansions of the more general model class (1). FPU models take into account the two first anharmonic corrections $\phi_{3,4}$ to the harmonic term ϕ_2. The case of a symmetric potential for FPU models is thus obtained by assuming $\phi_3=0$. Note that anharmonic terms in the Hamiltonian correspond to nonlinear terms in the equations of motion here. Equation (2) conserves both the total energy H (1) as well as the *total mechanical momentum* $P=\Sigma_l p_l$. Without loss of generality we will consider below the case $P=0$ only.

If we restrict our consideration to very small amplitudes and velocities only, we may neglect all nonlinear terms from the equations of motion, assuming $\phi_{m>2}=0$. The solution of the corresponding *linear* coupled differential equations

$$\ddot{x}_l = \phi_2(x_{l+1} + x_{l-1} - 2x_l) \tag{4}$$

can be written in the form of a superposition of plane waves each given by

$$x_l(t) = A_q \cos(\omega_q t - ql + B_q) \tag{5}$$

where q is the wave number, ω_q the plane wave frequency, and A_q and B_q are integration constants. The dispersion relation (Fig. 2)

$$\omega_q = \pm 2\sqrt{\phi_2}\sin\left(\frac{q}{2}\right) \tag{6}$$

is periodic in q and is characterized by an upper bound $|\omega_q| \leq \omega_\pi \equiv 2\sqrt{\phi_2}$. Moreover for small values of q $|\omega_q| \approx \sqrt{\phi_2}q$. Such an *acoustic* type of dispersion at small values of q is intimately connected to the above mentioned conservation of the total mechanical momentum P. Any spatially localized initial excitation on the lattice will ultimately disperse due to the q-dependence of the *group velocity*

$$v_q = \frac{d\omega_q}{dq} = \pm\sqrt{\phi_2}\cos\frac{q}{2}. \tag{7}$$

Taking into account weak anharmonic–nonlinear effects usually leads to a renormalization of plane wave properties such as frequencies and lifetimes. However, no principal change

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in the behavior of a spatially localized initial condition is expected from that perspective.

Some rigorous results exist for the study of stability of certain plane waves. Indeed, the corresponding modulational instability (cf. Refs. 13–18) is responsible for the appearance of localized structures. However, the linearization of the phase space flow around the plane wave in these studies limits possible conclusions about the appearance of strongly localized ILMs or DBs.

A nonperturbative and qualitatively new property of the evolution of spatially localized excitations takes place if the nonlinear terms become essential. Instead of observing a decay in space, robust and seemingly exact spatially localized vibrational excitations have been observed. Early results on ILMs or DBs in FPU chains have been obtained by Sievers, Takeno, and Kisoda.[19] These studies as well as their followups[20] provide three types of observations and results, among others.

First, they report on numerical evidence of the existence of long lived localized excitations, with lifetimes much larger than the typical oscillation times $\sim 2\pi/\omega_\pi$. The internal frequencies of such ILMs are *outside* the spectrum ω_q. In Figs. 4, 6, and 8 some of these excitations are shown (and will be discussed in more detail below). In fact, as will be discussed in the next sections, these excitations are *exact* solutions of the equations of motion.

Second, approximate numerical solutions were obtained using the *rotating wave approximation* which implies that a time-periodic solution is constructed taking into account only its first harmonics frequency contribution (and optionally also a dc component) and neglecting higher harmonics. The recipe is to use the ansatz $x_l(t)=c_l+a_l\cos(\Omega_b t)$, to insert it into the equations of motion (2) and to neglect all terms with higher harmonics which appear due to the nonlinear terms. The resulting set of coupled algebraic equations for the coefficients c_l, a_l can be solved numerically for finite numbers of sites, and yields solutions similar to those observed in numerical simulations. This approximation is strictly speaking valid only for small amplitudes of the displacements. In reality, however, it may serve as a good estimate to exact solutions for rather large amplitudes as well.

And third, for quite long simulation times *moving* ILMs have been observed, which in addition of being characterized by internal oscillations, propagate along the chain. Typically the observed propagation velocities are *smaller* than the maximum group velocity $\max(|v_q|)=\sqrt{\phi_2}$. Also the motion of these ILMs along the lattice leaves excited lattice parts behind, implying that in the course of time these moving structures will slow down or disappear due to radiation of energy.

While initially ILM excitations seemed to be connected to some specific properties of FPU chains, the observation of similar localized structures in Klein–Gordon chains as well as in higher dimensional lattices suggested that the existence of ILMs is a rather generic feature for various anharmonic Hamiltonian lattices.[4] This view became a well established fact due to numerous studies during the past decade. In the following we will discuss the existence and properties of ILMs or DBs in FPU chains using methods of the modern theory of localized excitations in discrete systems.

DISCRETE BREATHERS IN FPU CHAINS: SOME DEFINITIONS

Discrete breathers (intrinsic localized modes) are time-periodic spatially localized solutions of the equations of motion of a Hamiltonian lattice.[4] In mathematical terms we are searching for solutions of (2) satisfying

$$\hat{x}_l(t+T_b)=\hat{x}_l(t), \quad \hat{p}_l(t+T_b)=\hat{p}_l(t), \tag{8}$$

$$\hat{x}_{l\to\pm\infty}\to d_\pm, \quad \hat{p}_{l\to\pm\infty}\to 0. \tag{9}$$

The difference d_+-d_- characterizes the DB induced lattice deformation and is related to the abovementioned effects of thermal expansion (or contraction). Without loss of generality we may choose $d_-=0$ in the following. The period T_b is related to the DB frequency $\Omega_b=2\pi/T_b$. The DB solution can be thus represented as a Fourier series expansion with respect to time:

$$\hat{x}_l(t)=\sum_{k=-\infty}^{+\infty} A_{kl}e^{ik\Omega_b t}. \tag{10}$$

The localization property (9) implies

$$A_{k\neq 0,l\to\pm\infty}\to 0, \quad A_{k=0,l\to\pm\infty}\to d_\pm. \tag{11}$$

Inserting (10) into the equations of motion (2), and assuming a large distance from the DB core, the linearization of the algebraic equations for the coefficients A_{kl} together with the condition (11) leads to the *nonresonance* condition[21]

$$k\Omega_b \neq \omega_q \tag{12}$$

for all integer k. Excluding $k=0$ for a moment, that condition implies $\Omega_b>\omega_\pi$. The possible resonance for $k=0$ which induces nonzero static lattice deformations, will be discussed in more detail below.

