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Existence and stability of odd and even parity discrete breathers in Fermi-Pasta-Ulam lattices

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Abstract—Discrete breathers are spatially localized periodic solutions in nonlinear lattices. We have proved the existence of discrete breathers having odd and even parity symmetries, i.e., Sievers-Takeno and Page modes, in one-dimensional Fermi-Pasta-Ulam type lattices for a class of nonhomogeneous potentials. Moreover, we have proved that the Sievers-Takeno mode is spectrally unstable while the Page mode is spectrally stable.

1. Introduction

Spatially localized excitation in nonlinear space-discrete dynamical systems has attracted great interest since the ground-breaking work by Takeno *et al.* [1, 2]. The localized mode is called *discrete breather* (DB) or *intrinsic localized mode*. Considerable progress has been achieved in understanding the nature of DB so far (e.g., [3, 4] and references therein).

The DBs are time-periodic and spatially localized solutions of the equations of motion. From the mathematical point of view, fundamental issues are their existence and stability. The anti-continuous limit is a useful concept for proving the existence of DBs. Existence proofs based on this concept have been given for various lattice models [5, 6]. The stability of DBs also has been studied near the limit [7, 8, 9, 10].

The FPU lattice is one of the fundamental lattice models in physics, to which the anti-continuous limit approach is not applicable. Two types of fundamental DB solutions that have different spatial symmetries, i.e., odd and even parity DB solutions, are known for this model. The odd and even parity DBs are called Sievers-Takeno (ST) mode [1, 2] and Page (P) mode [11], respectively. Normalized spatial profiles of the ST and P modes in a one-dimensional FPU lattice are approximately given by $(\ldots, 0, -1/2, 1, -1/2, 0, \ldots)$ and $(\ldots, 0, -1, 1, 0, \ldots)$ in the regime of strong localization, respectively, provided that interaction potentials of the lattice are of hard type. These two modes were originally found by approximate analytical calculations and then numerically confirmed.

For the FPU model, the first existence proof of DB solutions with odd and even parity symmetries was given in the particular case of homogeneous potential [12]. For more general nonhomogeneous potentials, an existence proof has been given by using a center manifold reduction technique [13]: the existence of DB solutions with odd and even parity symmetries has been proved in a regime of weak localization, where the DBs have small amplitudes and frequencies close to the phonon band edge. In other regimes, no existence proof has been given. As for the stability of DBs, it has been clarified only numerically so far for the FPU lattices [14] and there has been no rigorous result.

In this study, we consider one-dimensional nonhomogeneous potential FPU lattices with periodic boundary conditions, and prove existence of the odd and even parity DBs, i.e., the ST and P modes, in the regime of strong localization. To this end, we develop a new approach which is based on the use of an associated homogeneous potential FPU lattice and Banach's fixed point theorem. Moreover, we prove that the odd and even parity DB solutions are spectrally unstable and stable, respectively.

2. Lattice model

We consider the one-dimensional FPU lattices described by the Hamiltonian

$$H = \sum_{i=-N}^{N} \frac{1}{2} p_i^2 + \sum_{i=-N}^{N} V(q_{i+1} - q_i), \tag{1}$$

where $q_i \in \mathbb{R}$, $p_i \in \mathbb{R}$, V is a potential function, and the periodic boundary conditions $q_{\pm(N+1)} = q_{\mp N}$ and $p_{\pm(N+1)} = p_{\mp N}$ are assumed. Let $N_0 = 2N + 1$, which represents the number of degrees of freedom. Hamiltonian (1) describes one-dimensional chains of unit-mass particles with nearest neighbour interactions by V. The position and momentum of the ith particle are represented by q_i and p_i, respectively.

Let $X \in \mathbb{R}$, $\mu \in \mathbb{R}^l$ be a set of parameters, and $O \subset \mathbb{R}^l$ be a neighbourhood of $\mu = 0$. We assume the interaction potential V to be defined by

$$V(X) = W(X, \mu) + \frac{1}{k} X^k, \tag{2}$$

where:

(P1) $k \geq 4$ is an even integer;
(P2) $W(X, \mu) : \mathbb{R} \times O \to \mathbb{R}$ is a C^2 function of X and μ;
(P3) $W(X, 0) = 0$ for all $X \in \mathbb{R}$.

