# Stability analysis of dynamical regimes in nonlinear systems with discrete symmetries

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We present a theorem that allows one to simplify the linear stability analysis of periodic and quasiperiodic nonlinear regimes in $N$-particle mechanical systems with different kinds of discrete symmetry. This theorem suggests a decomposition of the linearized system arising in the standard stability analysis into a number of subsystems whose dimensions can be considerably less than the dimension of the full system. As an example of such a simplification, we discuss the stability of bushes of modes (invariant manifolds) for the Fermi-Pasta-Ulam chains and prove another theorem about the maximal dimension of the above-mentioned subsystems.

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## I. INTRODUCTION

Different dynamical regimes in a mechanical system with discrete-symmetry group $G_0$ can be classified by subgroups $G_j \subseteq G_0$ of this group [1–3]. Actually, we can find an invariant manifold corresponding to each subgroup $G_j$ and decompose it into the basis vectors of the irreducible representations of the group $G_0$. As a result of this procedure, we obtain a *bush of modes* (see the above-cited papers) which can be considered as a certain physical object in a geometrical as well as a dynamical sense. The mode structure of a given bush is fully determined by its symmetry group $G_j$ and is independent of the specific type of interparticle interactions in the system. In Hamiltonian systems, bushes of modes represent dynamical objects in which the energy of the initial excitation turns out to be "trapped" (this is a phenomenon of energy localization in modal space). The number of modes belonging to a given bush (the bush dimension) does not change in time, while amplitudes of the modes do change, and we can find dynamical equations determining their evolution.

Being an *exact* nonlinear excitation, in the considered mechanical system, each bush possesses its own domain of *stability* depending on the value of its mode amplitudes. Beyond the stability threshold a phenomenon similar to parametric resonance occurs; the bush loses its stability and transforms into another bush of higher dimension. This process is accompanied by spontaneous lowering of the bush symmetry: $G_j \rightarrow \tilde{G}_j$, where $\tilde{G}_j \subset G_j$.

The concept of bushes of modes was introduced in [1,2], and the detailed theory of these dynamical objects was developed in [3]. Low-dimensional bushes in mechanical systems with various kinds of symmetry and structures were studied in [1–9]. The problem of bush stability was discussed in [3,7–9]. The two last papers are devoted to the vibrational bushes in Fermi-Pasta-Ulam (FPU) chains.

Note that dynamical objects equivalent to the bushes of modes were recently discussed for monoatomic chains in papers by different authors [10–12,15]. Let us emphasize that the group-theoretical methods developed in our papers [1–3] can be applied efficiently not only to monoatomic chains (as was illustrated in [8,9]), but to *all* other physical systems with discrete symmetry groups (see [1–7]).

In this paper, we present a theorem which can simplify essentially the stability analysis of the bushes of modes in complex systems with many degrees of freedom. The usefulness of this theorem is illustrated with the example of nonlinear chains with a large number of particles. Note that the simplification of the stability analysis in such systems actually originates from the well-known Wigner theorem about the block diagonalization of the matrix commuting with all matrices of a representation of a given symmetry group.

In Sec. II, we start with the simplest examples for introducing basic concepts and ideas. In Sec. III, we present a general theorem about invariance of the dynamical equations linearized near a given bush with respect to the bush symmetry group. In Sec. IV, we prove a theorem which turns out to be very useful for splitting the above-mentioned linearized dynamical equations for $N$-particle monoatomic chains. Some additional examples of the simplification of the bush stability analysis with the aid of group-theoretical methods are presented in Sec. V. The main results of this paper are discussed in the Conclusion (Sec. VI).

## II. SOME SIMPLE EXAMPLES

### A. FPU chains and their symmetry

We consider *longitudinal* vibrations of $N$-particle chains of identical masses ($m=1$) and identical springs connecting neighboring particles. Let $x_i(t)$ be the displacement of the $i$th particle ($i=1,2,\ldots,N$) from its equilibrium position at a given instance $t$. The dynamical equations of such a mechanical system (FPU chain) can be written as follows:

$$\ddot{x}_i = f(x_{i+1}-x_i) - f(x_i - x_{i-1}). \tag{1}$$

The nonlinear force $f(x)$ depends on the deformation $x$ of the spring as $f(x)=x+x^2$ and $f(x)=x+x^3$ for FPU-$\alpha$ and FPU-$\beta$ chains, respectively. We assume the periodic boundary conditions

$$x_0(t) \equiv x_N(t), \quad x_{N+1}(t) \equiv x_1(t) \tag{2}$$

to be valid. Let us also introduce the "configuration vector" $\boldsymbol{X}(t)$ which is the $N$-dimensional vector describing all the

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displacements of the individual particles at the moment $t$:

$$\boldsymbol{X}(t) = \{x_1(t), x_2(t), \ldots, x_N(t)\}. \qquad (3)$$

In the equilibrium state, a given chain is invariant under the action of the operator $\hat{a}$ which shifts the chain by the lattice spacing $a$. This operator generates the translational group

$$T_N = \{\hat{e}, \hat{a}, \hat{a}^2, \ldots, \hat{a}^{N-1}\}, \quad \hat{a}^N = \hat{e}, \qquad (4)$$

where $\hat{e}$ is the identity element and $N$ is the order of the cyclic group $T_N$. The operator $\hat{a}$ induces the cyclic permutation of all particles of the chain and, therefore, it acts on the "configuration vector" $\boldsymbol{X}(t)$ as follows:

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

The full symmetry group of the monoatomic chain contains also the inversion $\hat{i}$, with respect to the center of the chain, which acts on the vector $\boldsymbol{X}(t)$ in the following manner:

$$\hat{i}\boldsymbol{X}(t) \equiv \hat{i}\{x_1(t), x_2(t), \ldots, x_{N-1}(t), x_N(t)\} = \{-x_N(t), -x_{N-1}(t), \ldots, -x_2(t), -x_1(t)\}.$$

The complete set of all products $\hat{a}^k\hat{i}$ of the pure translations $\hat{a}^k$ ($k=0,1,2,\ldots,N-1$) with the inversion $\hat{i}$ forms the so-called dihedral group $D_N$ which can be written as the direct sum of two cosets $T_N$ and $T_N \cdot \hat{i}$:

$$D_N = T_N \oplus T_N \cdot \hat{i}. \qquad (5)$$

The dihedral group is a non-Abelian group induced by two generators ($\hat{a}$ and $\hat{i}$) with the following generating relations

$$\hat{a}^N = \hat{e}, \quad \hat{i}^2 = \hat{e}, \quad \hat{i}\hat{a} = \hat{a}^{-1}\hat{i}. \qquad (6)$$

We will consider different vibrational regimes in the FPU chains, which can be determined by the *specific forms* of the configuration vector. Each of these regimes depends on $m$ independent parameters ($m \leqslant N$), and this number is the *dimension* of the given regime.

The simplest case of one-dimensional vibrational regimes represents the so-called $\pi$ mode (zone boundary mode):[1]

$$\boldsymbol{X}(t) = \{A(t), -A(t) | A(t), -A(t) | A(t), -A(t) | \ldots\}, \qquad (7)$$

where $A(t)$ is a certain function of $t$. In our terminology, this is the one-dimensional bush $\mathrm{B}[\hat{a}^2, \hat{i}]$ (see below about notation of bushes of modes).

The vector

$$\boldsymbol{X}(t) = \{0, A(t), B(t), 0, -B(t), -A(t) | \ldots\} \qquad (8)$$

represents a two-dimensional vibrational regime that is determined by two time-dependent functions $A(t)$ and $B(t)$. This is the two-dimensional bush $\mathrm{B}[\hat{a}^6, \hat{a}\hat{i}]$ (see [9]).

[1]The dots in $\boldsymbol{X}(t)$ denote that the displacement fragment which is given explicitly must be repeated several times to form the full displacement pattern corresponding to the given bush.

In general, for the $m$-dimensional vibrational regime, we write $\boldsymbol{X}(t) = \boldsymbol{C}(t)$, where the $N$-dimensional vector $\boldsymbol{C}(t)$ depends on $m$ time-dependent functions only. Each specific dynamical regime $\boldsymbol{C}(t)$, being an invariant manifold, possesses its own symmetry group that is a subgroup of the parent symmetry group $G_0 = D_N$ of the chain in equilibrium.

### B. FPU-$\alpha$ chain with $N=4$ particles: Existence of the bush $\mathrm{B}[\hat{a}^2, \hat{i}]$

Let us consider the above-discussed equations for the simplest case $N=4$. The dynamical equations (1) read

$$\ddot{x}_1 = f(x_2 - x_1) - f(x_1 - x_4),$$

$$\ddot{x}_2 = f(x_3 - x_2) - f(x_2 - x_1),$$

$$\ddot{x}_3 = f(x_4 - x_3) - f(x_3 - x_2),$$

$$\ddot{x}_4 = f(x_1 - x_4) - f(x_4 - x_3). \qquad (9)$$

The symmetry group $G_0$ in the equilibrium state reads

$$G_0 = D_4 = [\hat{a}, \hat{i}] = \{\hat{e}, \hat{a}, \hat{a}^2, \hat{a}^3, \hat{i}, \hat{a}\hat{i}, \hat{a}^2\hat{i}, \hat{a}^3\hat{i}\}.$$

Hereafter, we write the generators of any symmetry group in square brackets, while all its elements (if it is necessary) are given in curly brackets.

The operators $\hat{a}$ and $\hat{i}$ act on the configuration vector $\boldsymbol{X} = \{x_1, x_2, x_3, x_4\}$ as follows:

$$\hat{a}\boldsymbol{X} = \{x_4, x_1, x_2, x_3\}, \quad \hat{i}\boldsymbol{X} = \{-x_4, -x_3, -x_2, -x_1\}.$$

Therefore, we can associate the following matrices $\mathrm{M}(\hat{a})$ and $\mathrm{M}(\hat{i})$ of the *mechanical representation*[2] with these generators:

$$\hat{a} \Rightarrow \mathrm{M}(\hat{a}) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\hat{i} \Rightarrow \mathrm{M}(\hat{i}) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \qquad (10)$$

Their action on the configuration vector $\boldsymbol{X}$ is equivalent to that of the operators $\hat{a}$ and $\hat{i}$, respectively.

Let us now make the transformations of variables in the system (9) according to the action of the matrices (10)—i.e.,

$$\mathrm{M}(\hat{a}): x_1 \to x_4, \quad x_2 \to x_1, \quad x_3 \to x_2, \quad x_4 \to x_3, \qquad (11)$$

[2]Here we consider only a special case: four-dimensional configuration space and the concrete symmetry group $G = [\hat{a}, \hat{i}]$. The general definition of the mechanical representation is given in the next section.

$$\mathrm{M}(\hat{i}): x_1 \to -x_4, \quad x_2 \to -x_3, \quad x_3 \to -x_2, \quad x_4 \to -x_1. \tag{12}$$

It is easy to check that both transformations (11) and (12) produce systems of equations which are *equivalent* to the system (9). Moreover, these transformations act on the individual equations $u_j$ $(j=1,2,3,4)$ of the system (9) exactly as on the components $x_j$ $(j=1,2,3,4)$ of the configuration vector $\boldsymbol{X}$. For example, for the operator $\hat{i}$ [or matrix $\mathrm{M}(\hat{i})$] we have

$$\hat{i}u_1 = -u_4, \quad \hat{i}u_2 = -u_3, \quad \hat{i}u_3 = -u_2, \quad \hat{i}u_4 = -u_1.$$

It is obvious that a certain transposition of these equations multiplied by $\pm 1$ will, indeed, produce a system fully identical to the original system (9). Thus, we are convinced that the symmetry group $G_0=D_4$ of our chain in equilibrium turns out to be the symmetry group (the group of invariance) of the dynamical equations of this mechanical system.

Let us now consider the vibrational regime (7)—i.e., $\pi$ mode—and check that it represents an invariant manifold for the dynamical system (9). Substituting $x_1(t)=x_3(t)=A(t)$ and $x_2(t)=x_4(t)=-A(t)$ into Eqs. (9), we reduce these equations to one and the same equation of the form

$$\ddot{A} = f(-2A) - f(2A). \tag{13}$$

In the case of the FPU-$\alpha$ model this equation turns out to be the equation of harmonic oscillator (for the FPU-$\beta$ model it reduces to the Duffing equation). Indeed, for the FPU-$\alpha$ chain, we obtain, from Eq. (13),

$$\ddot{A} + 4A = 0. \tag{14}$$

Using, for simplicity, the initial condition $A(0)=C_0$, $\dot{A}(0)=0$, we get the following solution to Eq. (14):

$$A(t) = C_0 \cos(2t). \tag{15}$$

Thus, the one-dimensional bush $\mathrm{B}[\hat{a}^2,\hat{i}]$ (or $\pi$ mode) (7) for the FPU-$\alpha$ chain represents the purely harmonic dynamical regime

$$\boldsymbol{X}(t) = C_0\{\cos(2t), -\cos(2t)|\cos(2t), -\cos(2t)\}. \tag{16}$$

On the other hand, the invariant manifold $\boldsymbol{X}(t)=\{A(t),-A(t),A(t),-A(t)\}$, corresponding to the bush $\mathrm{B}[\hat{a}^2,\hat{i}]$, can be obtained with the aid of the group-theoretical methods only, *without* consideration of the dynamical equations (9). Let us discuss this point in more detail.

