# Existence Condition and Stability of Rotating Intrinsic Localized Modes in FPU- $\beta$ Chain with Fixed Boundaries

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Abstract—Intrinsic localized mode (ILM) is a spatially localized and temporary periodic solution in nonlinear lattices. In this report, Rotating ILMs in onedimensional Fermi-Pasta-Ulam (FPU) chain placed in three-dimensional space are focused on. First we derive an equation of motion and dispersion relations of longitudinal and transverse waves. By using Newton-Raphson method, we investigate existence regions of the rotating ILMs in two-dimensional parameter space consisting of the rotational period and the initial extension of the chain. In addition, stability is evaluated for the rotating ILM in the regions by using characteristic multipliers. As a result, It is shown that the rotating P mode exist in wider region than that of ST mode. In addition, stability analysis also shows that the rotating P mode has wider stable region than the ST mode. Moreover, we derive the upper bound of the rotation period in the case of P mode.

## 1. Introduction

It is well known that a spatially localized and temporary periodic solution called intrinsic localized mode (ILM) exist in nonlinear lattice[1], such as graphene, protein, and DNA[2, 3]. It implies that ILM can be utilized to nanotechnology. We have focused on the carbon monoatomic chain in which carbon atoms are linearly-arranged. It has been reported that the carbon monoatomic chain can be fabricated from graphene sheet[4] and it will have very high heat conductivity at the room temperature[5]. Neighboring carbon atoms nonlinearly interact each other with respect to the distance between them[6]. Therefore, vibration of each carbon atom in the chain can be modeled as a nonlinear lattice. The aim of our research is to find ILM in the carbon monoatomic chain and to utilize it to control the heat conduction.

Although the carbon monoatomic chain can be modeled as a nonlinear lattice, there is the significant difference that each carbon atom can move not only the axial direction but also the radial direction. The degree of freedom of the radial direction will cause many differences from the traditional one-dimensional nonlinear lattice that the motions are constrained along the axis of the lattice. Then, we have first focused on the Fermi-Pasta-Ulam- $\beta$  (FPU- $\beta$ ) chain which is well-known model in which ILM exists[7]. In our previous research, two novel types of ILM was

found, namely, the transverse and the rotating ILMs[8]. In this paper, stability and existence parameter regions of the rotating ILMs are investigated.

## 2. FPU- $\beta$ chain in three dimensional space

Fermi-Pasta-Ulam chain is the one-dimensional nonlinear lattice that has linear and cubic interaction. Equilibrium state of the chain is shown Fig.1(a). In the figure,  $l_0$  is natural length of nonlinear spring connecting neighboring masses and a is displacement. If a is positive, the chain is initially extended, and *vice versa*. When the system is placed in three-dimensional space, any masses can move not only longitudinally (along the axis) but also transversely (perpendicular to the axis) (see Fig.1(b)). Therefore, the equation of motion of the masses is described as:

$$m\frac{d^{2}\mathbf{r}_{n}}{dt^{2}} = \alpha(|\mathbf{r}_{n+1} - \mathbf{r}_{n}| - l_{0})\frac{\mathbf{r}_{n+1} - \mathbf{r}_{n}}{|\mathbf{r}_{n+1} - \mathbf{r}_{n}|} + \beta(|\mathbf{r}_{n+1} - \mathbf{r}_{n}| - l_{0})^{3}\frac{\mathbf{r}_{n+1} - \mathbf{r}_{n}}{|\mathbf{r}_{n+1} - \mathbf{r}_{n}|} + \alpha(|\mathbf{r}_{n-1} - \mathbf{r}_{n}| - l_{0})\frac{\mathbf{r}_{n-1} - \mathbf{r}_{n}}{|\mathbf{r}_{n-1} - \mathbf{r}_{n}|} + \beta(|\mathbf{r}_{n-1} - \mathbf{r}_{n}| - l_{0})^{3}\frac{\mathbf{r}_{n-1} - \mathbf{r}_{n}}{|\mathbf{r}_{n-1} - \mathbf{r}_{n}|},$$
(1)

where  $r_n$  is the position vector from equilibrium position to each mass.  $\alpha$  and  $\beta$  are coefficients of the linear and cubic nonlinear interaction, respectively. In this paper,  $r_n$  is treated as a three-dimensional vector in the Cartesian coordinate system, namely,  $r_n = (n(l_0 + a) + x_n, y_n, z_n)$  where  $x_n$  is longitudinal displacement and  $y_n$  or  $z_n$  is transverse displacement of each mass.