A typical nonhomogeneous potential often used in the literature is polynomial potential. Equation (2) incorporates the polynomial potential $W(X,\mu) = \sum_{r=2}^{k-1} \mu_r X^r$, where $\mu = (\mu_2, \ldots, \mu_{k-1})$, as an example.

Hamiltonian (1) defines the equations of motion in the phase space $\mathbb{R}^{2N_0}$ which is endowed with the symplectic 2-form $\omega = \sum_{i=-N}^{N} dq_i \wedge dp_i$ as follows:

$$\dot{q}_i = p_i, \quad \dot{p}_i = V'(q_{i+1} - q_i) - V'(q_i - q_{i-1}), \tag{3}$$

where $i = -N, \ldots, N$. Let $\Gamma(t) = (q(t), p(t)) \in \mathbb{R}^{2N_0}$ be a T-periodic solution of Eq. (3), where $q = (q_{-N}, \ldots, q_N)$ and $p = (p_{-N}, \ldots, p_N)$ are the position and momentum vectors. Let ξ_i be the variation in q_i, and we use the notation $\xi = (\xi_{-N}, \ldots, \xi_N)$. Linearizing Eq. (3) along $\Gamma(t)$, we obtain the variational equations in the second-order differential equation form as follows:

$$\ddot{\xi} + A(t)\,\xi = 0, \tag{4}$$

where $A(t)$ is the Hessian matrix of the potential function evaluated on $\Gamma(t)$, i.e., its components are given by $[A(t)]_{ij} = \partial^2 U(q(t))/\partial q_i \partial q_j$, where $U = \sum_{i=-N}^{N} V(q_{i+1} - q_i)$.

Let $\{\xi_1, \ldots, \xi_{2N_0}\}$ be a system of fundamental solutions of Eq. (4). According to the Floquet theory, the fundamental solutions of Eq. (4) at t and $t + T$ are related via a $2N_0 \times 2N_0$ monodromy matrix M as

$$(\xi_1(t+T), \ldots, \xi_{2N_0}(t+T)) = (\xi_1(t), \ldots, \xi_{2N_0}(t))\, M. \tag{5}$$

Eigenvalues of M are called the characteristic multipliers and they are independent of the choice of fundamental solutions. Let ρ_i, $i = 1, \ldots, 2N_0$ be the characteristic multipliers of $\Gamma(t)$. The spectral stability of $\Gamma(t)$ is defined as follows.

Definition 1. *Periodic solution $\Gamma(t)$ is said to be spectrally unstable if there exists ρ_i such that $|\rho_i| > 1$, otherwise it is said to be spectrally stable.*

3. Symmetry of solution

We precisely describe the odd and even parity symmetries in this section. Let S_O and S_E be the linear mappings $S_O, S_E : \mathbb{R}^{N_0} \to \mathbb{R}^{N_0}$ defined by

$$S_O : (S_O \cdot x)_i = -x_{-i}, \quad i = -N, \ldots, N$$
$$S_E : (S_E \cdot x)_i = -x_{-(i+1)}, \quad i = -N, \ldots, N$$

where $x = (x_{-N}, \ldots, x_N) \in \mathbb{R}^{N_0}$ represents a point in the space $\mathbb{R}^{N_0}$ and $x_{-(N+1)} = x_N$ due to the periodic boundary conditions. These S_O and S_E are linear involutions, i.e., $S_O \circ S_O = S_E \circ S_E = \mathrm{id}$.

Let $\Gamma(t) = (q(t), p(t)) \in \mathbb{R}^{2N_0}$ denote a periodic solution of Eq. (3) with a period T. The solution $\Gamma(t)$ is said to have odd symmetry if it satisfies the relations

$$S_O \cdot q(t+T/2) = q(t), \quad S_O \cdot p(t+T/2) = p(t), \quad {}^\forall t \in \mathbb{R}. \tag{6}$$

When the interaction potential is an even function, i.e., $V(X) = V(-X)$, an additional symmetry $\Gamma(t+T/2) = -\Gamma(t)$ holds. Then equation (6) reduces to

$$-S_O \cdot q(t) = q(t), \quad -S_O \cdot p(t) = p(t), \quad {}^\forall t \in \mathbb{R}. \tag{7}$$

On the other hand, $\Gamma(t)$ is said to have even symmetry if it satisfies the relations

$$S_E \cdot q(t) = q(t), \quad S_E \cdot p(t) = p(t), \quad {}^\forall t \in \mathbb{R}. \tag{8}$$

Equations (6) and (8) correspond to the solution profiles centered at $i = 0$ site and that centered between $i = -1$ and 0 sites, respectively.

