BUSHES OF VIBRATIONAL MODES FOR FERMI-PASTA-ULAM CHAINS

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Abstract Some exact solutions and multi-mode invariant submanifolds were found for the Fermi-Pasta-Ulam (FPU) β-model by Poggi and Ruffo in Phys. D 103 (1997) 251. In the present paper we demonstrate how results of such a type can be obtained for an arbitrary N-particle chain with periodic boundary conditions with the aid of our group-theoretical approach [Phys. D 117 (1998) 43] based on the concept of bushes of normal modes in mechanical systems with discrete symmetry. The integro-differential equation describing the FPU-α dynamics in the modal space is derived. The loss of stability of the bushes of modes for the FPU-α model, in particular, for the limiting case \(N \to \infty\) for the dynamical regime with displacement pattern having period twice the lattice spacing (π-mode) is studied. Our results for the FPU-α chain are compared with those by Poggi and Ruffo for the FPU-β chain.

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1 Introduction

Fermi, Pasta and Ulam (FPU) introduced in [1] a simple nonlinear model for studying the problem of equipartition of energy among different degrees of freedom (linear normal modes) of an \(N\)-particle mechanical system for sufficiently large \(N\). This model represents a monatomic chain with interactions only between neighboring atoms. It may be also considered as a chain of identical masses connected with identical nonlinear springs. The
force \( F(\Delta x) \) produced by each spring can be expressed as a power series in its deformation \( \Delta x \):

\[
F(\Delta x) = -k \cdot \Delta x + \alpha \cdot (\Delta x)^2 + \beta \cdot (\Delta x)^3 + \ldots
\]  

(1)

The FPU-\( \alpha \) chain corresponds to the case \( \alpha \neq 0, \beta = 0 \), while the FPU-\( \beta \) chain corresponds to the case \( \alpha = 0, \beta \neq 0 \), and in the both models all terms of higher order than those written in (1) are neglected.

The FPU model played an important role in the development of some new concepts in the nonlinear dynamics of classical systems and helped to reveal a number of new nonlinear phenomena (see, for example, [2, 3, 25] and references cited therein). Let us specifically refer to the approximately recurrent behavior in time of the energy distribution among several of the first modes [1], to the introduction of the concept of solitons [4], to some important results concerning deterministic chaos [5], to breathing self-localized solitons [6], etc.

An interesting paper devoted to the FPU-\( \beta \) chain dynamics was published recently by Poggi and Ruffo [3]. These authors revealed some exact solutions for the considered mechanical system and demonstrated “the existence of subsets of normal modes where energy remains trapped for suitable initial conditions”, which they called “subsets of I-type”[1]. They also discussed the problem of stability of such solutions and appropriate multi-mode invariant submanifolds (with particular attention to the case of the thermodynamical limit \( N \to \infty \)).

In connection with the above mentioned paper we want to emphasize the following essential points:

- The analysis in [3] is based on the specific character of interaction between particles of the FPU-\( \beta \) chain and, therefore, such an analysis must be done once again for every other type of monatomic chain.

- Only one- and two-dimensional subsets of normal modes of “type I” were found for FPU-\( \beta \) in [3].

In the present paper we would like to demonstrate a simple group-theoretical method, based on our previous papers [7–10], for finding all subsets of modes of “type I” for

\[1\] We use another term for such objects - bushes of normal modes [7 - 10].
monatomic chains with periodical boundary conditions. This method, in its general form, can be used for any mechanical system with any space symmetry group $[10, 11]$. It is based on the concept of “bushes of normal modes” in nonlinear physical systems with discrete symmetry, which we consider to be as fundamental as the concepts of solitons, dissipative structures, etc. in modern nonlinear science. Apparently, bushes of modes play an important role in many physical phenomena of current interest $[10]$. For example,

- peculiarities of dielectric and optical spectra brought about by the interactions between different modes in crystals;
- critical dynamics, behavior of structural and thermodynamical parameters near phase transition points;
- phenomena induced by interaction between soft and hard modes, in particular, peculiarities of the temperature dependence of the Debye-Waller factor near phase transitions, which plays an important role in the interpretation of x-ray and neutron structural experiments, etc.

The present paper is devoted to the symmetry-determined bushes of vibrational modes in the monatomic chains. Let us explain these basic notions on the qualitative level. The more exact definitions we give in the next section.

**Modes.** We consider the symmetry group $G_0$ of a given mechanical system in equilibrium (“parent group”) and its irreducible representations (irreps). The basis vectors of these irreps, which describe the atomic displacements patterns, are called “symmetry-adapted coordinates”. In a particular case (the monatomic chain is precisely this case!), symmetry-adapted coordinates can be identical with normal coordinates. We mean by the term “mode” an arbitrary superposition (with time-dependent coefficients) of the above basis vectors of a given multidimensional irrep. All that was just said allows us to use for the monatomic chain the term “modes” (or “vibrational modes”) as a synonym of both the symmetry-adapted and normal modes.

In the most part of the paper, we treat $G_0$ as a cyclic group of pure translations.

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2 In particular, it can be used for multiatomic chains.
3 In more complicated cases when a given irrep enters several times into the full vibrational representation of the considered mechanical system, we must differentiate between the terms “symmetry-adapted” and “normal” coordinates (modes).
(only in Sec. 2.6, we consider $G_0$ as the dihedral group). All irreps of this group are one-dimensional, and each vibrational mode is simply a product of some time-dependent coefficient with the appropriate normal coordinate which can be introduced in the harmonic approximation by the conventional method.

**Bushes of modes.** Normal modes are independent of each other in the harmonic approximation, but the excitation from the initially excited mode (we call it “root” mode) can spread to a number of modes with zero amplitudes at the initial instant (we call them “secondary” modes), if anharmonic terms in the Hamiltonian of the considered mechanical system are taken into account.

It is essential that, in general, *not all modes* turn out to be excited as a result of the excitation of the given root mode, but only a very certain their collection. This phenomenon is a consequence of the specific selection rules for the excitation transfer between normal modes of different symmetry[7]. The bush of normal modes is a superposition of *all* modes, associated with different irreps of the parent group $G_0$, which are involved in the vibrational process as a result of exciting a given root mode.

Every bush describes an *exact* dynamical regime whose number of degrees of freedom can be essentially less than that of the considered mechanical system[4]. Note that one-dimensional bushes represent the similar nonlinear normal modes introduced by Rosenberg [15].

As was already stated, excitation of a primary (“root”) mode leads to the excitation of the bush as a single dynamical object. Amplitudes of modes belonging to the bush change in time and, as a rule, their evolution is not trivial. As a consequence, we can speak about a number of new types of excitations in systems with discrete symmetry.

The following propositions were justified in the previous papers [7-10]:

1. A certain subgroup $G$ of the symmetry group $G_0$ corresponds to a given bush, and this bush can be excited by imposing the appropriate initial conditions with the above symmetry group $G \subset G_0$.

2. Each mode belonging to the bush possesses its own symmetry group which is greater than or equal to the group $G$ of the whole bush.

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[4] Only in the special case, a given bush can possess the trivial symmetry and represent the general dynamical regime whose dimension coincides with that of the considered mechanical system.
3. In spite of evolving mode amplitudes, the complete collection of modes in the given bush is preserved in time and, in this sense, the bush can be considered as a geometrical object.

4. The energy of the initial excitation is trapped in the bush, i.e. it cannot spread to the modes which do not belong to the bush, because of the symmetry restrictions.

5. As an indivisible nonlinear object, the bush exists because of force interactions between the modes contained in it.

6. Taking into account the concrete type of interactions between particles of the considered mechanical system can only reduce the dimension of the given bush.

7. The extension of the bush can be realized as a result of the loss of its stability which is accompanied by spontaneous breaking of the bush symmetry (dynamical analog of phase transition).

In the present paper, we discuss symmetry-determined bushes of vibrational modes, i.e. bushes whose existence is brought about by the symmetry-related causes only. In other words, we do not take into account any information about the type of interactions between the particles of the mechanical system. Nevertheless, it should be noted that taking into account such information can lead to some additional selection rules for excitation transfer between different modes and, therefore, to the reduction of the dimension of the symmetry-determined bushes (we discuss this problem in Sec.2.5). Moreover, every additionally considered symmetry can result in a similar effect (see Sec.2.6.). Thus, one can be sure that the excitation of a given mode cannot spread out of the symmetry-determined bush having that mode as root, but there may exist additional causes actually restricting the excitation to a mode subset of this symmetry-determined bush.

Let us stress that the symmetry-determined bushes which are found in the present paper are valid for any of monatomic chains and, in some a sense, they can be applied to multiatomic chains as well (we explain this point in Sec.2.6).

The notion of bushes of normal modes was introduced in [7]. In the last paper and in [8, 9] we investigated the main properties of bushes of modes and developed the general group-theoretical method for their finding. The detailed discussion of our approach and some important theorems are presented in [10]. Bushes of small dimensionality for many structures with point and space groups of crystallographic symmetry are found, classified
and investigated in the above papers. Bushes of vibrational modes for the fullerene $C_{60}$ ("buckyball" structure) are discussed in \[22, 23\].

Since application of group-theoretical methods for finding bushes of modes for mechanical systems, described by space groups with multidimensional irreducible representations, is very difficult, we developed a set of appropriate computer programs for treating such problems (previously similar programs were used for studying structural phase transitions in crystals \[12\]).

All symmetry-determined “resonance subspaces” (see \[13, 14\]) and similar nonlinear normal modes were found in \[11\] for all mechanical systems with any of the 230 space groups. Setting up this problem and its solution became possible because of using the concept of “irreducible” bushes of modes and due to the employment of the remarkable computer program ISOTROPY, created by Stokes and Hatch. This program realizes a great number of group-theoretical methods used in the theory of crystals. Its modified version, including the possibility to treat bushes of modes, is now available on the Internet as free software \[16\].

The first part of the present paper is devoted to the problem of existence of bushes of normal modes in nonlinear chains, and the second part is devoted to the discussion of their stability. Considering the existence of a bush of modes in nonlinear periodical chains with arbitrary interaction between their atoms (not necessarily of nearest-neighbor type), we use the general group-theoretical method described in \[10\]. Discussing this problem we keep in mind not only the goal of obtaining some new results, but also the purpose of the exposition of our approach for studying dynamics of nonlinear systems with discrete symmetry using one-dimensional chains as the simplest case of such symmetry. Finally, we obtain for the FPU-\(\alpha\) model a new integro-differential equation in the modal space for the case of the continuum limit \((N \to \infty)\). This equation is valid for all wave lengths (not only for long wavelengths as in the KdV-equation obtained for the FPU-\(\alpha\) model by Zabusky and Kruskal \[4\]).

In the second part of the paper, we discuss the problem of bush stability using the FPU-\(\alpha\) chain as a concrete model (in contrast to the FPU-\(\beta\) chain considered in \[3\]). Different channels of the loss of bush stability for finite \(N\) are discussed. The appearance of “satellites” forbidden by symmetry are revealed for bushes of normal modes for sufficiently
large values of $N$. The simplest bush $B[2a]$, corresponding to the displacement pattern with periodicity twice the periodicity of the chain in the equilibrium state\footnote{This bush consists of only one zone boundary mode or $\pi$-mode, in another terminology.}, is studied for the limit $N \to \infty$.

2 Bushes of normal modes for nonlinear chains

We describe here the general method for finding bushes of vibrational modes \cite{10} using the one-dimensional FPU model with periodical boundary conditions as an illustrative example. The starting point of our approach is the expression of the set of atomic displacements as a sum of contributions from different irreducible representations (irreps) of the symmetry group of the considered mechanical system in equilibrium [see (3) below]. Therefore, we begin with the consideration of irreps and their basis vectors for the case of the monatomic chain.

2.1 Vibrations of monatomic chain in terms of irreducible representations of its symmetry group

Let us consider the many-particle Hamiltonian system moving near the single equilibrium state characterized by the parent group $G_0$ of point or space symmetry and introduce the $N$-dimensional vector $X(t)$ determining values of all of its $N$ degrees of freedom at a given instant $t$:

$$X(t) = \{x_1(t), x_2(t), \ldots, x_N(t)\}. \quad (2)$$

We can write the vector $X(t)$ as the superposition of basis vectors $\varphi_k^{(j)}$ of all those irreducible representations $\Gamma_j$ of the group $G_0$ which enter into the mechanical (reducible) representation of the considered system:

$$X(t) = \sum_{jk} \mu_k^{(j)}(t) \cdot \varphi_k^{(j)} = \sum_j \Delta_j(t). \quad (3)$$

Here the index $j$ corresponds to the irrep $\Gamma_j$ while the index $k$ corresponds to its different basis vectors because, in the general case, $\Gamma_j$ can be a multidimensional representation. The $N$-dimensional vector $\Delta_j(t)$ is the contribution to $X(t)$ from the irrep $\Gamma_j$. 
For an $N$-particle nonlinear chain, $X(t)$ is the complete set of displacements $x_i(t) (i = 1, 2, \ldots, N)$ of each particle (mass point) from its equilibrium position. [In accordance with the periodical boundary condition, we assume $x_{N+1}(t) \equiv x_1(t)$].

The translational group $T$ can be chosen as a simplest variant of the parent symmetry group $G_0$. Nevertheless, the monatomic chain is invariant under the action of inversion with respect to its center and, therefore, the full symmetry in this case is the dihedral group $D$. Certainly, this group is more relevant for the symmetry-based analysis of nonlinear vibrations in monatomic chains. On the other hand, the inversion can be absent for some multiatomic chains, and the full symmetry for such cases is represented by the group $T$. Since some important results can be obtained for any one-dimensional chain with the aid of the group $T$ only, we start our consideration with the more general and simple case $G_0 = T$. The influence of the different choice of the parent group ($G_0 = T$ or $G_0 = D$) on the group-theoretical analysis of nonlinear vibrations of monatomic chains will be considered in Sec. 2.6.

Thus, we suppose that the equilibrium state of our monatomic chain is described by the parent group $G_0 = T$ which, obviously, happens to be the cyclic group of order $N$ with generator $\hat{a}$:

$$G_0 = \{E, \hat{a}, \hat{a}^2, \hat{a}^3, \ldots, \hat{a}^{N-1}\}, \quad \hat{a}^N = E. \quad (4)$$

($E$ is the identity element of the group $G_0$). Here $\hat{a}$ is the operator translating all particles by the space period $a$ of the considered chain in equilibrium. This operator generates the cyclic permutation of all particles and, therefore, the permutation of the corresponding displacements $x_i(t)$:

$$\hat{a}\{x_1(t), x_2(t), \ldots x_{N-1}(t), x_N(t)\} = \{x_N(t), x_1(t), x_2(t), \ldots x_{N-1}(t)\}. \quad (5)$$

As is well known [17], the cyclic group $G_0$ of order $N$ has $N$ irreps and they are all one-dimensional. Moreover, the $1 \times 1$ matrices of its generator $\hat{a}$ for different irreps $\Gamma_k$ ($k = 1, 2, \ldots, N$) are simply the $N$th-degree roots of 1. As an example, we give all matrix irreps of the cyclic group $G_0$ for $N = 12$ in Table 1. (Since all $\Gamma_k$ are one-dimensional irreps, Table 1 coincides with the table of their characters).