At an arbitrary instant $t$, the displacement pattern $\{A(t),-A(t),A(t),-A(t)\}$ possesses its own symmetry group $G=D_2 \subset G_0=D_4$. Indeed, this pattern is conserved under inversion $(\hat{i})$ and under shifting all particles by $2a$. The latter procedure can be considered as a result of the action on the chain by the operator $\hat{a}^2$. These two symmetry elements ($\hat{a}^2$ and $\hat{i}$) determine the dihedral group $D_2$ which is a subgroup of order two of the original group $G_0=D_4$.[3]

It is obvious that the old element $\hat{a}$ of the group $G_0$, describing the chain in equilibrium, *does not survive* in the vibrational state described by the pattern (7). Note that this element $(\hat{a})$ transforms the regime (7) into its equivalent (but different) form $\{-A(t),A(t),-A(t),A(t)\}$. In the present paper, we will not discuss different equivalent forms of bushes of modes (a detailed consideration of this problem can be found in [9]). Thus, we encounter the *reduction* of symmetry $G_0=D_4 \to G=D_2$ when we pass from the equilibrium state to the vibrational state (7) for the considered mechanical system.

The dynamical regime (7) represents the one-dimensional bush consisting of only one mode ($\pi$ mode). We will denote it as $\mathrm{B}[G]=\mathrm{B}[\hat{a}^2,\hat{i}]:\{A,-A,A,-A\}$. In square brackets, the group of the bush symmetry is indicated by listing its generators ($\hat{a}^2$ and $\hat{i}$, in our case), while the characteristic fragment of the bush displacement pattern is presented next to the colon. The bush symmetry group $G$ fully determines the form (displacement pattern) of the bush $\mathrm{B}[G]$ (see, for example, [3,9]). Indeed, in the case of the bush $\mathrm{B}[\hat{a}^2,\hat{i}]$, it is easy to show that this form $\boldsymbol{X}=\{A(t),-A(t),A(t),-A(t)\}$ can be obtained as the general solution to the following linear algebraic equation representing the invariance of the configuration vector $\boldsymbol{X}: \hat{g}_1\boldsymbol{X}=\boldsymbol{X}$, $\hat{g}_2\boldsymbol{X}=\boldsymbol{X}$, where $\hat{g}_1=\hat{a}^2$ and $\hat{g}_2=\hat{i}$ are the generators of the group $G$. In our previous papers we often write these invariance conditions for the bush $\mathrm{B}[G]$ in the form

$$\hat{G}\boldsymbol{X} = \boldsymbol{X}. \tag{17}$$

It is very essential that the invariant vector $\boldsymbol{X}(t)$, which was found in such *geometrical* (group-theoretical) manner, turns out to be an invariant manifold for the considered dynamical system [3]. Thus, we can obtain the symmetry-determined invariant manifolds (bushes of modes) without any information on interparticle interactions in the mechanical system.

### C. FPU-$\alpha$ chain with $N=4$ particles: Stability of the bush $\mathrm{B}[\hat{a}^2,\hat{i}]$

We now turn to the question of the stability of the bush $\mathrm{B}[\hat{a}^2,\hat{i}]$, representing a *periodic* vibrational regime $\boldsymbol{X}=\{A(t),-A(t),A(t),-A(t)\}$, with $A(t)=C_0\cos(2t)$. According to the conventional prescription, we must linearize the dynamical system (9) in the *infinitesimal vicinity* of the given bush and then study the obtained system. For this goal, let us write

$$\boldsymbol{X}(t) = \boldsymbol{C}(t) + \boldsymbol{\delta}(t), \tag{18}$$

where $\boldsymbol{C}=\{A(t),-A(t),A(t),-A(t)\}$ represents our bush, while $\boldsymbol{\delta}(t)=\{\delta_1(t),\delta_2(t),\delta_3(t),\delta_4(t)\}$ is an infinitesimal vec-

[3]Let us recall that the order $m$ of the subgroup $G$ in the group $G_0$ is determined by the equation $m=\|G_0\|/\|G\|$, where $\|G_0\|$ and $\|G\|$ are numbers of elements in the groups $G_0$ and $G$, respectively.

tor. Substituting Eq. (18) into Eqs. (9) and neglecting all terms nonlinear in $\delta_j(t)$, we obtain the following linearized equations for the FPU-$\alpha$ model:

$$\ddot{\delta}_1 = [\delta_2 - 2\delta_1 + \delta_4] - 4A(t)[\delta_2 - \delta_4],$$

$$\ddot{\delta}_2 = [\delta_3 - 2\delta_2 + \delta_1] + 4A(t)[\delta_3 - \delta_1],$$

$$\ddot{\delta}_3 = [\delta_4 - 2\delta_3 + \delta_2] - 4A(t)[\delta_4 - \delta_2],$$

$$\ddot{\delta}_4 = [\delta_1 - 2\delta_4 + \delta_3] + 4A(t)[\delta_1 - \delta_3]. \tag{19}$$

The last system of equations can be written in the form

$$\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}, \tag{20}$$

where $\mathrm{J}(t)$ is the *Jacobi* matrix for the system (9) calculated by the substitution of the vector $\boldsymbol{X}=\{A(t),-A(t),A(t),-A(t)\}$. This matrix can be presented as follows:

$$\mathrm{J}(t) = \mathrm{L} + 4A(t) \cdot \mathrm{M}, \tag{21}$$

where

$$\mathrm{L} = \begin{pmatrix} -2 & 1 & 0 & 1 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 1 & 0 & 1 & -2 \end{pmatrix}, \quad \mathrm{M} = \begin{pmatrix} 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{pmatrix} \tag{22}$$

are two time-independent symmetric matrices.

It easy to check that matrices L and M commute with each other: $\mathrm{L}\cdot\mathrm{M}=\mathrm{M}\cdot\mathrm{L}$. Therefore, there exists a time-independent orthogonal matrix S that transforms the both matrices L and M to the diagonal form: $\tilde{\mathrm{S}}\cdot\mathrm{L}\cdot\mathrm{S}=\mathrm{L}_{dia}$, $\tilde{\mathrm{S}}\cdot\mathrm{M}\cdot\mathrm{S}=\mathrm{M}_{dia}$ (here $\tilde{\mathrm{S}}$ is the transposed matrix with respect to S). In turn, it means that the Jacobi matrix $\mathrm{J}(t)$ can be diagonalized at *any time t* by one and the same time-independent matrix S. Therefore, our linearized system (20) for the considered bush $\mathrm{B}[\hat{a}^2,\hat{i}]$ can be decomposed into four *independent* differential equations.

Let us discuss how the above matrix S can be obtain with the aid of the theory of irreducible representations of the symmetry group $G$ (in our case $G=D_2$).

In Sec. IV, we will consider a general method for obtaining the matrix S which reduces the Jacobi matrix $\mathrm{J}(t)$ to a block-diagonal form. This method uses the basis vectors of irreducible representations of the group $G$, constructed in the configuration space of the considered dynamical system. In our simplest case of the monoatomic chain with $N=4$ particles, this method leads to the result

$$\mathrm{S} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \tag{23}$$

The rows of the matrix S from Eq. (23) are simply the characters of four one-dimensional irreducible representations (irreps)—$\Gamma_1$, $\Gamma_2$, $\Gamma_3$, $\Gamma_4$—of the Abelian group $D_2$, because each of these irreps is contained once in the decomposition of the mechanical representation of the group $G=D_2$. Introducing new variables $\boldsymbol{y}=\{y_1,y_2,y_3,y_4\}$ instead of the old variables $\boldsymbol{\delta}=\{\delta_1(t),\delta_2(t),\delta_3(t),\delta_4(t)\}$ by the equation $\boldsymbol{y}=\mathrm{S}\cdot\boldsymbol{\delta}$ with S from Eq. (23), we arrive at the full splitting of the linearized equations (19) for the FPU-$\alpha$ model:

$$\ddot{y}_1 = 0, \tag{24a}$$

$$\ddot{y}_2 = -2[1 + 4A(t)]y_2, \tag{24b}$$

$$\ddot{y}_3 = -4y_3, \tag{24c}$$

$$\ddot{y}_4 = -2[1 - 4A(t)]y_4, \tag{24d}$$

where $A(t)=C_0\cos(2t)$.

With the aid of Eqs. (24), we can find the stability threshold in $C_0$ for loss of stability of the one-dimensional bush $\mathrm{B}[\hat{a}^2,\hat{i}]$. Indeed, according to Eqs. (24), the variables $y_j(t)$ $(j=1,2,3,4)$ are independent from each other, and we can consider them in turn. Equation (24a) for $y_1(t)$ describes the uniform motion of the center of masses of our chain, since it follows from the equations $\boldsymbol{y}=\mathrm{S}\cdot\boldsymbol{\delta}$ that $y_1(t)\sim\delta_1(t)+\delta_2(t)+\delta_3(t)+\delta_4(t)$. Therefore, considering *vibrational* regimes only, we may assume $y_1(t)\equiv 0$.

If only $y_3(t)$ appears in the solution to the system (24)—i.e., if $y_1(t)=0$, $y_2(t)=0$, $y_4(t)=0$—then we have from, the equation $\boldsymbol{\delta}=\tilde{\mathrm{S}}\cdot\boldsymbol{y}$ (note that S is the orthogonal matrix and, therefore, $\mathrm{S}^{-1}=\tilde{\mathrm{S}}$), $\boldsymbol{\delta}(t)=\{y_3(t),-y_3(t),y_3(t),-y_3(t)\}$, where $y_3(t)\sim\cos(2t)$. This solution leads only to deviations "along" the bush $\boldsymbol{X}(t)=C_0\{\cos(2t),-\cos(2t),\cos(2t),-\cos(2t)\}$ and does not signify instability.

Since $A(t)=C_0\cos(2t)$, Eq. (24b) reads $\ddot{y}_2+[2+8C_0\cos(2t)]y_2=0$ and can be transformed to the standard form of the Mathieu equation, as well as Eq. (24d). Therefore, the stability threshold of the considered bush $\mathrm{B}[\hat{a}^2,\hat{i}]$ for $N=4$ can be determined directly from the well-known diagram of the regions of stable and unstable motion of the Mathieu equation. In such a way we can find that critical value $C_c$ for the amplitude $C_0$ of the given bush for which it loses its stability is $C_c\approx 0.303$.

In conclusion, let us focus on the point that turns out to be very important for proving the general theorem in Sec. III. The system (19) was obtained by linearizing the original system (9), near the dynamical regime $\boldsymbol{C}(t)=\{A(t),-A(t),A(t),-A(t)\}$, and Eqs. (9) are invariant with respect to the parent group $G_0=[\hat{a},\hat{i}]$. Despite this fact, Eqs. (19) are invariant only with respect to its *subgroup* $G=\{\hat{e},\hat{a}^2,\hat{i},\hat{a}^2\hat{i}\}\subset G_0=\{\hat{e},\hat{a},\hat{a}^2,\hat{a}^3,\hat{i},\hat{a}\hat{i},\hat{a}^2\hat{i},\hat{a}^3\hat{i}\}$: the element $\hat{a}\in G_0$ (as well as $\hat{a}^3$, $\hat{a}\hat{i}$, $\hat{a}^3\hat{i}$) does not survive as a result of the symmetry reduction $G_0\to G$. Indeed, acting on Eqs. (19) by the operator $\hat{g}=\hat{a}$, which transposes variables $\delta_j$ as

$$\delta_1 \to \delta_4, \quad \delta_2 \to \delta_1, \quad \delta_3 \to \delta_2, \quad \delta_4 \to \delta_3, \tag{25}$$

we obtain the equations

$$\ddot{\delta}_4 = [\delta_1 - 2\delta_4 + \delta_3] - 4A(t)[\delta_1 - \delta_3],$$

$$\ddot{\delta}_1 = [\delta_2 - 2\delta_1 + \delta_4] + 4A(t)[\delta_2 - \delta_4],$$

$$\ddot{\delta}_2 = [\delta_3 - 2\delta_2 + \delta_1] - 4A(t)[\delta_3 - \delta_1],$$

$$\ddot{\delta}_3 = [\delta_4 - 2\delta_3 + \delta_2] + 4A(t)[\delta_4 - \delta_2]. \tag{26}$$

Obviously, this system is not equivalent to the system (19). [The equivalence between Eqs. (19) and (26) can be restored, if, besides the cyclic permutation (25) in Eqs. (19), we add the artificial transformation $A(t) \to -A(t)$].

What is the source of this phenomenon? The original nonlinear dynamical system, which can be written as $\ddot{\boldsymbol{X}} = \boldsymbol{F}(\boldsymbol{X})$, is invariant under the action of the operator $\hat{g} = \hat{a}$. Being linearized by the substitution $\boldsymbol{X}(t) = \boldsymbol{C}(t) + \boldsymbol{\delta}(t)$ and neglecting all the nonlinear in $\delta_j(t)$ terms, it becomes

$$\ddot{\boldsymbol{\delta}} = \left.\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{X}}\right)\right|_{\boldsymbol{X}=\boldsymbol{C}} \cdot \boldsymbol{\delta} = \mathrm{J}[\boldsymbol{C}(t)] \cdot \boldsymbol{\delta}, \tag{27}$$

where $\mathrm{J}[\boldsymbol{C}(t)]$ is the Jacobi matrix. The latter system is also invariant under the action of the operator $\hat{g} = \hat{a}$, but its transformation must be correctly written as follows:

$$\ddot{\boldsymbol{\delta}} = \hat{g}^{-1} \left.\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{X}}\right)\right|_{\boldsymbol{X}=\hat{g}\boldsymbol{C}} \cdot \hat{g}\boldsymbol{\delta} = \hat{g}^{-1}\mathrm{J}[\hat{g}\boldsymbol{C}(t)] \cdot \hat{g}\boldsymbol{\delta}. \tag{28}$$

In other words, we have to replace the vector $\boldsymbol{X}$ in the Jacobi matrix by a *transformed* vector, $\hat{g}\boldsymbol{C}$, near which the linearization is performed. Thus, we must write this matrix in the form $\mathrm{J}[\hat{g}\boldsymbol{C}(t)]$ instead of $\mathrm{J}[\boldsymbol{C}(t)]$. In our case, $\hat{g}\boldsymbol{C}(t) \equiv \hat{a}\boldsymbol{C}(t) = \{-A(t), A(t), -A(t), A(t)\}$ and, therefore, we indeed have to add the above-mentioned artificial transformation $A(t) \to -A(t)$.