4. Notations

We introduce some notations to state the main theorems. Consider the scalar differential equation

$$\ddot{\phi} + \phi^{k-1} = 0. \tag{9}$$

Equation (9) has the energy integral $\dot{\phi}^2/2 + \phi^k/k = h$, where h is an integration constant. Its solution is non-constant and periodic for any given $h > 0$. Let $\phi(t)$ be the solution of Eq. (9) with initial conditions $\phi(0) = (kh)^{1/k} > 0$ and $\dot{\phi}(0) = 0$. The period T of $\phi(t)$ depends on h, and it is obtained from the energy integral as follows:

$$T = 2\sqrt{2}\, h^{-(1/2-1/k)} \int_0^{k^{1/k}} \frac{1}{\sqrt{1 - x^k/k}}\, dx. \tag{10}$$

This indicates $T \propto h^{-(1/2-1/k)}$ and that T monotonically decreases from $T = +\infty$ to 0 as h varies from $h = 0$ to $+\infty$, since the integral in Eq. (10) is independent of h. Thus, for any given $T > 0$, there exists a non-constant periodic solution $\phi(t)$ with the period T, which corresponds to a value of h uniquely determined from Eq. (10). We denote this T-periodic solution of Eq. (9) with $\phi(t; T)$.

Let Π_O and Π_E be the subspaces of $\mathbb{R}^{N_0}$ defined by

$$\Pi_O = \left\{ x \in \mathbb{R}^{N_0} \,;\, -S_O \cdot x = x \right\}, \tag{11}$$
$$\Pi_E = \left\{ x \in \mathbb{R}^{N_0} \,;\, S_E \cdot x = x \right\}, \tag{12}$$

where $x = (x_{-N}, \ldots, x_N)$. These Π_O and Π_E are subspaces in the configuration space $\mathbb{R}^{N_0}$ that satisfy the odd and even symmetries, respectively (cf. Eqs. (7) and (8)).

Let $m \in \mathbb{N}$, $c > 0$, and $0 < r < 1$ be parameters. We define a closed subset $B_{m,c,r} \subset \mathbb{R}^{N_0}$ as follows:

$$B_{m,c,r} = \Big\{ x \in \mathbb{R}^{N_0} \,;\, |x_i| \le c \text{ for } 0 \le i \le m, \quad |x_i| \le c r^{(k-1)^{i-m}} \text{ for } m+1 \le i \le N \Big\}. \tag{13}$$

This subset $B_{m,c,r}$ is specified by the three parameters (m, c, r). Equation (13) shows that the interval of x_i rapidly decreases with increasing i in $B_{m,c,r}$.

Consider the phase space $\mathbb{R}^{2N_0}$ of Hamiltonian system (1). Let Π be the subspace of $\mathbb{R}^{2N_0}$ defined by

$$\Pi = \left\{ (q,p) \in \mathbb{R}^{2N_0} \,;\, \sum_{i=-N}^{N} q_i = \sum_{i=-N}^{N} p_i = 0 \right\}. \quad (14)$$

This is the subspace in which both the mass center and the total momentum are zero. Since $d(\sum_{i=-N}^{N} p_i)/dt = 0$ follows from Eq. (3) and the periodic boundary conditions, Π is an invariant subspace of Hamiltonian system (1).

5. Main results

Our main theorems for the existence and spectral stability are stated as follows. Theorems 1 and 2 are for the odd and even parity DB solutions, i.e., the ST and P modes, respectively.