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6We consider longitudinal vibrations of the chain.

7In contrast to many point and space groups which can possess multidimensional irreps.

8Note, that in this table and in some points of the text we neglect the hat over symbol $a$ for simplifi-
Let us construct the basis vectors of the irreps of the group $G_0$ in (4) which describe the different modes of vibration of our nonlinear chain. The basis vectors of the irreps are usually obtained by the method of the projection operator \cite{17}, but in our case it is simpler to make use of the “direct” method based on the definition of the group representation (see \cite{10}). Indeed, according to this definition

$$\hat{a}\Phi = \tilde{M}(a)\Phi,$$

where $M(a)$ is the matrix corresponding in the irrep $\Gamma_k$ to an element $\hat{a}$ of the group $G_0$, and $\Phi$ is the complete set of basis vectors $\varphi_k$ of this representation which are transformed under the action of the operator $\hat{a}$ [in \cite{6} we use tilde as a symbol of matrix transposition].

The matrix $M_k(a)$ of the generator $\hat{a}$ of the cyclic group $G_0$ for the irrep $\Gamma_k$ ($k = 0, 1, 2, \ldots, N - 1$) is equal to

$$M_k(a) = \gamma^k,$$

where $\gamma = e^{2\pi i/N}$ and, therefore, $\gamma^N = 1$.

The desired basis vector $\varphi_k$ of the irrep $\Gamma_k$ can be written in the form

$$\varphi_k = (x_1^{(k)}, x_2^{(k)}, \ldots, x_N^{(k)}),$$

where $x_i^{(k)}$ ($i = 1, \ldots, N$) are unknown displacements of the particles. From (6) and (7), we get the following equation which can be used for obtaining the basis vector $\varphi_k$:

$$\hat{a}\varphi_k = \gamma^k\varphi_k, \quad k = 0, 1, \ldots, N - 1.$$

Equation (9) leads us to a chain of simple algebraic equations for the components of the vector $\varphi_k$ in (8). Solving these equations, we obtain

$$\varphi_k = (x, \gamma^1 \cdot x, \gamma^2 \cdot x, \gamma^3 \cdot x, \ldots, \gamma^{2k} \cdot x),$$

where $x$ is an arbitrary constant determining the displacement of the first particle of the chain. (Hereafter, we denote complex conjugation by a bar over the appropriate value, for example, $\bar{\gamma} = e^{-2\pi i/N}$). The presence of only one arbitrary constant in the general form of each basis vector $\varphi_k$ means that every irrep $\Gamma_k$ of the group $G_0$ enters one and
only one time into the decomposition of the mechanical representation of the monatomic chain.

The above conclusion applies to the monatomic chain, but it is not valid for arbitrary physical systems: a given irrep may enter several times or not enter at all into the appropriate mechanical representation. The method of finding the basis vectors for multidimensional irreps and complex mechanical structures turns out to be very complicated and it is useful to use in this case the computer programs [12, 16].

Normalizing the vector \( \varphi_k \) from Eq. (10), we obtain the final form of the basis vectors of the irreps \( \Gamma_k \) of the group \( G_0 = T \):

\[
\varphi_k \equiv \varphi(\Gamma_k) = \frac{1}{\sqrt{N}}(1, \bar{\gamma}^k, \bar{\gamma}^{2k}, \bar{\gamma}^{3k}, \ldots, \bar{\gamma}^{(N-1)k}).
\]

These basis vectors provide us so-called symmetry-adapted coordinates. According to the Wigner theorem, they are normal coordinates associated with \( \Gamma_k \), if only one copy of this irrep (multidimensional, in general case) is contained in the decomposition of the mechanical representation into its irreducible parts.

As was shown above, the two notions — symmetry-adapted coordinates and normal coordinates — are identical when we characterize the monatomic chain by the translation group \( (G_0 = T) \). We will refer to the modes determined by the above coordinates as normal modes or vibrational modes.

Each basis vector \( \varphi_k \) determines a certain pattern of displacements of all \( N \) atoms of the chain and, in some cases, it is more convenient to consider real modes \( \psi_k \) instead of the complex modes \( \varphi_k \).

Note that two basis vectors, for which the sum of their indices is equal to \( N \), are complex conjugates of each other:

\[
\varphi_{N-k} = \overline{\varphi_k}, \quad k = 0, 1, 2, \ldots, \left[ \frac{N}{2} \right].
\]

9 Let us remember that in the opposite case, according to the Wigner theorem, additional linear transformation is required to diagonalize the force constant matrix. In our general approach we use symmetry-adapted coordinates since they can be obtained with the aid of the group-theoretical methods alone (without any information about concrete interactions in the mechanical system).

10 Modes differ from generalized coordinates \( \varphi_k \) by the appropriate time-dependent functions \( \mu_k(t) \) in front of the vectors \( \varphi_k \) as in Eq. (14). In further consideration, we will sometimes call by the term "modes" not only \( \mu_k(t) \cdot \varphi_k \), but also the vectors \( \varphi_k \) and even the functions \( \mu_k(t) \).
(Hereafter, \( \left[ \frac{N}{2} \right] \) denotes the integer part of \( \frac{N}{2} \).) Indeed,
\[
\varphi_{N-k} = \frac{1}{\sqrt{N}} (1, \tilde{\gamma}^{N-k}, \tilde{\gamma}^{2(N-k)}, \ldots) = \frac{1}{\sqrt{N}} (1, \tilde{\gamma}^{-k}, \tilde{\gamma}^{-2k}, \ldots) = \frac{1}{\sqrt{N}} (1, \gamma^k, \gamma^{2k}, \ldots) = \overline{\varphi_k},
\]
since \( \tilde{\gamma}^N = 1 \) and \( \tilde{\gamma}^{-k} = \gamma^k \).

Using the appropriate linear transformation in the space of these mutually conjugated vectors, we obtain the real normal modes in the form given by Poggi and Ruffo \cite{3}:
\[
\psi_k = \left\{ \frac{1}{\sqrt{N}} \left[ \sin \left( \frac{2\pi k}{N} n \right) + \cos \left( \frac{2\pi k}{N} n \right) \right] \right\}_{n = 1, 2, \ldots, N}.
\]
Here \( n \) is the number of the particle, and \( k (k = 0, 1, 2, \ldots, N - 1) \) is the number of the mode. We call the real vectors \( \psi_k \) and \( \psi_{N-k} \) “conjugate modes” similar to the term for pairs of complex modes \( \varphi_k \) and \( \varphi_{N-k} \).

Returning to the basic Eq. (3), we can rewrite it in the following form,
\[
X(t) = \sum_{k=0}^{N-1} \mu_k(t) \varphi_k = \sum_{k=0}^{N-1} \nu_k(t) \psi_k.
\]
Thus, the pattern of atomic displacements \( X(t) \) for the chain in the vibrational regime at any instant \( t \) can be represented as a superposition of complex (\( \varphi_k \)) or real (\( \psi_k \)) basis vectors with the coefficients \( \mu_k(t) \) or \( \nu_k(t) \) which depend on the time \( t \).

Let us emphasize that \( \psi_k \) from Eq. (13) are normal modes of the linear chain (they can be obtained in the harmonic approximation), but we use them in (14) as the basis of the configuration space for studying dynamics of the nonlinear chain.

2.2Bushes of normal modes

We continue to adapt the general method \cite{7–11} of studying nonlinear dynamics of mechanical systems with arbitrary discrete symmetry for the case of nonlinear chains. Every basis vector (normal mode) from Eqs. (11) or (13) determines a specific set of atomic displacements, and this pattern is characterized by a certain symmetry group \( G_k \) which is a subgroup of the group \( G_0 \) of the chain in equilibrium (\( G_k \subset G_0 \)). Let us excite a dynamical regime of the considered system using the set of atomic displacements corresponding to a given root mode \( \psi_k \) as initial conditions at the instant \( t = 0 \):
\[
x_i \big|_{t=0} = A \psi_{ki}; \quad \dot{x}_i \big|_{t=0} = 0 \quad (i = 1, 2, \ldots, N).
\]
Here $\psi_{ki}$ are components of the vector $\psi_k = (\psi_{k1}, \psi_{k2}, \ldots, \psi_{kN})$ and $A$ is a fixed constant.

The symmetry group of the mechanical system at an arbitrary later moment $t$ cannot be lower than the group $G_k$ at the initial moment determined by the vector $\psi_k$. Indeed, the symmetry of the system at some instant $t > t_0$ is determined by the intersection of the symmetry of its Hamiltonian and the symmetry of the initial conditions. On the other hand, $G_0$ can be considered as a symmetry group of the Hamiltonian, as well as of the equilibrium state, if this state is nondegenerate. Thus, every symmetry element $g \in G_k$ does not change the dynamical state $X(t)$ for $t > t_0$ (a more detailed consideration of this problem can be found in [7,8]).

Now we can pose the question: what modes $\psi_k$ from Eq. (14) can contribute to the considered dynamical regime $X(t)$ corresponding to the group $G_k \subset G$ for $t > t_0$? Obviously, because of nonlinear interactions between different modes, the root mode $\psi_k$ brings about the appearance of a number of “secondary” modes in the considered dynamical regime, and we can obtain all these modes by demanding that the symmetry $X(t)$ is equal to $G_k$ (at least, it must not be lower than $G_k$!):

$$\hat{G}_k X(t) = X(t).$$

This equation means that $X(t)$ is an invariant vector with respect to all elements of the group $G_k$. As a consequence, only those modes $\psi_j$ contribute to $X(t)$ whose symmetry group $G_j$ is higher than or equal to $G_k$ of the initial configuration of the mechanical system in hand. The complete set of these modes, i.e., the root mode and all secondary modes corresponding to it, forms the bush as the geometrical object.

Note that each subgroup $G' \subset G_0$ must be tried in finding bushes, but in general, some subgroups do not generate any vibrational bushes (see examples in Sec. 2.6).

Let us consider the symmetry group $G_k$ of different modes $\psi_k$ in more detail. We can

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11 We state this hypothesis at the beginning of Sec. 2.1. For the degenerate equilibrium state, i.e. when there exist several equivalent minimums of the potential energy, the symmetry group of the Hamiltonian is higher than that of the each of the appropriate equilibrium states.

12 Rigorously speaking, we must distinguish between the symmetry elements $g \subset G_k$, which act on three-dimensional vectors of the Euclidean space, and the operators $\hat{g}$, corresponding to them, which act on $N$-dimensional vectors $X(t)$ (see [10]). The complete set of the operators $\hat{g}$ associated with all $g \in G_k$ forms the group $\hat{G}_k$. 

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find the group $G_k \subset G_0$ of a given mode $\psi_k$ by selecting all elements $g \in G_0$ under which this mode is invariant:

$$\hat{g} \psi_k = \psi_k.$$  \hfill (17)

But there exists a more convenient method. Indeed, $X(t)$ was written in (3) as a sum of contributions $\Delta_j$ from different irreps $\Gamma_j$ of the dimension $n_j$. It is easy to show that the following consequence of Eq. (16) takes place for each individual irrep $\Gamma_j$:

$$\hat{G}_k \Delta_j = \Delta_j.$$  \hfill (18)

According to the definition (9) of the representation of the group $G_0$ we can act on the set of basis vectors $\psi_k^{(j)}$ by the matrix $\tilde{M}(g)$, instead of acting on them by the operator $\hat{g}$ ($g \in G_0$). This is a trivial procedure for the cyclic group $G_0$, since all of its irreps are one-dimensional and, therefore, these matrices are scalar values.\(^{13}\)

On the other hand, Eq. (17) can be true if and only if the $1 \times 1$ matrix $M(g)$, corresponding to the element $g \in G_0$, is equal to the unit matrix. Therefore, all elements $g \in G_0$ whose matrices of the irrep $\Gamma_k$ satisfy the condition

$$M_k(g) = 1$$  \hfill (19)

do not change the mode $\psi_k$ and, obviously, the complete set of such elements forms the subgroup $G_k$ of the group $G_k \subset G_0$.

Let us consider the case $N = 12$ as an illustrative example. All irreps of the corresponding cyclic group $G_0$ are given in Table 1, as well as the symmetry groups $G_k$ of modes $\varphi_k$ associated with these irreps. As was explained above, only those elements $g \in G_0$ belong to the group $G_k$ whose matrices in the irrep $\Gamma_k$ are equal to 1. In Table 1, we define the subgroups $G_k \subset G_0$ by putting their generators in square brackets. Hereafter, we write the element $a^p$ as $(p \cdot a)$: such notation is often used for cyclic groups. Note, that according to the well-known Lagrange theorem, the order $(M)$ of any subgroup is a divisor of the order $(N)$ of this group, and that every subgroup of the cyclic group is also a cyclic group which can be determined by the single generator. Irreps $\Gamma_{N-k}$ and $\Gamma_k$ are mutual conjugate representations: $\Gamma_{N-k} = \overline{\Gamma}_k$. It is easy to notice that all subgroups 

\(^{13}\)In the general case, the appropriate procedure can be realized using the notion of “invariant” vectors of the irreps of the group $G_0$.\]
$G_k$ of the original cyclic group $G_0$ with the order $N = 12$ are presented in Table 1, and that the subgroups corresponding to the conjugate irreps $\Gamma_k$ and $\Gamma_{N-k}$ are identical (more exactly, subgroups corresponding to the conjugate modes $\varphi_k$ and $\varphi_{N-k}$ associated with these irreps). Below we list subgroups $G_k$ of the group $G_0$ with $N = 12$, listing in braces all their elements (see footnote 8 on page 8), the order ($M$) and symbols of irreps whose basis vectors (modes) possess such a symmetry ($G_k$).

1. $G_0[a] = \{E, a, 2a, 3a, \ldots, 11a\}$, $M_0 = N = 12$.
   
   Only one mode $\varphi_0 = \frac{1}{\sqrt{12}}(1, 1, 1, \ldots, 1)$, corresponding to the irrep $\Gamma_0$, possesses this symmetry group. The mode $\varphi_0$ plays a special role: it corresponds to the movement of the chain as a whole. In the next sections, this mode is not taken into account since we consider only vibrational modes.

2. $G_1[2a] = \{E, 2a, 4a, 6a, 8a, 10a\}$, $M_1 = 6$.
   
   It can be found from Table 1 that only two modes $\varphi_0$ and $\varphi_6$ satisfy such symmetry, because the unit matrix (1) corresponds to the generator [2a] only for the irreps $\Gamma_0$ and $\Gamma_6$. We write this fact as follows

   $$G_1[2a] : \Gamma_0, \Gamma_6.$$  

   The symmetry group of the basis vector $\varphi_6$ is equal to $G_1[2a]$, while that of the basis vector $\varphi_0$ is higher (it is equal to $G_0[a]$). Therefore, $\varphi_6$ is the root mode, and $\varphi_0$ is a secondary mode corresponding to it.

   Proceeding in a similar way, we obtain:

3. $G_2[3a] = \{E, 3a, 6a, 9a\}$, $M_2 = 4 : \Gamma_0, \Gamma_4, \Gamma_8$.

4. $G_3[4a] = \{E, 4a, 8a\}$, $M_3 = 3 : \Gamma_0, \Gamma_3, \Gamma_6, \Gamma_9$.