On the other hand, dealing with the linearized system $\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}$, we conventionally consider the Jacobi matrix $\mathrm{J}[\boldsymbol{C}(t)] \equiv \mathrm{J}(t)$ as a fixed (but depending on $t$) matrix which *does not change* when the operator $\hat{g} = \hat{a}$ acts on the system $\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}$—this operator acts on the vector $\boldsymbol{\delta}$ only. The fact is that we try to split the system $\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}$ into some subsystems using the *traditional algebraic transformations* of the old variables $\delta_j$. Indeed, we introduce new variables $\boldsymbol{\delta}_{new} = \mathrm{S} \cdot \boldsymbol{\delta}$, where S is a suitable time-independent orthogonal matrix, and then obtain the new system $\ddot{\boldsymbol{\delta}}_{new} = (\tilde{\mathrm{S}} \cdot \mathrm{J}(t) \cdot \mathrm{S}) \cdot \boldsymbol{\delta}_{new}$ that decomposes into a number of subsystems.

### D. Stability of the bush $\mathrm{B}[\hat{a}^2, \hat{i}]$ for the FPU-$\alpha$ chain with $N > 4$ particles

Linearizing the dynamical equations of the FPU-$\alpha$ chain with $N=6$ in the vicinity of the bush $\mathrm{B}[\hat{a}^2, \hat{i}]$ ($\pi$ mode), we obtain the following Jacobi matrix in Eq. (20):

$$\mathrm{J}(t) = \mathrm{L} + 4A(t) \cdot \mathrm{M},$$

where

$$\mathrm{L} = \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 1 & -2 \end{pmatrix},$$

$$\mathrm{M} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}.$$

These two symmetric matrices, unlike the case $N=4$, *do not* commute with each other: $\mathrm{L} \cdot \mathrm{M} - \mathrm{M} \cdot \mathrm{L} \neq 0$. As a consequence, we cannot diagonalize both matrices L and M simultaneously—i.e., with the aid of one and the same orthogonal matrix S. Therefore, it is impossible to diagonalize the Jacobi matrix $\mathrm{J}(t)$ in the equation $\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}$ for all time $t$. In other words, there is no such matrix S that completely splits the linearized system for the bush $\mathrm{B}[\hat{a}^2, \hat{i}]$ for the chain with $N=6$ particles.

This difference between the cases $N=4$ and $N=6$ (generally, for $N > 4$) can be explained as follows. The group $G = [\hat{a}^2, \hat{i}]$ of the considered bush, in fact, determines *different* groups for the cases $N=4$ and $N=6$. Indeed, for $N=4$ $[\hat{a}^2, \hat{i}] \equiv \{\hat{E}, \hat{a}^2, \hat{i}, \hat{a}^2\hat{i}\} = D_2$, while for $N=6$, $[\hat{a}^2, \hat{i}] \equiv \{\hat{E}, \hat{a}^2, \hat{a}^4, \hat{i}, \hat{a}^2\hat{i}, \hat{a}^4\hat{i}\} = D_3$. The latter group ($D_3$) is non-Abelian ($\hat{i}\hat{a}^4 = a^2\hat{i}$), unlike the group $D_2$ ($\hat{i}\hat{a}^2 = a^2\hat{i}$), and as a consequence, it possesses not only one-dimensional irreducible representations, but two-dimensional irreps, as well. It will be shown in Sec. IV that precisely this fact does not permit us to split fully the above-discussed linearized system.[4]

In spite of this difficulty, we can simplify the linearized system $\ddot{\boldsymbol{\delta}} = \mathrm{J}(t) \cdot \boldsymbol{\delta}$ considerably with the aid of some group-theoretical methods, which are discussed in the two following sections. Now, we only would like to present the final result of the above splitting for the case $N=6$:

$$\ddot{y}_1 = -4y_1, \tag{29a}$$

$$\ddot{y}_2 = 0, \tag{29b}$$

$$\begin{aligned} \ddot{y}_3 + 2y_3 &= P(t)y_5, \\ \ddot{y}_5 + 2y_5 &= \bar{P}(t)y_3, \end{aligned} \tag{29c}$$

$$\begin{aligned} \ddot{y}_4 + 2y_4 &= P(t)y_6, \\ \ddot{y}_6 + 2y_6 &= \bar{P}(t)y_4. \end{aligned} \tag{29d}$$

[4]Actually, this fact can be understood if one takes into account that the two-dimensional irrep contains two times in the decomposition of the mechanical representation of the considered chain.

Here $P(t)=e^{i\pi/3}-4A(t)[1+e^{-i\pi/3}]$, while $\bar{P}(t)$ is the complex conjugate function with respect to $P(t)$. The two-dimensional subsystems (29c) and (29d) can be reduced to the real form by a certain linear transformation.

Note that the stability of the $\pi$ mode (the bush $\mathrm{B}[\hat{a}^2,\hat{i}]$) was discussed in a number of papers [8–10,12–15,18–20] by different methods and with an emphasis on different aspects of this stability. In particular, in our paper [8], a remarkable fact was revealed for the FPU-$\alpha$ chain: the stability threshold of the $\pi$ mode is one and the same for interactions with *all* the other modes of the chain. (For other one-dimensional nonlinear modes, for both the FPU-$\alpha$ and FPU-$\beta$ chains, the stability thresholds, determined by interactions with different modes, are essentially different [9].)

## III. GENERAL THEOREM AND ITS CONSEQUENCES

### A. Theorem about symmetry groups of linearized systems

We consider an $N$-degrees-of-freedom mechanical system described by $N$ autonomous differential equations

$$\ddot{\boldsymbol{X}} = \boldsymbol{F}(\boldsymbol{X}), \tag{30}$$

where the configuration vector $\boldsymbol{X}=\{x_1(t),x_2(t),\ldots,x_N(t)\}$ determines the deviation from the equilibrium state $\boldsymbol{X}=\{0,0,\ldots,0\}$, while vector function $\boldsymbol{F}(\boldsymbol{X})=\{f_1(\boldsymbol{X}),f_2(\boldsymbol{X}),\ldots,f_N(\boldsymbol{X})\}$ determines the right-hand sides of the dynamical equations.

We assume that Eq. (30) is invariant under the action of a discrete symmetry group $G_0$ which we call the "parent symmetry group" of our mechanical system. This means that, for all $g\in G_0$ Eq. (30) is invariant under the transformation of variables

$$\tilde{\boldsymbol{X}} = \hat{g}\boldsymbol{X}, \tag{31}$$

where $\hat{g}$ is the operator associated with the symmetry element $g$ of the group $G_0$ by the conventional definition

$$\hat{g}\boldsymbol{X} = \{g^{-1}x_1(t),\ldots,g^{-1}x_N(t)\}.$$

Using Eqs. (30) and (31), one can write $\boldsymbol{X}=\hat{g}^{-1}\tilde{\boldsymbol{X}}$, $\hat{g}^{-1}\ddot{\tilde{\boldsymbol{X}}}=\boldsymbol{F}(\hat{g}^{-1}\tilde{\boldsymbol{X}})$, and finally

$$\ddot{\tilde{\boldsymbol{X}}} = \hat{g}\boldsymbol{F}(\hat{g}^{-1}\tilde{\boldsymbol{X}}). \tag{32}$$

On the other hand, renaming $\boldsymbol{X}$ from Eq. (30) as $\tilde{\boldsymbol{X}}$, one can write $\ddot{\tilde{\boldsymbol{X}}}=\boldsymbol{F}(\tilde{\boldsymbol{X}})$. Comparing this equation with Eq. (32), we obtain $\boldsymbol{F}(\tilde{\boldsymbol{X}})=\hat{g}\boldsymbol{F}(\hat{g}^{-1}\tilde{\boldsymbol{X}})$ or

$$\boldsymbol{F}(\hat{g}\boldsymbol{X}) = \hat{g}\boldsymbol{F}(\boldsymbol{X}). \tag{33}$$

This is the condition of invariance of the dynamical equations (30) under the action of the operator $\hat{g}$. It must hold for all $g\in G_0$ (obviously, it is sufficient to consider such equivalence only for the *generators* of the group $G_0$).

Let $\boldsymbol{X}(t)=\boldsymbol{C}(t)$ be an $m$-dimensional specific dynamical regime in the considered mechanical system that corresponds to the bush $\mathrm{B}[G]$ ($G\subseteq G_0$). This means that there exist some functional relations between the individual displacements $x_i(t)$ ($i=1,2,\ldots,N$), and, as a result, the system (30) reduces to $m$ ordinary differential equations in terms of the independent functions [we denoted them by $A(t)$, $B(t)$, $C(t)$, etc., in the previous section; see, for example, Eqs. (7) and (8)].

The vector $\boldsymbol{C}(t)$ is a general solution to the equation [see Eq. (17)]

$$\hat{G}\boldsymbol{X} = \boldsymbol{X},$$

where $G$ is the symmetry group of the given bush $\mathrm{B}[G]$ ($G\subseteq G_0$).

Now, we want to study the *stability* of the dynamical regime $\boldsymbol{C}(t)$, corresponding to the bush $\mathrm{B}[G]$. To this end, we must linearize the dynamical equations (30) in a vicinity of the given bush or more precisely, in a vicinity of the vector $\boldsymbol{C}(t)$. Let

$$\boldsymbol{X} = \boldsymbol{C}(t) + \boldsymbol{\delta}(t), \tag{34}$$

where $\boldsymbol{\delta}(t)=\{\delta_1(t),\ldots,\delta_N(t)\}$ is an infinitesimal $N$-dimensional vector. Substituting $\boldsymbol{X}(t)$ from Eq. (34) into Eq. (30) and linearizing these equations with respect to $\boldsymbol{\delta}(t)$, we obtain

$$\ddot{\boldsymbol{\delta}} = \mathrm{J}[\boldsymbol{C}(t)]\cdot\boldsymbol{\delta}, \tag{35}$$

where $\mathrm{J}[\boldsymbol{C}(t)]$ is the Jacobi matrix of the system (30):

$$\mathrm{J}[\boldsymbol{C}(t)] = \left\| \left.\frac{\partial f_i}{\partial x_j}\right|_{\boldsymbol{X}=\boldsymbol{C}(t)} \right\|.$$

Now, we intend to prove the following

*Theorem 1*. The matrix $\mathrm{J}[\boldsymbol{C}(t)]$ of the linearized dynamical equations near a given bush $B[G]$, determined by the configuration vector $\boldsymbol{C}(t)$, commutes with all matrices $\mathrm{M}(g)$ ($g\in G$) of the mechanical representation of the symmetry group $G$ of the considered bush:

$$\mathrm{M}(g)\cdot\mathrm{J}[\boldsymbol{C}(t)] = \mathrm{J}[\boldsymbol{C}(t)]\cdot\mathrm{M}(g).$$

*Proof*. As was already discussed in Sec. II, the original nonlinear system $\ddot{\boldsymbol{X}}=\boldsymbol{F}(\boldsymbol{X})$ transforms into the system $\ddot{\boldsymbol{X}}=\hat{g}^{-1}\boldsymbol{F}(\hat{g}\boldsymbol{X})$ under the action of the operator $\hat{g}$ associated with the symmetry element $g\in G_0$ of the parent group $G_0$. According to Eq. (33), the invariance of our system with respect to the operator $\hat{g}$ can be written as follows:

$$\hat{g}^{-1}\boldsymbol{F}(\hat{g}\boldsymbol{X}) = \boldsymbol{F}(\boldsymbol{X}). \tag{36}$$

On the other hand, the system $\ddot{\boldsymbol{X}}=\boldsymbol{F}(\boldsymbol{X})$, linearized in the vicinity of the vector $\boldsymbol{X}=\boldsymbol{C}(t)$, reads $\ddot{\boldsymbol{\delta}}=\mathrm{J}[\boldsymbol{C}(t)]\cdot\boldsymbol{\delta}$ [see Eq. (35)]. Under the action of the operator $\hat{g}$, it transforms, according to Eq. (28), into the system

$$\ddot{\boldsymbol{\delta}} = \hat{g}^{-1}\mathrm{J}[\hat{g}\boldsymbol{C}(t)]\cdot\hat{g}\boldsymbol{\delta}. \tag{37}$$

Let us now consider the mechanical representation $\Gamma$ of the parent symmetry group $G_0$. To this end, we chose the "natural" basis $\boldsymbol{\Phi}=\{\boldsymbol{e}_1,\boldsymbol{e}_2,\ldots,\boldsymbol{e}_N\}$ in the space of all possible displacements of individual particles (configuration space):

$$\boldsymbol{e}_1=\begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix},\quad \boldsymbol{e}_2=\begin{pmatrix}0\\1\\0\\\vdots\\0\end{pmatrix},\ldots,\boldsymbol{e}_N=\begin{pmatrix}0\\0\\0\\\vdots\\1\end{pmatrix}. \tag{38}$$

Acting by an operator $\hat{g}$ $(g\in G)$ on the vector $\boldsymbol{e}_j$, we can write

$$\hat{g}\boldsymbol{e}_j=\sum_{i=1}^{N}\mathrm{M}_{ij}(g)\cdot\boldsymbol{e}_i,\quad j=1,2,\ldots,N. \tag{39}$$

This equation associates the matrix $\mathrm{M}(g)\equiv\|\mathrm{M}_{ij}\|$ with the operator $\hat{g}$ and, therefore, with the symmetry element $g\in G$:

$$g\Rightarrow\hat{g}\Rightarrow\mathrm{M}(g). \tag{40}$$

The set of matrices $\mathrm{M}(g)$ corresponding to all $g\in G$ forms the *mechanical representation* $\Gamma$ for our system.[5] As a consequence of this definition, the equation

$$\hat{g}\boldsymbol{C}=\mathrm{M}(g)\cdot\boldsymbol{C} \tag{41}$$

is valid for any vector $\boldsymbol{C}$ determined in the basis (38) as $\boldsymbol{C}=\sum_{k=1}^{N}C_k\boldsymbol{e}_k$.

