Paper

Existence regions of longitudinal and transverse intrinsic localized modes in Fermi–Pasta–Ulam chain in two-dimensional plane

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Abstract: We model the Fermi–Pasta–Ulam lattice, in which masses move in a two-dimensional plane, and identify different types of intrinsic localized modes (ILMs): longitudinal and transverse. The stability of the ILMs is evaluated by using characteristic multipliers. Longitudinal ILMs tend to be unstable because of the buckling effect of the chain. In contrast, transverse ILMs become stable if the chain is initially stretched. This difference between the longitudinal and the transverse ILMs is revealed by computing existence regions with respect to the angular frequency and the initial extension of the chain. The results show that the longitudinal ILMs tend to be stable in low-frequency and low-extension areas whereas the transverse ILMs become stable upon strongly stretching the chain.

Key Words: intrinsic localized mode, discrete breather, FPU chain, transverse ILM, stability

1. Introduction

Vibrations of atoms in crystals have attracted significant research efforts, and the nonlinear lattice model is frequently used to describe such phenomena in crystals [1]. The Fermi–Pasta–Ulam (FPU) chain is one such nonlinear lattice model and was proposed by Fermi *et al.* in 1955 to investigate equipartition of kinetic energy among the degrees of freedom [2]. In 1988, Sievers and Takeno identified theoretically that energy localized solutions exist in one-dimensional FPU chains [3]. The localized solutions are called intrinsic localized modes (ILMs) or discrete breathers (DBs). Since their discovery, the characteristics of ILMs have received considerable research attention [4, 5]. Recent decades have seen numerous experimental studies on the subject, such as optical wave guides [6], Josephson junction ladders [7, 8], micro-mechanical cantilever arrays [9], electric circuits [10, 11], coupled pendulums [12], and macro-magneto-mechanical cantilever arrays [13–15]. These experiments strongly suggest that ILMs may be used in practical engineering applications, especially in micro- or nanotechnologies.

Low-dimensional carbon materials are key materials in micro- and nanotechnologies. Recently, theo-

retical and numerical studies have focused on carbon nanotubes [16], graphene [17, 18], graphane [19], *etc.* These materials consist of two-dimensional carbon-atom lattices. Jin *et al.* fabricated a one-dimensional lattice in the form of a carbon monoatomic chain [20], which has interesting heat and electrical conductivities [21, 22]. Thus, the carbon chain is expected to become a key material in micro- and nanotechnologies, which motivates us to identify and control ILMs in the monoatomic carbon chains.

Monoatomic carbon chains consist of one-dimensionally arranged carbon atoms that interact non-linearly with their neighbors. These characteristics are very similar to those of a FPU chain, except that the degrees of freedom of each atom differ. In a FPU chain, each atom is constrained to move along the chain axis. In contrast, a monoatomic carbon chain may be located in three-dimensional space, so each atom can move not only along the chain axis but also perpendicular to it. The difference between lattice dimension and the degree of freedom of each element in the lattice plays a crucial role in ILMs. In fact, novel ILMs have been discovered in FPU chains in three-dimensional space; namely, transverse ILMs and rotating ILMs [23]. In addition, the difference in dimensions makes longitudinal ILMs, which correspond to traditional ILMs in FPU chains, unstable because of buckling effects [23].

This work investigates the existence region and stability of longitudinal and transverse ILMs. Section 2 introduces the FPU-chain model. Longitudinal and transverse ILMs are numerically obtained in Sec. 3, and their stability is discussed in Sec. 4. Section 5 computes the existence regions and the stability of ILMs with respect to their angular frequency and the initial chain extension. An area exists where ILMs become stable or marginally stable in each existence region. Finally, the results of this work are summarized in Sec. 6.

2. Fermi–Pasta–Ulam chain

This work considers a Fermi–Pasta–Ulam chain placed in a two-dimensional plane. The schematic configuration is shown in Fig. 1. Each mass can move not only in the axial direction but also in the radial direction. Therefore, the following equations of motion for the masses are derived from Newton’s second law of motion [23]:

$$m\ddot{\mathbf{r}}_n = \frac{\mathbf{d}_n}{\|\mathbf{d}_n\|} \left\{ -\alpha (\|\mathbf{d}_n\| - \ell_0) - \beta (\|\mathbf{d}_n\| - \ell_0)^3 \right\} - \frac{\mathbf{d}_{n+1}}{\|\mathbf{d}_{n+1}\|} \left\{ -\alpha (\|\mathbf{d}_{n+1}\| - \ell_0) - \beta (\|\mathbf{d}_{n+1}\| - \ell_0)^3 \right\} \quad (1)$$