5. $G_4[6a] = \{E, 6a\}$, $M_4 = 2 : \Gamma_0, \Gamma_2, \Gamma_4, \Gamma_6, \Gamma_8, \Gamma_{10}$.

6. $G_5[12a] = \{E\}$, $M_5 = 1 : \Gamma_j$ for $j = 0, 1, 2, \ldots, 11$.

Now we can write all possible bushes for the chain with $N = 12$ particles using Eq. (14) and the above results. Each bush corresponds to the appropriate subgroup $G_k$ of the
parent group \(G_0\), and it embraces all modes with symmetry equal to (for root modes) or higher than (for secondary modes) \(G_k\).

\[
G_1[2a]: \quad x^{(1)}(t) = \mu_0(t)\varphi_0 + \mu_6(t)\varphi_6,
\]

\[
G_2[3a]: \quad x^{(2)}(t) = \mu_0(t)\varphi_0 + \mu_4(t)\varphi_4 + \mu_8(t)\varphi_8,
\]

\[
G_3[4a]: \quad x^{(3)}(t) = \mu_0(t)\varphi_0 + \mu_3(t)\varphi_3 + \mu_6(t)\varphi_6 + \mu_9(t)\varphi_9,
\]

\[
G_4[6a]: \quad x^{(4)}(t) = \mu_0(t)\varphi_0 + \mu_2(t)\varphi_2 + \mu_4(t)\varphi_4 + \mu_6(t)\varphi_6 + \mu_8(t)\varphi_8 + \mu_{10}(t)\varphi_{10},
\]

\[
G_5[12a] = E: \quad x^{(5)}(t) = \sum_{j=0}^{11} \mu_j(t)\varphi_j, \quad \text{(the trivial bush)}.
\]

Thus there exist four nontrivial vibrational bushes (besides the trivial bush with \(G_5[12a] = E\)) for the nonlinear chain with \(N = 12\) particles. The modes (basis vectors of appropriate irreps) \(\varphi_k\) determine the pattern of atomic displacements, and the time-dependent coefficients \(\mu_k(t)\) characterize the evolution of these displacements in time.

It easy to find from (20) that every bush with symmetry group \(G_k\) contains the contributions from modes with this symmetry \(G_k\) and from all other modes whose symmetry is higher than \(G_k\). This is the geometrical cause of the spreading of the initial excitation from the root mode to other (secondary) modes with \(G_k\) equal to or higher than that of the root mode. The dynamical reason for such a phenomenon will be considered below in Sec. 2.3.

Returning to the general case, we obtain that the numbers and the types of possible bushes for any nonlinear chain with \(N\) particles depend essentially on divisibility properties of the integer \(N\). Indeed, the total number of bushes for an \(N\)-particle chain is equal to the number of divisors of \(N\). The number of modes contained in the concrete bush corresponding to the divisor \(M\) (this divisor determines the order of the appropriate cyclic group \(G_k\)) is equal to \(N/M\). In particular, for prime number \(N\) there exists only one (trivial) bush with \(G_1 = \{E\}\) which contains all modes \(\varphi_j\) \((j = 0, 1, 2, ..., N - 1)\).\(^{15}\)

\(^{14}\)Note, that \(\mu_k(t)\) associated with different bushes are not related. Indeed, we may introduce the additional index \(i\) for these coefficients \(\mu_k^{(i)}(t)\), which corresponds to the number of the bush, but this index is omitted for simplification of the notation.

\(^{15}\)Moreover, it is easy to verify that the order \(M\) of the group \(G_j[ma]\) equals \(N/m\) and, therefore, the number of modes of the bush with such symmetry is simply equal to \(m\).

\(^{16}\)In this case of trivial symmetry, the bush describes the full dynamics of the considered mechanical
Therefore, the bush structure for the chain with \( N = 12 \) differs in principle from that for \( N = 11 \) or \( N = 13 \).

In conclusion, let us note that all possible symmetry-determined bushes of normal modes can be found for arbitrary mechanical system with discrete symmetry by the regular group-theoretical methods described in detail in our previous papers (see [10] and [11]). We will not consider these methods in the present paper, but we want to extract their main points.

A certain subgroup \( G \) of the parent group \( G_0 \) corresponds to a given bush \( B[G] \). This subgroup must be fixed for singling out the complete collection of the normal modes contained in \( B[G] \). Then the structure of the given bush, i.e. the list of all modes belonging to \( B[G] \), can be found as a result of solving the following systems of linear algebraic equations for each of the irreps \( \Gamma_j \) of the group \( G_0 \):

\[
(\Gamma_j \downarrow G) \mathbf{C}_j = \mathbf{C}_j.
\]  

Here \( \Gamma_j \downarrow G \) is the restriction of the irrep \( \Gamma_j \) of the parent group \( G_0 \) to the subgroup \( G \) of this group. In other words, we must solve the equations

\[
M_j(g_i) \mathbf{C}_j = \mathbf{C}_j
\]

for all matrices \( M_j(g_i) \) corresponding to the generators \( g_i \) of the subgroup \( G \) in the irrep \( \Gamma_j \).

The invariant vectors \( \mathbf{C}_j \) from (21) determine the set of coefficients in the superposition of the basis vectors of the given irrep \( \Gamma_j \) which is compatible with the symmetry group \( G \) of the given bush \( B[G] \). In particular, the invariant vectors can turn out to be zero vectors for some irreps \( \Gamma_j \), and this means that such irreps do not contribute to the given bush.

For obtaining the bushes of vibrational modes, in addition to the above results, we must find the explicit form of the basis vectors constructed from the set of atomic system without any simplification.

17 In particular, the subgroup \( G \) can be fixed by indication of the initially excited root mode, since the definite group is associated with each normal mode.

18 There exist bushes of modes of very different physical nature.
displacements, for all irreps which contribute to the given bush. (This can be done for example, with the aid of the method of projection operators).

As we already noted, the above procedures are simple for the monatomic chain, but special group-theoretical computer programs are needed for the general case (see references [12] and [16]).

If the complete list of modes of a given bush is known, the root mode can be frequently defined as that with the lowest symmetry of all other bush modes. Nevertheless, there exist cases where the root mode of the bush can be chosen in different ways and there exist cases where the symmetry group of the bush is determined by the intersection of the symmetry groups of the modes associated with several different irreps of the parent group. In the last case, we speak about a bush with several root modes (see [10] and, especially, [23] and [24]). In general, the set of root modes must uniquely determine the symmetry group of the whole bush. The excitation of this set of root modes leads by necessity to the excitation of all other modes of the bush.

### 2.3 Bushes of modes as dynamical objects

Considering bushes of modes in the previous section, we made use of geometrical (group-theoretical) methods only. Now let us consider the concrete mechanical model—the FPU-α chain described by the Hamiltonian

\[
H = \frac{1}{2} \sum_{n=1}^{N} p_n^2 + \frac{1}{2} \sum_{n=1}^{N} (x_{n+1} - x_n)^2 + \frac{\alpha}{3} \sum_{n=1}^{N} (x_{n+1} - x_n)^3. \tag{22}
\]

Here \(x_n(t)\) is the displacement of \(n\)th particle from its equilibrium state at the instant \(t\), and \(p_n(t)\) is the corresponding momentum.

As in the original paper by Fermi-Pasta-Ulam [1], the nonlinearity of the chain is assumed to be weak. It depends on two different factors — on the coefficient \(\alpha\) in (22) and on the energy of the initial excitation of the system. We can remove \(\alpha\) from (22) by means of a scaling transformation of \(x_n(t)\), i.e., the coefficient \(\alpha\) can be made equal to 1. Nevertheless, sometimes it is convenient to write \(\alpha (|\alpha| \ll 1)\) in Eq. (22) explicitly to stress the weakness of the nonlinearity of the chain.

As was already stated, the basis vectors \(\varphi_j\) (11) of irreps of the group \(G_0\) are (linear) normal modes of the FPU chain in the harmonic approximation \((\alpha = 0)\), and we can use
them in (14) as a basis for studying nonlinear dynamics of the system (22) with $\alpha \neq 0$.

We consider the equations of motion in the form,

$$\ddot{x}_n = -\frac{\partial U}{\partial x_n}, \quad (n = 1, 2, \ldots, N), \quad (23)$$

where $U(x_1, \ldots, x_N)$ is the potential energy of the FPU chain. This system of differential equations becomes linear in the harmonic approximation ($\alpha = 0$), and reduces to the set of independent oscillators

$$\ddot{\mu}_j + \omega_j^2 \mu_j = 0, \quad (j = 0, 1, 2, \ldots, N - 1) \quad (24)$$

with frequencies

$$\omega_j = 2 \sin \left( \frac{\pi j}{N} \right) \quad (25)$$

as a result of the transition from the initial variables $x_n(t)$ to the normal modes in the complex (11) or real (13) form. From this point, we call the time-dependent coefficients $\mu_j(t)$ [or $\nu_j(t)$] from Eq. (14) by the term, “normal modes”, even though this term corresponds really to $\mu_j(t)\varphi_j$. This is convenient because $\varphi_j$ are constant vectors and $\mu_j(t)$ are our new dynamical variables. Substituting (14) into equations (23) and solving them with respect to variables $\mu_j(t)$, we obtain the following nonlinear differential equations (see details of such a transition in the general case in the Appendix of Ref. [10]):

$$\ddot{\mu}_j + \omega_j^2 \mu_j = \gamma \sum_{k=0}^{N-1} \mu_k \mu_{j-k} \left[ 2 \sin \left( \frac{2\pi}{N}(j - k) \right) - \sin \left( \frac{2\pi}{N}j \right) \right], \quad (26)$$

$$\gamma = \frac{2\alpha i}{\sqrt{N}}, \quad j = 0, 1, 2, \ldots, N - 1.$$ 

Hereafter, we use the following convention about indices of normal modes: these indices must belong to the interval $[0, N - 1]$ and, therefore, the value of the mode index of the type $\pm j \pm k$ $(j, k = 0, 1, \ldots, N - 1)$ must be reduced to this interval by adding or subtracting $mN$, where $m$ is an integer number.

The transition from initial variables $x_n(t)$ to normal modes $\nu_j(t)$ in the real form (13) leads to the following dynamical equations for the FPU-$\alpha$ model:

$$\ddot{\nu}_j + \omega_j^2 \nu_j = -\frac{\alpha}{\sqrt{N}} \sum_{k=0}^{N-1} \nu_k \left[ (\nu_{j+k} + \nu_{j-k}) \left( 2 \sin \frac{2\pi}{N}k + \sin \frac{2\pi}{N}j \right) \right. \left. + (\nu_{j+k} - \nu_{j-k}) \left( 2 \sin \frac{2\pi}{N}k - \sin \frac{2\pi}{N}j \right) \right], \quad j = 0, 1, 2, \ldots, N - 1. \quad (27)$$
Now we can consider the dynamical cause of the existence of bushes of normal modes. First of all, let us remember that the mode $\mu_0$ corresponds to the movement of the FPU chain as a whole object and, therefore, to the movement of its center of mass. Vibrations associated with all other modes $\mu_j(t)$, ($j = 1, 2, ..., N - 1$) cannot move the center of mass because of the specific type of displacement patterns described by basis vectors $\varphi_j$. Therefore, the excitation of any mode $\mu_j(t)$ with $j \neq 0$ cannot lead to the excitation of the mode $\mu_0$, as a consequence of the conservation of momentum. This general conclusion can be easy verified using the dynamical equations (26). Indeed, we obtain the following equation of motion for the mode $\mu_0$:

$$\ddot{\mu}_0 + 0\mu_0 = 0.$$ 

It is also easy to verify that mode $\mu_0(t)$ cannot excite any other mode, and, therefore, we can forget about $\mu_0(t)$ when discussing dynamical equations.

On the other hand, this mode enters into each bush of the nonlinear chain (see, for example, Eqs. (20)). What does it mean? We obtain bushes, as geometrical objects, from the idea of invariance of vibration patterns with respect to the subgroups of the cyclic group $G_0$ only. But there can exist further causes for reducing of the number of modes in a given bush because of some additional symmetry properties of the concrete dynamical system and because of its specific character (we discuss this problem in Secs. 2.5 and 2.6). In the above case of the mode $\mu_0(t)$, such cause is provided by the law of conservation of momentum which is the consequence of homogeneity of the space.

Let us assume that only one mode $\mu_6(t)$ is excited in the FPU-\( \alpha \) chain with $N = 12$ particles. In other words, we suppose that all modes except mode $\mu_6(t)$, are equal to zero identically (we call them “sleeping modes”):

$$\mu_j(t) \equiv 0, \text{ for } j \neq 6.$$ 

Can such a dynamical regime exist in our nonlinear chain? Using the above assumption, it is easy to obtain from Eqs. (26),

$$\ddot{\mu}_6 + 4\mu_6 = 0,$$

$$\ddot{\mu}_j + \omega_j^2\mu_j = 0, \text{ for all } j \neq 6.$$ 

The following analysis will be based on studying equations (26) for complex modes $\mu_j(t)$, but the same results can be obtained using equations (27) for real modes $\nu_j(t)$ as well.
Therefore, the hypothesis that \( \mu_6(t) \neq 0 \) while \( \mu_j(t) \equiv 0 \) for \( j \neq 6 \) is self-consistent, and we have a pure harmonic regime \( \mu_6(t) = A \cos(\sqrt{2} t + \delta) \) for the FPU-\( \alpha \) chain (\( A, \delta \) are arbitrary constants). It corresponds to the one-dimensional bush \( \{ \varphi_6 \} \) with symmetry group \( G_1[2a] \) [see Eqs. (20)].

Let us consider the bush with symmetry \( G_2[3a] \) corresponding to the second equation of (20). We must now assume that \( \mu_4 \neq 0, \mu_8 \neq 0 \) while all other modes are equal to zero identically. Then, we obtain from Eqs. (26):

\[
\ddot{\mu}_4 + 3 \mu_4 = -2.598 \gamma \mu_8^2, \tag{30a}
\]

\[
\ddot{\mu}_8 + 3 \mu_8 = 2.598 \gamma \mu_4^2, \tag{30b}
\]

(\( \mu_j \equiv 0 \) for \( j \neq 4, 8 \)).

These equations describe the two-mode dynamical regime where both modes \( \mu_4(t) \) and \( \mu_8(t) \) (they form a conjugate pair) are connected with each other by the force interaction. Indeed, if the first oscillator, described by Eq. (30a) was excited (\( \mu_4(t) \neq 0 \)), then the force \( 2.598 \gamma \mu_4^2 \), acting on the second oscillator, appears in the right-hand side (rhs) of Eq. (30b) and, therefore, \( \mu_8(t) \) cannot be equal to zero identically (\( \mu_8(t) \neq 0 \)). Conversely, the excitation of the mode \( \mu_8(t) \) leads to the excitation of the mode \( \mu_4(t) \) because of the force term \( -2.598 \gamma \mu_8^2 \) in Eq. (30a). Therefore, the dynamical regimes \( \mu_4(t) \neq 0, \mu_8(t) \equiv 0 \) and \( \mu_4(t) \equiv 0, \mu_8(t) \neq 0 \) cannot exist, and we may speak about the force interaction between modes \( \mu_4(t) \) and \( \mu_8(t) \) (for more details, see [7, 10]).