Using Eq. (41), we can rewrite Eq. (37) in terms of matrices $\mathrm{M}(g)\equiv\mathrm{M}_g$ $(g\in G_0)$ of the mechanical representation of the group $G_0$:

$$\ddot{\boldsymbol{\delta}}=\mathrm{M}_g^{-1}\cdot\mathrm{J}[\mathrm{M}_g\boldsymbol{C}(t)]\cdot\mathrm{M}_g\boldsymbol{\delta}. \tag{42}$$

Comparing this equation with Eq. (35), we conclude that the invariance of the system $\ddot{\boldsymbol{\delta}}=\mathrm{J}[\boldsymbol{C}(t)]\cdot\boldsymbol{\delta}$ with respect of the operator $\hat{g}$ (matrix $\mathrm{M}_g$) can be written as the relation

$$\mathrm{M}_g^{-1}\cdot\mathrm{J}[\mathrm{M}_g\boldsymbol{C}(t)]\cdot\mathrm{M}_g=\mathrm{J}[\boldsymbol{C}(t)]. \tag{43}$$

Now, let us suppose that $g$ is an element of the symmetry group $G$ of a given bush $\mathrm{B}[G]$ $(G\subseteq G_0)$. By the definition, all the elements of this group $(g\in G)$ leave invariant the vector $\boldsymbol{C}(t)$ that determines the displacement pattern of this bush:

$$\hat{g}\boldsymbol{C}(t)=\mathrm{M}_g\cdot\boldsymbol{C}(t)=\boldsymbol{C}(t),\quad g\in G. \tag{44}$$

Taking into account this equation, we obtain from Eq. (43) the relation

$$\mathrm{M}_g^{-1}\cdot\mathrm{J}[\boldsymbol{C}(t)]\cdot\mathrm{M}_g=\mathrm{J}[\boldsymbol{C}(t)], \tag{45}$$

which holds for each element $g$ of the symmetry group $G$ of the considered bush.

Rewriting Eq. (45) in the form

$$\mathrm{J}[\boldsymbol{C}(t)]\cdot\mathrm{M}_g=\mathrm{M}_g\cdot\mathrm{J}[\boldsymbol{C}(t)], \tag{46}$$

we arrive at the conclusion of our theorem: all the matrices $\mathrm{M}_g$ of the mechanical representation of the group $G$ *commute* with the Jacobi matrix $\mathrm{J}[\boldsymbol{C}(t)]$ of the linearized (near the given bush) dynamical equations $\ddot{\boldsymbol{\delta}}=\mathrm{J}[\boldsymbol{C}(t)]\cdot\boldsymbol{\delta}$. □

In what follows, we will introduce a simpler notation for the Jacobi matrix:

$$\mathrm{J}[\boldsymbol{C}(t)]\equiv\mathrm{J}(t). \tag{47}$$

*Remark*. We have proved that all the matrices $\mathrm{M}_g$ with $g\in G$ commute with the Jacobi matrix $\mathrm{J}(t)$ of the system (35). But if we take a symmetry element $g\in G_0$ that is not contained in $G$ $(g\in G_0\backslash G)$, the matrix $\mathrm{M}_g$ corresponding to $g$ *may not* commute with $\mathrm{J}(t)$. An example of such noncommutativity and the source of this phenomenon were presented in Sec. II C.

### B. Application of the Wigner theorem

Taking into account theorem 1, we can apply the well-known Wigner theorem (see, for example, [17]) to split the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ into a certain number of independent subsystems. We will formulate this theorem in a form convenient for our present purposes.

Let us have a reducible representation $\Gamma$ of the group $G$ which can be decomposed into a direct sum of the irreducible representations $\Gamma_j$ of this group:

$$\Gamma=\sum_j{}^{\oplus}m_j\Gamma_j. \tag{48}$$

Here $m_j$ is the number of times that $\Gamma_j$ enters into this decomposition. We denote the dimension of the irrep $\Gamma_j$ by $n_j$. Then the Wigner theorem asserts the following.

*Any matrix* H *commuting with all the matrices of a representation* $\Gamma$ *of the group G can be reduced to the block-diagonal form*

$$\mathrm{H}=\sum{}^{\oplus}\mathrm{D}_j \tag{49}$$

*such that* (1) *the dimension of the each block* $\mathrm{D}_j$ *is equal to* $m_j\cdot n_j$ *and* (2) *the block* $\mathrm{D}_j$ *consists of subblocks representing matrices proportional to the identity matrix* $\mathrm{I}_n$ *of dimension* $n_j$ *which are repeated* $m_j$ *times along the rows and columns of the block* $\mathrm{D}_j$.

We can illustrate the structure of a certain block $\mathrm{D}_j=\mathrm{D}$ characterized by the numbers $n_j=n$, $m_j=m$ as follows:

$$\mathrm{D}=\begin{pmatrix}\mu_{11}\mathrm{I}_n & \mu_{12}\mathrm{I}_n & \ldots & \mu_{1m}\mathrm{I}_n\\ \mu_{21}\mathrm{I}_n & \mu_{22}\mathrm{I}_n & \ldots & \mu_{2m}\mathrm{I}_n\\ \ldots & \ldots & \ldots & \ldots\\ \mu_{m1}\mathrm{I}_n & \mu_{m2}\mathrm{I}_n & \ldots & \mu_{mm}\mathrm{I}_n\end{pmatrix}, \tag{50}$$

Now, let us adapt the Wigner theorem for splitting the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ near the dynamical regime (a bush of modes) with symmetry group $G$. To this end, we assume for H and $\Gamma$, occurring in the Wigner theorem, that H is the Jacobi matrix $\mathrm{J}(t)$, while $\Gamma$ is the mechanical representation of the group $G$.

[5]According to the traditional definition of the $n$-dimensional matrix representation of the group $G$, a matrix $\mathrm{M}(g)$ is associated with the element $g\in G$, if $\hat{g}\boldsymbol{\Phi}=\widetilde{\mathrm{M}}(g)\boldsymbol{\Phi}$. Here $\boldsymbol{\Phi}=\{\phi_1(\boldsymbol{r}),\phi_2(\boldsymbol{r}),\ldots,\phi_N(\boldsymbol{r})\}$ is the set of basis vectors, $\hat{g}$ is the operator acting on the vectors as $\hat{g}\phi_i(\boldsymbol{r})=\phi_i(g^{-1}\boldsymbol{r})$, and $\widetilde{\mathrm{M}}(g)$ is the matrix transposed with respect to the matrix $\mathrm{M}(g)$.

To implement this splitting explicitly one must pass from the old basis $\mathbf{\Phi}_{old}=\{\boldsymbol{e}_1,\boldsymbol{e}_2,\ldots,\boldsymbol{e}_N,\}$ of the mechanical space to the new basis $\mathbf{\Phi}_{new}=\{\phi_1,\phi_2,\ldots,\phi_N,\}$ formed by the complete set of the basis vectors $\phi_k$ $(k=1,2,\ldots,N)$ of all the irreps of the group $G$. If $\mathbf{\Phi}_{new}=\mathrm{S}\cdot\mathbf{\Phi}_{old}$, then the unitary transformation[6]

$$\mathrm{J}_{new}(t)=\mathrm{S}^{\dagger}\cdot\mathrm{J}_{old}(t)\cdot\mathrm{S} \tag{51}$$

produces the above-discussed block-diagonal matrix $\mathrm{J}_{new}(t)$ of the linearized system $\ddot{\boldsymbol{\delta}}_{new}=\mathrm{J}_{new}(t)\cdot\boldsymbol{\delta}_{new}$ (here $\boldsymbol{\delta}_{old}=\mathrm{S}\cdot\boldsymbol{\delta}_{new}$).

In the next section, we will search the basis vectors $\phi_i[\Gamma_j]$ $(i=1,2,\ldots,n_j)$ of each irreducible representation $\Gamma_j$ in the form

$$\phi_i[\Gamma_j]=\{x_{ij}^{(1)},x_{ij}^{(2)},\ldots,x_{ij}^{(N)}\}, \tag{52}$$

where $x_{ij}^{(k)}$, $(k=1,2,\ldots,N)$ determines the displacement of the $k$th particle corresponding to the $i$th basis vector $\phi_i[\Gamma_j]$ of the $j$th irrep $\Gamma_j$. Actually, this means that we search $\phi_i[\Gamma_j]$ as a superposition of the old basis vectors $\boldsymbol{e}_k$ $(k=1,2,\ldots,N)$ of the mechanical space [see Eq. (38)]:

$$\phi_i[\Gamma_j]=\sum_{k=1}^{N}x_{ij}^{(k)}\cdot\boldsymbol{e}_k. \tag{53}$$

If we find all the basis vectors $\phi_i[\Gamma_j]$ in such a form, the coefficients $x_{ij}^{(k)}$ are obviously the elements of the matrix S that determines the transformation $\mathbf{\Phi}_{new}=\mathrm{S}\cdot\mathbf{\Phi}_{old}$ from the old basis $\mathbf{\Phi}_{old}=\{\boldsymbol{e}_k|k=1,2,\ldots,N\}$ to the new basis $\mathbf{\Phi}_{new}=\{\phi_i[\Gamma_j]|i=1,2,\ldots,n_j;j=1,2,\ldots\}$. Here $j=1,2,\ldots$ are indices of the irreducible representations that contribute to the reducible mechanical representation $\Gamma$.

Thus, finding all the basis vectors $\phi_i[\Gamma_j]$ of the irreps $\Gamma_j$ in the form (52) provides us directly with the matrix S that decomposes the Jacobi matrix $\mathrm{J}(t)$ of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$.

### C. Splitting schemes

The above-discussed implicit decomposition of the Jacobi matrix $\mathrm{J}(t)$ is a cumbersome procedure and, therefore, it is interesting to know beforehand to what extent this decomposition will be useful. This can be easily determined by means of the theory of *characters* of group representations. Let us consider such an approach in more detail.

We want to determine the *splitting scheme* of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$; namely, we want to find out how many subsystems of different dimensions one can obtain as a result of the decomposition of the Jacobi matrix.

Each block $\mathrm{D}_j$ from the decomposition (49) of the matrix $\mathrm{H}\equiv\mathrm{J}(t)$ generates an independent subsystem with $n_j\cdot m_j$ equations in the decomposition of the linearized system. However, each of these subsystems automatically splits into $n_j$ new subsystems consisting of $m_j$ differential equations, as a consequence of the specific structure of the block $\mathrm{D}_j$ [see Eq. (50)]. Indeed, for example, if a certain D block for the matrix $\mathrm{J}(t)$ possesses the form $(n_j=3,\ m_j=2)$

$$\mathrm{J}_j(t)=\begin{pmatrix}\mu_{11}\mathrm{I}_3 & \mu_{12}\mathrm{I}_3\\ \mu_{21}\mathrm{I}_3 & \mu_{22}\mathrm{I}_3\end{pmatrix},$$

it is easy to check that we obtain the following three independent pairs of the equations from the system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$:

$$\begin{cases}\ddot{\delta}_1=\mu_{11}\delta_1+\mu_{12}\delta_4,\\ \ddot{\delta}_4=\mu_{21}\delta_1+\mu_{22}\delta_4,\end{cases}\quad\begin{cases}\ddot{\delta}_2=\mu_{11}\delta_2+\mu_{12}\delta_5,\\ \ddot{\delta}_5=\mu_{21}\delta_2+\mu_{22}\delta_5,\end{cases}$$

$$\begin{cases}\ddot{\delta}_3=\mu_{11}\delta_3+\mu_{12}\delta_6,\\ \ddot{\delta}_6=\mu_{21}\delta_3+\mu_{22}\delta_6.\end{cases} \tag{54}$$

We see that the dimension of each subsystem (54) is equal to $m_j=2$, while the total number of these subsystems is equal to $n_j=3$. Moreover, these subsystems can be written in the form $\ddot{\boldsymbol{\delta}}=\mathrm{M}\cdot\boldsymbol{\delta}$ with one and the same matrix

$$\mathrm{M}=\begin{pmatrix}\mu_{11} & \mu_{12}\\ \mu_{21} & \mu_{22}\end{pmatrix}.$$

Thus, to obtain the splitting scheme of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$, for each irrep $\Gamma_j$ of the bush symmetry group $G$, we must find two numbers—$n_j$ (the dimension of $\Gamma_j$) and $m_j$ [the multiplicity number from Eq. (48)].

The multiplicity numbers $m_j$ can be found by means of the well-known formula from the theory of the group representations [17]:

$$m_j=\frac{1}{\|G\|}\sum_{g\in G}\chi_{\Gamma}(g)\bar{\chi}_j(g). \tag{55}$$

Here $\|G\|$ is the number of elements of the group $G$, $\chi_{\Gamma}(g)$ and $\chi_j(g)$ are the traces of the matrices associated with the group element $g\in G$ in the reducible representation $\Gamma$ (mechanical representation, in our case) and in the irreducible representation $\Gamma_j$, respectively [the bar over $\chi_j(g)$ denotes complex conjugation].

On the other hand, $\chi_j(g)$ can be obtained from the standard tables of characters of the irreducible representations for many groups of discrete symmetry (in particular, for all the point symmetry groups), while $\chi_{\Gamma}(g)$ can be obtained without the explicit construction of the matrices of the mechanical representation $\Gamma$.

The method for obtaining $\chi_{\Gamma}(g)$ is discussed in many textbooks (see, for example, [21]) in connection with studying the small vibrations of multiatomic molecules. The main point of the method is that, for a fixed $g\in G$, only those atoms whose positions do not change under the action of $g$ on the considered molecule contribute to $\chi_{\Gamma}(g)$. Moreover, this contribution is determined by the trace of the three-dimensional matrix associated with the symmetry element $g$. For example, the contribution to $\chi_{\Gamma}(g)$ from any atom invariant under the action of a rotation by an angle $\phi$ is $1+2\cos(\phi)$, while that for a mirror rotation is $-1+2\cos(\phi)$.

