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Weakly nonlinear localization for a 1-D FPU chain with clustering zones

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Abstract. We study weakly nonlinear spatially localized solutions of a Fermi-Pasta-Ulam model describing a unidimensional chain of particles interacting with a number of neighbors that can vary from site to site. The interaction potential contains quadratic and quartic terms, and is derived from a nonlinear elastic network model proposed by Juanico et al. [1]. The FPU model can be also derived for arbitrary dimensions, under a small angular displacement assumption. The variable interaction range is a consequence of the spatial inhomogeneity in the equilibrium particle distribution. We here study some simple one-dimensional examples with only a few, well defined agglomeration regions. These agglomerations are seen to lead to spatially localized linear modes and gaps in the linear spectrum, which in turn imply a normal form that has spatially localized periodic orbits.

1 Introduction

We study weakly nonlinear oscillations of a quartic FPU-type lattice system where the number of interacting neighbors depends on the site. This "inhomogeneous FPU" system is derived from the nonlinear elastic network model proposed by Juanico et al. [1]. Elastic networks are systems of particles interacting through binary elastic forces, and the model of [1] was proposed to study some qualitative features of protein vibrations, especially the possibility of spatially localized nonlinear oscillations. Some related works on network models and protein vibrations are [8,9,12–14].

In this article we derive the multidimensional inhomogeneous FPU model from the nonlinear elastic network model of [1] under a small angular displacement assumption, and present some preliminary semi-analytical results on one-dimensional inhomogeneous FPU models. We restrict our attention to approximate spatially localized solutions of some simple one-dimensional models. The general idea is to first look for spatially localized linear modes, and then look for approximate expressions for the continuation of these solutions in the weakly nonlinear regime using a combination of tools from normal form theory, and the study of relative equilibrium solutions of systems with S^1 symmetry.

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The existence of localized linear modes comes from the inhomogeneity of the particle interactions, and we see modes localized in the regions where particles agglomerate and interact with more neighbors. The continuation argument uses resonance arguments that rely on a frequency gap between separating the higher frequency localized modes from the rest of the spectrum. The result is the existence of spatially localized periodic orbits in a normal form (i.e. approximate) system. Further information on these orbits is left for future work.

The frequency gap is special to the configurations we study here, and is absent from more general 1-D configurations, and in 3-D protein models, where we have agglomeration regions of different sizes. The idea of the present paper may be extended to these more interesting cases, but this will require a more detailed study of the overlap between certain modes. This work is still in progress.

Normal form and periodic orbits of FPU lattices have been studied extensively, especially low frequency modes, and the transfer of energy to higher modes, see e.g. [2–4,6,10] and references. In the present work we follow the ideas of [1,12] and look at higher frequency modes. Note however that the localization scenario of [1] is more general, since it involves more localization regions and more pronounced nonlinear effects, for instance localization does not always coincide with regions of linear localization. Some further remarks can be found in the discussion section.

The paper is organized as follows. In Sect. 2 we outline the derivation of the inhomogeneous FPU model, and write the equations in normal mode coordinates. In Sect. 3 we discuss the linear normal modes for some one-dimensional models with agglomeration regions. In Sect. 4 we outline the normal form argument.

2 Elastic network model and inhomogeneous FPU lattice

Consider N particles, with positions $\mathbf{r}_i \in \mathbb{R}^D$, $i = 1, \ldots, N$ (we are interested in $D = 1, 2, 3$). To describe the oscillation of each particle around its equilibrium position $\mathbf{R}_i$, we consider the potential energy U proposed by [1]

$$U = \sum_{i,j=1}^{N} c_{ij} \Big[\frac{k_2}{2} (|\mathbf{q}_i - \mathbf{q}_j + \mathbf{R}_{ij}| - |\mathbf{R}_{ij}|)^2 + \frac{k_4}{4} (|\mathbf{q}_i - \mathbf{q}_j + \mathbf{R}_{ij}| - |\mathbf{R}_{ij}|)^4 \Big], \qquad (1)$$

where $\mathbf{q}_i = \mathbf{r}_i - \mathbf{R}_i$ is the displacement of particle i, $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$, and $|\cdot|$ is the Euclidean distance in $\mathbb{R}^D$.

The c_{ij} are defined as follows: $c_{ij} = 1$, if $|\mathbf{R}_i - \mathbf{R}_j| < R_c$, and $c_{ij} = 0$ otherwise, so that R_c represents a pairwise interaction range. k_2 and k_4 are positive constants. The equilibrium of this potential is $\mathbf{q}_i = 0$ (equivalently $\mathbf{r}_i = \mathbf{R}_i$), for all $i = 1, \ldots, N$.