The existence of the exact equations (30) for the FPU-\( \alpha \) chain with \( N = 12 \) means that there exists a two-dimensional subspace \( S_{4,8} \) of the twelve-dimensional configuration space spanned by the basis vectors \( \varphi_4 \) and \( \varphi_8 \) (these vectors are associated with the modes \( \mu_4 \) and \( \mu_8 \)) which is dynamically invariant. Indeed, the trajectory corresponding to the dynamical regime (30) in the configuration space remains in the subspace \( S_{4,8} \) for every time \( t \).

We do not discuss the problem of finding the analytical solution of Eqs. (30) in the present paper, and only want to note that these equations describe the two-dimensional

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\( ^{20} \)Let us remember once more that the mode \( \mu_0 \) is excluded from our consideration.

\( ^{21} \)Hereafter, we keep in the coefficients of the dynamical equations only three figures after the decimal point.
bush with symmetry group $G_2[3a]$ as a *dynamical* object.

Now let us consider the bush with $G_3[4a]$ from Eqs. (20). Assuming that $\mu_3(t) \neq 0$, $\mu_6(t) \neq 0$, $\mu_9(t) \neq 0$, and all other modes are equal to zero, we obtain from (20) the following dynamical system with only three degrees of freedom:

\[
\begin{align*}
\ddot{\mu}_3 + 2\mu_3 &= -4\gamma\mu_9\mu_6, \\
\ddot{\mu}_6 + 4\mu_6 &= 2\gamma(\mu_3^2 - \mu_9^2), \\
\ddot{\mu}_9 + 2\mu_9 &= 4\gamma\mu_3\mu_6.
\end{align*}
\]

Note that modes $\mu_3$ and $\mu_9$ are conjugate. They have the identical symmetry groups $G_3[4a]$, while the mode $\mu_6$ possesses higher symmetry $G_1[2a] \supseteq G_3[4a]$. Either mode $\mu_3$ or $\mu_9$ can be the root mode, and $\mu_6$ is the secondary mode. Indeed, if we excite the mode $\mu_3(t)$ at the instant $t = 0$ using the appropriate initial conditions, the force $2\gamma\mu_3^2$ acts on the mode $\mu_6$ according to Eq. (31b) and, therefore, this mode turns out to be excited as well. (We can say this in another way: Eq. (31b) cannot be satisfied in the opposite case $\mu_3(t) \neq 0$, $\mu_6(t) \equiv 0$.) On the other hand, it follows from Eq. (31c) that $\mu_9(t)$ will be also excited when $\mu_3(t) \neq 0$ and $\mu_6(t) \neq 0$ because of the force $4\gamma\mu_3\mu_6$ in the right-hand side of this equation.

Thus, the excitation of the root mode $\mu_3(t)$ brings about the excitation of the *secondary* mode $\mu_6$, but the opposite statement is not correct as a consequence of the specific asymmetric structure of bush dynamical equations with respect to the root and secondary modes. Indeed, the excitation of only the secondary mode $\mu_6$ does not produce forces acting on modes $\mu_3$ and $\mu_9$, because the forces $4\gamma\mu_6\mu_9$ and $4\gamma\mu_6\mu_3$ are equal to zero if $\mu_3(t) \equiv 0$ and $\mu_9(t) \equiv 0$. Note that the previous geometrical analysis based on the consideration of the symmetry groups of modes (the symmetry of $\mu_6$ is higher than that of $\mu_3$, $\mu_9$) leads to the same conclusion which was obtained above by the studying of the structure of the dynamical equations (31). This is the general result proved by us in [10] (see Theorem 1): dynamical arguments must confirm the geometrical (group-theoretical) arguments\(^{22}\). The similar consideration of the bush with symmetry $G_4[6a]$ leads to the

\(^{22}\) Indeed, it follows as a consequence of this Theorem that when the group-theoretical method permits the existence of a nonzero invariant vector and, therefore, the existence of the secondary mode
following dynamical system with five degrees of freedom describing the evolution of modes $\mu_2, \mu_4, \mu_6, \mu_8$ and $\mu_{10}$:

\begin{align}
\ddot{\mu}_2 + \mu_2 &= \gamma \left[ -1.732 \mu_4 \mu_{10} - 3.466 \mu_6 \mu_8 \right], \\
\ddot{\mu}_4 + 3\mu_4 &= \gamma \left[ 0.866 \mu_2^2 - 2.598 \mu_8^2 - 3.466 \mu_6 \mu_{10} \right], \\
\ddot{\mu}_6 + 4\mu_6 &= 3.466 \gamma \left[ \mu_2 \mu_4 - \mu_8 \mu_{10} \right], \\
\ddot{\mu}_8 + 3\mu_8 &= \gamma \left[ 2.598 \mu_4^2 - 0.866 \mu_{10}^2 + 3.466 \mu_2 \mu_6 \right], \\
\ddot{\mu}_{10} + \mu_{10} &= \gamma \left[ 1.732 \mu_2 \mu_8 + 3.466 \mu_4 \mu_6 \right].
\end{align}

Here conjugate modes $\mu_2$, $\mu_{10}$ are root modes because they have the lowest symmetry $G_4[6a]$. Conjugate modes $\mu_4$, $\mu_8$ with the group $G_2[3a] \supset G_4[6a]$ and mode $\mu_6$ with $G_1[2a] \supset G_4[6a]$ are secondary modes. This geometrical fact can be again checked by the appropriate consideration of the structure of equations (32). Indeed, the excitation of the mode $\mu_2(t)$ implies the appearance of the mode $\mu_4$ because of the force $0.866 \gamma \mu_2^2$ in Eq. (32b), and then the mode $\mu_8$ appears due to the force $2.598 \gamma \mu_4^2$ in Eq. (32d). The presence of modes $\mu_2$, $\mu_4$, $\mu_8$ in the dynamical process leads to the excitation of the mode $\mu_6$, due to the force $3.466 \gamma \mu_2 \mu_4$ in Eq. (32c), and to the excitation of the mode $\mu_{10}$ because of the force $\gamma(1.732 \mu_2 \mu_8 + 3.466 \mu_4 \mu_6)$ in Eq. (32e). Thus, the dynamical equations (32) describe the evolution of the five-dimensional bush with symmetry $G_4[6a]$.

The last bush from Eqs. (20) is the trivial one, because it contains all 12 modes and describes the dynamics of the FPU-\(\alpha\) chain with twelve particles in the general case.

Thus, we found all possible bushes of modes for the case $N = 12$ generated by the subgroups of the parent group $G_0 = T$ of pure translations, and it is clear that anyone can proceed in the similar way for considering the case of an arbitrary $N$.

In conclusion, let us consider the thermodynamical limit $N \to \infty$ for the equation of motion (27) in the real modal space.
2.4 Integro-differential equation for the FPU-α chain in the limit \( N \rightarrow \infty \)

As usual in the physics of crystals, it is convenient to introduce the wave number \( k \) instead of the mode number \( j \) for the case \( N \gg 1 \),

\[
k = \frac{2\pi}{N} j, \quad j = 0, 1, 2 \ldots, N - 1.
\]

(33)

All values of \( k \) belong to the interval \([0, 2\pi)\) which corresponds to the primitive cell of the reciprocal lattice with the period \( b = \frac{2\pi}{a} \), where \( a \) is a period of the one-dimensional lattice associated with the FPU chain in equilibrium (we assume \( a = 1 \)). The density of the \( k \)-points from Eq. (33) increases with increasing of \( N \). These points are distributed continuously and uniformly on the interval \([0, 2\pi)\) in the limit \( N \rightarrow \infty \).

The number of terms on the right-hand side of each Eqs. (27) increases as \( N \rightarrow \infty \), and we can transform the sum into a definite integral, assuming \( \nu_k(t) \) to be a smooth function of its index \( k \). As a result of this procedure, the following integro-differential equation instead of the system of ordinary differential equations (27) can be obtained:

\[
\ddot{z}(x,t) + \omega^2(x)z(x,t) = \int_0^{2\pi} z(y,t) \left\{ \left[ z(x+y,t) + z(-x-y,t) \right] K_+(x,y) + \left[ z(x-y,t) - z(-x+y,t) \right] K_-(x,y) \right\} dy,
\]

where

\[
\omega(x) = 2\sin\left(\frac{x}{2}\right), \quad K_\pm(x,y) = 2\sin(y) \pm \sin(x), \quad 0 \leq x < 2\pi.
\]

(34)

(35)

The function \( z(x,t) \) was introduced in Eq. (34) instead of \( \nu_k(t) \) and, therefore, \( z(x,t) \) signifies the value of the mode with wave number \( x \) at time \( t \). Thus, we use different notations for the wave number in the discrete case \( (k) \) and in the continuous case \( (x) \). It is easy to verify the correctness of Eqs. (34, 35) by replacing the integral on the right-hand side of Eq. (34) with its Darboux sum and using the following relation between \( z(x,t) \) and \( \nu_k(t) \):

\[
z(x,t) = \frac{\sqrt{N}}{2\pi} \nu_k(t), \quad (x = k).
\]

(36)

\[23\] Note that the coefficient \( \alpha \) can be removed from Eqs. (27) as well as from Eq. (34) by the appropriate scale transformation of the functions \( \nu_k(t) \) and \( z(x,t) \), respectively. In Eq. (34) we also imply that the variables \( \pm x \) and \( \pm y \) are reduced to the interval \([0, 2\pi)\) with the aid of cyclic conditions, \( x \equiv x \pm 2\pi \) and \( y \equiv y \pm 2\pi \).
Such a procedure returns us to the discrete model (27).

Note that Eqs. (34, 35) correspond to the continuum limit for the FPU-α model in modal space, while the well-known Korteweg-deVries equation (KdV) corresponds to the continuum limit in ordinary space \[4\]. Besides the form of above mentioned equations, there exists a principal difference between these two equations. Indeed, Eqs. (34, 35), in contrast to the KdV-equation, is valid not only for long waves, but for short waves as well. We can make use of this fact for considering bushes of modes which often correspond namely to sufficiently short waves. The application of the integro-differential equation (34) for studying some problems of the FPU-α dynamics will be considered elsewhere.

2.5 On the difference between bush structures for FPU-α and FPU-β chains

Let us compare our results, which are based on the group-theoretical method (Sec. 2.2), with those by Poggi and Ruffo \[3\], which are based on specific dynamical properties of the FPU-β chain. Naturally, taking into account concrete properties of a given mechanical system, we can obtain some additional selection rules as compared with general symmetry-related results. Poggi and Ruffo found for the FPU-β model five one-mode solutions corresponding to the following numbers of modes

$$j = \frac{N}{4}, \frac{N}{3}, \frac{N}{2}, \frac{2N}{3}, \frac{3N}{4}$$

(37)

and two types of solutions associated with the pairs of modes \(\{\frac{N}{4}, \frac{3N}{4}\}\) and \(\{\frac{N}{3}, \frac{2N}{3}\}\). Our results differ from these, and we want to discuss the problem using the example of the chain with \(N = 12\) considered in Sec. 2.2.

According to Eqs. (20) there exists only one one-dimensional bush \(B[2a]\) associated with the excitation of the mode with \(j = \frac{N}{2} = 6\) (remember that we, as well as Poggi and Ruffo, neglect the mode \(\mu_0\)). But the excitation of the mode with \(j = \frac{N}{3} = 4\) leads to the appearance of the two-dimensional bush \(B[3a]\) with \(j = 4, 8\) (modes \(\mu_4\) and \(\mu_8\) are conjugate). Thus, in contrast to the FPU-β model, the one-dimensional dynamical regime with only \(\mu_4\) (or \(\mu_8\)) does not exist. Moreover, this conclusion is confirmed also by the dynamical consideration for the FPU-α model in the Sec. 2.3. The difference between
structures of the bush \( B[3a] \) for the FPU-\( \beta \) and for the FPU-\( \alpha \) chains is brought about namely by their specific dynamical properties.

Because of the same reason, the excitation of the mode \( \mu_3(j = \frac{N}{4}) \) leads, for the FPU-\( \alpha \) chain and for the general case as well, to the excitation of the conjugate mode \( \mu_9(j = \frac{3N}{4}) \) and to the secondary mode \( \mu_6(j = \frac{N}{2}) \). We see, therefore, that some modes in the list (37), obtained by Poggi and Ruffo for the FPU-\( \beta \) chain, combine into the three-dimensional bush \( B[4a] \) for the FPU-\( \alpha \) model, as well as for the arbitrary nonlinear chain. In other words, the three-dimensional symmetry-determined bush \( B[4a] \), being an indivisible nonlinear dynamical object for FPU-\( \alpha \) model, can be split into smaller invariant manifolds (i.e., bushes of modes in general sense) by imposing the appropriate initial conditions. Indeed, the one-dimensional bush with \( j = \frac{N}{4} \) can exist in the FPU-\( \beta \) model according to Eq. (37), but it does not exist in the FPU-\( \alpha \) model because it follows from Eq. (38b) that excitation of the mode \( \mu_3(j = \frac{N}{4}) \) always leads to the excitation of the (secondary) mode \( \mu_6(j = \frac{N}{2}) \).

Let us stress once again that our results, obtained by the group-theoretical method, are general: they are correct for any nonlinear monatomic chain. Nevertheless, the specific character of interatomic interactions can reduce the dimensionality of bushes found by this method, as we have just seen comparing the structures of bushes of modes for FPU-\( \alpha \) and FPU-\( \beta \) chains.

### 2.6 Bushes of normal modes associated with dihedral symmetry of nonlinear chains

Introducing the concept of bushes of normal modes, we started with a certain symmetry group \( G_0 \) (parent group) of the considered mechanical system and basis vectors of its irreducible representations. Each given bush corresponds to some subgroup \( G_k \) of the group \( G_0(G_k \subset G_0) \).

In previous sections, the group \( T = E, \hat{a}, \hat{a}^2, \ldots, \hat{a}^{N-1} \) (see Eq.(4)) was chosen as the symmetry group \( G_0 \) of the monatomic chain in equilibrium. But the full symmetry of such a system is higher, because space inversion \( \hat{i} \) with respect to the center of the

\(^{24}\)In some sense, they are also valid for multiatomic chains (see Sec. 2.6).
finite monatomic chain also is a symmetry element, as well as the product \( \hat{a}^k \cdot \hat{i} \) of the translation \( \hat{a}^k(k = 0, 1, \ldots, N - 1) \) with the inversion \( \hat{i} \). Therefore, the full symmetry group \( D \) (dihedral group) of the monatomic chain possesses twice as many elements as the translational group \( T \) which is its subgroup of index 2. We can write the group \( D \) as the direct sum of two cosets with respect to the subgroup \( T \):

\[
D = T + T \cdot \hat{i}.
\]

It is convenient for our purpose to rewrite this equation in the form

\[
\tilde{G}_0 = G_0 + G_0 \cdot \hat{i},
\]

where \( G_0 = T \) and \( \tilde{G}_0 = D \).

We will discuss the connection between bushes of modes associated with the group \( G_0 \) and those associated with its supergroup \( \tilde{G}_0 \). The irreducible representations of the groups \( G_0 \) and \( \tilde{G}_0 \) will be denoted by \( \Gamma_j \) and \( \tilde{\Gamma}_j \), respectively.