The stability of a DB (as for any periodic orbit) can be accounted for by linearizing the phase space flow around a given DB solution $\hat{x}_l(t)$, i.e., by adding a small perturbation to it $x_l(t)=\hat{x}_l(t)+\epsilon_l(t)$, inserting this expression into the equations of motion (2) and keeping only terms linear in ϵ_l:

$$\begin{aligned}\dot{\epsilon}_l &= \pi_l,\\ \dot{\pi}_l &= -W''(\hat{x}_l-\hat{x}_{l-1})(\epsilon_l-\epsilon_{l-1})+W''(\hat{x}_{l+1}-\hat{x}_l)(\epsilon_{l+1}-\epsilon_l).\end{aligned} \tag{13}$$

Equations (13) define a map

$$\begin{pmatrix}\vec{\pi}(T_b)\\ \vec{\epsilon}(T_b)\end{pmatrix}=\mathcal{F}\begin{pmatrix}\vec{\pi}(0)\\ \vec{\epsilon}(0)\end{pmatrix} \tag{14}$$

which maps the phase space of perturbations onto itself by integrating each point over the DB period T_b. Here we used the abbreviation $\vec{x}\equiv(x_1,x_2,\ldots,x_l,\ldots)$. The map (14) is characterized by a symplectic Floquet matrix $\mathcal{F}$, whose complex eigenvalues λ and eigenvectors $\vec{y}$ provide information about the stability of the DB. For details we refer to Ref. 22. Here we note that if all eigenvalues λ are of length one, then the DB is linearly (marginally) *stable*. Otherwise perturbations exist which will grow in time (typically exponentially) and correspond to a linearly *unstable* DB. Upon changing a control parameter (e.g., the DB frequency) stable DBs can be-

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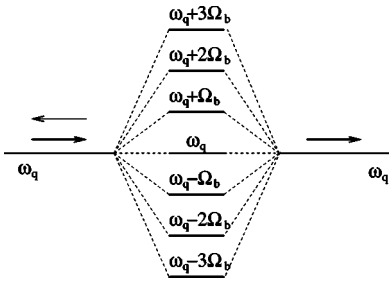

FIG. 3. Schematic representation of the one-channel scattering of a wave by a discrete breather.

come unstable (and vice versa). Such a change of stability is appearing because two (or more) Floquet eigenvalues collide on the unit circle and depart from it. If one of the two associated eigenvectors (or both) is spatially localized, such a collision and the corresponding instability are independent of the size of the lattice. If both eigenvectors are spatially delocalized, the strength of the instability depends on the size of the system and vanishes in the limit of an infinite system.[23]

The absence of a cubic term ϕ_3 (or more generally the case of a symmetric potential W) implies a parity symmetry of the interaction potential W. Consequently DB solutions will contain only odd harmonics in a Fourier expansion with respect to time, $A_{2k,l}=0$. That implies $d_+=0$ (we remind the reader that $d_-=0$ as well). For such a case the Floquet problem (13) is periodic with period $T_b/2$, because the time-periodic coefficients in (13) contain only even harmonics $2k\Omega_b$ in a Fourier expansion with respect to time.

Two eigenvectors of the Floquet matrix are corresponding to homogeneous shifts in all coordinates or likewise velocities (due to the conservation of P). Their eigenvalues are always located at +1 in the complex plane. Two more eigenvectors of the Floquet matrix are corresponding to perturbations along the DB periodic orbit (phase mode) or along the family of DB solutions. Their eigenvalues are located either at +1 for asymmetric potentials W (since the Floquet mapping is performed for one period T_b) or at −1 for symmetric potentials W (since the Floquet mapping is performed for $T_b/2$).

Finally we will also use the linearized phase space flow dynamics around a DB solution (13) in order to compute the transmission coefficient for a small amplitude plane wave launched into the DB. It is a special Bloch-type solution of Eq. (13) of the form[24]

$$\epsilon_l(t) = \sum_{k=-\infty}^{\infty} \epsilon_{lk} e^{i(\omega_q + k\Omega_b)t}. \tag{15}$$

The DB solution acts as a time-periodic scattering potential for an incoming wave with frequency ω_q and generates new *channels* at frequencies $\omega_q + k\Omega_b$. If $\omega_q + k\Omega_b \neq \omega_{q'}$ for nonzero k then all channels are *closed* except for the open channel $k=0$. Such a situation corresponds to *elastic* scattering, i.e., the energies of the incoming and the outgoing (transmitted and reflected) waves are equal. Otherwise we are confronted with *inelastic* scattering. The scattering setup is schematically represented in Fig. 3. For computational details the reader is referred to Ref. 25.

EXISTENCE PROOFS

The pioneering DB existence proof of MacKay and Aubry[26] was designed to apply for networks of weakly coupled oscillators using the implicit function theorem. The extension of this technique to FPU systems turned out to be complicated because one needs a limiting case where DB solutions are compact. Nevertheless it was applied successfully to the case of a *diatomic* FPU chain with alternating heavy and light masses.[27] DB solutions were shown to exist close to the limit where the ratio of light to heavy masses vanishes.