The pairwise potentials here describe "hyper-elastic" interactions (as in classical elasticity), since by $|\mathbf{q}_i - \mathbf{q}_j + \mathbf{R}_{ij}| - |\mathbf{R}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j| - |\mathbf{R}_i - \mathbf{R}_j|$.

Let θ_{ij} be the angle between $\mathbf{R}_{ij}$ and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and

$$h = \max\{\theta_{ij} | \forall\ i, j = 1, \ldots, N\}. \qquad (2)$$

We then find that

$$\begin{aligned} (|\mathbf{q}_i - \mathbf{q}_j + \mathbf{R}_{ij}| - |\mathbf{R}_{ij}|)^2 &= |\mathbf{q}_i - \mathbf{q}_j|^2 + \mathrm{O}(h^2), \\ (|\mathbf{q}_i - \mathbf{q}_j + \mathbf{R}_{ij}| - |\mathbf{R}_{ij}|)^4 &= |\mathbf{q}_i - \mathbf{q}_j|^4 + \mathrm{O}(h^2), \end{aligned} \qquad (3)$$

so that

$$U = \sum_{i,j=1}^{N} c_{ij}\Big[\frac{k_2}{2}|\mathbf{q}_i - \mathbf{q}_j|^2 + \frac{k_4}{4}|\mathbf{q}_i - \mathbf{q}_j|^4\Big] + \mathrm{O}(h^2). \tag{4}$$

The above approximation of small angular displacements of the particles is relevant for $D > 1$. For $D = 1$, we have $h = 0$, provided that $\mathbf{R}_i < \mathbf{R}_j$ implies $\mathbf{r}_i < \mathbf{r}_j$ for all i, j.

We can then consider the Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\sum_{i=1}^{N}|\mathbf{p}_i|^2 + \sum_{i,j=1}^{N} c_{ij}\Big[\frac{k_2}{2}|\mathbf{q}_i - \mathbf{q}_j|^2 + \frac{k_4}{4}|\mathbf{q}_i - \mathbf{q}_j|^4\Big], \tag{5}$$

where $\mathbf{p}_i$ is the momentum of particle i.

This is a multidimensional FPU-type model where the number of interacting neighbors is variable. The model is valid for small displacements of the particles around of equilibrium position.

In what follows we consider the $D = 1$ case, motivated by the examples in the next section. The formalism applies to higher dimensions with small changes.

The potential energy has two components, the quadratic and quartic parts, U_2 and U_4, respectively.

Let $\mathbf{p} = (p_1, p_2, \ldots, p_N)$, $\mathbf{q} = (q_1, q_2, \ldots, q_N)$.

Consider the *interaction matrix* C, defined as

$$\mathrm{C} = \begin{pmatrix} n_1 & -c_{21} & \cdots & -c_{N1} \\ -c_{12} & n_2 & \ddots & \vdots \\ \vdots & \ddots & n_{N-1} & -c_{NN-1} \\ -c_{1N} & \cdots & -c_{N-1N} & n_N \end{pmatrix}, \tag{6}$$

where the c_{ij} are as in (1), and $n_i = \sum_j^N c_{ij}$, is the number particles interacting with particle i, then

$$U_2 = \frac{k_2}{2}\sum_{i,j=1}^{N} c_{ij}|\mathbf{q}_i - \mathbf{q}_j|^2 = k_2\langle \mathbf{q}, \mathrm{C}\mathbf{q}\rangle, \tag{7}$$

where $\langle\cdot,\cdot\rangle$ denotes the Euclidean inner product in $\mathbb{R}^N$, so that the quadratic part $\mathcal{H}_0$ of the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H}_0 = \frac{1}{2m}\langle \mathbf{p}, \mathbf{p}\rangle + k_2\langle \mathbf{q}, \mathrm{C}\mathbf{q}\rangle. \tag{8}$$