Up to this point we discussed bushes for monatomic chains in terms of the irreps \( \Gamma_j \) of the translational group \( G_0 = T \), although the full symmetry group of these systems is \( \tilde{G}_0 = D \). Why did we proceed in such a manner and how is the list of bushes of normal modes modified if we consider the complete symmetry group \( \tilde{G}_0 \) instead of its subgroup \( G_0 \)? We give the brief answer to this question below, while the detailed consideration will be given in another paper devoted to multiatomic chains.

The group \( \tilde{G}_0 = D \) is a non-Abelian group since some its elements do not commute with each other (for example, \( \hat{i} \cdot \hat{a} = \hat{a}^{-1} \cdot \hat{i} \)). As a consequence, the number of classes of conjugate elements of this group is less than the total number \((2N)\) of its elements and some irreps \( \tilde{\Gamma}_j \) are not one-dimensional.

Let us discuss the monatomic chain with \( N = 12 \) particles in more detail. The appropriate group \( \tilde{G}_0 = D \) has nine classes of conjugate elements and, therefore, nine irreducible representations \( \tilde{\Gamma}_j \). Four of these irreps \((\tilde{\Gamma}_1, \tilde{\Gamma}_2, \tilde{\Gamma}_3, \tilde{\Gamma}_4)\) are one-dimensional and five other irreps \((\tilde{\Gamma}_5, \tilde{\Gamma}_6, \tilde{\Gamma}_7, \tilde{\Gamma}_8, \tilde{\Gamma}_9)\) are two-dimensional.

To determine a given irrep \( \tilde{\Gamma}_j \) of the group \( \tilde{G}_0 \) defined by Eq. (39), we must write matrices of this representation for elements of the first coset \( G_0 \) and of the second coset \( G_0 \cdot \hat{i} \). They form the first half \( \tilde{\Gamma}_j^{(1)} \) and the second half \( \tilde{\Gamma}_j^{(2)} \) of the irrep \( \tilde{\Gamma}_j \), respectively.\(^{25}\)

\(^{25}\)Obviously, \( \tilde{\Gamma}_j^{(1)} \) is the restriction of the irrep \( \tilde{\Gamma}_j \) of the group \( \tilde{G}_0 \) onto the subgroup \( G_0 \).
\( \tilde{\Gamma}_j^{(1)} \) for one-dimensional irreps coincides with either irrep \( \Gamma_0 \) or irrep \( \Gamma_6 \) of the group \( G_0 \) (see Eq. (11) below). \( \tilde{\Gamma}_j^{(1)} \) for two-dimensional irreps can be written as a direct sum of two conjugate irreps of group \( G_0 \), for example, \( \tilde{\Gamma}_5^{(1)} = \begin{pmatrix} \Gamma_1 \\ \Gamma_{11} \end{pmatrix} \). All matrices of the second half \( \tilde{\Gamma}_j^{(2)} \) of the irrep \( \tilde{\Gamma}_j \) are products of the appropriate matrices of \( \tilde{\Gamma}_j^{(1)} \) with the matrix corresponding to the inversion \( \hat{i} \). For one-dimensional irreps \( \tilde{\Gamma}_j \) this matrix is equal to \( (+1) \) or \( (-1) \), while for two-dimensional irreps \( \tilde{\Gamma}_j \) it is equal to \( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \). Therefore, the irrep \( \tilde{\Gamma}_5 \) has the following form

\[
\tilde{\Gamma}_5 = \begin{pmatrix} \Gamma_1 \\ \Gamma_{11} \end{pmatrix} + \begin{pmatrix} \Gamma_1 \\ \Gamma_{11} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{40}
\]

This view of the irrep \( \tilde{\Gamma}_j \) must be compared with the definition (39) of group \( \tilde{G}_0 \); it allows one to determine the explicit form of all matrices of the both cosets from Eq. (39).

Using the above notation we can write all irreps \( \tilde{\Gamma}_j \) \((j = 1, ..., 9)\) of the group \( \tilde{G}_0 \) as follows:

\[
\begin{align*}
\tilde{\Gamma}_1 &= \Gamma_0 + \Gamma_0 \cdot (1); \\
\tilde{\Gamma}_2 &= \Gamma_0 + \Gamma_0 \cdot (-1); \\
\tilde{\Gamma}_3 &= \Gamma_6 + \Gamma_6 \cdot (1); \\
\tilde{\Gamma}_4 &= \Gamma_6 + \Gamma_6 \cdot (-1); \\
\tilde{\Gamma}_k &= \begin{pmatrix} \Gamma_{k-4} \\ \Gamma_{16-k} \end{pmatrix} + \begin{pmatrix} \Gamma_{k-4} \\ \Gamma_{16-k} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad k = 5, 6, 7, 8, 9. \tag{41}
\end{align*}
\]

Note that irreps \( \Gamma_{k-4} \) and \( \Gamma_{16-k} \) in Eq. (31) are mutually conjugate for any \( k \):

\[
\begin{align*}
\Gamma_1 - \Gamma_{11}, \quad \Gamma_2 - \Gamma_{10}, \quad \Gamma_3 - \Gamma_9, \quad \Gamma_4 - \Gamma_8, \quad \Gamma_5 - \Gamma_7. \tag{42}
\end{align*}
\]

As was already discussed, bushes of normal modes correspond to different subgroups of the parent symmetry group of the considered mechanical system in equilibrium. For monatomic chains, bushes associated with the parent group \( G_0 \) were considered in Sec. 2.2. Now we want to discuss bushes associated with the parent group \( \tilde{G}_0 \).

There are 34 subgroups of the group \( \tilde{G}_0 \) for the chain with \( N = 12 \) particles. Note that since \( G_0 \subset \tilde{G}_0 \), all subgroups of \( G_0 \) are also subgroups of \( \tilde{G}_0 \). Therefore, all bushes found in Sec. 2.2 are valid not only for the parent group \( G_0 \), but for the parent group \( \tilde{G}_0 \), too. In addition to these bushes, some new bushes of normal modes can appear when we consider \( \tilde{G}_0 \) as the parent group. To find them we must examine those subgroups of

\[^{26}\text{Henceforth, we will omit zero elements of all matrices.}\]
The subgroup \{ \hat{a}^4, \hat{i} \} of the group \tilde{G}_0 is determined by two generators \hat{a}^4 and \hat{i} (hereafter we write down in braces only generators of the appropriate group instead of all its elements). This subgroup is obtained from the subgroup \{ \hat{a}^4 \} of the group \tilde{G}_0 = T by adding inversion \hat{i}. As was shown in Sec. 2.2, the three-dimensional vibrational bush \[ B\{\hat{a}^4\} = \mu_6(t)\varphi_6 + \mu_3(t)\varphi_3 + \mu_9(t)\varphi_9 \] (43) corresponds to the subgroup \{ \hat{a}^4 \} where three functions \mu_6(t), \mu_3(t) and \mu_9(t) are independent of each other. Thus, three one-dimensional irreps \Gamma_6, \Gamma_3 and \Gamma_9 contribute to the bush \( B\{\hat{a}^4\} \) associated with the parent group \( G_0 = T \) (namely their basis vectors \( \varphi_j \) are contained in Eq. (43). In terms of irreps of the parent group \( \tilde{G}_0 \), the same bush is formed by basis vectors of one-dimensional irrep \( \tilde{\Gamma}_3 \) and two-dimensional irrep \( \tilde{\Gamma}_7 \) (note that restrictions of these irreps to the subgroup \{ \hat{a}^4 \} give us the above mentioned irreps \( \Gamma_6, \Gamma_3 \) and \( \Gamma_9 \) of the group \( G_0 = T \)). The additional generator \( \hat{i} \) which appears when we pass from the subgroup \{ \hat{a}^4 \} to the subgroup \{ \hat{a}^4, \hat{i} \} introduces the matrix (1) for the irrep \( \tilde{\Gamma}_3 \) and the matrix \[ \begin{pmatrix} 1 \\ 1 \end{pmatrix} \] for the irrep \( \tilde{\Gamma}_7 \), and the new bush \( B\{\hat{a}, \hat{i}\} \) must be invariant with respect to these matrices. This invariance condition leads to the following transformation under the action of \( \hat{i} \): \[ \mu_6(t) \rightarrow \mu_6(t), \ \mu_3(t) \rightarrow \mu_9(t), \ \mu_9(t) \rightarrow \mu_3(t) . \] (44) As a result, we obtain the restriction \( \mu_3(t) = \mu_9(t) \) on previously independent functions \( \mu_3(t) \) and \( \mu_9(t) \). In other words, the old three-dimensional bush \( B\{\hat{a}^4\} \) from Eq. (43) transforms into the new two-dimensional bush \[ B\{\hat{a}^4, \hat{i}\} = \mu_6(t)\varphi_6 + \mu_3(t)[\varphi_3 + \varphi_9] \] (45) Let us emphasize that the transition from the parent group \( G_0 = T \) to the parent group \( \tilde{G}_0 = D \) results in new superpositions of one and the same set of normal modes.
\[ \varphi_j \quad (j = 0, 1, \ldots, 11) \]

when we find the appropriate bushes of modes and, therefore, we can compare bushes associated with different parent groups.

Thus, all bushes associated with the group \( G_0 \) are also bushes associated with the group \( \tilde{G}_0 \), but there appears a set of new bushes for \( \tilde{G}_0 \) because of additional restrictions on time-dependent functions \( \mu_j(t) \) for some old bushes. The detailed analysis of this phenomenon will be published elsewhere, while we give the appropriate results in Table 2 of the present paper.

The dimensions of the bushes are indicated in the first column of this table. The list of the appropriate irreps \( \Gamma_j \) in square brackets in column 2 corresponds to a certain bush. Such a list determines the bush uniquely, since a quite definite basis vector \( \varphi_j \) corresponds to the irrep \( \Gamma_j \) of the group \( G_0 \).

For bushes associated with the parent group \( \tilde{G}_0 = D \) (column 3) we give in square brackets not only individual irreps \( \Gamma_j \) (of the group \( G_0 = T! \)) but also the pairs \( \Gamma_i - \Gamma_j \) of conjugate irreps (the irreps of such pairs are connected by hyphens). Only one function \( \mu_i(t) \) corresponds to each pair \( \Gamma_i - \Gamma_j \). The above discussed bushes (43) and (45) can be written in this notation as follows:

\[
B\{\hat{a}^4\} = [\Gamma_6, \Gamma_3, \Gamma_4],
\]

\[
B\{\hat{a}^4, \hat{i}\} = [\Gamma_6, \Gamma_3 - \Gamma_4].
\]

The relation between \( \mu_3(t) \) and \( \mu_9(t) \) for the bush \( B\{\hat{a}^4, \hat{i}\} \) (see Eq. (43)) is very simple (\( \mu_3(t) = \mu_9(t) \)), while for some other bushes the similar relations can be more complicated. Namely because of this reason we do not define concretely the relation between functions \( \mu_i(t) \) and \( \mu_j(t) \), and write simply \( \Gamma_i - \Gamma_j \), indicating by the same token only that such a relation does exist and, therefore, instead of two independent functions \( \mu_i(t) \) and \( \mu_j(t) \) only one function \( \mu_i(t) \) corresponds to the pair \( \Gamma_i - \Gamma_j \).

Moreover, each square brackets in the third column of Table 3 can correspond to several bushes which differ from each other by different relations between \( \mu_i(t) \) and \( \mu_j(t) \) associated with pairs \( \Gamma_i - \Gamma_j \). By the way, this is one of the causes why the number of bushes in Table 3 is less than the total number (34) of subgroups of the group \( \tilde{G}_0 = D \). There exist also another cause of the above phenomenon. Indeed, there are no vibrational bushes for some subgroups of the parent group \( \tilde{G}_0 = D \). As examples we can point to
subgroups \( \{ \hat{a}, \hat{i} \} \) and \( \{ \hat{a}^2, \hat{a} \hat{i} \} \). Finally, it is possible that adding a new generator does not change the appropriate old bush (for example, \( B\{ \hat{a}^2, \hat{i} \} = B\{ \hat{a}^2 \} \)).

To conclude the discussion of relations between bushes associated with parent groups \( G_0 \) and \( \tilde{G}_0 \), which are indicated in Table 2, let us say that besides five bushes associated with \( G_0 \) there exist seven new types of bushes in accordance with their classification under the parent group \( \tilde{G}_0 \): 2 one-dimensional, 2 two-dimensional, 1 three-dimensional, 1 five-dimensional and 1 six-dimensional.

Let us stress that for some multiatomic chains inversion is not a symmetry element and \( G_0 = T \) is the full symmetry group of these mechanical systems. In such cases we only need to use \( G_0 = T \) as the parent group for finding normal modes. For monatomic chains and for multiatomic chains with inversion, using \( G_0 \) as a parent group provides more rich information about possible bushes and, therefore, is preferable. In most sections of the present paper, we restrict ourselves to studying only bushes associated with the group \( G_0 = T \), since this case is more general and more simple.

It is very essential that our list of bushes given in Sec. 2.2 (see also the second column of Table 2) is valid for every one-dimensional structure with the symmetry group \( G_0 = T \), independently of how many particles are in its primitive cell: the difference appears only in the form of basis vectors, but not in the bush structure. Let us discuss this point using as an example the bush with subgroup \( G_3[4a] \) from Eq. (20) which was denoted in the present section as \( B\{ \hat{a}^4 \} \) (Eq. (43)).

The bush of such type can be excited in various chains, but the basis vectors \( \varphi_j \) from (43) will be different for different structures of the primitive cell. In particular, the dimension of the vectors \( \varphi_j \) and \( X(t) \) is equal to \( k \cdot N \) if there are \( k \) particles in the primitive cell. Moreover, the dimension of the bush also can change, because, in general, basis vectors \( \varphi_j \) depend on a number of arbitrary constants and this number is equal to the number of copies of the appropriate irreps in the decomposition of the full vibrational representation of our mechanical system into its irreducible parts [10].

Thus, the group-theoretical methods give us a possibility to divide the problem of finding all types of symmetry-determined nonlinear vibrations into two independent parts:

\[\text{27} \text{In terms of crystallography, we can say that it is possible for a given crystal to not have inversion even though its Bravais lattice does.}\]
1) obtaining the list of bushes using group-subgroup relations only;

2) taking into account the concrete structure of the considered mechanical systems.

We will discuss bushes of normal modes for multiatomic chains in more detail in a special paper.

3 Stability of bushes of normal modes

Some aspects of the stability of exact solutions for the FPU-β chain were discussed by Poggi and Ruffo in [3]. They used the standard method based on the idea of the linearization of appropriate dynamical equations in the vicinity of a given solution. We also make use of this method, as well as of a direct numerical study of the dynamical equations for the FPU-α chain in the ordinary and in the modal space.

The loss of the stability of bushes for small $N$ and for large $N$ can occur in different ways. It is convenient to discuss these cases separately.

3.1 Stability of bushes of modes for small $N$

Let us consider the problem of bush stability using as an example the FPU-α chain with $N = 12$. All numerical data on thresholds of the bush stability, given in the present section, correspond namely to this case.