[6]Here $\mathrm{S}^{\dagger}$ is the Hermite conjugated matrix with respect to the matrix S.

The above method for finding the multiplicity numbers $m_j$ is very quick and simple. We apply it in Sec. V in connection with the simplification of the stability analysis of some nonlinear dynamical regimes in an octahedral molecule with symmetry group $G=O_h$.

## IV. STABILITY ANALYSIS OF DYNAMICAL REGIMES IN MONOATOMIC CHAINS

### A. Setting up the problem and theorem 2

In general, the study of the stability of periodic and, especially, quasiperiodic dynamical regimes in mechanical systems with many degrees of freedom presents considerable difficulties. Indeed, for this purpose, we must integrate a large linearized (near the considered regime) system of differential equations with time-dependent coefficients. In the case of the periodic regime, one can use the Floquet method requiring integration over only one time period to construct the monodromy matrix. But for the quasiperiodic regime this method is inapplicable, and one often needs to solve a system of a great number of differential equations for very large time intervals to reveal instability (especially, near the stability threshold).

In such a situation, a decomposition (splitting) of the full linearized system into a number of independent subsystems of small dimensions proves to be very useful. Moreover, this decomposition can provide valuable information on the generalized degrees of freedom responsible for the loss of stability of the given dynamical regime for the first time. Let us note that the number of such "critical" degrees of freedom can frequently be rather small.

We want to illustrate the above idea with the case of $N$-particle monoatomic chains for $N \gg 1$. Let us introduce the following notation. The bush $\mathrm{B}[G]$ with the symmetry group $G$ containing the translational subgroup $[\hat{a}^m]$ will be denoted by $\mathrm{B}[\hat{a}^m, \ldots]$, where the ellipsis stands for other generators of the group $G$. (Note that any $m$-dimensional bush can exist only for the chain with $N$ divisible by $m$.)

*Theorem 2*. Linear stability analysis of any bush $B[\hat{a}^m, \ldots]$ in the $N$-degrees-of-freedom monoatomic chain can be reduced to stability analysis of isolated subsystems of the second-order differential equations with time-dependent coefficients whose dimensions do not exceed the integer number $m$.

*Corollary*. If the bush dimension is $d$, one can pass on to subsystems of *autonomous* differential equations with dimensions not exceeding $(m+d)$.

Before proving these propositions we must consider the procedure of constructing the basis vectors of the irreducible representations of the translational group $T$.

### B. Basis vectors of irreducible representations of the translational groups

The basis vectors of irreducible representations of different symmetry groups are usually obtained by the method of projection operators [17], but in our case, it is easier to make use of the "direct" method based on the definition of the group representation.[7]

Let $\Gamma$ be an $n$-dimensional representation (reducible or irreducible) of the group $G$, while $V[\Gamma]$ be the invariant subspace corresponding to the representation determined by the set $\mathbf{\Phi}$ of $N$-dimensional basis vectors $\phi_j$ $(j=1,\ldots,n)$:

$$\mathbf{\Phi} = \{\phi_1, \phi_2, \ldots, \phi_n\}. \tag{56}$$

Acting on any basis vector $\phi_j$ by an operator $\hat{g}$ $(g \in G)$ and bearing in mind the invariance of the subspace $V[\Gamma]$, we can represent the vector $\hat{g}\phi_j$ as a superposition of all basis vectors from Eq. (56). In other words,

$$\hat{g}\mathbf{\Phi} \equiv \{\hat{g}\phi_1, \hat{g}\phi_2, \ldots, \hat{g}\phi_n\} = \widetilde{\mathrm{M}}(g)\mathbf{\Phi}, \tag{57}$$

where $\mathrm{M}(g)$ is the matrix corresponding, in the representation $\Gamma$, to the element $g$ of the group $G$. [In Eq. (57), we use a tilde as the symbol of matrix transposition.] Equation (57) associates with any $g \in G$ a certain $n \times n$ matrix $\mathrm{M}(g)$ and encapsulates the definition of matrix representation

$$\Gamma = \{\mathrm{M}(g_1), \mathrm{M}(g_2), \ldots\}. \tag{58}$$

The above-mentioned "direct" method is based precisely on this definition. Let us use it to obtain the basis vectors of the irreducible representations for the translational group $T \equiv [\hat{a}^m]$. We will construct these vectors in the configuration space of the $N$-particle monoatomic chain and, therefore, each vector $\phi_j$ can be written as follows:

$$\phi_j = \{x_1, x_2, \ldots, x_N\}, \tag{59}$$

where $x_i$ is a displacement of the $i$th particle from its equilibrium.

The group $T \equiv [\hat{a}^m]$ represents a *translational subgroup* corresponding to the bush $\mathrm{B}[G] = \mathrm{B}[\hat{a}^m, \ldots]$. For an $N$-particle chain,[8] $T \equiv [\hat{a}^m]$ is a subgroup of the order $k=N/m$ of the full translational group $T_N \equiv [\hat{a}]$, and we can write the complete set of its elements as follows:

$$T_k = \{\hat{e}, \hat{a}^m, \hat{a}^{2m}, \hat{a}^{3m}, \ldots, \hat{a}^{(k-1)m}\} \quad (\hat{a}^{km} = \hat{a}^N = \hat{e}). \tag{60}$$

Being cyclic, the group $T_k$ from Eq. (60) possesses only one-dimensional irreps and their total number is equal to the order $(k=N/m)$ of this group.

Below, for simplicity, we consider the case $m=3$ and $N=12$. The generalization to the case of arbitrary values of $m$ and $N$ turns out to be trivial.

As is well known, the one-dimensional irreps $\Gamma_i$ of the $k$th order cyclic group can be constructed with the aid of the $k$th degree roots of 1 and, therefore, for our case $N=12$, $m=3$, $k=4$, we obtain the irreducible representations listed in Table I.

In accordance with the definition (57), the basis vector $\phi$ of the one-dimensional irrep $\Gamma$, for which $\mathrm{M}(g)=\gamma$, must satisfy the equation

[7] We already use this method in our previous papers (see, for example, [8]).

[8] Note that the relation $N \bmod m = 0$ must hold.

TABLE I. Irreducible representations of the cyclic group $T_4$.

| | $\hat{e}$ | $\hat{g}$ | $\hat{g}^2$ | $\hat{g}^3$ |
|---|---|---|---|---|
| $\Gamma_1$ | 1 | 1 | 1 | 1 |
| $\Gamma_2$ | 1 | $i$ | $-1$ | $-i$ |
| $\Gamma_3$ | 1 | $-1$ | 1 | $-1$ |
| $\Gamma_4$ | 1 | $-i$ | $-1$ | $i$ |

$$\hat{g}\phi = \gamma\phi. \tag{61}$$

In our case, $\hat{g}=\hat{a}^3$, this equation can be written as follows:

$$\hat{g}\phi \equiv \{x_{10},x_{11},x_{12}|x_1,x_2,x_3|x_4,x_5,x_6|x_7,x_8,x_9\} = \gamma\{x_1,x_2,x_3|x_4,x_5,x_6|x_7,x_8,x_9|x_{10},x_{11},x_{12}\}. \tag{62}$$

Here $\gamma=1$, $i$, $-1$, and $-i$ for the irreps $\Gamma_1$, $\Gamma_2$, $\Gamma_3$, and $\Gamma_4$, respectively. Equating the sequential components of both sides of Eq. (62), we obtain the *general solution* to the equation $\hat{g}\phi=\gamma\phi$, which turns out to depend on three arbitrary constants—say, $x$, $y$, and $z$:

$$\begin{aligned}\phi &= \{x,y,z|\gamma^{-1}x,\gamma^{-1}y,\gamma^{-1}z|\gamma^{-2}x,\gamma^{-2}y,\gamma^{-2}z|\gamma^{-3}x,\gamma^{-3}y,\gamma^{-3}z\}\\ &= x\{1,0,0|\gamma^{-1},0,0|\gamma^{-2},0,0|\gamma^{-3},0,0\}\\ &\quad + y\{0,1,0|0,\gamma^{-1},0|0,\gamma^{-2},0|0,\gamma^{-3},0\}\\ &\quad + z\{0,0,1|0,0,\gamma^{-1}|0,0,\gamma^{-2}|0,0,\gamma^{-3}\}.\end{aligned} \tag{63}$$

Here we write the vector $\phi$ as the superposition (with coefficients $x$, $y$, $z$) of *three basis vectors*. It means that the irrep $\Gamma$ is contained *thrice* in the decomposition of the mechanical representation into irreducible representations of the group $G=[\hat{a}^3]$.

This result can be generalized to the case of arbitrary $N$ and $m$ in a trivial manner: each irrep of the group $G=[\hat{a}^m]$ enters *exactly m times* into the decomposition of the mechanical representation for an $N$-particle chain, and the rule for constructing $m$ appropriate basis vectors is fully obvious from Eq. (63).

### C. Decomposition of the Jacobi matrix

The basis vectors of all irreps $\Gamma_i$, listed for the case $N=12$, $m=3$ in Table I, can be obtained from Eq. (63) setting $\gamma=1$, $i$, $-1$, $-i$, respectively [these values are one-dimensional matrices corresponding in $\Gamma_i$ $(i=1,2,3,4)$ to the generator $\hat{g}\equiv\hat{a}^3$].

Let us write the above basis vectors sequentially, as it is done in Table II. The $12\times12$ matrix, determined by this table, is precisely the matrix S that splits the linearized dynamical equations $\ddot{\delta}=\mathrm{J}(t)\cdot\delta$ for the considered case. In Table II, we denote the basis vectors $\phi_j(\Gamma_i)$ by the symbol of the irrep $\Gamma_i$ $(i=1,2,3,4)$ and the number $j=1,2,3$ of the basis vector of this irrep. The normalization factor $\left(\frac{1}{2}\right)$ must be associated with each row of this table to produce the normalized basis vectors [because of this fact, we mark the rows as $2\phi_j(\Gamma_i)$ in the last column of Table II].

Obviously, we can use the matrix S from Table II (the rows of this matrix are the basis vectors of all the irreps of the group $T_4$) not only for the action on the vectors in the $\boldsymbol{X}$ space of the full nonlinear system, but on the vectors in the $\delta$ space of the linearized system $\ddot{\delta}=\mathrm{J}(t)\cdot\delta$, as well. It is essential that in the latter case the matrix S reduce the Jacobi matrix $\mathrm{J}(t)$ to a certain block-diagonal form. Indeed, as was shown in theorem 1, the matrix $\mathrm{J}(t)$ commutes with all the matrices of the mechanical representation of the bush symmetry group. Therefore, according to the Wigner theorem, it can be reduced, using unitary transformation by the matrix S, to the block-diagonal form with blocks whose dimension is equal to $n_j\cdot m_j$. Here $n_j$ is the dimension of the irrep $\Gamma_j$, while $m_j$ is the number of times that this irrep enters into the decomposition of the mechanical representation (constructed, in our case, in the $\delta$ space).

TABLE II. Basis vectors of the irreducible representations of the cyclic group $T_4$.

| $\delta_1$ $x_1$ | $\delta_2$ $x_2$ | $\delta_3$ $x_3$ | $\delta_4$ $x_4$ | $\delta_5$ $x_5$ | $\delta_6$ $x_6$ | $\delta_7$ $x_7$ | $\delta_8$ $x_8$ | $\delta_9$ $x_9$ | $\delta_{10}$ $x_{10}$ | $\delta_{11}$ $x_{11}$ | $\delta_{12}$ $x_{12}$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | $2\phi_1(\Gamma_1)$ |
| 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | $2\phi_2(\Gamma_1)$ |
| 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 1 | $2\phi_3(\Gamma_1)$ |
| 1 | 0 | 0 | $-i$ | 0 | 0 | $-1$ | 0 | 0 | $i$ | 0 | 0 | $2\phi_1(\Gamma_2)$ |
| 0 | 1 | 0 | 0 | $-i$ | 0 | 0 | $-1$ | 0 | 0 | $i$ | 0 | $2\phi_2(\Gamma_2)$ |
| 0 | 0 | 1 | 0 | 0 | $-i$ | 0 | 0 | $-1$ | 0 | 0 | $i$ | $2\phi_3(\Gamma_2)$ |
| 1 | 0 | 0 | $-1$ | 0 | 0 | 1 | 0 | 0 | $-1$ | 0 | 0 | $2\phi_1(\Gamma_3)$ |
| 0 | 1 | 0 | 0 | $-1$ | 0 | 0 | 1 | 0 | 0 | $-1$ | 0 | $2\phi_2(\Gamma_3)$ |
| 0 | 0 | 1 | 0 | 0 | $-1$ | 0 | 0 | 1 | 0 | 0 | $-1$ | $2\phi_3(\Gamma_3)$ |
| 1 | 0 | 0 | $i$ | 0 | 0 | $-1$ | 0 | 0 | $-i$ | 0 | 0 | $2\phi_1(\Gamma_4)$ |
| 0 | 1 | 0 | 0 | $i$ | 0 | 0 | $-1$ | 0 | 0 | $-i$ | 0 | $2\phi_2(\Gamma_4)$ |
| 0 | 0 | 1 | 0 | 0 | $i$ | 0 | 0 | $-1$ | 0 | 0 | $-i$ | $2\phi_3(\Gamma_4)$ |

### D. Proof of theorem 2

In Sec. IV B, we have shown that for the translational group $T=[\hat{a}^m]$ all $n_j=1$ and all $m_j=m$. Therefore, the matrix S, constructed according to the prescription of Sec. IV C, decomposes the Jacobi matrix $\mathrm{J}(t)$ into blocks whose dimension is equal to $m$. As a consequence of this decomposition, the system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ splits into $k=N/m$ independent subsystems $L_j$ $(j=1,2,\ldots,k)$, each consisting of $m$ differential equations of the second order. The coefficients of these equations are time-dependent functions, and this time dependence is determined by the functions $A(t)$, $B(t)$, $C(t)$, etc., entering into the bush displacement pattern [see, for example, Eqs. (7) and (8)]. For the one-dimensional bushes, the coefficients of the above subsystems $L_j$ turn out to be periodic functions with identical period, while for the many-dimensional bushes they possess different periods (such bushes describe quasiperiodic motion).