The interaction matrix C is symmetric because the interaction between particles is symmetric. Therefore it is possible to find a diagonal matrix Λ such that $\mathrm{C} = M\Lambda M^T$, where M is an orthogonal matrix, i.e. $M = M^T$. We can then define a symplectic transformation from the variables $(\mathbf{q}, \mathbf{p})$ to the variables $(\mathbf{Q}, \mathbf{P})$ by

$$\mathbf{P} = M\mathbf{p}, \quad \mathbf{Q} = M\mathbf{q}, \tag{9}$$

where $\mathbf{P} = (P_1, P_2, \ldots, P_N)$ and $\mathbf{Q} = (Q_1, Q_2, \ldots, Q_N)$. The quadratic part $\mathcal{H}_0$ of the Hamiltonian in the $(\mathbf{Q}, \mathbf{P})$ variables is then

$$\mathcal{H}_0 = \frac{1}{2m}\langle \mathbf{P}, \mathbf{P}\rangle + k_2\langle \mathbf{Q}, \Lambda\mathbf{Q}\rangle. \tag{10}$$

The quartic part U_4 of the Hamiltonian $\mathcal{H}$ is

$$U_4 = \frac{k_4}{4} \sum_{l_1,l_2,l_3,l_4=1}^{N} \Gamma_{l_1 l_2 l_3 l_4} Q_{l_1} Q_{l_2} Q_{l_3} Q_{l_4}, \tag{11}$$

where

$$\Gamma_{l_1 l_2 l_3 l_4} = \sum_{i,j=1}^{N} c_{ij} \big(M_{il_1} - M_{jl_1}\big)\big(M_{il_2} - M_{jl_2}\big)\big(M_{il_3} - M_{jl_3}\big)\big(M_{il_4} - M_{jl_4}\big). \tag{12}$$

Let λ_i be the eigenvalues of the matrix C, $\lambda_1 \leqslant, \ldots, \leqslant \lambda_N$.
Note that $\lambda_1 = 0$, with corresponding eigenvector $1/\sqrt{N}[1, \ldots, 1]^T$.
Then, by Hamilton's equations it follows that

$$\dot{Q}_1 = \frac{\partial \mathcal{H}}{\partial P_1} = \frac{1}{m} P_1, \tag{13}$$

$$\dot{P}_1 = -\frac{\partial \mathcal{H}}{\partial Q_1} = -2k_2\lambda_1 Q_1 - \frac{k_4}{4}\frac{\partial}{\partial Q_1} \sum_{l_1,l_2,l_3,l_4=1}^{N} \Gamma_{l_1 l_2 l_3 l_4} Q_{l_1} Q_{l_2} Q_{l_3} Q_{l_4} = 0,$$

since $\Gamma_{l_1 l_2 l_3 l_4} = 0$ when at least one of the $l_i = 1$, $i = 1, 2, 3, 4$, is unity. We have that P_1 is a constant. This is the conservation of the total lineal momentum.

Setting $P_1 = 0$ in $\mathcal{H}$, we may consider Hamilton's equations for $Q_2, \ldots, Q_N$ and $P_2, \ldots, P_N$, and the Hamiltonian

$$\mathcal{H} = \frac{1}{2m} \sum_{l=2}^{N} P_l^2 + k_2 \sum_{l=2}^{N} \lambda_l Q^2 + \frac{k_4}{4} \sum_{l_1,l_2,l_3,l_4=2}^{N} \Gamma_{l_1 l_2 l_3 l_4} Q_{l_1} Q_{l_2} Q_{l_3} Q_{l_4}. \tag{14}$$

Using the symplectic change of variables

$$\begin{pmatrix} Q'_l \\ P'_l \end{pmatrix} = \begin{pmatrix} \sqrt{m} & 0 \\ 0 & \frac{1}{\sqrt{m}} \end{pmatrix} \begin{pmatrix} Q_l \\ P_l \end{pmatrix}, \tag{15}$$

$l = 2, \ldots, N$, we have

$$\mathcal{H}_0 = \sum_{l=2}^{N} \frac{1}{2} P_l'^2 + \sum_{l=2}^{N} \frac{1}{2} \omega_l^2 Q_i'^2, \quad \text{with} \quad \omega_l^2 = 2\frac{k_2 \lambda_l}{m}\cdot \tag{16}$$

The ω_l are the frequencies of the linear normal modes. Introducing the spectral variables

$$\begin{pmatrix} a_k \\ a_k^* \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{\omega_k}{2}} & \frac{\mathrm{i}}{\sqrt{2\omega_k}} \\ \sqrt{\frac{\omega_k}{2}} & -\frac{\mathrm{i}}{\sqrt{2\omega_k}} \end{pmatrix} \begin{pmatrix} Q'_k \\ P'_k \end{pmatrix}, \tag{17}$$