$$(n = 1, \dots, N),$$

where $\mathbf{r}_n = (x_n, y_n)$ is the two-dimensional displacement vector of the n th mass and $\mathbf{d}_n = \mathbf{r}_n - \mathbf{r}_{n-1}$ is the two-dimensional distance vector between mass $n - 1$ and mass n . In a FPU chain, each mass is connected by a nonlinear spring. The natural length of the spring is denoted ℓ_0 , and α and β are the linear spring coefficient and the cubic spring coefficient, respectively. In this work, all masses and the linear spring constant are set to unity, and the cubic spring constant is set to 25. The chain size is $N = 8$ and the boundaries are assumed to be periodic; namely, $\mathbf{r}_0 = \mathbf{r}_N$ and $\mathbf{r}_{N+1} = \mathbf{r}_1$.

As shown in Fig. 1, all masses are initially arranged in a straight line with equal intervals. This work assumes an initial extension of the chain. Thus, the initial distance vector can be $\mathbf{d}_n = \ell_n = (\ell_0, 0) + (\ell_1, 0)$, where $\ell_1 > 0$ is the initial extension of the nonlinear spring. The natural length of the nonlinear spring is set to unity, and ℓ_1 denotes the ratio of the initial extension to the natural length.

Fig. 1. Fermi–Pasta–Ulam chain in a two-dimensional plane. Adjacent masses are connected by nonlinear springs.

3. Intrinsic localized modes

Intrinsic localized modes have spatially localized profiles in the amplitude distribution. Only a few masses oscillate with large amplitude while the others remain almost at rest at their equilibrium positions. In the region where the masses are at rest, the equation of motion (1) can be linearized around $\mathbf{r}_n = 0$. Therefore, the necessary condition for ILM to exist is non-resonance with respect to the solutions of the linearized equations. Resonance will cause energy to propagate from the ILM core to the outside, and finally the ILM will decay.

The FPU chain is in two-dimensional plane, so the longitudinal and the transverse plane waves should be considered. To simplify the analysis, let the chain be of infinite length. The longitudinal and transverse plane waves are described as $x_n(t) = a_x e^{-i\kappa_x n \pm i\omega_x t}$ and $y_n(t) = a_y e^{-i\kappa_y n \pm i\omega_y t}$, respectively. By substituting the plane-wave solutions for $\mathbf{r}_n$ into the linearized equation, the relationship between the wave number κ and the angular frequency ω (*i.e.*, dispersion relations) are obtained:

$$\omega_x = 2\sqrt{1 + 3\beta\ell_1^2} \sin\left|\frac{\kappa_x}{2}\right|, \quad (2)$$

$$\omega_y = 2\sqrt{\frac{\ell_1 + \beta\ell_1^3}{1 + \ell_1}} \sin\left|\frac{\kappa_y}{2}\right|. \quad (3)$$

For both plane waves, the angular frequency goes to zero as the wave number goes to zero. However, ω_x and ω_y become maximal at $\kappa_x = \pi$ and $\kappa_y = \pi$, respectively:

$$\omega_{x,\max} = 2\sqrt{1 + 3\beta\ell_1^2}, \quad (4)$$

$$\omega_{y,\max} = 2\sqrt{\frac{\ell_1 + \beta\ell_1^3}{1 + \ell_1}}. \quad (5)$$

Therefore, the angular frequency of the ILMs should be greater than these maxima.

The angular frequency of the longitudinal ILM $\omega_{\text{L-ILM}}$ should be greater than $\omega_{x,\max}$. In this case, $\omega_{y,\max}$ is not related to the existence condition because no motion occurs in the transverse direction [23]. However, for the transverse ILM, both $\omega_{x,\max}$ and $\omega_{y,\max}$ should be considered because transverse motion will cause longitudinal motion. Let mass n oscillate transversely with a frequency ω ; namely, $\mathbf{r}_n = (0, a_n \cos \omega t)$, with the other masses fixed at zero. The nonlinear springs connected between mass n and the neighboring masses generate restoring forces of equal magnitude and that vary with the same frequency as the motion of mass n . The restoring forces have an x component and a y component because the angle between the springs and the axis is nonzero. At the neighboring mass, the transverse force changes with frequency ω . However, the longitudinal force becomes reaches its maximum twice during each period of the moving mass because it peaks at $\mathbf{r}_n = (0, a_n)$ and $(0, -a_n)$. The longitudinal force oscillates with the frequency 2ω . Therefore, the angular frequency of the transverse ILM should simultaneously satisfy the conditions $\omega_{\text{T-ILM}} > \omega_{y,\max}$ and $2\omega_{\text{T-ILM}} > \omega_{x,\max}$.