Theorem 1. *Suppose potential function (2) and (P1)-(P3). Let $\{a_i\}_{i=-N}^{N}$ and (m,c,r) be constants given in Table 1 for k. Then, for any $N \geq 4$ and any $T > 0$, there exists a unique $x \in B_{m,c,r} \cap \Pi_O$ such that $\Gamma^0_{\mathrm{ST}}(t;T) = (u\phi(t;T), u\dot{\phi}(t;T)) \in \mathbb{R}^{2N_0}$ is a T-periodic solution of FPU lattice (1) with $\mu = 0$, where $u = a + x$ and $a = (a_{-N}, \ldots, a_N)$. Moreover, there exist a neighbourhood $U \subset \mathbb{R}^l$ of $\mu = 0$ and a unique family $\Gamma_{\mathrm{ST}}(t;T,\mu)$ of T-periodic solutions of FPU lattice (1) for $\mu \in U$ such that $\Gamma_{\mathrm{ST}}(t;T,\mu)$ is C^1 with respect to t and μ, $\Gamma_{\mathrm{ST}}(t;T,\mu) \in \Pi$, $\Gamma_{\mathrm{ST}}(t;T,0) = \Gamma^0_{\mathrm{ST}}(t;T)$, and it satisfies odd symmetry (6). The periodic solution $\Gamma_{\mathrm{ST}}(t;T,\mu)$ is spectrally unstable with one unstable characteristic multiplier.*

$k=4$	$a_0 = 0.3762$ $a_{\pm1} = -0.1968$ $a_{\pm2} = 8.67 \times 10^{-3}$ $a_i = 0$ (otherwise) $(m,c,r) = (\,3,\ 9\times10^{-5},\ 3\times10^{-3}\,)$
$k=6$	$a_0 = 0.5057$ $a_{\pm1} = -0.2539$ $a_{\pm2} = 1.1 \times 10^{-3}$ $a_i = 0$ (otherwise) $(m,c,r) = (\,3,\ 8\times10^{-5},\ 7\times10^{-4}\,)$
$k \geq 8$	$a_0 = 2\times3^{-(k-1)/(k-2)}$ $a_{\pm1} = -3^{-(k-1)/(k-2)}$ $a_i = 0$ (otherwise) $(m,c,r) = (\,2, 2.02\times3^{-(k-1)^2/(k-2)}, 5\times10^{-3}\,)$

Table 1

Theorem 2. *Suppose potential function (2) and (P1)-(P3). Let $\{a_i\}_{i=-N}^{N}$ and (m,c,r) be constants given in Table 2 for k. Then, for any $N \geq 4$ and any $T > 0$, there exists a unique $x \in B_{m,c,r} \cap \Pi_E$ such that $\Gamma^0_{\mathrm{P}}(t;T) = (u\phi(t;T), u\dot{\phi}(t;T)) \in \mathbb{R}^{2N_0}$ is a T-periodic solution of FPU lattice (1) with $\mu = 0$, where $u = a + x$ and $a = (a_{-N}, \ldots, a_N)$. Moreover, there exist a neighbourhood $U \subset \mathbb{R}^l$ of $\mu = 0$ and a unique family $\Gamma_{\mathrm{P}}(t;T,\mu)$ of T-periodic solutions of FPU lattice (1) for $\mu \in U$ such that $\Gamma_{\mathrm{P}}(t;T,\mu)$ is C^1 with respect to t and μ, $\Gamma_{\mathrm{P}}(t;T,\mu) \in \Pi$, $\Gamma_{\mathrm{P}}(t;T,0) = \Gamma^0_{\mathrm{P}}(t;T)$, and it satisfies even symmetry (8). The periodic solution $\Gamma_{\mathrm{P}}(t;T,\mu)$ is spectrally stable.*

$k=4$	$a_0 = -a_{-1} = 0.323$ $a_1 = -a_{-2} = -0.0535$ $a_i = 0$ (otherwise) $(m,c,r) = (\,2,\ 3\times10^{-4},\ 6\times10^{-3}\,)$
$k=6$	$a_0 = -a_{-1} = 0.4166$ $a_1 = -a_{-2} = -0.015$ $a_i = 0$ (otherwise) $(m,c,r) = (\,2,\ 9\times10^{-5},\ 7\times10^{-4}\,)$
$k=8$	$a_0 = -a_{-1} = 0.44484$ $a_1 = -a_{-2} = -3.65\times10^{-3}$ $a_i = 0$ (otherwise) $(m,c,r) = (\,2,\ 2\times10^{-5},\ 2\times10^{-4}\,)$
$k=10$	$a_0 = -a_{-1} = 0.45839$ $a_1 = -a_{-2} = -9.1\times10^{-4}$ $a_i = 0$ (otherwise) $(m,c,r) = (\,2,\ 2\times10^{-5},\ 8\times10^{-5}\,)$
$k \geq 12$	$a_0 = -a_{-1} = (1+2^{k-1})^{-1/(k-2)}$ $a_i = 0$ (otherwise) (m,c,r) $= (\,1,\ 2.02\,(1+2^{k-1})^{-(k-1)/(k-2)},\ 2\times10^{-3}\,)$