In general, it is impossible to obtain the explicit form of the functions $A(t)$, $B(t)$, $C(t)$, etc., determining the bush displacement pattern. Therefore, we can add the bush dynamical equations to the $m$ differential equations of each subsystems $L_j$. These additional $d$ equations determine the functions $A(t)$, $B(t)$, $C(t)$, etc., *implicitly*, where $d$ is the dimension of the considered bush $\mathrm{B}[\hat{a}^m,\ldots]$.

On the other hand, we can give the following estimate for the bush dimension $d$:

$$d \leq m. \tag{64}$$

Here $m$ is the index of the translational symmetry of the bush $\mathrm{B}[\hat{a}^m,\ldots]$ (it determines the ratio between the size of the primitive cell in the vibrational state and in the equilibrium). Indeed, the bush displacement pattern can be found as the solution to the equation $\hat{G}\boldsymbol{X}=\boldsymbol{X}$. If we take into account only translational symmetry group of the bush $\mathrm{B}[\hat{a}^m,\ldots]$—i.e., $G=[\hat{a}^m]$—this equation reduces to the equation $\hat{g}\phi=\phi$ $(\hat{g}=\hat{a}^m)$ for the basis vector $\phi$ of the *identity* irrep [$\gamma=1$ in Eq. (61)] of the group $T=[\hat{a}^m]$. As it has been already shown in Sec. IV B, such a vector $\phi$ depends on exactly $m$ arbitrary parameters. But some additional symmetry elements, denoted by the ellipsis in the bush symbol $\mathrm{B}[\hat{a}^m,\ldots]$, can lead to a decrease in the number $m$ of the above parameters.[9] As a consequence, for all cases, $d\leq m$, and we can state that $m$ equations of each $L_j$, extended by $d$ additional equations of the given bush, provide us with $k=N/m$ independent subsystems $\tilde{L}_j$ of $m+d$ *autonomous* differential equations. Thus, the linear stability analysis of the bush $\mathrm{B}[\hat{a}^m,\ldots]$ in the $N$-particle chain indeed reduces to studying the stability of individual subsystems whose dimension does not exceed $m+d$. We have arrived at the conclusion of theorem 2 and its corollary. The proof is completed.

The authors of Ref. [22], studying the synchronization of the chaotic oscillators in chains with shift-invariant symmetry and using for this purpose the discrete Fourier transformation method, arrived at a conclusion equivalent to the statement of our theorem 2. We would like to note that this theorem is only a part of the general group-theoretical approach developed in the present paper. In the framework of this approach, we can easily take into account any additional symmetries of a considered dynamical system. In particular, below we study the stability problem for chains with inversion and/or with even potential (see also [8,9]) and for the molecule with octahedral symmetry. Moreover, the authors of [22] discussed only the stability of the *synchronization manifold* which corresponds, in our terminology, to the trivial bush $\{A(t), A(t),\ldots,A(t)\}$, while our approach has been used, in particular, for *all* possible one-dimensional bushes in the FPU chains [9].

### E. Example 1: Splitting the linearized system for the bush $\mathrm{B}[\hat{a}^3]$

We consider the splitting of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for the bush $\mathrm{B}[\hat{a}^3]$ in a chain with $N=12$ particles. The original nonlinear system, for this case, reads

$$\ddot{x}_i = f(x_{i+1}-x_i) - f(x_i - x_{i-1}),$$
$$i=1,2,\ldots,12 \quad (x_0=x_{12},\ x_{13}=x_1). \tag{65}$$

The displacement pattern of the bush $\mathrm{B}[\hat{a}^3]$, obtained from the equation $\hat{a}^3\,\boldsymbol{X}=\boldsymbol{X}$, reads

$$\boldsymbol{X}=\{x(t),y(t),z(t)|x(t),y(t),z(t)|x(t),y(t),z(t)|x(t),y(t),z(t)\}. \tag{66}$$

Substituting this form of vibrational pattern into (65), we obtain three differential equations for the functions $x(t)$, $y(t)$, and $z(t)$ [all the other equations of (65) turn out to be equivalent to these equations]:

$$\ddot{x}=f(y-x)-f(x-z),$$
$$\ddot{y}=f(z-y)-f(y-x),$$
$$\ddot{z}=f(x-z)-f(z-y). \tag{67}$$

The linearization of Eqs. (65) near the dynamical regime determined by Eq. (66) leads to the system

$$\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}, \tag{68}$$

with the following Jacobi matrix:

$$\mathrm{J}(t)=\begin{pmatrix}
\alpha & A & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & B\\
A & \beta & C & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & C & \gamma & B & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & B & \alpha & A & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & A & \beta & C & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & C & \gamma & B & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & B & \alpha & A & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & A & \beta & C & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & C & \gamma & B & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & B & \alpha & A & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A & \beta & C\\
B & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C & \gamma
\end{pmatrix}, \tag{69}$$

where

$$A(t)=f'[y(t)-x(t)],$$
$$B(t)=f'[x(t)-z(t)],$$
$$C(t)=f'[z(t)-y(t)],$$
$$\alpha(t)=-[A(t)+B(t)],$$
$$\beta(t)=-[A(t)+C(t)],$$
$$\gamma(t)=-[B(t)+C(t)]. \tag{70}$$

Using Table II, the matrix S that splits up the system (68) can be written as follows:

[9]Moreover, these additional symmetry elements lead not only to reducing the bush dimension, but to a further splitting of the above discussed subsystems $L_j$.

$$\mathrm{S} = \frac{1}{2}\begin{pmatrix} \mathrm{I} & \mathrm{I} & \mathrm{I} & \mathrm{I} \\ \mathrm{I} & -i\mathrm{I} & -\mathrm{I} & i\mathrm{I} \\ \mathrm{I} & -\mathrm{I} & \mathrm{I} & -\mathrm{I} \\ \mathrm{I} & i\mathrm{I} & -\mathrm{I} & -i\mathrm{I} \end{pmatrix}, \tag{71}$$

where I is the $3\times 3$ identity matrix.

With the aid of the unitary transformation

$$\mathrm{J}_{new}(t) = \mathrm{S}^{\dagger}\cdot \mathrm{J}(t)\cdot \mathrm{S}, \tag{72}$$

we obtain

$$\mathrm{J}_{new}(t) = \begin{pmatrix} \mathrm{D}_1 & 0 & 0 & 0 \\ 0 & \mathrm{D}_2 & 0 & 0 \\ 0 & 0 & \mathrm{D}_3 & 0 \\ 0 & 0 & 0 & \mathrm{D}_4 \end{pmatrix}, \tag{73}$$

where

$$\mathrm{D}_k = \begin{pmatrix} -(A+B) & A & \gamma_k B \\ A & -(A+C) & C \\ \bar{\gamma}_k B & C & -(B+C) \end{pmatrix} \quad (k=1,2,3,4), \tag{74}$$

with $\gamma_1=1$, $\gamma_2=i$, $\gamma_3=-1$, and $\gamma_4=-i$ ($\bar{\gamma}_k$ is the complex conjugate value of $\gamma_k$).

This means that the linear transformation

$$\boldsymbol{\delta} = \mathrm{S}\cdot \boldsymbol{\delta}_{new} \tag{75}$$

reduces the old equations (68) to the following form:

$$\ddot{\boldsymbol{\delta}}_{new} = \mathrm{J}_{new}(t)\cdot \boldsymbol{\delta}_{new}, \tag{76}$$

with the block-diagonal matrix $\mathrm{J}_{new}(t)=\mathrm{S}^{\dagger}\cdot\mathrm{J}(t)\cdot\mathrm{S}$ determined by Eqs. (73) and (74).

Assuming

$$\boldsymbol{\delta}_{new} = \{\delta_1^{(1)},\delta_2^{(1)},\delta_3^{(1)}|\delta_1^{(2)},\delta_2^{(2)},\delta_3^{(2)}|\delta_1^{(3)},\delta_2^{(3)},\delta_3^{(3)}|\delta_1^{(4)},\delta_2^{(4)},\delta_3^{(4)}\},$$

we can present Eq. (76) in a more explicit form

$$\ddot{\delta}_1^{(k)} = -(A+B)\delta_1^{(k)} + A\delta_2^{(k)} + \gamma_k B\delta_3^{(k)},$$

$$\ddot{\delta}_2^{(k)} = A\delta_1^{(k)} - (A+C)\delta_2^{(k)} + C\delta_3^{(k)},$$

$$\ddot{\delta}_3^{(k)} = \bar{\gamma}_k B\delta_1^{(k)} + C\delta_2^{(k)} - (B+C)\delta_3^{(k)}, \tag{77}$$

where $\gamma_k=1,i,-1,-i$ for $k=1,2,3,4$, respectively.

Thus, we obtain four independent $3\times 3$ systems of linear differential equations with time-dependent coefficients $A(t)$, $B(t)$, and $C(t)$, which are determined by Eqs. (70).

Let us write down these equations for the FPU-$\alpha$ chain. For this case, the function $f(x)$ in Eq. (65) reads $f(x)=x+x^2$. Therefore, $f'(x)=1+2x$, and we obtain, from Eqs. (70),

$$A(t) = 1 + 2[y(t) - x(t)],$$

$$B(t) = 1 + 2[x(t) - z(t)],$$

$$C(t) = 1 + 2[z(t) - y(t)].$$

Substituting these functions into Eqs. (77) one can finally obtain the following equations for the FPU-$\alpha$ chain:

$$\ddot{\boldsymbol{\delta}}^{(k)} = \mathrm{J}_k(t)\cdot \boldsymbol{\delta}^{(k)},$$

where

$$\mathrm{J}_k(t) = \begin{pmatrix} -2(1+y-z) & 1+2(y-x) & \gamma_k[1+2(x-z)] \\ 1+2(y-x) & -2(1+z-x) & 1+2(z-y) \\ \bar{\gamma}_k[1+2(x-z)] & 1+2(z-y) & -2(1+x-y) \end{pmatrix}$$

$$(k=1,2,3,4). \tag{78}$$

Here $\gamma_1=1$, $\gamma_2=i$, $\gamma_3=-1$, and $\gamma_4=-i$ and $x\equiv x(t)$, $y\equiv y(t)$, and $z\equiv z(t)$ are functions determined by the dynamical equations of the bush $\mathrm{B}[\hat{a}^3]$:

$$\ddot{x} = (y-2x+z)(1+y-z),$$

$$\ddot{y} = (z-2y+x)(1+z-x),$$

$$\ddot{z} = (x-2z+y)(1+x-y). \tag{79}$$

These equations can be obtained from Eqs. (67) taking into account the relation $f(x)=x+x^2$ for the case of the FPU-$\alpha$ model.

*Remark*. According to Eqs. (66) and (67) [see also Eqs. (79)], the vibrational bush $\mathrm{B}[\hat{a}^3]$ is three dimensional. However, it actually turns out to be a *two-dimensional* bush. Indeed, there is no *on-site* potential in the FPU-$\alpha$ chains and, therefore, the conservation law of the total momentum of such system holds. Assuming that the center of mass is fixed, we obtain an additional relation $x(t)+y(t)+z(t)=0$ which reduces the dimension of the bush $\mathrm{B}[\hat{a}^3]$ from 3 to 2.

### F. Further decomposition of linearized systems based on higher-symmetry groups

Up to this point, we have discussed the decomposition of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ using only the *translational* part of the bush symmetry group. In general, one can arrive at a more detailed splitting, if one takes into account the additional bush symmetries.

#### *1. Example 2: Splitting of the linearized system for the bush* $\mathrm{B}[\hat{a}^3,\hat{i}]$

Let us consider the decomposition of the linearized system for the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ in the case of an arbitrary monoatomic chain. Since the translational part of the symmetry group $G=[\hat{a}^3,\hat{i}]$, which turns out to be the dihedral group, is the same as that of the early considered bush $\mathrm{B}[\hat{a}^3]$, we can take advantage of all the results obtained in Sec. IV E and add only some restrictions originating from the presence of the additional generator $\hat{i}$ of the group $[\hat{a}^3,\hat{i}]$.

Substituting the vector $\boldsymbol{X}(t)$ in the form (66) into the equation $\hat{i}\boldsymbol{X}(t)=\boldsymbol{X}(t)$, we obtain $z(t)\equiv -x(t)$, $y(t)\equiv -y(t)$ and, therefore, $y(t)\equiv 0$. The displacement pattern for the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ then can be written as follows:

$$\boldsymbol{X}(t)=\{x(t),0,-x(t)|x(t),0,-x(t)|x(t),0,-x(t)|x(t),0,-x(t)\}. \tag{80}$$

Thus, the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ turns out to be *one dimensional*.