Dispersion relation can be obtained by linearizing Eq.(1)

$$\omega_x = 2\sqrt{\frac{\alpha + 3\beta a^2}{m}} \sin\left|\frac{k_x}{2}\right|,\tag{2}$$

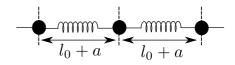
$$\omega_y = 2\sqrt{\frac{\alpha a + \beta a^3}{m(l_0 + a)}} \sin\left|\frac{k_y}{2}\right|,\tag{3}$$

where  $\omega_x$  and  $\omega_y$  denote angular frequency of longitudinal and transverse waves, respectively. Since the chain is cylindrically symmetric,  $\omega_z$  is the same as  $\omega_y$ . Eqs.(2) and (3) show that there are upper bound for the frequencies  $\omega_x$  and  $\omega_y$ . To exist an ILM, the ILM should avoid to resonate with

linear plain waves, namely, the frequency of the ILM  $\omega_b$  should be greater than  $\omega_x = 2\sqrt{\frac{\alpha+3\beta a^2}{m}}$  or  $\omega_y = 2\sqrt{\frac{\alpha a+\beta a^3}{m(l_0+a)}}$ . In this paper, m,  $\alpha$ , and  $l_0$  are set unity, and  $\beta$  is fixed at 25. The number of masses is chosen to be eight.

## 3. Rotating ILM

In the FPU- $\beta$  chain placed in three-dimensional space, three kind of ILM exist, namely, longitudinal, transverse, and rotating ILMs (see Fig.2)[8]. The longitudinal ILM coincides with the traditional ILM in which each mass move only along the axis of the chain. On the other hand, transverse ILM mainly consists of perpendicular oscillation to the axis. For more details of these two types otational period of ILMs, see Ref.[8]. The rotating ILM which is focused on in this paper is also a spatially localized and temporary periodic solution of Eq.(1) in which each mass rotates around the axis of the chain. An example of the rotating ILM is shown Fig.3. As shown in the Fig.3, a few masses have large amplitude and the phase difference between  $y_n$  and  $z_n$  equal  $\pi/2$ . Thus, each mass rotates around the axis, and the radii of the rotations are localized. In addition, in Fig.3(a), two neighboring masses (4th and 5th) oscillate in antiphase with the same amplitude while the other masses show very small amplitude motion. Therefore, the amplitude distribution correspond to Page mode[7]. In this paper, rotating P mode is abbreviated as R-P mode. Fig.3(b) shows a different ILM from R-P mode in spatial symmetry of the amplitude distribution. The 4th mass has the largest amplitude and the 3rd and 5th masses have the same amplitude which rather smaller than that of the 4th mass but sufficiently large comparing with the other masses. This amplitude distribution correspond to Sievers-Takeno mode[7]. The rotating Sievers-Takeno mode is also abbreviated as R-ST mode. Note that, the length of all the nonlinear springs connecting nearest neighbor masses are time-invariant while the rotating ILM is oscillating. That is, all the masses do not oscillate with changing the length of the nonlinear springs like the longitudinal and transverse ILMs. Therefore, another existence condition should be considered instead of the non-resonant condition Eqs.(2) and (3).