A special case of *homogeneous* potentials W with $\phi_m = \mu\delta_{m,2n}$ where n is a given positive integer, was treated in Ref. 28 to separate time and space dependence. This feature was then used in Ref. 29 to provide a constructive proof of existence of DBs. As shown recently,[30] this proof can be extended to systems with onsite potentials by adding $\Sigma_l\left(\frac{1}{2}\omega_0^2 x_l^2 + \nu x_l^{2n}\right)$ to the Hamiltonian (1).

An implicit proof of existence of DBs in FPU models was provided by Aubry *et al.* in Ref. 31 using a variational method. Discrete breathers are obtained as loops in phase space which maximize a certain average energy function for a fixed pseudoaction. More recently James[32] proved existence of DBs in FPU models for low amplitudes (energies).

All these results provide the certainty of existence of DB solutions in infinite FPU models. However, due to the implicit character of most of these proofs a detailed study of DB properties has to be obtained, e.g., using advanced computational methods.

DB SOLUTIONS AND THEIR STABILITY

Computational tools for studying DB properties are confined to the case of a finite lattice size. The typically exponential spatial degree of localization of DBs yields reliable results which apply for infinite lattice size as well. In terms of the dynamics in phase space $\{x_l, p_l\}$ we are searching for a starting point of a trajectory such that after integrating over a given period of time the trajectory reaches the starting point again. Of course all points on the corresponding one-dimensional manifold generated by the trajectory fulfill this condition. Discrete breathers are so-called isolated periodic orbits. That implies that fixing the total energy and mechanical momentum for a given DB solution, no other DB solutions are found in an infinitesimal neighborhood of the DB loop. In other words, DB solutions do not belong to higher dimensional *resonant* tori in the model phase space. However, if changes in the energy are allowed, then generically infinitesimal deformations of the original DB loop will result in a new DB loop with slightly changed parameters such as energy, frequency or amplitude. Sliding along such a family of DB solutions may lead to a stability change of the solutions. Here we use a Newton method to find a DB solution at a chosen frequency together with open boundary conditions.

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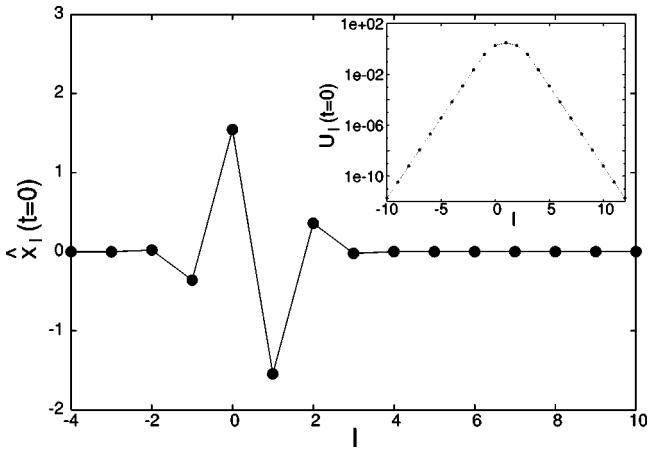

FIG. 4. Displacements $\hat{x}_l(t=0)$ for $\phi_2=\phi_4=1$, $\phi_3=0$ and $\Omega_b=4.5$ vs lattice site number l for an antisymmetric DB. Inset: Staggered deformation $u_l(t=0)$ for the same solution on a logarithmic scale vs lattice site number l. This DB is stable.

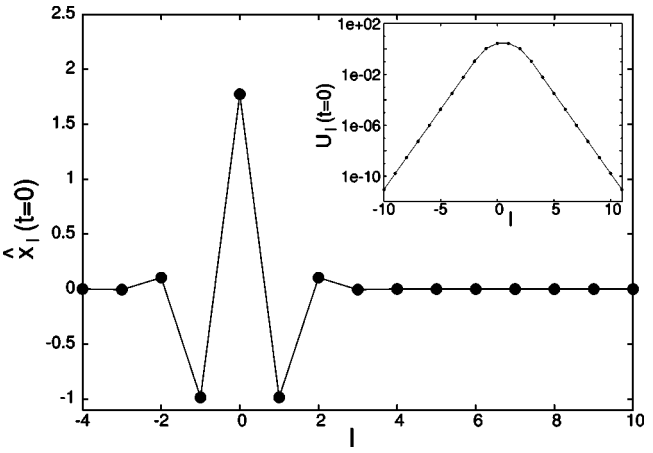

FIG. 6. Displacements $\hat{x}_l(t=0)$ for $\phi_2=\phi_4=1$, $\phi_3=0$ and $\Omega_b=4.5$ vs lattice site number l for a symmetric DB. Inset: Staggered deformation $u_l(t=0)$ for the same solution on a logarithmic scale vs lattice site number l. This DB is unstable.

For details on this method as well as on numerical evaluations of the Floquet matrix we refer to Ref. 22.

The Page mode for $\phi_3=0$

In Fig. 4 we show the profile of a *stable* DB solution $\hat{x}_l(t=0)$ for $\phi_2=\phi_4=1$, $\phi_3=0$, $\Omega_b=4.5$ and 80 sites, the index l running from $l=-39$ to $l=40$ with open boundary conditions. Note that $\hat{p}_l(t=0)=0$. Because $\Omega_b>\omega_\pi$, the amplitudes stagger.[21] The solution is antisymmetric in space, and likewise coined *centered between sites* and also *Page mode*. In the inset we plot the profile of the corresponding *staggered deformation* $u_l=(-1)^l(x_l-x_{l-1})$ on a logarithmic scale. The DB is strongly localized, and only a part of the chain is shown. The inset shows that the DB is localized exponentially. The exponent depends on the model parameters and the DB frequency.[21] In the left part of Fig. 5 we show the location of the Floquet eigenvalues λ in the complex plane. All eigenvalues reside on the unit circle. The two pairs of degenerate eigenvalues located at +1 and −1 on the real axis (see discussion above) are shown with diamonds. Besides the Floquet continuum of extended eigenstates (crosses) two pairs of stable spatially localized eigenstates are observed (shown by squares and circles). In the two right panels of Fig. 5 the real part of the displacement components of these localized eigenstates are plotted.