Table 2

Remark 1. If $\Gamma(t)$ is a periodic solution of autonomous Hamiltonian system (1), then so is a phase-shifted solution $\Gamma(t+\tau)$ for $^\forall\tau \in \mathbb{R}$ and it has the same orbit as $\Gamma(t)$ in the phase space. Two periodic solutions are identified if they differ only by a phase-shift.

Remark 2. We assumed the μ-dependent potential W of nearest-neighbor interaction type in Eqs. (1) and (2), focusing on the FPU lattices. This assumption is not essential. The statements of Theorems 1 and 2 hold for a more general Hamiltonian $H = \sum_{i=-N}^{N} p_i^2/2 + \sum_{i=-N}^{N}(q_{i+1}-q_i)^k/k + W(q,\mu)$, provided that W is a C^2 function of q and μ such that $W(q,0) = 0$ and $W(q + c\epsilon, \mu) = W(q,\mu)$ for $^\forall c \in \mathbb{R}$, where $\epsilon = (1,\ldots,1) \in \mathbb{R}^{N_0}$

Remark 3. Theorems 1 and 2 imply the existence of spatially periodic array of odd or even parity DB solutions in the infinite FPU lattices.

In Theorem 1, the approximation vector a has non-zero components on only a small number of sites with the indices satisfying $|i| < m$, and it represents a strongly localized profile. The theorem states that the profile vector u of

$\Gamma^0_{\mathrm{ST}}(t;T)$ is close to a and satisfies

$$|u_i - a_i| \le \begin{cases} c & \text{if } |i| \le m, \\ c\, r^{(k-1)^{|i|-m}} & \text{otherwise.} \end{cases}$$

In addition, the latter inequality indicates rapid decrease of $|u_i|$ with increasing $|i|$, since it is equivalent to $|u_i| \le c\, r^{(k-1)^{|i|-m}}$ due to $a_i = 0$, $|i| \ge m$. Thus $\Gamma^0_{\mathrm{ST}}(t;T)$ is a strongly localized solution. The solution $\Gamma_{\mathrm{ST}}(t;T,\mu)$ is also strongly localized for small μ because of its continuity with respect to μ. Similarly, Theorem 2 shows that both $\Gamma^0_{\mathrm{P}}(t;T)$ and $\Gamma_{\mathrm{P}}(t;T,\mu)$ have strongly localized profiles. The approximations $\{a_i\}_{i=-N}^{N}$ play a crucial role in the theorems.

6. Strategy of proofs of the theorems

We outline our strategy for proving Theorems 1 and 2. First, we consider the homogeneous potential FPU lattice which is described by Hamiltonian (1) with the potential $V(X) = X^k/k$, i.e., $\mu = 0$ in Eq. (2). In this particular lattice, it is possible to find a DB solution in the form $q = u\phi(t)$, where $u \in \mathbb{R}^{N_0}$ is a constant vector describing the spatial profile of the solution. The problem of finding a DB solution is reduced to a set of algebraic equations for u, and we solve it by using Banach's fixed point theorem in a neighborhood of the approximation $\{a_i\}_{i=-N}^{N}$. This fixed point approach enables one to obtain a precise quantitative estimation of u that has odd or even parity symmetry. Using this estimation of u, we evaluate the characteristic multipliers, i.e., the spectral stability, of the DB solution.

Next, we consider the nonhomogeneous potential FPU lattice, i.e., $\mu \ne 0$ in Eq. (2). The DB solution in the homogeneous potential lattice is continued to a nonhomogeneous potential one for small $\mu \ne 0$ by using the implicit function theorem, based on the characteristic multipliers for $\mu = 0$. We show that this continuation retains odd or even parity symmetry of the DB solution. Finally, we evaluate variations of the characteristic multipliers under the perturbation in μ to determine the spectral stability of the DB solution for $\mu \ne 0$.

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