Intrinsic localized modes are found numerically by using the Newton-Raphson method, which is also called the shooting method [4]. The ILMs studied in this paper are temporary periodic solutions of Eq. (1), so they correspond to fixed points on an appropriately defined Poincaré map. Let $\mathbf{X}^* \in \mathbb{R}^{4N}$ be an ILM solution. The precision goal in our numerical simulation was set to $\|\mathbf{X}^* - P(\mathbf{X}^*)\| < \epsilon = 10^{-10}$, where the map P is computed by integrating the equation of motion (1) until the trajectory starting at $\mathbf{X}^*$ transverse the Poincaré section.

Two types of longitudinal ILMs (L-ILMs) are found numerically at $T = 2\pi/\omega_{\text{L-ILM}} = 1.5$. The first is the longitudinal Page mode (L-P mode) and the second is the longitudinal Sievers-Takeno mode (L-ST mode), as shown in Figs. 2(a) and 2(b), respectively. The L-P mode is centered between masses four and five, whereas the L-ST mode is centered mass four. The blue lines in Figs. 2(a)–2(d) indicate the trajectories of each mass. Each mass oscillates longitudinally (*i.e.*, in the x direction) with no bias; namely, the mean position of mass $\bar{x}_n$ is zero. The motions of the L-ILMs are the same as those of ILMs in a traditional one-dimensional FPU chain.

Figure 3 shows transverse ILMs. Similarly to the L-ILMs, two different types of ILM are obtained at $T = 2\pi/\omega_{\text{T-ILM}} = 1.5$. As shown in Figs. 3(e) and 3(f), the distributions of amplitude y_n resemble

(a) L-P mode

(b) L-ST mode

(a) T-P mode

(b) T-ST mode

(c) x_n of L-P

(d) x_n of L-ST

(c) x_n of T-P

(d) x_n of T-ST

(e) y_n of L-P

(f) y_n of L-ST

(e) y_n of T-P

(f) y_n of T-ST

Fig. 2. Longitudinal ILMs. Open circles correspond to masses and blue lines indicate trajectories of each mass.

Fig. 3. Transverse ILMs.

those of x_n for L-ILMs, shown in Figs. 2(c) and 2(d). However, as shown in Figs. 3(c) and 3(d), each mass oscillates with biases in the longitudinal direction. The biases are positive to the left of the center of the ILM and negative to the right, which means that the chain is compressed toward the center of the ILM. Because of this static compression, the energy distribution of T-ILMs is not strictly localized in space. Usually, both the energy and the amplitude decrease exponentially with distance from the center of ILM [24]. For the T-ILMs, the kinetic energy of masses decreases exponentially in its distribution. Thus, the T-ILMs consist of exponentially localized vibrations and the static compression.

4. Stability

The stability of ILMs can be determined by the characteristic or Floquet multipliers. These are the eigenvalues of the Jacobian $DP(\mathbf{X}^*)$, which is a linearized map around ILM solution $\mathbf{X}^*$ [4]. An ILM is unstable if a characteristic multiplier exists outside the unit circle in the complex plane. A perturbation along the corresponding eigenvector or eigenspace will grow exponentially. In general, a temporally periodic solution is a stable solution when all the characteristic multipliers are inside the unit circle. Let λ be a characteristic multiplier of a solution that satisfies $|\lambda| < 1$. Because Eq. (1) is conservative, the inverse $1/\lambda$ and the complex conjugates $\bar{\lambda}$ and $1/\bar{\lambda}$ are also characteristic multipliers of the solution. Therefore, a temporally periodic solution is not unstable if and only if all characteristic multipliers are located on the unit circle. In this work, we simply call such solutions stable.