$k = 2, \ldots, N$, The Hamiltonian then becomes

$$\mathcal{H} = \sum_{k=2}^{N} \omega_k a_k a_k^* + \frac{k_4}{4} \sum_{k_1,k_2,k_3,k_4=2}^{N} \tilde{\Gamma}_{k_1 k_2 k_3 k_4} \Big[a_{k_1} a_{k_2} a_{k_3} a_{k_4} + 4a_{k_1} a_{k_2} a_{k_3} a_{k_4}^* + 6a_{k_1} a_{k_2} a_{k_3}^* a_{k_4}^* + 4a_{k_1} a_{k_2}^* a_{k_3}^* a_{k_4}^* + a_{k_1}^* a_{k_2}^* a_{k_3}^* a_{k_4}^* \Big], \tag{18}$$

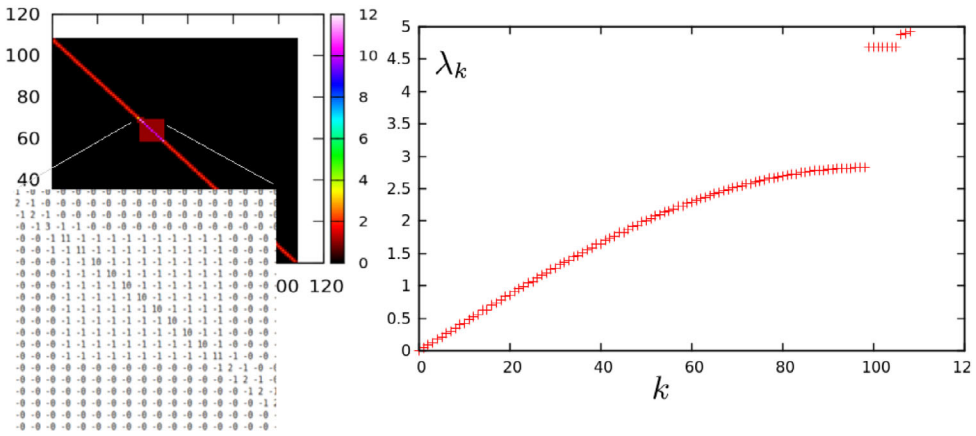

Fig. 1. a) Detail of the block in the interaction matrix C. b) Mode k vs λ_k (dispersion relation) for the interaction matrix C. These graphs are for example A.

where

$$\tilde{\Gamma}_{k_1k_2k_3k_4} = \frac{\Gamma_{k_1k_2k_3k_4}}{4\sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}}. \tag{19}$$

The coefficient $\tilde{\Gamma}_{k_1k_2k_3k_4}$ is a product of factors $F_{i,j;l} = (M_{il} - M_{jl})/\sqrt{\omega_l}$. $\sqrt{\omega_l}$ vanishes for small l, and large N, but we expect that the $M_{il} - M_{jl}$ vanish faster. For instance, in the case of the chain with nearest-neighbor interactions we have $|F_{j+1,j;1}| \leq C/\sqrt{N}$ for large N.

3 Numerical study of normal modes

We examine some 1-D examples of inhomogeneous FPU lattices. We choose $\mathbf{R}_i$ with $i = 1, \ldots, N$, along a line, and R_c so that particles $i = 2, \ldots, N-1$ interact with at least two neighbors, and particles $i = 1$, N interact with at least one neighbor. By varying the density of the particles we can have regions of agglomeration, where particles interact with more neighbors.

3.1 Example A: Chain with one region of agglomeration

This example corresponds to $N = 112$ particles, with one agglomeration region. The position of this region is slightly off the center of the chain. Away from the agglomeration region, which consists of approximately ten particles, those particles interact with their nearest neighbors. The interaction matrix C is indicated in Fig. 1a, where we see a tridiagonal matrix and one larger block, representing the agglomeration zone. In Fig. 1a we can see a detail of the block of the C matrix and its interaction with the tridiagonal part. This shows clearly the coupling between the large block and the tridiagonal region.