(a) Equilibrium state

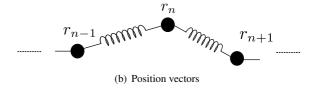


Figure 1: FPU- $\beta$  chain place in 3D space

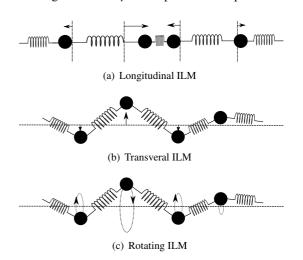


Figure 2: Three kinds of ILM in FPU- $\beta$  chain

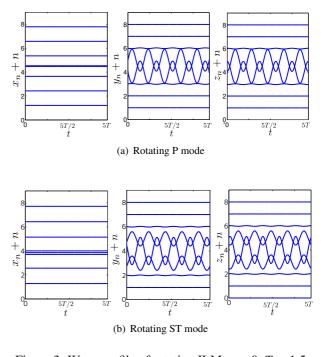


Figure 3: Wave profile of rotating ILM. a = 0, T = 1.5

## 4. Analysis of rotating ILM

In this section, we focus on the rotating ILMs mentioned in the previous section. Stability and existence region of the rotating ILM will be discussed below.

### 4.1. Dependence on parameter and bifurcation

Figure 4(a) shows R-P modes with respect to the rotation period when the initial extension a is fixed at 0.1. In the figure, the vertical axis shows the maximum radius of the R-P mode and horizontal axis shows the rotation period. The radius of the R-P mode decreases as the rotation period increases and disappears at about T=9.5 through a bifurcation. On the other hand, as shown in Fig.4(b), the R-ST mode disappear at about T=4.7, at which two branches coalesce. The other branch consist of the R-P modes that the 3rd and the 4th masses have the largest radius (see inset of Fig.4(b)). Thus, it seems that existence regions of R-P mode are strongly related to the position where the ILM stands.

## 4.2. Existence regions and stability

For the stability analysis, the characteristics multipliers are computed for each rotating ILM. Since the system of Eq.(1) is a conservative system, ILM is stable if and only if all the characteristic multipliers are located on the unit circle in the complex plane. Otherwise, the rotating ILM is unstable[9].

Figure 5 shows the parameter regions and stability of the ILMs. In the figure, the vertical axis shows the rotation period and horizontal axis shows the initial extension. The colors of the regions correspond to the maximum absolute values of the characteristic multipliers. As shown in the figure, there is the tendency that the range of the rotation period become narrow as the initial extension increases. In addition, the region of the central R-P modes in Fig3(a) are larger than those of the R-ST modes. The difference may come from the position of ILM and the size of the chain. R-P mode in Fig.3(a) is located exactly at the center of the chain, while another R-ST R-P modes shown in Fig.4(b) is not. If the size of the chain is sufficiently large, the difference of existence region will decrease unless R-P mode stands near the boundaries of the chain. The stability analysis shows that there is a relatively large area, which is colored by blue, where the R-P modes are almost stable. On the other hand, such stable region does not exist for the R-ST modes. Therefore, it is implied that the stability of the rotating ILMs depends on the spatial symmetry of amplitude distribution.

## 4.3. Existence condition for R-P mode

In the case of the R-P mode, the bifurcation diagram shows that the radius of the rotation approaches zero as the period increases. In the small amplitude regime, Eq.(1) can be linearized. Here we assume the uniform solution that

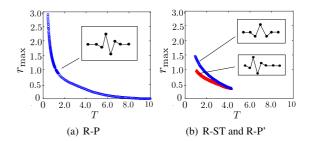


Figure 4: Dependence on parameter T. a=0.1. The insets indicate displacement distributions. (a) R-P mode at the center of the chain (b)R-ST and R-P'mode.