Firstly, we discuss the stability of the one-dimensional bush $B[2a]$ with the symmetry group $G = [2a]$. It contains only one mode $\nu_6(t)$. Therefore, we must consider all other modes ($j \neq 6$) in Eqs. (27) to be equal to zero in the exact solution corresponding to the given bush. Bearing in mind the intention to study the bush stability, we suppose that these “sleeping” modes are not exactly equal to zero, but are sufficiently small quantities (for example, at about $10^{-10}$ for the numeric investigation). Then the terms of Eqs. (27) differ from each other by the order of their smallness:

$$|\nu_j\nu_6| \gg |\nu_i\nu_k| \quad \text{for } i, j, k \neq 6.$$  \hspace{1cm} (48)

As a result, we can keep only those terms in the right-hand sides of Eqs. (27), which contain the mode $\nu_6(t)$. Thus, these equations can be reduced for $N = 12$ to the following form (hereafter all numerical coefficients are given up to the third figure after the decimal
\[\begin{align*}
\ddot{\nu}_1 + \omega^2_1 \nu_1 &= -1.155 \alpha \nu_5 \nu_6, \\
\ddot{\nu}_2 + \omega^2_2 \nu_2 &= -2 \alpha \nu_4 \nu_6, \\
\ddot{\nu}_3 + \omega^2_3 \nu_3 &= -2.309 \alpha \nu_3 \nu_6, \\
\ddot{\nu}_4 + \omega^2_4 \nu_4 &= -2 \alpha \nu_2 \nu_6, \\
\ddot{\nu}_5 + \omega^2_5 \nu_5 &= -1.155 \alpha \nu_1 \nu_6, \\
\ddot{\nu}_6 + \omega^2_6 \nu_6 &= 0, \\
\ddot{\nu}_7 + \omega^2_7 \nu_7 &= 1.155 \alpha \nu_1 \nu_6, \\
\ddot{\nu}_8 + \omega^2_8 \nu_8 &= 2 \alpha \nu_1 \nu_6, \\
\ddot{\nu}_9 + \omega^2_9 \nu_9 &= 2.309 \alpha \nu_9 \nu_6, \\
\ddot{\nu}_{10} + \omega^2_{10} \nu_{10} &= 2 \alpha \nu_8 \nu_6, \\
\ddot{\nu}_{11} + \omega^2_{11} \nu_{11} &= 1.155 \alpha \nu_7 \nu_6,
\end{align*}\] 

where

\[\omega_j^2 = 4 \sin^2 \left( \frac{\pi j}{12} \right), \quad j = 1, 2, \ldots, 11.\] (50)

The system (49) of eleven equations splits into seven independent subsystems. Moreover, it follows from the equation (49f)

\[\ddot{\nu}_6 + \omega^2_6 \nu_6 = 0 \quad (\omega^2_6 = 4)\] (51)

that the root mode \(\nu_6(t)\) vibrates in harmonic manner,

\[\nu_6(t) = A \cos(2t + \delta),\] (52)

and, therefore, we can substitute \(\nu_6(t)\) in this form into all of the other equations in (49).

Thus, we obtain

\[\begin{align*}
\ddot{\nu}_1 + \omega^2_1 \nu_1 &= -1.155 (\alpha A) \nu_5 \cos(2\tau), \\
\ddot{\nu}_5 + \omega^2_5 \nu_5 &= -1.155 (\alpha A) \nu_1 \cos(2\tau),
\end{align*}\] (53a)

---

\[28\] Let us emphasize that this is the exact equation of the one-dimensional bush \(B[2a]\) (see also Eq. (29)).
\[ \ddot{v}_2 + \omega_2^2 v_2 = -2(\alpha A)\nu_4 \cos(2\tau), \quad (53b) \]

\[ \ddot{v}_4 + \omega_4^2 v_4 = -2(\alpha A)\nu_2 \cos(2\tau), \]

\[ \ddot{v}_3 + \omega_3^2 v_3 = -2.309(\alpha A)\nu_3 \cos(2\tau), \quad (53c) \]

\[ \ddot{v}_7 + \omega_7^2 v_7 = 1.155(\alpha A)\nu_{11} \cos(2\tau), \quad (53d) \]

\[ \ddot{v}_{11} + \omega_{11}^2 v_{11} = 1.155(\alpha A)\nu_7 \cos(2\tau), \]

\[ \ddot{v}_8 + \omega_8^2 v_8 = 2(\alpha A)\nu_{10} \cos(2\tau), \quad (53e) \]

\[ \ddot{v}_{10} + \omega_{10}^2 v_{10} = 2(\alpha A)\nu_8 \cos(2\tau), \]

\[ \ddot{v}_9 + \omega_9^2 v_9 = 2.309(\alpha A)\nu_9 \cos(2\tau). \quad (53f) \]

The initial phase \( \delta \) was removed from the above equations by introducing the new time variable

\[ \tau = t + \frac{\delta}{2}. \quad (54) \]

Individual subsystems (53) describe different ways that the stability of the original bush \( B[2a] \) can be lost. Indeed, we obtain conditions of the loss of stability with respect to the modes \( \nu_3(t) \) and \( \nu_9(t) \) from Eqs (53c) and (53f), respectively, which can be easily reduced to the standard form of the Mathieu equation [18]:

\[ \ddot{y} + [a - 2q \cos(2\tau)]y = 0. \quad (55) \]

The set of stable and unstable regions correspond to this equation in the plane \( (a, q) \) of its pertinent parameters. Using the stability chart of the Mathieu equation in the same manner as in [3] we obtain, for the considered way of the loss of stability, that the bush \( B[2a] \), describing by the mode \( \nu_6(t) \), is stable for

\[ | \alpha A | < (\alpha A)_c = 1.049. \quad (56) \]

Moreover, it can be stable for larger values of \( | \alpha A | \), as well (for example, for the interval 16.465 < \( | \alpha A | < 16.474 \)), but in this paper we study only the first (basic) zone of stability for all bushes of modes.
Appearance of the modes $\nu_3$ and $\nu_9$ means that the original one-dimensional bush $B[2a]$ enlarges up to the three-dimensional bush $B[4a]$ which embraces the root modes $\nu_3, \nu_9$ and the secondary mode $\nu_6$ [see Eq. (20)]. Let us rewrite Eqs. (49c), (49f) and (49i), describing the dynamics of this bush:

\[
\ddot{\nu}_3 + 2\nu_3 = -2.309 \alpha \nu_3 \nu_6, \quad (57a)
\]
\[
\ddot{\nu}_6 + 4\nu_6 = 0, \quad (57b)
\]
\[
\ddot{\nu}_9 + 2\nu_9 = 2.309 \alpha \nu_9 \nu_6. \quad (57c)
\]

Eqs. (57) represent the linearized equations (with respect to the “sleeping” modes $\nu_3$ and $\nu_6$) of the exact equations of the bush $B[4a]$ in terms of real modes.$^{29}$

\[
\ddot{\nu}_3 + \omega_3^2 \nu_3 = -\frac{8\alpha}{\sqrt{12}} \nu_3 \nu_6, \quad (58a)
\]
\[
\ddot{\nu}_6 + \omega_6^2 \nu_6 = -\frac{4\alpha}{\sqrt{12}} (\nu_3^2 - \nu_9^2), \quad (58b)
\]
\[
\ddot{\nu}_9 + \omega_9^2 \nu_9 = \frac{8\alpha}{\sqrt{12}} \nu_9 \nu_6. \quad (58c)
\]

In contrast to the equations (31) for the bush $B[4a]$ in terms of complex modes $\mu_3, \mu_6, \mu_9,$ Eqs. (58a) and (58c) are independent from each other. Nevertheless, the parametric excitation of the mode $\nu_3(t)$, brought about by the mode $\nu_6(t) = A \cos(2t + \delta)$, leads simultaneously to the excitation of the mode $\nu_9(t)$. Indeed, the same condition of the loss of the stability corresponds to both equations (57a) and (57c), because they can be converted to the identical form using the transformation (54) with the initial phase shifted by $\pi$.

Equations (53b) for modes $\nu_2(t), \nu_4(t)$ and (53e) for conjugate modes $\nu_{10}(t), \nu_8(t)$ describe the transition from the original bush $B[2a]$ to the embracing bush $B[6a]$ because of the parametric resonance with the mode $\nu_6(t)$ [see (22)]. Note that Eqs. (53b) and (53e) can be converted to the same form using the above mentioned transformation reducing Eqs. (57c) to the form of Eqs (57a) and, therefore, we may discuss equations for modes $\nu_2(t)$ and $\nu_4(t)$ only.

It is interesting to stress that we cannot consider the parametric excitation of the bush $B[3a]$ by the mode $\nu_6(t)$ belonging to the bush $B[2a]$. Indeed, according to Eq.(20) the

$^{29}$Compare these equations with those in terms of complex modes (31).
two-dimensional vibrational bush \( B[3a] \) consist of two modes, \( \nu_4 \) and \( \nu_8 \), whose symmetry group is \( G = 3a \). On the other hand, the new bush \( B \), appearing as a result of the loss of stability of the old bush \( B[2a] \), must include the last bush and, therefore, must contain the mode \( \nu_6 \). Thus, the above mentioned loss of stability can induce only bushes \( B[6a] \) and \( B[12a] \), but not the bush \( B[3a] \) (see Eq. (20)). This geometrical fact can be confirmed by the following dynamical arguments.

We find from Eqs. (53) that the active mode \( \nu_6(t) \) (see Eq. (52)) can excite the following pairs of the sleeping modes \( \nu_1, \nu_5 \) (Eq. (53a)), \( \nu_2, \nu_4 \) (Eq. (53b)), \( \nu_7, \nu_11 \) (Eq. (53d)) and \( \nu_8, \nu_{10} \) (Eq. (53c)). All modes in the pairs \((\nu_1, \nu_5)\) and \((\nu_7, \nu_{11})\) possess the same symmetry group \( G = 12 \), while the modes from each other pair, i.e. \((\nu_2, \nu_4)\) and \((\nu_8, \nu_{10})\), have different symmetry groups: the group \( G = 3a \) corresponds to \( \nu_4, \nu_8 \) and \( G = 6a \) corresponds to \( \nu_2, \nu_{10} \). Since both modes of each of the above mentioned pairs must appear simultaneously (this can be seen from the structure of Eqs. (53a), (53b), (53d) and (53c), respectively), the bush \( B[3a] \), in its pure form, cannot be excited in connection with the loss of stability of the bush \( B[2a] \).

Indeed, as was just stated, according to, for example, equation (53b), the excitation of the mode \( \nu_4 \) with \( G = 3a \) leads necessarily to excitation of the root mode \( \nu_2 \) \( (G = 6a) \) of the larger bush \( B[6a] \). Thus, equations (53b)

\[
\ddot{\nu}_2 + \omega_2^2 \nu_2 = -2(\alpha A) \nu_4 \cos(2\tau), \\
\ddot{\nu}_4 + \omega_4^2 \nu_4 = -2(\alpha A) \nu_2 \cos(2\tau)
\]

describe the transition from the original bush \( B[2a] \) to the bush \( B[6a] \) \{root modes \( \nu_2(t), \nu_{10}(t) \)\}, when \( (\alpha A) \) reaches the appropriate critical value \( (\alpha A)_c \). Direct numerical computations for Eqs. (53) lead to the following result:

\[
(\alpha A)_c = 1.049.
\]

Comparing the critical values (56) and (60) of \( (\alpha A) \) providing the transition to the bushes \( B[4a] \) and \( B[6a] \) respectively, we see that these bushes are excited by the mode \( \nu_6(t) \) at the same threshold (up to the numerical accuracy).

\(^{30}\)See Table 1.
Similar to the above analysis, we can consider the stability of the bush $B[2a]$ with respect to interactions with the root modes of the bush $B[12a]$. There are four such modes: $\nu_1, \nu_5$ and $\nu_7, \nu_{11}$ conjugate to them. Nevertheless, it is sufficient to take into account only two equations (53a) for $\nu_1$ and $\nu_5$ because Eqs. (53d) for $\nu_7, \nu_{11}$ can be transformed to the form (53a). The critical value $(\alpha A)_c$ which corresponds to the transition $B[2a] \rightarrow B[12a]$ also coincides with the above values (56) and (60) for transitions $B[2a] \rightarrow B[4a]$ and $B[2a] \rightarrow B[6a]$: 

\[(\alpha A)_c = 1.049.\] (61)

We will return to this surprising coincidence in the next section of the present paper.

Comparing all three variants [see Eqs. (56), (60), (61)] of the loss of the stability of the original bush $B[2a]$, which brought about its extension up to the bushes $B[4a], B[6a]$ and $B[12a]$, respectively, we find that as the amplitude $A$ of the mode $\nu_6(t)$ is increased, the transition $B[2a] \rightarrow B[12a]$ must occur because the bush $B[12a]$ embraces both bushes $B[4a]$ and $B[6a]$. This result, obtained from approximate Eqs. (53), was confirmed by direct numerical computation of the exact dynamical equations for the FPU-$\alpha$ model.

We wrote two variants of the appropriate computer programs: the program P1 solves Eqs. (23) in ordinary space and then decomposes the vector $X(t)$, defined by Eq. (3), into the set of modes, while the program P2 solves Eqs. (27) for the FPU-$\alpha$ chain in modal space. Both programs give the same estimation for the value of $(\alpha A)_c$: 

\[1.04 < (\alpha A)_c < 1.05,\]

and confirm the above conclusion that the bush $B[2a]$ really transmutes into the bush $B[12a]$ as a result of the loss of its stability.

Below we give the critical values of $(\alpha A)$ for the loss of stability of all other bushes for the FPU-$\alpha$ chain with $N = 12$:

\[B[4a] \rightarrow B[12a] : (\alpha A)_c \approx 1.05,\] (62)

\[B[3a] \rightarrow B[6a] : (\alpha A)_c \approx 0.60,\] (63)

\[B[6a] \rightarrow B[12a] : (\alpha A)_c \approx 1.29.\] (64)

Let us pay attention to the loss of the stability of the bush $B[3a]$. As follows from Eq. (53), this bush transmutes at $(\alpha A)_c = 0.60$ into the embracing bush $B[6a]$. This
transformation is accompanied by the lowering of symmetry \((G[3a] \supset G[6a])\) twice. The new bush \(B[6a]\), arising as a result of this process, exists as an individual stable object for the following interval of its own root mode

\[
0.60 < \alpha A < 1.29. \tag{65}
\]

In turn, the bush \(B[6a]\) loses stability for \((\alpha A) > (\alpha A)_c = 1.29\) and transmutes into the largest bush \(B[12a]\) containing all modes \(\nu_j (j = 1, 2, \ldots, 11)\), also with lowering of symmetry twice \((G[6a] \supset G[12a])\).

Thus, we have considered the stability of all possible bushes for the FPU-\(\alpha\) chain with \(N = 12\) particles. All other cases with sufficiently small \(N\) can be studied by similar methods. But some new phenomena appear when \(N\) becomes very large, and we consider them in the next section.