The Sievers–Takeno mode for $\phi_3=0$

For the same parameters we show in Fig. 6 an *unstable* DB solution which is symmetric in space, or *centered on a site* and also known as the *Sievers–Takeno mode*.

In the left part of Fig. 7 we show the location of the Floquet eigenvalues λ in the complex plane. Not all eigenvalues reside on the unit circle. At variance with the Page mode, one of the pairs of localized eigenstates (circles) is located on the real axis off the unit circle. In the two right panels of Fig. 5 the real part of the displacement components of these localized eigenstates are plotted. The instability is caused by a spatially localized Floquet eigenvector, which deforms the Sievers–Takeno mode in Fig. 6 in the direction of the Page mode in Fig. 4. Indeed the Sievers–Takeno mode, when perturbed in the full nonlinear equations of motion along the unstable Floquet eigenvector, starts to perform additional oscillations around the stable Page mode for times large compared to the DB period.

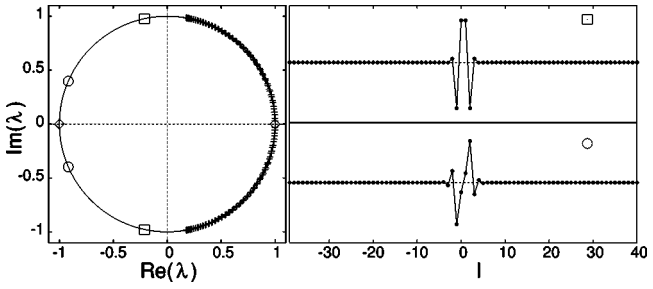

FIG. 5. Left panel: Location of Floquet eigenvalues λ in the complex plane for the DB in Fig. 4 (crosses, diamonds, squares, circles). The unit circle is shown to guide the eye. Right panels: Real part of the displacement components of the Floquet eigenvectors marked with the corresponding symbols (square and circle).

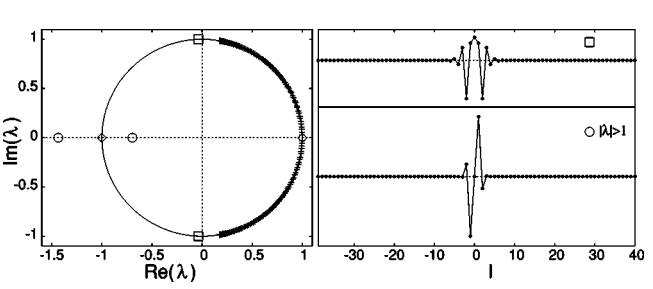

FIG. 7. Left panel: Location of Floquet eigenvalues λ in the complex plane for the DB in Fig. 6 (crosses, diamonds, squares, circles). The unit circle is shown to guide the eye. Right panels: Real part of the displacement components of the Floquet eigenvectors marked with the corresponding symbols (square and circle).

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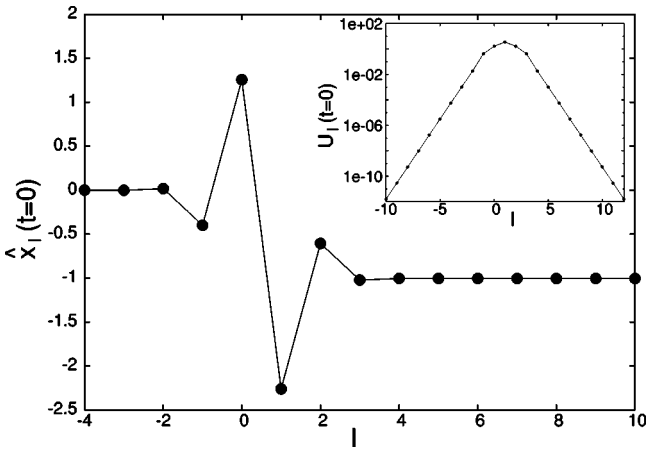

FIG. 8. Displacements $\hat{x}_l(t=0)$ for $\phi_2=\phi_3=\phi_4=1$ and $\Omega_b=4.5$ vs lattice site number l. Inset: Staggered deformation $u_l(t=0)$ for the same solution on a logarithmic scale vs lattice site number l. This DB is unstable.

The Page mode for $\phi_3 \neq 0$

If $\phi_3 \neq 0$, then the interaction potential W becomes asymmetric. DB solutions will now contain in general all Fourier harmonics $k\Omega_b$ including $k=0$. Depending on the sign of ϕ_3 this will cause either a contraction or expansion of the chain. In Fig. 8 we show a DB solution which can be continued from the Page mode in Fig. 4 up to $\phi_3=1$. For that particular case $d_+ \approx -1.005$. The DB solution can be thus viewed as a localized vibration which induces a nonzero kink-shaped lattice distortion. This DB solution turns out to be *unstable*. The reason for that is the interaction of *localized* Floquet eigenstates with the Floquet continuum (the eigenstates which correspond to plane waves far away from the DB). Such *oscillatory instabilities* can be characterized by the wave numbers q_{os} which correspond to the extended Floquet state interacting with the originally localized one.[23] In the left part of Fig. 9 we show the location of the Floquet eigenvalues λ in the complex plane. Not all eigenvalues reside on the unit circle. The two pairs of degenerate eigenvalues, which were located at +1 and −1 on the real axis (see discussion above) for $\phi_3=0$, are now all located at +1 and shown with diamonds. Besides the Floquet continuum of extended eigenstates two pairs of eigenstates (which were localized for the Page mode with $\phi_3=0$) are observed to strongly interact with the Floquet continuum (shown by squares and circles). While the small deviation of the corresponding eigenvalues from the unit circle is of the order of 0.01…0.03, we checked that it is independent of the system size by increasing the number of sites from 80 to 640 (see also Ref. 23). In the two right panels of Fig. 9 the real part of the displacement components of these resonating and unstable eigenstates are plotted.