As a result of the substitution $z(t)\equiv -x(t)$, $y(t)\equiv 0$, the three equations (67) reduce to only one equation

$$\ddot{x}=f(-x)-f(2x). \tag{81}$$

For the FPU-$\alpha$ chain [see Eqs. (79)], this equation transforms to

$$\ddot{x}+3x+3x^2=0. \tag{82}$$

Unlike the purely translational group $[\hat{a}^3]$, of the three-dimensional bush $\mathrm{B}[\hat{a}^3]$, the symmetry group $[\hat{a}^3,\hat{i}]$ of the one-dimensional bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ is the dihedral group with another set of the irreps and basis vectors. It can be shown (see the next section) that taking into account that $[\hat{a}^3,\hat{i}]$ is the supergroup with respect to group $[\hat{a}^3]$ allows one to obtain the following splitting scheme of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$:

$$1{:}(\delta_1);\quad 1{:}(\delta_6);\quad 2{:}(\delta_2,\delta_3);$$

$$2{:}(\delta_4,\delta_5);\quad 3{:}(\delta_7,\delta_9,\delta_{11});\quad 3{:}(\delta_8,\delta_{10},\delta_{12}). \tag{83}$$

Here we present the dimension of each independent subsystem (before the colon) and the list of its variables (after the colon). From the scheme (83), one can see that two of four three-dimensional subsystems corresponding to the splitting provided by group $[\hat{a}^3]$ [see Eqs. (77)], in the case of the supergroup $[\hat{a}^3,\hat{i}]$, are decomposed into new independent subsystems of dimensions equal to 1 and 2. In concise notation, the splitting scheme (83) can be written as follows:

$$2(1),\quad 2(2),\quad 2(3). \tag{84}$$

Each term of this sequence is of the form $b_j(d_j)$ where $b_j$ is the number of independent subsystems whose dimension is equal to $d_j$.

#### *2. Irreducible representations and their basis vectors for the dihedral group*

Hereafter, for simplicity, we will discuss only chains with an *even* number ($N$) of particles and illustrate the main ideas with the example $N=12$.

The symmetry of an $N$-particle (monoatomic) chain is completely described by the *dihedral* group $G_0=D_N$ which can be written as the union of two cosets with respect to its translational subgroup $T_N=\{\hat{e},\hat{a},\hat{a}^2,\ldots,\hat{a}^{N-1}\}$:

$$D_N=T_N\oplus T_N\cdot\hat{i}. \tag{85}$$

Here $\hat{i}$ is the inversion relative to the center of the chain. The group $D_N$ is a non-Abelian group, since some of its elements do not commute with each other (for example, $\hat{i}\hat{a}=\hat{a}^{-1}\hat{i}$). 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 $\Gamma_j$ are not one dimensional. The irreps of the dihedral group $D_N$ can be obtained by the well-known induction procedure from those of its subgroup $T_N$. It turns out that for $D_N$ with *even N* there are four one-dimensional irreps, while all the other $(N/2-1)$ irreps are two dimensional. We discussed the construction of these irreps in [8], where the following results were obtained.

Every irrep can be determined by two matrices $\mathrm{M}_j(\hat{a})$ and $\mathrm{M}_j(\hat{i})$ corresponding to its generators $\hat{a}$ and $\hat{i}$, where $j$ is the number of this irrep. Four one-dimensional irreps $(j=1,2,3,4)$ are real and are determined by the matrices[10]

$$\mathrm{M}_j(\hat{a})=\pm 1,\quad \mathrm{M}_j(\hat{i})=\pm 1. \tag{86}$$

All other irreps are two dimensional and are determined by the matrices

$$\mathrm{M}_j(\hat{a})=\begin{pmatrix}\mu_j & 0\\ 0 & \bar{\mu}_j\end{pmatrix},\quad \mathrm{M}_j(\hat{i})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$$

with $\mu_j=e^{2\pi ij/N}$ and $\bar{\mu}_j=e^{-2\pi ij/N}$ $(j\neq 0,\ N/2)$.[11]

Let us find the basis vectors of the irreducible representations of the dihedral group $[\hat{a}^m,\hat{i}]$ for the case $m=3$ which corresponds to the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$. Let $\phi$ and $\psi$ be the basis vectors of the two-dimensional invariant subspace corresponding to the irrep with the matrix

$$\mathrm{M}(\hat{g})=\begin{pmatrix}\gamma & 0\\ 0 & \bar{\gamma}\end{pmatrix},$$

where $\hat{g}=\hat{a}^m$ is the translational generator of the dihedral group. They can be obtained from the equations $\hat{g}\phi=\gamma\phi$ and $\hat{g}\psi=\bar{\gamma}\psi$, respectively. For example, using Eq. (63) for the case $m=3$, we find $\phi=\{x,y,z|\gamma^{-1}x,\gamma^{-1}y,\gamma^{-1}z|\gamma^{-2}x,\gamma^{-2}y,\gamma^{-2}z|\ldots\}$ and $\psi=\{\tilde{x},\tilde{y},\tilde{z}|\bar{\gamma}^{-1}\tilde{x},\bar{\gamma}^{-1}\tilde{y},\bar{\gamma}^{-1}\tilde{z}|\bar{\gamma}^{-2}\tilde{x},\bar{\gamma}^{-2}\tilde{y},\bar{\gamma}^{-2}\tilde{z}|\ldots\}$. Here $(x,y,z)$ and $(\tilde{x},\tilde{y},\tilde{z})$ are arbitrary constants which these vectors depend on.

Taking into account the presence of the matrix

$$\mathrm{M}(\hat{i})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

in every two-dimensional irrep, one can state that

$$\hat{i}\phi=\psi,\quad \hat{i}\psi=\phi. \tag{87}$$

Because of these relations, there appear certain connections between the arbitrary constants $(x,y,z)$ and $(\tilde{x},\tilde{y},\tilde{z})$. As a consequence, the basis vectors $\phi$ and $\psi$, for each two-dimensional irrep of the group $[\hat{a}^3,\hat{i}]$, depend on only three arbitrary parameters $x$, $y$, and $z$. In turn, this means that each two-dimensional irrep enters exactly 3 times into the decomposition of the mechanical representation of the dihedral group $[\hat{a}^3,\hat{i}]$.

[10]All combinations of signs are allowed in Eqs. (86).

[11]For the values $j=0$ and $j=N/2$, two-dimensional representations turn out to be reducible and they decompose into two pairs of one-dimensional irreps listed in Eqs. (86).

Unlike this, the one-dimensional irreps of the dihedral group $[\hat{a}^3,\hat{i}]$ are contained in the mechanical representation less than 3 times. Indeed, let us consider the basis vectors $\phi$ and $\psi$ of the one-dimensional irreps of the group $[\hat{a}^3]$ determined by the matrices $\mathrm{M}(a^3)=1$ and $\mathrm{M}(a^3)=-1$, respectively, for the case $m=3$, $N=12$:

$$\phi=\{x,y,z|x,y,z|x,y,z|x,y,z\},$$

$$\psi=\{x,y,z|-x,-y,-z|x,y,z|-x,-y,-z\}.$$

These vectors can be obtained from Eq. (63) by letting $\gamma=1$ and $\gamma=-1$. If the vector $\phi$ is not only the basis vector of the irrep of the group $[\hat{a}^3]$, but also is the basis vector of a certain one-dimensional irrep of the dihedral group $[\hat{a}^3,\hat{i}]$, it must satisfy the equations $\hat{i}\phi=\phi$, for the irrep $\Gamma_1$ $(\mathrm{M}(\hat{i})=1)$ and $\hat{i}\phi=-\phi$, for the irrep $\Gamma_2$ $(\mathrm{M}(\hat{i})=-1)$. We obtain $z=-x$, $y=0$ from the former equation and $z=x$ from the latter equation. Thus

$$\phi[\Gamma_1]=\{x,0,-x|x,0,-x|x,0,-x|x,0,-x\},$$

$$\phi[\Gamma_2]=\{x,y,x|x,y,x|x,y,x|x,y,x\}.$$

In the same manner, we obtain the basis vectors $\psi[\Gamma_3]$ and $\psi[\Gamma_4]$ from the equations $\hat{i}\psi=\psi$ and $\hat{i}\psi=-\psi$, respectively:

$$\psi[\Gamma_3]=\{x,y,x|-x,-y,-x|x,y,x|-x,-y,-x\},$$

$$\psi[\Gamma_4]=\{x,0,-x|-x,0,x|x,0,-x|-x,0,x\}.$$

From the above results, we conclude that the irreps $\Gamma_1$ and $\Gamma_4$ are contained once, while the irreps $\Gamma_2$ and $\Gamma_3$ are contained twice in the decomposition of the mechanical representation for the considered chain.

The generalization of these results to the case of the dihedral group $[\hat{a}^m,\hat{i}]$ with *arbitrary m* is trivial.

The splitting scheme (83) for the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ for the monoatomic chain with $N=12$ particles can be now explained as follows. There are five irreps $(\Gamma_1,\Gamma_2,\Gamma_3,\Gamma_4,\Gamma_5)$ of the group $[\hat{a}^3,\hat{i}]\equiv\{\hat{e},\hat{a}^3,\hat{a}^6,\hat{a}^9|\hat{i},\hat{i}\hat{a}^3,\hat{i}\hat{a}^6,\hat{i}\hat{a}^9\}\equiv D_4$. As we have just shown, the one-dimensional irreps $\Gamma_1$ $(n_1=1)$ and $\Gamma_4$ $(n_4=1)$ are contained once $(m_1=1,\ m_4=1)$ in the decomposition of the mechanical representation $\Gamma$ for our chain. On the other hand, the one-dimensional irreps $\Gamma_2$ $(n_2=1)$ and $\Gamma_3$ $(n_3=1)$ are contained twice $(m_2=2,\ m_3=2)$ in $\Gamma$, while the two-dimensional irrep $\Gamma_5$ $(n_5=2)$ is contained thrice $(m_5=3)$ in $\Gamma$. The 12 variables $\delta_j$ from Eq. (83) are associated with the irreps of the group $D_4$ in the following manner:

$$\delta_1\to\Gamma_1(1),\quad \delta_2\to\Gamma_2(1),\quad \delta_3\to\Gamma_2(2),$$

$$\delta_4\to\Gamma_3(1),\quad \delta_5\to\Gamma_3(2),\quad \delta_6\to\Gamma_4(1),$$

$$(\delta_7,\delta_8)\to\Gamma_5(1),\quad (\delta_9,\delta_{10})\to\Gamma_5(2),\quad (\delta_{11},\delta_{12})\to\Gamma_5(3). \tag{88}$$

Here, in parentheses, we give the index of the copy of the irrep $\Gamma_i$ (whose dimension is equal to $n_i$) in the decomposition of the mechanical representation $\Gamma$. Note that the total number of such copies determines how many times $m_i$ the irrep $\Gamma_i$ is contained in $\Gamma$. On the other hand, as we already know, $m_i$ shows us the dimension of the subsystems $L_j$, while $n_i$ determines the total number of $L_j$ with the same dimension associated with $\Gamma_i$. As a result, we obtain the splitting scheme (83).

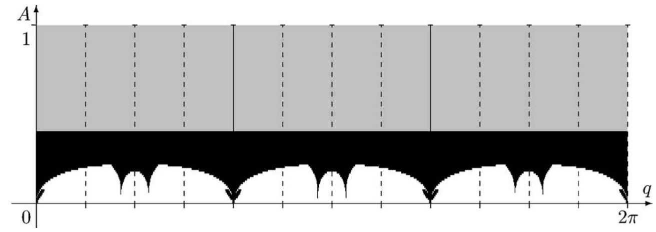


FIG. 1. Regions of stability (white color) of different modes of the FPU-$\alpha$ chain, interacting parametrically with the one-dimensional bush $\mathrm{B}[a^3,i]$.

The above-discussed decomposition of the full linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ into independent subsystems $L_j$ of small dimensions permits one to analyze efficiently the stability of a given bush in the monoatomic chain with an arbitrarily large number of particles $(N)$.

Using this idea, the stability diagrams for all the one-dimensional bushes in both FPU-$\alpha$ and FPU-$\beta$ chains were obtained in [9]. As an example, in Fig. 1, we reproduce the stability diagram for the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$ for the FPU-$\alpha$ chain from that paper. In this diagram, each point $(A,q)$ determines a certain value of the bush mode amplitude $A$ and a certain value of the wave number $q=2\pi j/N$ that is associated with the index $j$ of a fixed mode. The black points $(A,q)$ correspond to the case where the mode $j=qN/2\pi$ becomes excited because of its parametric interaction with the mode of the bush $\mathrm{B}[\hat{a}^3,\hat{i}]$. The white color denotes the opposite case: the corresponding mode $j$, being zero at the initial instant, continues to be zero in spite of its interaction with the considered bush. Such a diagram allows one to study stability of one-dimensional bushes not only for finite $N$, but also for the case $N\to\infty$ (some more details can be found in [9]).