### 3.2 Stability of bushes of modes for large \(N\)

Let us consider the stability of the bush \(B[2a]\) for an arbitrary even value of \(N\) (its stability for the case \(N = 12\) was discussed in Section 3.1). This bush consists of only one mode with \(j = N/2\) and the appropriate dynamical equation

\[
\ddot{\nu}_{N/2} + \omega_{N/2}^2 \nu_{N/2} = 0 \tag{66}
\]

can be obtained from Eqs. (27) assuming that all modes different from \(\nu_{N/2}(t)\) are equal to zero. This is equation of the harmonic oscillator with \(\omega_{N/2} = 2\) [see Eq. (24)], and we can write its solution in the form:

\[
\nu_{N/2}(\tau) = A \cos(2\tau) \tag{67}
\]

\(^{31}\)Transition from one bush \(B_1\) to another bush \(B_2\) with higher dimensionality (with more degrees of freedom) as a result of the loss of stability of \(B_1\) is always associated with spontaneous breaking of symmetry of the original dynamic regime described by the bush \(B_1\). This is one of the central conclusions of the bush theory since every bush possesses its own symmetry group \([7, 8]\). In connection with this, let us note that some aspects of the loss of permutational symmetry of the vibrating chains are considered in \([21]\).

\(^{32}\)In this paper, we consider stability of the bushes associated with the translational parent group \(G_0 = T\) only.
Linearizing the system (27) near the exact solution (67) leads to the following approximate equations:

\[ \ddot{\nu}_j + \omega_j^2 \nu_j = -\frac{8\alpha}{\sqrt{N}} \sin \left( \frac{2\pi j}{N} \right) \nu_{N/2-j} , \quad j = 1, 2, \ldots, N - 1 \]

\[ \omega_j^2 = 4 \sin^2 \left( \frac{\pi j}{N} \right) , \quad j = 1, 2, \ldots, \frac{N}{2} - 1, \frac{N}{2} + 1, \ldots, N - 1 . \]

Note, that right-hand sides of these equations contain only the term \( \nu_{N/2-j} \) (the coefficients before similar terms \( \nu_{N/2+j} \) turns out to be zero). It is easy to see that the system (68) splits into a number of subsystems containing one or two equations only. Indeed, the mode \( \nu_j \) in (68) is connected with the mode \( \nu_{\tilde{j}} \) where \( \tilde{j} = \frac{N}{2} - j \), and vice versa, the mode \( \nu_j \) is connected with \( \nu_{\tilde{j}} \equiv \nu_j \). Therefore, we have for \( j = 1, 2, \ldots, \frac{N}{2} - 1 \) in Eq. (68) the following pairs of equations which are independent from all other equations:

\[ \ddot{\nu}_j + 4 \sin^2 \left( \frac{\pi j}{N} \right) \nu_j = -\gamma \sin \left( \frac{2\pi j}{N} \right) \nu_{\tilde{j}} \cos(2\tau) , \quad \tilde{j} = \frac{N}{2} - j \]  

\[ \ddot{\nu}_{\tilde{j}} + 4 \cos^2 \left( \frac{\pi j}{N} \right) \nu_{\tilde{j}} = -\gamma \sin \left( \frac{2\pi j}{N} \right) \nu_j \cos(2\tau) , \]

where

\[ \gamma = \frac{8\alpha A}{\sqrt{N}} , \quad j = 1, 2, \ldots, \left( \frac{N}{4} - 1 \right) . \]

Here we made use of the explicit form of \( \nu_{N/2}(t) \) from Eq. (67). For \( j = \frac{N}{2} + 1, \ldots, N - 1 \) we obtain from (68) the equations similar to (68), but with the changing of the sign of the constant \( \gamma \). As was discussed in the previous section, this case can be reduced to Eqs. (69) by replacing \( \tau \rightarrow \tau + \frac{\pi}{2} \). (Note, that for \( j > \frac{N}{2} \), the index \( \tilde{j} = \frac{N}{2} - j \) becomes negative and then we can use the cyclic condition \( j + N \equiv j \) for obtaining positive values of \( \tilde{j} \)). When \( j = \frac{N}{2} - j \), both modes \( \nu_j \) and \( \nu_{\tilde{j}} \) reduce to the same mode \( \nu_{\frac{N}{4}} \) and (68) reduces to the pair of identical equations of the form

\[ \ddot{\nu}_{\frac{N}{4}} + 2 \nu_{\frac{N}{4}} = -\gamma \nu_{\frac{N}{4}} \cos(2\tau) . \]

Obviously, this equation can be transformed to the standard form of the Mathieu equation (53) with \( y(\tau) = \nu_{\frac{N}{4}}(\tau), a = 2, q = -\gamma/2 \).

Thus, the system (68) of \( N - 2 \) differential equations splits into the subsystems (69) or (71) according to the diagram shown in Fig. 1, where indices \( j \) corresponding to pairs of equations (69) are connected with the arches of different size.
It is convenient to rewrite Eqs. (69) as follows:\textsuperscript{33}

\[\begin{align*}
\ddot{x} + 4 \sin^2(k)x &= \gamma \sin(2k)y \cos(2\tau), \\
\ddot{y} + 4 \cos^2(k)y &= \gamma \sin(2k)x \cos(2\tau).
\end{align*}\] (72)

where \(k = \pi j/N, x(\tau) = \nu_j(\tau), y(\tau) = \nu_{N/2-j}(\tau)\). Thus, studying the loss of stability of the bush \(B[2a]\), brought about by its interactions with the modes \(\nu_{N/4}\) and \(\nu_{3N/4}\) is reduced to analyzing the Mathieu equation (71), and the loss of its stability with respect to all other modes reduces to analyzing Eqs. (72).

We begin to study the stability of the bush \(B[2a]\) by considering its interaction with the mode \(\nu_{N/4}\) [let us remember that \(B[2a]\) consists of only one mode \(\nu_{N/2}\) described by Eq. (67)]. It is clear that \(B[2a]\) must be a stable object for very small values of \(\alpha A\) and we are interested in the lower boundary \(A_c\) of the loss of its stability, because of the parametric excitation of the mode \(\nu_{N/4}\), when the amplitude \(A\) of the mode \(\nu_{N/2}\) increases from zero. This problem can be solved easily with the aid of the Mathieu equation (71). Using its well known stability chart and analytical formulas for boundaries of unstable regions in the \((a,q)\) plane \[18\], and independently by direct numerical investigation of Eq. (71), we found the following threshold value \(\gamma_c\) for the coefficient \(\gamma\) entering into this equation:

\[\gamma_c = 2.42332.\] (73)

Then from Eq. (70) we obtain:

\[\alpha A_c = 0.30292\sqrt{N}.\] (74)

Thus, the bush \(B[2a]\) is stable with respect to the interaction with the mode \(\nu_{N/4}\) for \(|\alpha A| < \alpha A_c\) given by Eq. (74). It is obvious that the same value of \(\alpha A_c\) corresponds to the loss of stability of \(B[2a]\) because of parametric excitation of the mode \(\nu_{3N/4}\).

Now we must take into account interactions of the bush \(B[2a]\) with all other modes \(\nu_j(t)\). As was already stated, studying the stability of \(B[2a]\) leads, in this case, to the equations (72). They are linear differential equations with periodic coefficients and, therefore, the Floquet theory can be applied to them. Unfortunately, we did not obtain any

\textsuperscript{33} As was already noted, the sign before \(\gamma\) in Eqs. (8) is not essential.
exact solutions of Eqs. (72) and can now give only results of the appropriate numerical analysis. Our computation of the multiplicators for the system (72) as eigenvalues of the monodromic matrix reveals a surprising fact! Indeed, it seems that the critical value \( \gamma_c \) of the constant \( \gamma \) from (69) [see also Eqs. (72)], corresponding to the loss of stability of the bush \( B[2a] \), must depend on the mode number \( j \), since the coefficients of these equations depend explicitly on \( j/N \). However, this is not true. We found that \( \gamma_c \) does not depend on \( j/N \), at least up to \( 10^{-5} \), and coincides with that of the Mathieu equation (71):
\[
\gamma_c = 2.42332.
\]

This nontrivial fact means that the original bush \( B[2a] \) loses its stability with respect to all modes \( \nu_j \) \( (j \neq N/2) \) simultaneously, i.e., for the same value \( A_c \) of the amplitude of the mode \( \nu_{N/2}(t) \). In other words, all modes of an \( N \)-particle FPU-\( \alpha \) chain are excited parametrically because of interaction with \( B[2a] \) when \( \alpha A \) reaches its critical value \( \alpha A_c = 0.30292\sqrt{N} \) and, therefore, \( B[2a] \) transforms at once into the bush \( B[Na] \) of trivial symmetry.\(^{34}\)

The above results obtained by studying Eqs. (69, 71) were verified with the aid of the program P1 for solving the dynamical equations (23) for the atomic displacements \( x_i(t) \), \( i = 1, 2, \ldots, N \). Indeed, for \( N = 50, 100, 200 \), we obtained in such a way the relation \( \alpha A_c = 0.303\sqrt{N} \) which is in the excellent agreement with Eq. (74). Moreover, it was also found that all modes \( \nu_j(t), j = 1, 2, \ldots, N - 1 \) are present in the decomposition (14) of the configurational vector \( \mathbf{X}(t) \) from Eq. (2). This fact confirms the above discussed conclusion about the appearance of the bush \( B[Na] \) from the original bush \( B[2a] \) when the amplitude \( A \) exceeds the critical value \( A_c \) from Eq. (74).

Note that using the program P1 for studying the stability of the bush \( B[2a] \), we try \( N \) only up to 1024, but analyzing this problem with the aid of Eqs. (69) we try very great values of \( N \), such as \( N = 10^4, 10^5 \) allowing \( j/N \) to approach sufficiently close to the “dangerous” zero value.

Now let us consider the configuration vector \( \mathbf{X}(t) \) from Eq. (14) which determines displacements of all \( N \) particles from their equilibrium states expressed in terms of the

\(^{34}\) We already met this phenomenon [see Eqs. (56), (60) and (61)] for the special case \( N = 12 \). The value \( \alpha A_c = 1.049 \) from the above mentioned equations is obtained from our present formula \( \alpha A_c = 0.30292\sqrt{N} \) for \( N = 12 \).
modes $\nu_j(t)$. The bush $B[2a]$ consists of only one mode $\nu_{N/2}$ and, therefore,

$$X(t)\big|_{B[2a]} = \nu_{N/2}(t) \psi_{N/2}.$$ \hspace{1cm} (75)

The components $(\psi_{N/2})_n$ of the N-dimensional vector $\psi_{N/2}$ can be obtained from Eq. (13):

$$(\psi_{N/2})_n = \frac{1}{\sqrt{N}} \cos(\pi n), \quad n = 1, 2, \ldots, N. \hspace{1cm} (76)$$

Then we have

$$\psi_{N/2} = \frac{1}{\sqrt{N}} c, \text{ where } c = (-1, 1, -1, 1, \ldots, -1, 1) \hspace{1cm} (77)$$

and

$$X(t)\big|_{B[2a]} = \frac{A}{\sqrt{N}} \cos(2t) \ c. \hspace{1cm} (78)$$

Here, for simplicity, we choose such an initial condition for the excitation of the bush $B[2a]$ that $\delta$ from Eq. (52) is equal to zero. It is clear from (77), (78) that the displacement pattern of the FPU chain, corresponding to arbitrary instant $t$, possesses the translational symmetry $2a$ (see Fig.2), since displacements of every two particles $2a$ apart from each other are identical.

The dynamical regime (78) loses its stability when the amplitude $A$ becomes larger then $A_c$ determined by Eq. (74):

$$A_c \approx 0.303 \frac{\sqrt{N}}{\alpha}. \hspace{1cm} (79)$$

Substituting this value into Eq. (78) we obtain the critical form $X(t)$ for the considered bush $B[2a]$:

$$X_c(t)\big|_{B[2a]} = \frac{0.303}{\alpha} c \cos(2t). \hspace{1cm} (80)$$

Note that $X_c(t)$ from (80) does not depend on the number of particles ($N$) in the FPU chain! It follows from (80) that amplitudes of all atomic displacements for critical $X_c(t)$ must be larger for lesser values of $\alpha$ and, formally, they tend to infinity when $\alpha \to 0$. Such a behavior reflects the fact that there are no interactions between normal modes in the limit $\alpha = 0$ and, therefore, the normal mode $\nu_{N/2}(t)$ becomes stable in this case for any arbitrary amplitude $A$. To avoid a possible misunderstanding, let us note that for a FPU-\(\alpha\) system, considered as an abstract exact model, any distance $a$ between particles in equilibrium is permitted and, as a result, atomic displacements can be large. From
this point of view, the presence $\alpha$ in the denominator in Eq. (80) must not be striking. However, when we consider the FPU-$\alpha$ model as an approximation to the real physical system, only sufficiently small atomic displacements are assumed because we must neglect, in such a case, the higher terms in the Taylor series (11) for $F(\Delta x)$. We must also take into account that the value of the amplitude $A$ of the oscillatory regime is restricted because the nonlinear term with $\alpha$ in the FPU-$\alpha$ Hamiltonian (22) can be negative with absolute value larger than the quadratic term (the height of this barrier and its distance from zero are proportional to $1/\alpha^2$ and $1/\alpha$, respectively).

There was a discussion on the loss of stability of the zone-boundary mode (ZBM) in [20, 21, 19]. In our terms, this problem is identical to the problem of the loss of stability of the bush $B[2a]$, since this bush consists of only one above mentioned mode. In the present paper, we do not want to give detailed comparisons of the results by different authors and restrict ourselves by the following short comments.

In the paper [19] by Sandusky and Page, the interrelation between the loss of stability of the zone-boundary mode (ZBM) and existence of intrinsic localized modes (ILM’s) is discussed for different nonlinear monatomic chains. It was found that there can exist two different types of the loss of stability of the ZBM in the $(k_2, k_3, k_4)$ chains. One of these types is connected with the appearance of the ILM’s, while the other, the so called “period-doubling” type, is not related to ILM’s.

Only the “time-doubling” type of the loss of stability of ZBM occurs when the coefficient $k_3$ is sufficiently large, in particular, when $k_3 \neq 0$, $k_4 = 0$ (this case corresponds to the FPU-$\alpha$ model). Namely this phenomenon is discussed in the present paper for the FPU-$\alpha$ chain, and we can compare the values of the amplitude threshold for the loss of stability of the ZBM (the bush $B[2a]$, in our terms) obtained by us and by Sandusky and Page.

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35 We are very grateful for the referee of our paper for these references which we did not know previously.

36 In some papers, the zone-boundary mode is called by the term “$\pi$-mode”.

37 The term “breathers” is usually used for ILM’s at the present time.

38 Here, $k_2, k_3, k_4$ are coefficients in front of the harmonic term ($k_2$) and in front of the anharmonic terms of the third ($k_3$) and fourth ($k_4$) orders.

39 This term means that the new mode which appears because of the loss of stability of the ZBM possesses a time period two times larger than that of ZBM.
Page. The following estimate was found in [19]:

\[ 0.302 < |\Lambda_3| < 0.303, \]  

(81)

where \( \Lambda_3 = k_3A/k_2 \) with \( A \) being the non-normalized amplitude of the ZBM.

Taking into account Eq. (22), we can express \( \Lambda_3 \) in terms of our paper:

\[ \Lambda_3 = \alpha A/\sqrt{N}, \]  

(82)

where \( A \) is the mode amplitude with respect to normalized basis vectors (13). Then, with the aid of the Eq. (74)

\[ \alpha A_c = 0.30292\sqrt{N} \]

we obtain

\[ \Lambda_3 = 0.30292 \]  

(83)

This value of the threshold of the loss of stability of the ZBM is in the excellent agreement with estimation (81) obtained in the paper [19] for the case \( N = 100 \). Our result (83) is valid for arbitrary value of \( N \) and, moreover, as was already discussed in the text of the present paper, we found that all modes appear simultaneously\(^\text{40}\) when \( \Lambda_3 \) exceeds the remarkable threshold (83). This threshold was obtained by another method, as compared to [19], and with the higher precision.