The spectrum of the interaction matrix C in Fig. 1b shows a gap separating the higher frequencies. In Fig. 3a we see the eigenfunctions M_{ln} ordered from high to

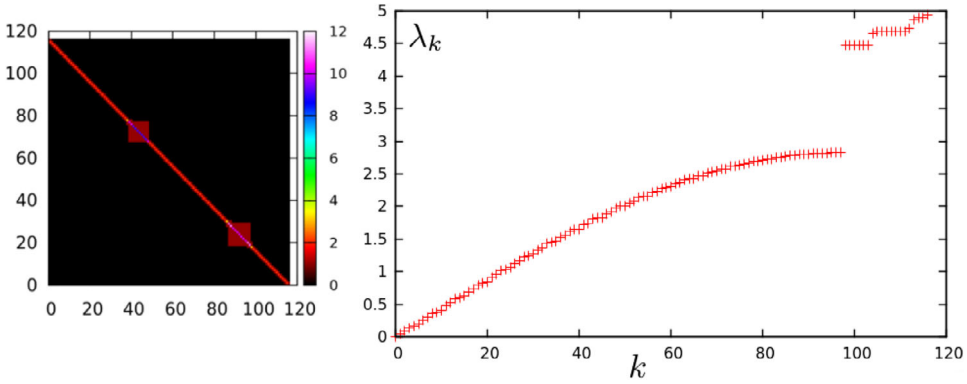

Fig. 2. a) Representation of interaction matrix C for a chain with two agglomeration regions. b) Mode k vs. λ_k for the chain with two agglomeration regions.

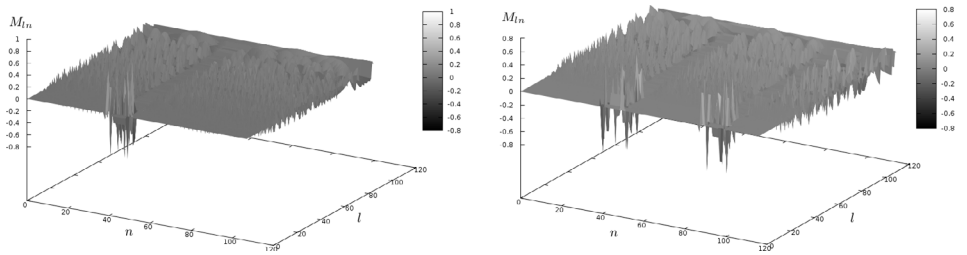

Fig. 3. a) M_{ln} is the amplitude of normal mode with index l ordered of high to lower modes (normalized eigenvector of C corresponding to eigenvalue λ_l) at site n, example A. b) Same for example B.

lower frequencies. The graph shows spatial localization of the vibrational modes of the higher frequencies, moreover the high frequency modes are localized at the region of agglomeration. The vibrational modes belonging to the lowest frequencies are not localized, for them the agglomeration zone is almost "transparent". In Fig. 3a we can also see that the medium frequency vibrational modes cannot pass the agglomeration zone.

3.2 Example B: Chain with two regions of agglomeration

This example corresponds to $N = 120$ particles in a chain with two agglomeration regions. These regions are at asymmetrically opposite off-center positions. The rest of the chain is homogeneous, and the particles only have interaction with their nearest neighbors. The interaction matrix for this example is indicated in Fig. 2a. In this matrix we see two blocks over the diagonal. Each agglomeration contains approximately 12 particles.

Figure 2b shows the dispersion relation for the matrix of interaction. This relation has essentially the same shape as the dispersion relation of the previous example, i.e. there exists a gap in the dispersion relation but with the difference that we have more higher frequencies. Figure 3b shows the eigenfunctions M_{ln} ordered from highest vibrational modes to lowest modes. We can observe again the spatial localization of the high vibrational modes in the regions of agglomeration.

The factor $\tilde{\Gamma}_{k_1k_2k_3k_4}$ for these two examples was calculated numerically and satisfies $\tilde{\Gamma}_{k_1k_2k_3k_4} < 1$, for all indices.

4 Birkhoff normal forms and invariant subspaces

In this section we discuss some properties of Birkhoff normal forms for 1-D systems. The general idea of Birkhoff normal forms, applied to the present problem, is that some quartic terms in the Hamiltonian can be removed by near-identity canonical transformations that are defined near the origin, e.g. in a ball of radius ρ near the origin. The change of coordinates should make some aspects of the dynamics more transparent.

Following the general theory, see e.g. [16], we may produce a canonical transformations as the time-1 of the Hamiltonian flow of a function χ, where to eliminate a monomial $\tilde{\Gamma}_{k_1k_2k_3k_4}b_{k_1}b_{k_2}b_{k_3}b_{k_4}$ in $\mathcal{H}$, with $b_{k_j}=a_{k_j}$, or $a^*_{k_j}$, χ must contain a corresponding monomial

$$\frac{\tilde{\Gamma}_{k_1k_2k_3k_4}}{\sum_{j=1}^4\sigma(k_j)\omega_{k_j}}b_{k_1}b_{k_2}b_{k_3}b_{k_4}, \tag{20}$$

(up to a constant). The quartic monomials that can not be eliminated, i.e. the resonant monomials, are the ones for which $\sum_{j=1}^4\sigma(k_j)\omega_{k_j}=0$, where $\sigma_{k_j}=1$ if $b_{k_j}=a_{k_j}$, and $\sigma_{k_j}=-1$ if $b_{k_j}=a^*_{k_j}$.