## V. SOME ADDITIONAL EXAMPLES

### A. Stability of the two-dimensional bush $\mathrm{B}[\hat{a}^4,\hat{i}]$ in the FPU-$\alpha$ chain

Let us consider the stability of the two-dimensional bush $\mathrm{B}[\hat{a}^4,\hat{i}]$ for the case $N=12$. It can be determined by the displacement pattern [9]

$$\boldsymbol{X}(t)=\{A(t),B(t),-B(t),-A(t)|A(t),B(t),-B(t),-A(t)|A(t),B(t),-B(t),-A(t)\}. \tag{89}$$

The symmetry group of this bush is the dihedral group $D_3$ with the translational subgroup

$$T_3=\{\hat{e},\hat{a}^4,\hat{a}^8\}\quad(\hat{a}^{12}=\hat{e}). \tag{90}$$

Using the techniques developed in the previous sections, one can obtain the following results on the decomposition of

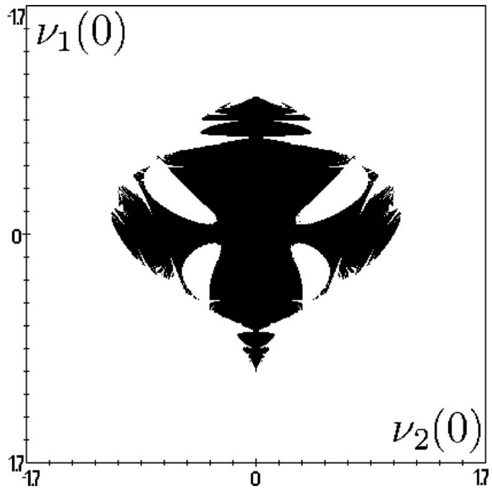


FIG. 2. Stability diagram for the bush $\mathrm{B}[a^4,i]$ in the FPU-$\alpha$ chain with $N=12$ particles.

the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ (for computational details see [24]). The linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for studying the stability of the bush $\mathrm{B}[\hat{a}^4,\hat{i}]$, in the case $N=12$, splits into two $2\times 2$ and two $4\times 4$ independent systems $L_j$ $(j=1,2,3,4)$ of differential equations of the second order. These systems can be written in the form $\ddot{\boldsymbol{\nu}}_j=\mathrm{M}_j(t)\cdot\boldsymbol{\nu}_j$. Here $\boldsymbol{\nu}_j$ are two-dimensional or four-dimensional vectors and $\mathrm{M}_j(t)$ are $2\times 2$ or $4\times 4$ matrices. The explicit forms of these matrices for systems $L_j$ $(j=1,2,3,4)$ are

$$\mathrm{M}_1(t)=\begin{pmatrix}-K_3(t) & K_1(t)\\ K_1(t) & -K_4(t)\end{pmatrix},\quad \mathrm{M}_2(t)=\begin{pmatrix}-K_1(t) & K_1(t)\\ K_1(t) & -K_1(t)\end{pmatrix},$$

$$\mathrm{M}_3(t)=\mathrm{M}_4(t)=\begin{pmatrix}-K_6(t) & K_1(t) & K_2(t) & 0\\ K_1(t) & -K_3(t) & 0 & 0\\ K_2(t) & 0 & -K_5(t) & K_1(t)\\ 0 & 0 & K_1(t) & -K_1(t)\end{pmatrix}, \tag{91}$$

where

$$K_1(t)=1-2A(t)+2B(t),\quad K_2(t)=\sqrt{3}\left(\frac{1}{2}-2B(t)\right),$$

$$K_3(t)=3+6A(t)+2B(t),\quad K_4(t)=3-2A(t)-6B(t),$$

$$K_5(t)=\frac{5}{2}-2A(t)-4B(t),\quad K_6(t)=\frac{3}{2}-2A(t).$$

In conclusion, in Fig. 2 we reproduce the stability diagram for the two-dimensional bush $\mathrm{B}[\hat{a}^4,\hat{i}]$ from our paper [9]. This diagram corresponds to the FPU-$\alpha$ chain with $N=12$ particles. It represents a planar section of the four-dimensional stability domain in the space of the initial conditions $\nu_1(0)$, $\nu_2(0)$, $\dot{\nu}_1(0)$, and $\dot{\nu}_2(0)$, where $\nu_1(t)$ and $\nu_2(t)$ are two modes of the considered bush. In producing this figure, we specify $\dot{\nu}_1(0)=0$ and $\dot{\nu}_2(0)=0$ and change $\nu_1(0)$ and $\nu_2(0)$ in some interval near their zero values. The stability domain, resembling a beetle, is drown in *black* color in the plane $\nu_1(0)$-$\nu_2(0)$. The bush $\mathrm{B}[\hat{a}^4,\hat{i}]$ loses its stability (and transforms into another bush of higher dimension) when we cross the boundary of the black region in any direction. From Fig. 2 it is obvious how nontrivial the stability domain for a bush of modes can be.

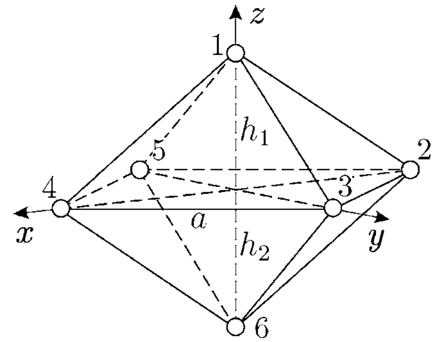


FIG. 3. Octahedral structure with the symmetry group $O_h$.

A detailed description of the stability domains for one-dimensional and two-dimensional bushes of modes in both FPU-$\alpha$ and FPU-$\beta$ chains can be found in [9].

### B. Stability of bushes of modes for the octahedral molecule

As was already discussed, the group-theoretical method developed in the present paper can be applied not only to the monoatomic chains, but to any dynamical systems with discrete symmetry. Below, we demonstrate this idea using a mechanical system with the point symmetry group $O_h$ as one possible example. Let us consider the model of an octahedral molecule depicted in Fig. 3. It is formed by six equal atoms situated at the vertices of a regular octahedron whose edges we denote by $a$. The origin of coordinates is chosen as the center of the octahedron. Four atoms (2,3,4,5) in the plane $XY$ form a square, while two other atoms (1,6) are situated on the $Z$ axis.

In [7], we have considered nonlinear vibrations of the above molecule structure supposing that interatomic interactions are described by the Lennard-Jones potential. All possible bushes of modes and a certain stability analysis of these dynamical objects, based on the direct numeric calculations, have been presented in that paper. We can simplify this stability analysis and, at the same time, deepen our insights into the bush stability problem using the above-discussed group-theoretical approach.

Let us split the full linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for the octahedral structure (Fig. 3) in the vicinity of the three bushes: one-, two-, and three-dimensional bushes $\mathrm{B}1[O_h]$, $\mathrm{B}2[D_{4h}]$, and $\mathrm{B}3[C_{4v}]$ with point symmetry groups $O_h$, $D_{4h}$, and $C_{4v}$, respectively.

Note that simple *geometric forms* of the vibrational states of the considered molecule correspond to these bushes [7]. The bush $\mathrm{B}1[O_h]$ describes evolution of the regular octahedron whose edge length $a=a(t)$ changes periodically in time. In the vibrational state corresponding to the bush $\mathrm{B}2[D_{4h}]$

the atoms situated in the $XY$ plane, as before, form a square for any time $t$, while the distances (heights) $h_1=h_1(t)$, $h_2=h_2(t)$ of the top and bottom atoms (see Fig. 3) from this plane, being equal to each other $[h_1(t)=h_2(t)]$, become different from those in the regular octahedron. The form of the vibrational state for the bush B3$[C_{4v}]$ differs from that for the bush B2$[D_{4h}]$ by inequality $[h_1(t)\neq h_2(t)]$ of the two heights.

The dynamics of the considered octahedral structure is characterized by 18 degrees of freedom, but only 12 of them correspond to vibrations (one can eliminate 6 degrees of freedom associated with the translation and rotation of the molecule as a whole unit).

Thus, we have a nonlinear system of 12 differential equations describing vibrations of our mechanical structure. The dimension of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ near any specific vibrational regime is also equal to 12, but we can split it into a number of independent subsystems. Using a group-theoretical approach, we have obtained the following splitting schemes (details of the calculation can be found in [24]):

$$\text{For B1}[O_h]: \quad 12(1);$$

$$\text{For B2}[D_{4h}]: \quad 6(1), \quad 3(2);$$

$$\text{For B3}[C_{4v}]: \quad 1(1), \quad 1(2), \quad 3(3). \tag{92}$$

Let us comment on these splitting schemes. The linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for the bush B1$[O_h]$ can be decomposed into 12 independent equations

$$\ddot{\nu}_j = K_j(t)\nu_j \quad (j=1,\ldots,12), \tag{93}$$

where $K_j(t)$ are functions depending on the time-periodic solution $a(t)$ to the dynamical equation of the considered one-dimensional bush (see [7]):

$$\ddot{a} = -4u'(a) - \sqrt{2}u'(\sqrt{2}a). \tag{94}$$

Here $u(r)$ is the potential of the center two-particle interaction [for example, it can be the Lennard-Jones potential $u(r)=A/r^{12}-B/r^6$], while $u'(r)$ is the derivative of this potential.

The linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for the bush B2$[D_{4h}]$ can be decomposed into six independent equations of the form (93) and three two-dimensional subsystems

$$\ddot{\boldsymbol{\nu}}_j = \mathrm{K}_j(t)\boldsymbol{\nu}_j \quad (j=1,2,3), \tag{95}$$

where $\boldsymbol{\nu}_j$ are two-dimensional vector variables, while $\mathrm{K}_j(t)$ are $2\times 2$ matrices. All the coefficients of these matrices, as well as scalar coefficients $K_j(t)$ from the one-dimensional equations of the form (93), are quasiperiodic functions depending on the two variables $a(t)$ and $h(t)$, which represent the solution to the dynamical equations of the bush B2$[D_{4h}]$:

$$\ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - 2u'(b)\frac{a}{b},$$

$$\ddot{h} = -4u'(b)\frac{h}{b} - u'(2h). \tag{96}$$

[For the definition of the function $b(t)$ see below].

The linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ for the bush B3$[C_{4v}]$ can be decomposed into one individual equation of the form (93), one two-dimensional subsystem of the form (95), and three three-dimensional subsystems which we also can write as Eq. (95) assuming that $\boldsymbol{\nu}_j$ and $\mathrm{K}_j(t)$ are, in this case, three-dimensional vectors and $3\times 3$ matrices, respectively. All the elements of matrices $\mathrm{K}_j(t)$ depend on the three functions $a(t)$, $h_1(t)$, and $h_2(t)$, describing the dynamics of the bush B3$[C_{4v}]$. These functions represent the solution to the following equations of the considered bush [7]:

$$\ddot{a} = -2u'(a) - \sqrt{2}u'(\sqrt{2}a) - u'(b)\frac{a}{b} - u'(c)\frac{a}{c},$$

$$\ddot{h}_1 = -u'(b)\frac{5h_1-h_2}{b} - u'(h_1+h_2),$$

$$\ddot{h}_2 = -u'(c)\frac{5h_2-h_1}{c} - u'(h_1+h_2). \tag{97}$$

Here

$$b = \sqrt{\frac{a^2}{2} + \left(\frac{5}{4}h_1 - \frac{1}{4}h_2\right)^2}, \quad c = \sqrt{\frac{a^2}{2} + \left(\frac{5}{4}h_2 - \frac{1}{4}h_1\right)^2}$$

(note that for the bush B2$[D_{4h}]$ $h_1=h_2=h$).

The explicit form of the coefficients of Eqs. (93) and (95) can be found in [24].

## VI. CONCLUSION

All the exact dynamical regimes in $N$-particle mechanical systems with discrete symmetry can be classified by the *subgroups* $G_j$ of the parent group $G_0$—i.e., the symmetry group of its equations of motion. Actually, each subgroup $G_j$ singles out a certain *invariant manifold* which, being decomposed into the basis vectors of the irreducible representations of the group $G_0$, is termed a "bush of modes"[1–3].

The bush B$[G_j]$, representing an $n$-dimensional vibrational regime, can be considered as a dynamical object characterized by its displacement pattern of all the particles from their equilibrium positions, by the appropriate dynamical equations and the domain of the stability. One-dimensional bushes are symmetry-determined similar nonlinear normal modes introduced by Rosenberg [16] (see also [4]). For Hamiltonian systems, the energy of the initial excitation turns out to be "trapped" in the bush and this is a phenomenon of energy localization in modal space.

The different aspects of the bush theory were developed in [1–7]. Bushes of vibrational modes (invariant manifolds) in the FPU chains were discussed in [8–12].

The stability analysis of a given bush B$[G]$ reduces to studying the linearized (in the vicinity of the bush) dynamical equations $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$. In the present paper, we prove (theorem 1) that the symmetry group of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ turns out to be precisely the symmetry group $G$ of the considered bush $\mathrm{B}[G]$. This result allows one to apply the well-known Wigner theorem about the specific structure of the matrix [$\mathrm{J}(t)$, in our case] commuting with all the matrices of a fixed representation (mechanical representation, in our case) of a given group. According to the above theorem one can split effectively the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ into a number of independent subsystems of differential equations with time-dependent coefficients.

We want to emphasize that this symmetry-related method for splitting the linearized systems arising in the linear stability analysis of the dynamical regimes is suitable for *arbitrary* nonlinear mechanical systems with discrete symmetry. Such a decomposition (splitting) of the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$ is especially important for the *multidimensional* bushes of modes, describing *quasiperiodic* vibrational regimes, which cannot be treated with the aid of the Floquet method. Indeed, in this case, we need to integrate the differential equations with time-dependent coefficients over a large time interval, unlike the case of periodic regimes where we can solve the appropriate differential equations over only one period to construct the monodromy matrix.

The above method is applied for studying the stability of some dynamical regimes (bushes of modes) in the monoatomic chains. For this specific mechanical systems, we prove theorem 2 which allows one to find very simply the upper bound of dimensions of the independent subsystems obtained after splitting the linearized system $\ddot{\boldsymbol{\delta}}=\mathrm{J}(t)\cdot\boldsymbol{\delta}$. Indeed, according to this theorem, the dimension of each such subsystem does not exceed the integer $m$ determining the ratio of the volumes of the primitive cell of the chain in the vibrational state, corresponding to the given bush $\mathrm{B}[G]=\mathrm{B}[\hat{a}^m,\ldots]$, and the equilibrium state. Taking into account any other symmetry elements of the considered bush allows one to reduce the dimensions of at least some of the above-discussed subsystems.

In conclusion, let us mention a particular research field where the group-theoretical approach developed in the present paper would be relevant. For an investigation of the integrability of the Hamiltonian systems with a large number of degrees of freedom, one may study the integrability of the reduced Hamiltonian system on low-dimensional invariant manifolds (see [23] and references therein). In particular, it is important to single out one-dimensional manifolds and split the linearized Hamiltonian systems in the vicinity of such manifolds. Evidently, the group-theoretical methods can be useful for studying these problems for the dynamical systems with discrete symmetries. For example, the invariant manifold corresponding to the two-dimensional bush $\mathrm{B}[\hat{a}^4,\hat{i}]$ has been already used for such a purpose and the nonintegrability of nonlinear lattices with generic polynomial interaction and on-site potentials has been proved in the paper by Yoshimura and Umeno [23].

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