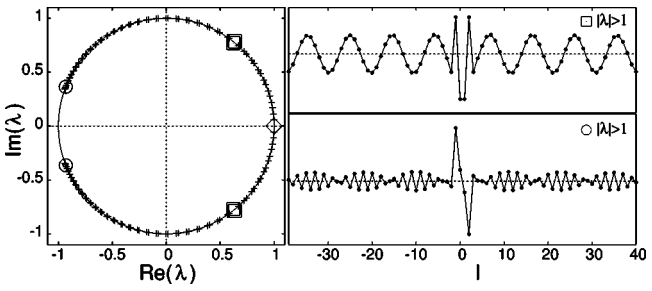

FIG. 9. Left panel: Location of Floquet eigenvalues λ in the complex plane for the DB in Fig. 8 (crosses, diamonds, squares, circles). The unit circle is shown to guide the eye. Right panels: real part of the displacement components of the Floquet eigenvectors marked with the corresponding symbols (square and circle).

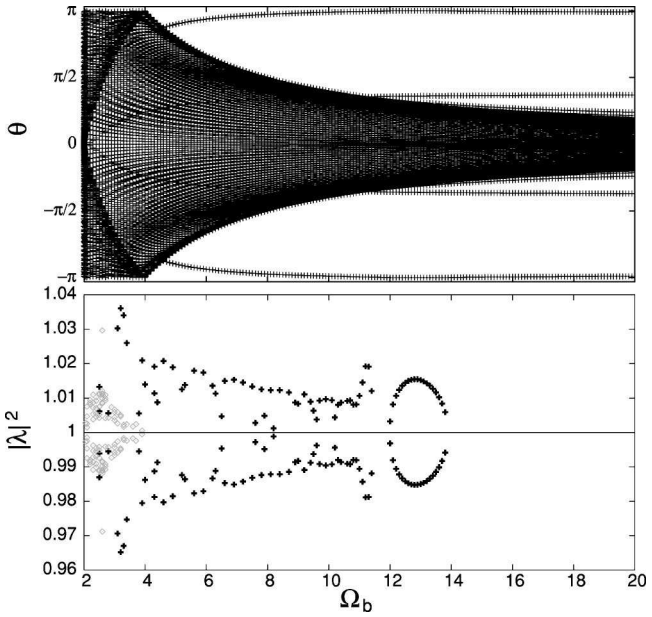

FIG. 10. All Floquet phases θ and the squared eigenvalue length $|\lambda|^2$ of the unstable Floquet eigenvectors for a DB with $\phi_2=\phi_4=1$ and $\phi_3=0.5$ as a function of the DB frequency Ω_b. Eigenvalues which correspond to finite size instabilities are shown using gray symbols.

When the Page mode is perturbed along the oscillatory instability eigenvector in the full nonlinear equations of motion, it deforms initially very slowly compared to the DB period, due to the weak amplitude of the instability. After reaching a critical threshold in the perturbation amplitude, the mode depins from its original lattice site position and starts to move along the lattice.

The Sievers–Takeno mode for $\phi_3 \neq 0$

When continuing the Sievers–Takeno mode from $\phi_3=0$ to nonzero values of ϕ_3, the strong instability caused by a localized Floquet eigenstate for $\phi_3=0$ remains. It also acquires the above discussed oscillatory instabilities of the Page mode. At the same time the spatial profile of the mode ceases to show up with any symmetry.

DB stability properties for different frequencies

In the following we present results on the stability of the Page mode DB upon variation of the DB frequency Ω_b. The Sievers–Takeno mode DB yields similar results, except for keeping its strong localized instability discussed above.

In Fig. 10 we plot the dependence of the arguments θ and the squared absolute values $|\lambda|^2$ of the irreducible part of the Floquet matrix eigenvalue spectrum $\lambda=|\lambda|\exp(i\theta)$ as a function of the DB frequency Ω_b for $\phi_2=\phi_4=1$ and ϕ_3

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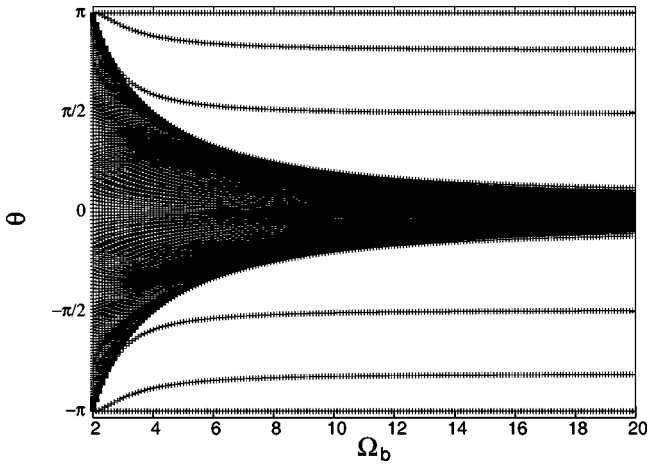

FIG. 11. All Floquet phases θ for a DB with $\phi_2=\phi_4=1$ and $\phi_3=0$ as a function of the DB frequency Ω_b. Note that the Floquet map is obtained here by integrating (13) over the time $T_b/2$.