In this finite problem all non-resonant monomials can be eliminated, provided ρ is sufficiently small. The size of ρ is however controlled by the coefficient of the monomials in (20), and we only seek to eliminate certain non-resonant quartic monomials whose coefficients are in some sense "not too large". We will in fact only try to eliminate monomials $b_{k_1}b_{k_2}b_{k_3}b_{k_4}$ for which the frequency sum denominator satisfies $\sum_{i=1}^g\sigma(k_j)\omega_{k_i}\geq \mathrm{O}(1)$, i.e. "not too small", for some reasonable notion of O(1) discussed below. In this we will assume that $\tilde{\Gamma}_{k_1k_2k_3k_4}\leq \mathrm{O}(1)$ (this is verified in the examples of the previous section).

We will not consider here the question of eliminating monomials with both $\tilde{\Gamma}_{k_1k_2k_3k_4}$ and $\sum_{i=1}^g\sigma(k_j)\omega_{k_i}$ small. This analysis requires information on the overlap of the different modes and seems important for more general examples.

Motivated by the experiments A, B and the observation of the gap separating low and high frequencies we define two sets of indices $\mathcal{I}_-$ and $\mathcal{I}_+$ representing modes of frequencies that are below and above the gap, respectively. Let

$$\omega_c=\max_{j\in\mathcal{I}_-}(\omega_j),\quad \Omega_c=\min_{j\in\mathcal{I}_+}(\Omega_j), \tag{21}$$

with $\omega_c<\Omega_c$, and $\mathcal{I}_+\cup\mathcal{I}_-=\{2,\ldots,N\}$. Also let

$$\mathrm{G}=\Omega_c-\omega_c,\qquad \Delta=\max_{i,j\in\mathcal{I}_+}|\Omega_i-\Omega_j|. \tag{22}$$

The discussion of the $\tilde{\Gamma}_{k_1k_2k_3k_4}$ in Sect. 2 suggests that a reasonable small parameter for the problem is the smallest frequency ω_2 (i.e. the inverse of the size of the chain), and that O(1) means independent of ω_2 (i.e. the size of the chain).

Following the above considerations we assume that

$$\Omega_c-\Delta\geq \mathrm{O}(1),\quad \mathrm{G}\geq \mathrm{O}(1),\quad \mathrm{G}-\Delta\geq \mathrm{O}(1). \tag{23}$$

Proposition 1. *We can define a symplectic change of coordinates $a=f(\tilde{a})$, $a=\tilde{a}+$ cubic terms, $a=(a_2,\ldots,a_N)$, $\tilde{a}=(\tilde{a}_2,\ldots,\tilde{a}_N)$, that is generated by a function χ that is the sum of monomials of the form (20) with $\sum_{i=1}^g\sigma(k_j)\omega_{k_i}\geq \mathrm{O}(1)$ so that (i) the subspace V_+ defined by $\tilde{a}_j=0$, $\forall j\in\mathcal{I}_-$, is invariant under the Hamiltonian flow of $\tilde{\mathcal{H}}(\tilde{a})=\mathcal{H}(f(\tilde{a}))$, and (ii) the quartic part of $\tilde{\mathcal{H}}(\tilde{a})$, restricted to V_+, is invariant under the action $\tilde{a}_j\mapsto\tilde{a}_je^{i\phi}$, for all $j\in\mathcal{I}_+$, $\phi\in\mathbb{R}$.*

Table 1. Monomials in the equations of motion and their origin in the Hamiltonian.