Thus, we confirmed the validity of the results on the loss of the ZBM stability for the FPU-\( \alpha \) chain by Sandusky and Page from the paper [19] in contrast to those obtained in [20,21] (the discussion on the causes of the incorrectness of the appropriate results reported in [20,21] can be found in [19]).

In many papers, the energy density \( \epsilon = E(0)/N \) of the initial excitation, i.e. the energy \( E(0) \) per one particle, is considered as a relevant control parameter characterizing the loss of stability of different modes in nonlinear chains. Substituting \( X_c(0) \) from (80) into the Hamiltonian (22) leads to vanishing the sum of anharmonic (cubic) terms, and we obtain the following expression for the threshold \( \epsilon_c \) of the loss of stability of the bush \( B[2a] \):

\[ \epsilon = 0.18325/\alpha^2. \]

\(^{40}\)We suspect that this phenomenon leads, as a final result, to equipartition of the energy between different modes of the FPU-\( \alpha \) chain, but we did not study this fact.
Let us emphasize that this value does not depend on the number $N$ of the particles in the FPU-α chain.

We want to note that unlike one-dimensional bushes, the energy density $\epsilon$ is not a relevant parameter for characterizing bush stability in the general case. Indeed, it can be shown that if a given bush contains several modes, the threshold of the loss of stability depends not only on $\epsilon$ but on the distribution of the energy among its modes at the initial instant. Because of this reason, we prefer to fix this initial energy distribution in a certain way, namely, we assume that the energy is completely localized only in the root mode of the bush and then we look for the threshold value $A_c$ of this mode.

In conclusion, let us note that the rigorous stability analysis of all bushes of vibrational modes cannot be fulfilled on the basis of the Floquet theory\footnote{Note that the threshold of the loss of stability of the ZBM, i.e. of the bush $B[2a]$, was obtained in \cite{19} and in the present paper with the aid of the Floquet theory.}, because, in general, dynamical regimes corresponding to them are not periodical. Indeed, a given bush can contain modes with incommensurable frequencies (for example, the bush $B[4a]$ contains the modes with the harmonic frequencies $\omega_{3,9} = \sqrt{2}$ and $\omega_6 = 2$).

Now let us compare our results on stability of the bush $B[2a]$ for the FPU-α model with those by Poggi and Ruffo obtained in \cite{3} for the FPU-β model [remember that $B[2a]$ is the simplest bush consisting of only one mode $\nu_{N/2}(t)$]. The dynamical equation describing the evolution of the mode $\nu_{N/2}(t)$ is the equation of the harmonic oscillator for the FPU-α chain and the Duffing equation for the FPU-β chain, respectively. The problem of the loss of stability of the bush $B[2a]$ according to the parametric excitation of the other modes reduces in the linear approximation to studying the differential equations (69,71) for the FPU-α case and to studying the Lamé equation for the FPU-β case. In both cases, coefficients of the above mentioned equations depend on $j/N$ only, where $j$ is a number of the excited mode and $N$ is the total number of particles in the FPU chain.

Let us consider the main difference in stability properties of the bush $B[2a]$ for the two discussed mechanical systems. There are different threshold values of the energy localized in the mode $\nu_{N/2}$ for exciting the different modes $\nu_j$ for the FPU-β chain and, moreover, the modes for which $\sin^2(\frac{\pi j}{N}) < \frac{1}{3}$ cannot be excited parametrically at all \cite{3}. In contrast to this, we found that in the FPU-α model all modes with $j \neq \frac{N}{2}$ are excited by the
mode $\nu_{N/2}$ simultaneously, i.e., the same threshold value $\alpha A_c$ corresponds to them. When $|\alpha A| > \alpha A_c$ all modes $\nu_j (j \neq N/2)$ begin to increase at once, and, as a result, the original bush $B[2a]$ loses its stability.

The studying of stability of the bushes other than $B[2a]$ for arbitrary $N$ (which are multidimensional) is the more complicated problem, and we will not discuss it in the present paper. Let us point out only one interesting result. As was discussed in Sec. 2, every bush possesses a certain symmetry group $G$ and contains a number of modes whose symmetry is higher or equal to $G$. These modes $\nu_j$ are depicted as sticks in Fig.3a for the case of the bush $B[8a]$ and we will refer to them, using the spectroscopic terminology, as “lines” (note that some modes of the bush are too small to be shown on this picture). The height of each such stick (line) is determined by the value of $\nu_j(t)$ at the instant $t$. When $N$ becomes sufficiently large (using the program P1, we considered the cases $N = 128, 256, 512, 1024$) a number of satellites, forbidden by the above mentioned symmetry restriction, appear near every line of a given bush (see Fig. 3b) for the amplitude of the root mode exceeding a certain critical value. This phenomenon may be described in the following manner.

Let $j_0$ correspond to one of the modes $\nu_{j_0}$ belonging to a given bush. Then several “forbidden” modes $\nu_j$ with $j = j_0 \pm 1, j_0 \pm 2, j_0 \pm 3, \ldots$ arise above a certain threshold for $\alpha A_c$ of a root mode. It must be stressed that the appearance of such “satellites” of different orders is not connected with any symmetry related principles. The excitation of the satellites brought about by the approach of frequencies of the appropriate modes to each other when $N \to \infty$ and this phenomenon, in turn, results in resonance interactions between modes. The time evolution of the satellites can be very nontrivial, in particular for large $N$, amplitudes of satellites of higher orders can be greater than those of lesser orders. In Fig 3.b, we show schematically the satellite structure of the bush $B[8a]$ for $N=128$ at $t \approx 2500 T_L$, where $T_L$ is the period of oscillations of the root mode. Note, that “first” modes, i.e. modes $\nu_j$ with $j$ near the beginning and near the end of the interval of permissible values of mode numbers, are also present on the Fig.3.b. The appearance of the satellite structure corresponds to the beginning of the process of the loss of stability of the given bush, but this structure can be observed for a sufficiently long time as a metastable state.
In connection with the above mentioned metastable states, let us note that there are a number of papers devoted to studying the dynamics of nonlinear chains above the threshold of the loss of stability of the zone-boundary mode, i.e. the bush $B[2a]$, in our terms (see, for example, [13] and [27] where some types of localized states were revealed in the certain cases). In particular, the very interesting phenomenon of the emergence of “chaotic breathers” as a kind of metastable dynamical regime was reported in [27]. We do not study such phenomena in the present paper.

4 Conclusion

In the present paper we demonstrate how to obtain the invariant submanifolds in the modal space of an $N$-particle chain with periodic boundary conditions by regular group-theoretical methods based on the concept of bushes of normal modes developed by us in [7-11] for arbitrary mechanical systems with discrete symmetry. Bushes of modes appear under certain initial conditions and they can be considered as geometrical objects with their own symmetry and as dynamical objects, as well. For the last case, differential equations corresponding to the dynamical systems whose dimensionality is frequently essentially less than $N$ can be obtained. The energy localized in the very definite set of modes, corresponding to a given bush, remains trapped. The object of such a type were revealed recently for the FPU-$\beta$ chain by Poggi and Ruffo [3]. We show that these objects do correspond to our concept of bushes of normal modes and that the group-theoretical methods developed by us earlier allow one to find easily all these objects for arbitrary chains (not for the FPU models only). We also compare the classification of the bushes of vibrational modes according with the different choice of the parent symmetry group $G_0$ (it can be the cyclic group of pure translations or the dihedral group).

For a concrete chain—FPU-$\alpha$ model—we derive the integro-differential equation which describes the dynamics of this chain in the modal space in the limit $N \to \infty$. In contrast to the KdV equation obtained by Zabusky and Kruskal for the FPU-$\alpha$ model in the continuum limit in the ordinary space, the above mentioned integro-differential equation is correct for all wave lengths, not only for long waves.

We study the stability of all possible bushes of normal modes for the case $N = 12$. 

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For the bush $B[2a]$ to which the pattern of atomic displacements with translational symmetry twice that of the equilibrium state corresponds, we found the boundary of the loss of stability in the limit $N \to \infty$. It was found that the bush $B[2a]$ loses its stability with respect to all other modes *simultaneously* when the amplitude of atomic displacements exceeds the value $(0.303/\alpha)$. Let us stress that this result corresponds only to the FPU-\(\alpha\) model. Indeed, Poggi and Ruffo found essentially different results for the FPU-\(\beta\) chain \(\mathbb{3}\) (we give the appropriate comparison in Sec. 3.2 of the present paper). We also briefly discussed the appearance of the metastable satellite structure of symmetry forbidden lines near the permitted lines of the bush $B[ma]$ where $m \neq 2$ for sufficiently large $N$.

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Fig. 1. Splitting of Eqs. (68).

Fig. 2. The monatomic chain in the equilibrium state and the pattern of atomic displacements for the bush $B[2a]$.

Fig. 3. Satellites near the modes of the bush $B[8a]$ (schematically). (a) Absence of the satellite structure for $N = 32$. (b) Appearance of the satellite structure for $N = 128$. 
Table 1. Irreducible representations of the cyclic group $G_0$ for $N = 12$

| Irreps $\Gamma$ | $E$ | $a$ | $a^2$ | $a^3$ | $a^4$ | $a^5$ | $a^6$ | $a^7$ | $a^8$ | $a^9$ | $a^{10}$ | $a^{11}$ | Symmetry groups $G_k$ | Modes |
|-----------------|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------------------|-------|
| $\Gamma_0$     | 1   | 1   | 1     | 1     | 1     | 1     | 1     | 1     | 1     | 1     | 1     | 1     | $[a]$            | $\nu_0$|
| $\Gamma_1$     | 1   | $\gamma$ | $\gamma^2$ | $\gamma^3$ | $\gamma^4$ | $\gamma^5$ | $\gamma^6$ | $\gamma^7$ | $\gamma^8$ | $\gamma^9$ | $\gamma^{10}$ | $\gamma^{11}$ | $[12a]$          | $\nu_1$|
| $\Gamma_2$     | 1   | $\gamma^2$ | $\gamma^4$ | $\gamma^6$ | $\gamma^8$ | $\gamma^{10}$ | 1     | $\gamma^2$ | $\gamma^4$ | $\gamma^6$ | $\gamma^8$ | $\gamma^{10}$ | $[6a]$           | $\nu_2$|
| $\Gamma_3$     | 1   | $\gamma^3$ | $\gamma^6$ | $\gamma^9$ | 1     | $\gamma^3$ | $\gamma^6$ | $\gamma^9$ | 1     | $\gamma^3$ | $\gamma^6$ | $\gamma^9$ | $[4a]$          | $\nu_3$|
| $\Gamma_4$     | 1   | $\gamma^4$ | $\gamma^8$ | 1     | $\gamma^4$ | $\gamma^8$ | 1     | $\gamma^4$ | $\gamma^8$ | 1     | $\gamma^4$ | $\gamma^8$ | $[3a]$          | $\nu_4$|
| $\Gamma_5$     | 1   | $\gamma^5$ | $\gamma^{10}$ | $\gamma^3$ | $\gamma^8$ | $\gamma$ | $\gamma^6$ | $\gamma^{11}$ | $\gamma^4$ | $\gamma^9$ | $\gamma^2$ | $\gamma^7$ | $[12a]$         | $\nu_5$|
| $\Gamma_6$     | 1   | $\gamma^6$ | 1     | $\gamma^6$ | 1     | $\gamma^6$ | 1     | $\gamma^6$ | 1     | $\gamma^6$ | 1     | $\gamma^6$ | $[2a]$          | $\nu_6$|
| $\Gamma_7$     | 1   | $\gamma^7$ | $\gamma^2$ | $\gamma^9$ | $\gamma^4$ | $\gamma^{11}$ | $\gamma^6$ | $\gamma^1$ | $\gamma^8$ | $\gamma^3$ | $\gamma^{10}$ | $\gamma^5$ | $[12a]$         | $\nu_7$|
| $\Gamma_8$     | 1   | $\gamma^8$ | $\gamma^4$ | 1     | $\gamma^8$ | $\gamma^4$ | 1     | $\gamma^8$ | $\gamma^4$ | 1     | $\gamma^8$ | $\gamma^4$ | $[3a]$          | $\nu_8$|
| $\Gamma_9$     | 1   | $\gamma^9$ | $\gamma^6$ | $\gamma^3$ | 1     | $\gamma^9$ | $\gamma^6$ | $\gamma^3$ | 1     | $\gamma^9$ | $\gamma^6$ | $\gamma^3$ | $[4a]$          | $\nu_9$|
| $\Gamma_{10}$  | 1   | $\gamma^{10}$ | $\gamma^8$ | $\gamma^6$ | $\gamma^4$ | $\gamma^2$ | 1     | $\gamma^{10}$ | $\gamma^8$ | $\gamma^6$ | $\gamma^4$ | $\gamma^2$ | $[6a]$          | $\nu_{10}$|
| $\Gamma_{11}$  | 1   | $\gamma^{11}$ | $\gamma^{10}$ | $\gamma^9$ | $\gamma^8$ | $\gamma^7$ | $\gamma^6$ | $\gamma^5$ | $\gamma^4$ | $\gamma^3$ | $\gamma^2$ | $\gamma^1$ | $[12a]$         | $\nu_{11}$|

Here $\gamma = e^{2\pi i/12}$ and, therefore, $\gamma^3 = i$, $\gamma^6 = -1$, $\gamma^9 = -i$, $\gamma^{12} = 1$

Table 2. Bush classification in accordance with the parent groups $G_0 = T$ and $\tilde{G}_0 = D$

| Dim | $G_0 = T$ | $\tilde{G}_0 = D$ (new bush) |
|-----|-----------|------------------|
| 1   | $[\Gamma_6]$ | $[\Gamma_4 - \Gamma_8]; [\Gamma_3 - \Gamma_9]$ |
| 2   | $[\Gamma_4, \Gamma_8]$ | $[\Gamma_6, \Gamma_3 - \Gamma_9]; [\Gamma_2 - \Gamma_{10}, \Gamma_4 - \Gamma_8]$ |
| 3   | $[\Gamma_6, \Gamma_3, \Gamma_9]$ | $[\Gamma_6, \Gamma_2 - \Gamma_{10}, \Gamma_4 - \Gamma_8]$ |
| 5   | $[\Gamma_6, \Gamma_2, \Gamma_{10}, \Gamma_4, \Gamma_8]$ | $[\Gamma_1 - \Gamma_{11}, \Gamma_2 - \Gamma_{10}, \Gamma_3 - \Gamma_9, \Gamma_4 - \Gamma_8, \Gamma_5 - \Gamma_7]$ |
| 6   | - | $[\Gamma_6, \Gamma_1 - \Gamma_{11}, \Gamma_2 - \Gamma_{10}, \Gamma_3 - \Gamma_9, \Gamma_4 - \Gamma_8, \Gamma_5 - \Gamma_7]$ |
| 11  | $[\Gamma_1, \Gamma_2, \ldots, \Gamma_{11}]$ | - |