$=0.5$. These results are obtained for a DB family which is continued from the Page mode in Fig. 4. We first note that $\omega_\pi \equiv 2$ and for $\omega_\pi < \Omega_b < 2\omega_\pi$ the arguments θ cover the whole unit circle interval. The corresponding interactions between different extended Floquet eigenstates lead to finite size instabilities[23,31] which are marked with gray symbols in the lower panel of Fig. 10. These instabilities will disappear for an infinite system, i.e., the corresponding values $|\lambda|-1 \sim 1/N$ where N is the number of sites.[23] For that DB frequency interval scattering of waves will be inelastic for wavenumbers q, q' satisfying $\omega_q+\Omega_b=\omega_{q'}$.[24] Note that this inelastic two-channel scattering will survive in the limit of an infinite system, opposite to the finite size instabilities of the DB itself.

The mentioned oscillatory instabilities induced by the interaction between two pairs of originally localized eigenstates and the continuum are clearly observable, and cause deviations of the corresponding absolute values $|\lambda|$ from unity. As conjectured in Ref. 33, these instabilities survive in the limit of an infinite lattice. The first pair of these eigenstates exits the continuum at $\Omega_b \approx 4.6$. The corresponding eigenvalues return to the unit circle and approach -1 in the complex plane at $\Omega_b \approx 12$, collide with each other, separate on the real axis causing another instability (cf. the corresponding ellipse structure in Fig. 10) and merge again at -1 for $\Omega_b \approx 14$. The second pair exits the continuum at $\Omega_b \approx 11.5$. For sufficiently large values of $\Omega_b > 14$ the DB becomes *stable*.

The discussed instabilities for the Page mode are solely caused by the asymmetric term ϕ_3. Indeed, for $\phi_3=0$ the abovementioned periodicity of (13) with $T_b/2$ excludes the possibility of finite size instabilities or equally inelastic multichannel scattering, since the condition $\omega_q+2\Omega_b=\omega_{q'}$ can not be satisfied due to $\Omega_b > \omega_\pi$. The oscillatory instabilities caused by the interaction of localized Floquet eigenstates with the Floquet continuum are removed for the same reason. The dependence of the eigenvalue phases Θ on Ω_b for a Floquet matrix defined by integrating (13) over T_b for $\phi_3=0$ is practically identical to the case $\phi_3=0.5$ (upper panel in Fig. 10). However, the correct irreducible Floquet matrix for $\phi_3=0$ is obtained by integrating (13) over the true period $T_b/2$. The phase variation shown in Fig. 11 demonstrates that the localized Floquet states are indeed separated from the Floquet continuum.

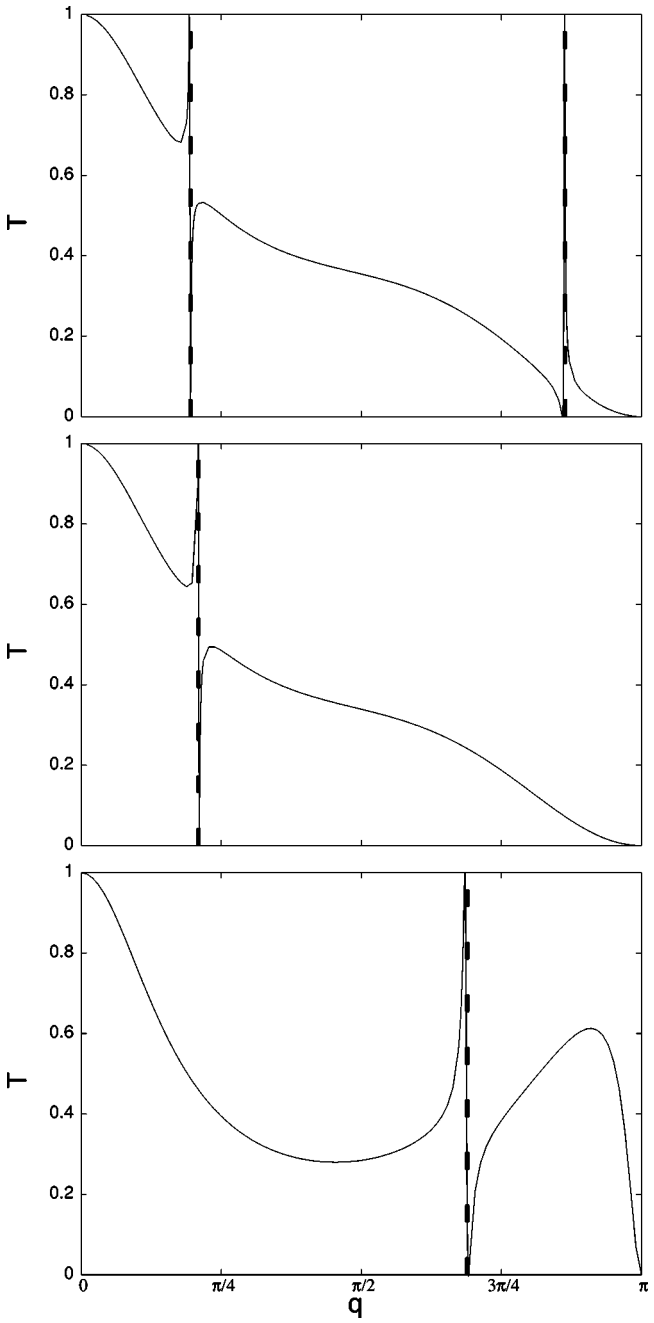

FIG. 12. Transmission coefficient T vs wave number q of an incident wave for $\phi_2=\phi_4=1$ and $\phi_3=0.5$ scattered by a Page mode DB. From top to bottom: $\Omega_b=4.5, 4.7, 10$. The vertical dashed line indicates the position of the oscillatory instabilities q_{os}.