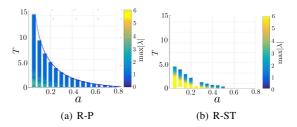


Figure 5: Existence regions of rotating ILMs and stability. The colorbar indicates the maximum absolute value of multipliers. (a) R-P mode. The curve expresses Eqs.(6) (b) R-ST mode.

each mass has the same radius of rotation  $r_0$  (see Fig.6). For the uniform solution, we obtain the following equaitons from Eq.(1):

$$l^2 = (1+a)^2 + (2r_0)^2, (4)$$

$$r_0 \left(\frac{2\pi}{T}\right)^2 = 2\left\{(l-1) + 25(l-1)^3\right\} \frac{2r_0}{l}.$$
 (5)

These equations mean that the restoring force of the spring and centrifugal force of angular frequency  $\frac{2\pi}{T}$  are balanced. By linearizing the equations around  $r_0 = 0$ , we obtain a relational expression between the rotation period and initial extension as follows:

$$T = \pi \sqrt{\frac{1+a}{a+25a^3}}. (6)$$

The curve in Fig.5(a) is drawn by Eq.(6). As shown in Fig.5(a), the boundary of the existence region of the R-P mode is almost coincide with the theoretical curve. Therefore, it seems that Eq.(6) gives the upper bound of the rotation period of the rotating ILM. Interestingly, Eq.(6) has the same form as Eq.(3) when  $\omega_y = \frac{2\pi}{T}$ .

## 5. Conclusion

In this paper, we have focused on the rotating ILM in the FPU- $\beta$  chain and discussed the existence condition and the stability. We have revealed parameter regions where the rotating ILM can exit. As a result, it has been found

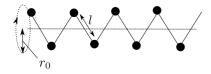


Figure 6: Displacement distribution near the bifurcation we assume in the case of R-P mode.

that the region for the R-P mode is wider than that of the R-ST mode. Stability analysis has also shown that the R-P mode has wider stable region than the R-ST mode. In addition, the upper bound of the rotation period has successfully been obtained for the R-P mode which stands at the center of the chain by using a uniform solution and the small amplitude approximation. However, the upper bound is not well-fit to the case of R-ST mode which does not stand on the center. The bifurcation occurs before the amplitude becomes sufficiently small. An analysis without the small amplitude approximation would be required. From the results of the paper, one can expect that a stable or nearly stable rotating ILM exist in a realistic system in which masses are connected nonlinearly, such as the carbon monoatomic chain. In the future, we will search localized solutions in a nonlinear lattice model of the carbon monoatomic chain.

#### References

- [1] A. J. Sievers, S. Takeno, "Intrinsic Localized Modes in Anharmonic Crystals," *Phys. Rev. Lett.*, vol. 61, pp. 970-973, 1988.
- [2] Y. Yamayose, Y. Kinoshita, Y. Doi, A. Nakatani and T. Kitamura, "Excitation of intrinsic localized modes in a graphene sheet," *EPL*., vol. 80, pp. 1-6, 2007.
- [3] M. Ibañes, M. Sancho, G. P. Tsironis, "Dynamical properties of discrete breathers in curved chains with first and second neighbor interactions," *Phys. Rev. E.*, vol.65, p. 041902, 2002.
- [4] C. Jin, H. Lan, L. Peng, K. Suenaga, S. Iijima, "Deriving Carbon Atomic Chains from Graphene," *Phys. Rev. Lett.*, vol.102, p. 205501, 2009.
- [5] N. Wei, G. Wu, J. Dong, "Heat conduction in a carbon chain," *Phys. Lett. A.*, vol. 325, pp.403-406, 2004.
- [6] W. Brenner, "Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films," *Phys. Rev. B.*, vol. 42, pp. 9458-9471, 1999.
- [7] S. Flach, A. Gorbach, "Discrete breathers in Fermi-PastaUlam lattices," *CHAOS*., vol. 15, pp. 015112-5, 2005.
- [8] M. Kimura, A. Mitani, S. Doi, "Existence and stability of intrinsic localized modes in a finite FPU chain

- placed in three-dimensional space," *Letters on materials.*, vol. 6, pp. 22-26, 2016.
- [9] S. Flach, A. Gorbach, "Discrete breathers Advances in theory and applications," *Phys. Rep.*, vol. 467, pp.13-26, 2008.