For longitudinal ILMs, the red circles in Figs. 4(a) and 4(b) show the characteristic multipliers of L-P and L-ST, respectively. The figures show several characteristic multipliers outside the unit circle and on the real axis, so the L-P and L-ST modes are unstable. In a traditional FPU chain, the stability of ILM depends on the spatial symmetry of the ILM [24]. The blue crosses in the figures show

characteristic multipliers computed by fixing the transverse motions. In this case, the P mode becomes stable whereas the ST mode remains unstable. This fact implies that the transverse-direction degree of freedom makes the longitudinal ILMs unstable. The eigenvectors of the characteristic multipliers that exceed unity have nonzero y components. For example, the eigenvectors of $\lambda_{\max}$ in Figs. 4(a) and 4(b) are shown in Figs. 5(a) and 5(b), respectively. Localized y - and $\dot{y}$ -components are observed while all x - and $\dot{x}$ -components are zero. Therefore, the longitudinal ILM will deform transversely if a small noise is added to the original ILM solution. Phenomenologically, the longitudinal ILMs are rendered unstable by the buckling of the chain. Around the center of the longitudinal ILM, masses oscillate in antiphase with relatively large amplitudes. Thus, the chain is locally compressed for a moment. Initially extending the chain is an effective way to reduce the influence of the buckling instability. This is discussed in the next section.

Figures 4(c) and 4(d) show characteristic multipliers of the transverse ILMs. Similarly to the longitudinal ILMs, both P and ST modes are unstable because three characteristic multipliers are located outside the unit circle. One of them is on the real axis, and the other two form a complex-conjugate pair located in the left half complex plane. The instability of the transverse ILMs may also be due to the buckling effect. In Figs. 3(a) and 3(b), the trajectories of masses drawn by blue curves show that two neighboring masses approach each other on the chain axis. Figures 5(c) and 5(d) also show localized y - and $\dot{y}$ -components in the eigenvectors of $\lambda_{\max}$ in Figs. 4(c) and 4(d). It implies that the buckling effect affects the stability of the transverse ILMs, as well as the longitudinal ILMs.

As shown in Fig. 4, all the ILMs considered in this paper are unstable. Although the absolute value of the maximum characteristic multiplier of the T-P mode is less than that of the T-ST and other longitudinal modes, the T-P mode would be difficult to observe in a real system. The T-P mode will decay over several tens of periods of oscillation, because a small random perturbation increases about threefold each period. The instability is attributed to the frequency of the ILMs begins too high compared with those of the zone-boundary modes, $\omega_{x,\max}$ and $\omega_{y,\max}$. The next section discusses

Fig. 4. Characteristic multipliers of ILMs. The dashed curves correspond to the unit circle in the complex plane. The red circles indicate the characteristic multipliers of ILMs in Eq. (1). The blue crosses are obtained from the corresponding ILMs in the traditional FPU chain.

(a) L-P mode

(b) L-ST mode

(c) T-P mode

(d) T-ST mode

Fig. 5. Eigenvectors of $\lambda_{\max}$ in Fig. 4. x - and $\dot{x}$ -components are shown in the upper panels, y - and $\dot{y}$ -components are in the lower panels. Note that the eigenvectors shown here are real vectors.

ILM stability with respect to frequency and initial chain extension.

5. Existence regions

This section discusses the regions in which ILMs exist and the stability of the ILMs. To compute the regions, we first prepare a set of ILM solutions, which is obtained by gradually changing the initial extension while the ILM period is fixed at $T = 1$. From each solution in the set, another set of ILM solutions is obtained by increasing the period from 1. The parameters are held constant if the ILM solutions disappear or lose their localization.

Figures 6(a) and 6(b) show the regions where the longitudinal P and ST modes exist, respectively. In the figures, the colored areas indicate where the Newton–Raphson method converges and satisfy the condition $\|\mathbf{X}^* - P(\mathbf{X}^*)\| < 10^{-10}$. The darkness corresponds to the inverse of the maximum absolute value of the characteristic multipliers $1/|\lambda_{\max}|$. Therefore, ILMs in darker regions survive for a longer time. In addition, the region where the all characteristic multipliers satisfy the condition $||\lambda| - 1| < 10^{-6}$ is emphasized by green color, *i.e.*, ILMs in the green regions are stable. In contrast, brighter regions indicate the parameter regions where ILMs rapidly decay. The red curve is calculated by using Eq. (4). For longitudinal ILMs, the angular frequency should be greater than $\omega_{x,\max}$. All ILM solutions obtained satisfy the condition. As the initial extension ℓ_1 increases, the gap between the bottom boundary of the existence region and the red curve also increases. When the initial extension becomes large, another mechanism for the existence condition should be considered instead of $\omega_{L-ILM} > \omega_{x,\max}$.

Fig. 6. Existence regions of ILMs in Eq. (1). The stable regions are indicated by green.