Case	Monomial in $\dot{a}_k$, $k \in \mathcal{I}_-$ $k_1, k_2, k_3 \in \mathcal{I}_+$	Monomial in quartic Hamiltonian
(1)	$a_{k_1} a_{k_2} a_{k_3}$	$a_{k_1} a_{k_2} a_{k_3} a^*_{k_4}$
(2)	$a_{k_1} a_{k_2} a^*_{k_3}$	$a_{k_1} a_{k_2} a^*_{k_3} a^*_k$
(3)	$a_{k_1} a^*_{k_2} a^*_{k_3}$	$a_{k_1} a^*_{k_2} a^*_{k_3} a^*_k$
(4)	$a_{k_1} a_{k_2} a^*_{k_3}$	$a_{k_1} a_{k_2} a^*_k a^*_{k_3}$
(5)	$a_{k_1} a^*_{k_2} a^*_{k_3}$	$a_{k_1} a^*_{k_2} a^*_k a^*_{k_3}$
(6)	$a_{k_1} a^*_{k_3} a^*_{k_2}$	$a_{k_1} a^*_k a^*_{k_3} a^*_{k_2}$

Table 2. Frequency sums for quartic monomials of degree 3 in the variables a_k, a^*_k, $k \in \mathcal{I}_-$, and degree 1 in the variables a_k, a^*_k, $k \in \mathcal{I}_+$.

Case	frequency sum denominator
(1)	$\Omega_{l_1} + \Omega_{l_2} + \Omega_{l_3} - \tilde{\omega}_{l_4} \geq \Omega_c + G > \mathrm{O}(1)$
(2)	$\Omega_{l_1} + \Omega_{l_2} - \Omega_{l_3} - \tilde{\omega}_{l_4} = 0 \geq G + \Delta > \mathrm{O}(1)$
(3)	$\Omega_{l_1} - \Omega_{l_2} - \Omega_{l_3} - \tilde{\omega}_{l_4} \geq G - \Delta > \mathrm{O}(1)$
(4)	$\Omega_{l_1} + \Omega_{l_2} - \tilde{\omega}_{l_3} - \Omega_{l_4} \geq G - \Delta > \mathrm{O}(1)$
(5)	$\lvert\Omega_{l_1} - \Omega_{l_2} - \tilde{\omega}_{l_3} - \Omega_{l_4}\rvert \geq G - \Delta \geq \mathrm{O}(1)$
(6)	$\lvert\Omega_{l_1} - \tilde{\omega}_{l_2} - \Omega_{l_3} - \Omega_{l_4}\rvert \geq G - \Delta \geq \mathrm{O}(1)$

The idea for (i) is that from

$$\begin{aligned}\dot{a}_k = -\mathrm{i}\omega_k a_k - \mathrm{i}\frac{k_4}{4}\Bigg\{ &\sum_{k_1,k_2,k_3=2}^{N} \tilde{\Gamma}_{k_1 k_2 k_3 k}\left(4a_{k_1}a_{k_2}a_{k_3} + 6a_{k_1}a_{k_2}a^*_{k_3} + 4a_{k_1}a^*_{k_2}a^*_{k_3}\right) \\ &+ \sum_{k_1,k_2,k_4=2}^{N} \tilde{\Gamma}_{k_1 k_2 k k_4}\left(6a_{k_1}a_{k_2}a^*_{k_4} + 4a_{k_1}a^*_{k_2}a^*_{k_4}\right) + \sum_{k_1,k_3,k_4=2}^{N} \tilde{\Gamma}_{k_1 k k_3 k_4} 4a_{k_1}a^*_{k_3}a^*_{k_4} \\ &+4\sum_{k_2,k_3,k_4=2}^{N} \tilde{\Gamma}_{k k_2 k_3 k_4} a^*_{k_2}a^*_{k_3}a^*_{k_4}\Bigg\} \end{aligned} \tag{24}$$

with $k \in \mathcal{I}_-$, it is sufficient to eliminate monomials $b_{k_1}b_{k_2}b_{k_3}$ with $b_{k_j} = a_{k_j}$ or $b_{k_j} = a^*_{k_j}$ and $k_1, k_2, k_3 \in \mathcal{I}_+$. These monomials come from the monomials of $\mathcal{H}$ indicated in Table 1. By (21), (22), these monomials have frequency sum denominators that are of O(1), as indicated in Table 2, where we use the notation $\Omega_l = \omega_l$, if $l \in \mathcal{I}_+$, and $\tilde{\omega}_l = \omega_l$, if $l \in \mathcal{I}_-$.