RESONANT WAVE SCATTERING BY DBS

As mentioned above, the linearized phase space flow equations (13) give also information about the complex transmission amplitude t_q and the transmission coefficient $T(q) \equiv |t_q|^2$. While the numerical technique and also a num-

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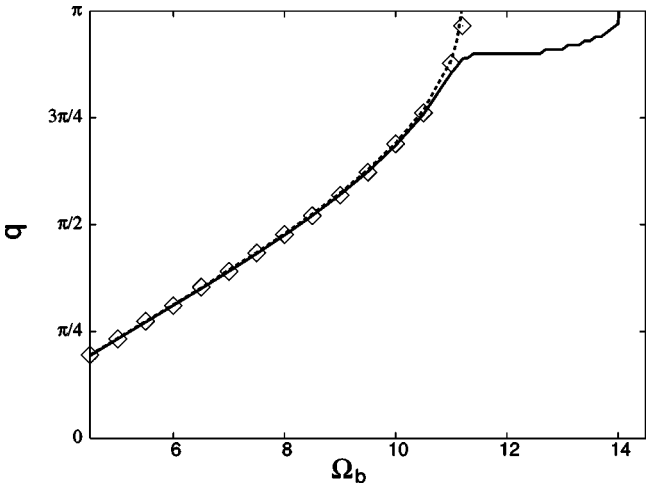

FIG. 13. The dependence of the position of an oscillatory instability q_{os} (diamonds) and the associated locations of perfect transmission (solid line) and perfect reflection (dashed line) on Ω_b for a Page mode DB with $\phi_2 = \phi_4 = 1$ and $\phi_3 = 0.5$.

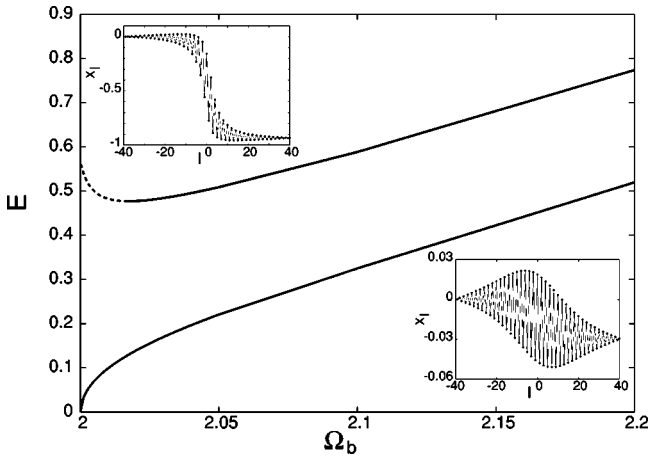

FIG. 14. DB energy E vs DB frequency Ω_b for $\phi_2 = \phi_4 = 1$ and $\phi_3 = 0.5$ (lower curve) and $\phi_3 = 1$ (upper curve). Insets: Displacements $\hat{x}_l(t=0)$ for $\Omega_b = 2.001$ vs lattice site number l. Upper left inset for $\phi_3 = 1$, lower right inset for $\phi_3 = 0.5$.

ber of results concerning wave scattering by FPU breathers have been reported recently,[24,25,34] we want to address here one aspect which was not yet discussed.

We show in Fig. 12 the q-dependence of $T(q)$ for three different frequencies $\Omega_b = 4.5, 4.7, 10$ of the Page mode DB with $\phi_2 = \phi_4 = 1$ and $\phi_3 = 0.5$, for which we gave the Floquet spectral data in Fig. 10. The perfect transmission $T(q=0) = 1$ for all cases is due to the conservation of total mechanical momentum.[25] Equally the vanishing of the transmission $T(q=\pi) = 0$ is due to the vanishing of the group velocity (7) at the band edge $q = \pi$.[24] However, the resonant perfect transmission and reflection peaks observed for $q \neq 0, \pi$ are due to *Fano resonances*.[25,34] We remind the reader that Fano resonances are induced by localized states interacting with a continuum of scattering states.[35]

This is precisely the situation observed in the case of an asymmetric FPU potential. For $\phi_3 = 0$ the Page mode DB has a localized Floquet eigenstate well separated from the Floquet continuum. However any nonzero value of ϕ_3 induces an interaction between this localized state and the continuum mediated by the DB. This interaction causes an oscillatory instability in the Floquet matrix spectrum. The dashed vertical lines in all three panels in Fig. 12 indicate the location of the oscillatory instability q_{os} as observed in Fig. 10. In all three cases the value of q_{os} is very close to the locations of perfect transmission and reflection. In Fig. 13 we plot the q-values of the oscillatory instability of the DB q_{os} from Fig. 10 together with the positions of the perfect transmission and reflection as functions of Ω_b. The obtained correlation between these resonant q-values is evident.