The longitudinal ILMs tend to be stable when the frequency approaches $\omega_{x,\max}$ and the initial extension is less than 0.1 but not zero. Comparing Fig. 6(a) with Fig. 6(b) show that the green region is wider for the P mode than for the ST mode. In fact, there is no green region for ST mode. This difference seems to come from the difference in stability between longitudinal ILMs in a traditional FPU chain.

The regions where the T-ILMs exist have different shapes with respect to the regions where L-ILMs exist. The existence condition for the T-ILMs is $\omega_{\text{T-ILM}} > \omega_{x,\max}/2$ and $\omega_{\text{T-ILM}} > \omega_{y,\max}$. In this case, $\omega_{x,\max}/2$ always exceeds $\omega_{y,\max}$. As shown in Figs. 6(c) and 6(d), the colored regions are located above the red curve drawn by $\omega = \omega_{x,\max}/2$. Unlike for longitudinal ILMs, the gap between the lower boundary of the regions and the red curve does not become large with respect to the initial extension ℓ_1 , which implies that the nonresonance condition $\omega_{\text{T-ILM}} > \omega_{x,\max}$ is significant for transverse ILMs.

Relatively large green regions appear for $\ell_1 \geq 0.2$, as shown in Figs. 6(c) and 6(d). In contrast with the L-ILMs, the initial extension stabilizes the T-ILMs. The T-P mode has a larger stable area than does the T-ST mode; these characteristics are similar to the stability of the longitudinal ILMs in a traditional FPU chain.

The lower boundary of the existence region in Fig. 6(c) is almost straight at $\ell_1 < 0.18$, $\omega \simeq 3.17$, which is caused by the collision of neighboring masses at the center of the T-P mode. In Eq. (1), the distance between neighboring masses exists in the denominators of the coefficient $\mathbf{d}_n/||\mathbf{d}_n||$. If two masses become very close to each other, the numerical error becomes large, and the Newton–Raphson method fails to converge. Why the boundary is a straight line is unclear so far. In addition, the existence of T-P modes below the straight line for $\ell_1 \simeq 0$ remains to be confirmed.

6. Conclusions

This work investigates intrinsic localized modes in a Fermi–Pasta–Ulam (FPU) lattice placed in a two-dimensional plane. In addition to the traditional FPU chain, longitudinal ILMs, in which masses oscillate along the chain axis, are identified. The amplitude distributions of the longitudinal ILMs are rigorously consistent with those in traditional FPU chains. However, the stability characteristics differ because of the buckling effect. For the traditional ILM, the ST mode is unstable whereas the P mode is stable. For the longitudinal ILMs, almost all solutions are unstable. This result implies that the longitudinal ILM would be difficult to use in practical engineering applications.

However, transverse ILMs, in which masses mainly oscillate normal to the chain axis, only exist in a FPU chain placed in two- or three-dimensional space. Interestingly, existence regions and stability are quite different between ST- and P-type ILMs. The T-P mode has a larger area where the maximum eigenvalue is equal to unity, which is similar to the traditional longitudinal ILMs. In addition, the initial extension stabilizes both ST- and P- type ILMs. Therefore, in a stretched lattice, transverse ILMs play a significant role because the lifetime is much longer than the period of harmonic lattice oscillations.

Removing the constraint on motion of masses in a one-dimensional lattice renders longitudinal ILMs unstable and causes transverse ILMs. The instability caused by the buckling effect also occurs in carbon nanotubes [25]. Thus, the buckling effect is a common problem for stabilizing ILMs in low-dimensional materials. In addition to the FPU chain, transversely oscillating ILMs are identified in a polymer chain with secondary structure [26] and in polyethylene chains [27]. Therefore, one can expect that transverse ILMs also exist in carbon monoatomic chains.

The mobility of ILMs is also important for practical applications because moving ILMs carry kinetic energy. In fact, the existence and mobility of longitudinal ILMs have already been discussed in curved biopolymer chains [28], where the curvature strongly affects the mobility of moving ILMs. Future work will investigate the mobility of longitudinal and transverse ILMs in FPU chains.

To investigate ILMs in carbon monoatomic chains, more realistic interaction potentials, such as the Morse, Lennard–Jones, and Brenner potentials, should be considered. Longitudinal ILMs exist in one-dimensionally constrained Morse and Lennard–Jones lattices [29]. In future work, transverse ILMs will be investigated for realistic one-dimensional lattices.

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