Part (ii) follows from the fact that we can eliminate all monomials $a_{l_1}a_{l_2}a_{l_3}a^*_{l_4}$, $a_{l_1}a_{l_2}a_{l_3}a_{l_4}$ (and their complex conjugates), with $l_1, l_2, l_3, l_4 \in \mathcal{I}_+$, from $\mathcal{H}$. The frequency denominator for the monomial $a_{l_1}a_{l_2}a_{l_3}a^*_{l_4}$, $l_1, l_2, l_3, l_4 \in \mathcal{I}_+$ (and its complex conjugate) is

$$\Omega_{l_1} + \Omega_{l_2} + \Omega_{l_3} - \Omega_{l_4} \geq 2\Omega_c - \Delta > \mathrm{O}(1).$$

Similarly the denominator for $a_{l_1}a_{l_2}a_{l_3}a_{l_4}$, $l_1, l_2, l_3, l_4 \in \mathcal{I}_+$ (and its complex conjugate) is

$$\Omega_{l_1} + \Omega_{l_2} + \Omega_{l_3} + \Omega_{l_4} \geq 4\Omega_c > \mathrm{O}(1).$$

Therefore the quadratic and quartic part of $\tilde{\mathcal{H}}(a)$, restricted to V_+, and denoted by $\overline{\mathcal{H}}(a)$, is

$$\overline{\mathcal{H}} = \sum_{l\in\mathcal{I}_+} \omega_l a_l a_l^* + \frac{3k_4}{2} \sum_{l_1,l_2,l_3,l_4\in\mathcal{I}_+} \tilde{\Gamma}_{l_1 l_2 l_3 l_4} a_{l_1} a_{l_2} a_{l_3}^* a_{l_4}^*. \tag{25}$$

This concludes the argument. A more precise statement, e.g. an estimate of ρ, is left for future work.

It is clear that (25) implies $\overline{\mathcal{H}}(ae^{\mathrm{i}\phi}) = \overline{\mathcal{H}}(a)$, for all $a \in V_+$, $\phi \in \mathbb{R}$, so that the Hamiltonian flow of $\overline{\mathcal{H}}$ has the additional constant of motion

$$\mathcal{P}_+ = \sum_{l\in\mathcal{I}_+} |a_l|^2. \tag{26}$$

Then to look for periodic orbits of the Hamiltonian flow of $\overline{\mathcal{H}}$ in V_+, we seek solutions of the form $a_l = e^{\mathrm{i}\lambda t} A_l$, $l \in \mathcal{I}_+$. Such $A \in \mathbb{C}^{|\mathcal{I}_+|}$ are critical points of $\overline{\mathcal{H}}$ on the spheres $\mathcal{P}_+(A) = c$, $c > 0$. It is a topological fact [15] that we have at least $|\mathcal{I}_+|$ families of such critical points A at each sphere $\mathcal{P}_+(A) = c$, $c > 0$. These families of critical points are circles, since if A is critical point then so is $e^{\mathrm{i}\theta} A$. Relative equilibria for S^1 Hamiltonian systems have been studied extensively, in discrete NLS equations, and other contexts, see e.g. [11].

Note also that we have at least two such periodic orbits at each $\mathcal{P}_+(A) = c$, $c > 0$, that are stable in the subspace V_+, they correspond to the maxima and minima of $\overline{\mathcal{H}}$ in $\mathcal{P}_+(A) = c$. These solutions may have however unstable directions in the remaining directions. Their numerical computation and stability analysis is left for future work. This analysis should also be useful in determining whether these solutions persist under inclusion of the higher order terms of $\tilde{\mathcal{H}}$.

5 Discussion

We have studied weakly nonlinear spatially localized modes in some inhomogeneous FPU lattices. The localization is related to the presence of well defined regions of particle agglomerations, that is rather special to the configurations we consider, but may point to a mechanism that is applicable to more general inhomogeneities, where the absence of spectral gaps is compensated by small overlap of the eigenmodes. This scenario will be examined in future work.

The existence of nonlinear normal modes (periodic orbits) near the origin of a Hamiltonian system with definite quadratic Hamiltonian is a robust phenomenon, predicted by the Weinstein-Moser theorem, and other well-known generalizations, see e.g. [5]. The computation and continuation of these orbits generally requires numerical computations as in [12], and the existence of spatially localized periodic orbits is a concept that should make use of some extra structure in the system. In the particular problem this structure is provided by the interaction matrix characterizing the system, and a first idea is to combine the spectral data of this matrix with normal form ideas.

These and related matrices have been studied quite extensively in spectral graph theory, and we hope that certain features of the numerical dispersion and mode overlap factors can be explained by theoretical arguments. Also of interest is the use of this linear information in normal forms involving more general non-linear interactions. In particular, the absence of cubic interactions seems crucial for our argument on high-low frequency interactions, and a natural question is whether cubic interactions among certain ranges of modes can be non-resonant. The studies of [8,9,14],

also suggest a convex dispersion profile for the low modes of protein models that is different from the one arising in 1-D. Thus it seems that there are several related questions for different ranges of frequencies.

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