From a general point of view, the DB acts as a time-periodic scattering potential for incoming waves. The time-periodic scattering potential generates locally new frequencies from an incoming wave which correspond to closed channels. These closed channels provide additional propagation ways for the incoming wave. In that sense a time-periodic scattering potential in a strictly one-dimensional system acts similar to a local enlargement of the system dimensionality around the scatterer.[24,25] Such additional propagation channels allow for wave interference, and may also cause a total *destructive interference* leading to a total reflection of the incoming wave, which is another way of understanding the origin of the observed Fano resonance.[34] Note that in a strict sense the correlation between an oscillatory instability of a DB solution and a corresponding Fano resonance holds only for the limit of weak coupling between the localized Floquet state and the Floquet continuum.[25] And only in that limiting case we can expect a nearby location of perfect reflection (Fano resonance) and perfect transmission. The case of strong interaction can lead to the disappearance of an oscillatory instability in the Floquet spectrum and of the perfect transmission peak, but simultaneously to a remaining of the Fano resonance of perfect reflection.[34]

THE FREQUENCY LIMITS OF THE DB SOLUTION FAMILIES

When the frequency Ω_b is varied along a DB family, we may consider the two limiting cases $\Omega_b \to \infty$ and $\Omega_b \to \omega_\pi$. The high frequency limit implies large amplitudes inside the DB core. The leading order contribution in the equations of motion will then be due to the ϕ_4 term. The core profile of these high frequency DBs will be very similar to the DB cores in Figs. 4 and 6 regardless the values of ϕ_2 and ϕ_3 which will only affect the tail characteristics.[21,29,36,37] Opposite to that, the low frequency limit is depending on the value of ϕ_3.[33,38]

In Fig. 14 we plot the dependence of the DB energy (1) on its frequency for $\phi_3 = 1$ and $\phi_3 = 0.5$ and 80 sites. For $\phi_3 = 0.5$ the energy tends to zero as Ω_b tends to ω_π. However, for $\phi_3 = 1$ the DB energy passes through a minimum as the frequency is lowered, and increases again with further approaching the limiting value ω_π.[33,38] These results are intimately connected with the modulational instability of plane waves at small amplitudes.[13,15,16] Assuming that a DB family has a zero amplitude limit, it follows that in a one-dimensional chain as discussed here its energy will also vanish in that limit.[39] It has been conjectured[16] (and later con-

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firmed numerically[15]) that a small-amplitude DB occurs due to an instability (bifurcation) of the $q=\pi$ plane wave. The rigorous analysis of this plane wave bifurcation gives an inequality[13,15,16,32]

$$3\phi_2\phi_4 - 4\phi_3^2 > 0 \tag{16}$$

which has to hold in order to obtain the modulational instability of the $q=\pi$ mode and by conjecture a low-amplitude DB solution. Since inequality (16) is satisfied for $\phi_2=\phi_4=1$ and $\phi_3=0.5$, we do observe the low amplitude (and thus low energy) limit of the DB family in Fig. 14. However, choosing $\phi_2=\phi_4=1$ and $\phi_3=1$, the inequality (16) is violated. Consequently the $q=\pi$ mode does not experience a low amplitude modulational instability, and low amplitude (and low energy) DBs do not exist. Nevertheless, as explained above, the high frequency limit of such an FPU model will always allow for DB solutions of a well known asymptotic shape. Consequently the energy versus frequency curve in Fig. 14 has to show up with a minimum. It is instructive to compute the DB profiles for Ω_b close to ω_π for the two cases. These profiles are shown in the insets in Fig. 14. For $\phi_3=0.5$ the low energy DB delocalizes and takes the shape of a $q=\pi$ plane wave (or better to say a standing wave, due to the open boundary conditions). The lattice deformation $d_+\approx -0.03$ tends to zero when increasing the system size and further approaching $\Omega_b \to 2$. For $\phi_3=1$ the DB with frequency close to ω_π has still large amplitudes, including a nonzero and well pronounced lattice distortion $d_+\approx -1$. While both DB branches have weak oscillatory instabilities as shown in Fig. 10, the dashed part of the upper curve in Fig. 14 indicates that DBs from that part of the branch experience an additional instability with corresponding eigenvalues located on the real axis. When decreasing ϕ_3 and approaching $\phi_3^{(cr)}=\sqrt{3\phi_2\phi_4}/2$, which changes the sign of the l.h.s. of inequality (16), the value of d_+ for DBs with frequencies close to the linear spectrum ($\Omega_b \to 2$) tends to zero and the energy threshold disappears.

DISCUSSION

The results of this work can be continued—and have been continued—in many different directions. The unstable Sievers–Takeno mode DB, when properly perturbed, lead to DB-like excitations which propagate along the lattice.[20,40] Some perturbative analytical results give a partial understanding of this effect.[41] Still there is strong evidence of the *nonexistence* of exact and spatially localized moving DBs.[42]

The inequality (16) can be used to predict the existence or noexistence of DB solutions for various other FPU-like models. A consequence is that DB excitations are not expected to exist for the Toda chain. A similar conclusion can be obtained for a so-called *Roto-FPU* model with $W(x)=1-\cos x$. However, such a system of coupled rotors allows for *rotobreathers*, i.e., solutions where a few degrees of freedom are in a rotating state, while the rest of the system is in a spatially localized oscillating state[43] [cf. Fig. 1(b)].

Discrete breathers are not an exclusive property of one-dimensional lattices. They exist equally in higher dimensional lattices,[4] where they show up with nonzero lower energy thresholds,[39] independent on further model parameters. This is true also for generalizations of FPU models to higher lattice dimensions. An interesting result concerns the case of asymmetric interaction potentials W and higher-dimensional FPU lattices. As shown in,[44] the requirement to have a finite energy for a DB leads to a static lattice deformation with a dipole symmetry and a spatial decay law $\sim r^{1-d}$ where r is the distance from the breather core and d the lattice dimension.

Finally we mention a number of studies of FPU breathers emerging from perturbed extended states via modulational instability or induced by fluctuations in thermal equilibrium.[18,45] These studies show clearly that DB solutions are not only interesting mathematical objects, but essential in order to understand and describe the properties of nonlinear lattice dynamics in thermal equilibrium and during relaxational processes.

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