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Interaction of Lower and Higher Order Hamiltonian Resonances

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The tools of normal forms and recurrence are used to analyze the interaction of low and higher order resonances in Hamiltonian systems. The resonance zones where the short-periodic solutions of the low order resonances exist are characterized by small variations of the corresponding actions that match the variations of the higher order resonance; this yields cases of embedded double resonance. The resulting interaction produces periodic solutions that in some cases destabilize a resonance zone. Applications are given to the three dof 1 : 1 : 4 resonance and to periodic FPU-chains producing unexpected nonlinear stability results and quasi-trapping phenomena.

Keywords: Symmetry; Hamiltonian; double resonance; quasi-trapping.

1. Introduction

The presence of low (prominent) and higher order resonances in Hamiltonian systems enables the possibility of a special kind of double resonance. In such a case the higher order resonance zone will, if it exists, be embedded in the primary resonance zone of the low order resonance.

Consider a n degrees-of-freedom (dof) Hamiltonian system in a neighborhood of stable equilibrium. We assume the Hamiltonian $H(p, q)$ can be expanded in a Taylor series of the form

$$H(p, q) = H_2(p, q) + H_3(p, q) + H_4(p, q) + \cdots$$

where the $H_m, m = 2, 3, \ldots$ are homogeneous polynomials in p, q of degree m. The quadratic form $H_2(p, q)$ is Morse in $(p, q) = (0, 0)$. Suppose that we have:

$$H_2 = \frac{1}{2}\sum_{m=1}^{n} \omega_m (p_m^2 + q_m^2)$$

or equivalently

$$H_2 = \frac{1}{2}\sum_{m=1}^{n} (p_m^2 + \omega_m^2 q_m^2)$$

with positive frequencies $\omega_m, m = 1, 2, \ldots, n$. Often it is convenient to scale the coordinates near the stable origin of the system by putting $p, q \to \varepsilon p, \varepsilon q$ and dividing by ε^2. This leads to the Hamiltonian $H = H_2 + \varepsilon H_3 + \varepsilon^2 H_4 + \varepsilon^3 \ldots$.

If necessary, we can approximate the frequencies $\omega_m, m = 1, 2, \ldots, n$ by rational numbers as the rationals are dense in the set of real numbers. This will add a perturbation term to the Hamiltonian.

A powerful theorem on the stability of Hamiltonian systems in the sense of exponentially-long time invariance of the actions was formulated and proved in [Nekhoroshev, 1977]. This theorem presupposes the absence of first or second order resonances in the system so it cannot be applied in our cases. In many applications in physics and engineering a combination of low and higher order resonances takes place. To avoid this problem one usually concentrates on the low order resonances neglecting the higher order ones. The purpose of our paper is to explore cases of combined low and higher order resonances to analyze the variation of the nonresonant actions (or amplitudes). The resulting dynamics turns out to be interesting, it throws new light on quasi-trapping phenomena and delayed recurrence.

The formulation of Hamiltonian resonance is well-known, see [Sanders *et al.*, 2007, Chapter 10, Tables 10.3–4]. For two dof, the low order resonances are $1:2$, $1:3$ and $1:1$. A combination of low and high order would for example be the three dof resonances $1:2:7$ or $1:1:9$. A three dof first order resonance like $1:2:2$ can be part of the resonance $1:2:2:7$. A basic observation is that in a large part of phase-space, the dynamics of the low order resonance dominates. However, in the absence of theoretical results that the orbits will remain in these low order resonance regions, we have to include and identify parts of phase-space, the resonance zones (introduced in Sec. 3), where the higher order resonances become important. The essence of the problems we are faced with arise already at three dof. So to understand the phenomena and theory we will in most cases restrict to three dof.

Our main tools will be normal form theory and the use of the Poincaré recurrence theorem from [Poincaré, 1892, 1893, 1899, Vol. 3] to characterize the dynamics in resonance zones. The emphasis is on the analysis of dynamics with numerics for illustration. Recurrence in time-independent Hamiltonian systems on bounded domains implies that orbits cannot be trapped in a region that does not contain the initial position in phase-space. However, quasi-trapping, as described by [Zaslavsky, 2007], plays an important part with consequences for the recurrence times. Suppose that an orbit travels through a resonance zone M. The zone may contain periodic and quasi-periodic solutions, homo- and heteroclinic solutions, tori and other geometric structures. The complexity of M will determine the length of the time interval to pass the resonance zone. It turns out that in the case of three dof with one low order resonance involving two dof, we have two possibilities. In the first case the resonance zone M may contain higher order resonances (see Sec. 3) that complicate the dynamics within the zone. This is a case of secondary or embedded double resonance. An example is found in our treatment of the $1:1:4$ resonance. In the second case no higher order resonance will be active in M because of strong detuning, but a nonresonant forcing corresponding to a simple torus structure may impede and delay transition of the zone.

To characterize recurrence we will use the Euclidean distance d in phase-space which is the distance of a phase-point with respect to its initial conditions as a function of time. When considering the solutions of the initial value problem

$$\dot{x} = f(x), \quad x(0) = x(0)$$

in $\mathbb{R}^n$, this Euclidean distance written in components $x_i(t), x_i(0), i = 1, \ldots, n$ will be at time t:

$$d = \sqrt{\sum_{i=1}^{n}(x_i(t) - x_i(0))^2}.$$

Near stable equilibrium, the dynamics of two dof Hamiltonian systems is dominated by a foliation of the energy manifold in tori that separate the phase-flow. This excludes diffusion phenomena. To study recurrence and quasi-trapping we consider mainly the simplest Hamiltonian context that allows for this phenomenon, three dof autonomous Hamiltonian systems. It follows from the proof of the recurrence theorem that for a fixed return distance d the recurrence time on a bounded energy manifold will always be bounded by an upper limit except for a set of initial conditions of measure zero.

A formulation for these systems will be given in Sec. 2; Sec. 4 will introduce secondary resonances that may be active in so-called resonance zones. We find a typical example of these phenomena in the $1:1:4$ resonance of Sec. 5; another example, the $2:2:3$ resonance, was discussed in [Verhulst, 2018]. An application of the $1:1:\omega$ resonance with ω nonresonant will be the periodic FPU-chain with four particles in Sec. 6. In this problem, the α- and the β-chains behave quite differently. It was shown in [Bruggeman & Verhulst, 2018] that a periodic FPU-chain with four particles will be found again as a submanifold in a chain with $4n$ particles. This motivates us to consider the dynamics of the periodic FPU-chain with eight particles in Secs. 7 and 8.

Many papers were written on FPU-chains, we cannot do justice to these. A useful modern reference is [Christodoulidi *et al.*, 2010]. Regarding the existence of invariant manifolds (called "bushes") in classical FPU-chains, basic results are found in [Chechin & Sakhnenko, 1998; Chechin *et al.*, 2002; Chechin *et al.*, 2005]. In these papers group-theoretical methods were used for coupled oscillator systems with special attention to α- and β FPU-chains. See for the existence of invariant manifolds additional manifolds also [Rink, 2001]. We will focus on examples of existence and stability of invariant manifolds for the classical periodic FPU-chain and for the FPU-chain with alternating masses. A remarkable result is that the linear or spectral stability concluded in the papers by [Chechin & Sakhnenko, 1998; Chechin *et al.*, 2002; Chechin *et al.*, 2005] is in a number of cases destroyed by the nonlinearities. For this nonlinear analysis the idea of interaction of low and higher order resonances in resonance zones is essential.

Apart from chains of oscillators there is also an extensive literature on passage through resonance. Again we cannot do justice to all contributions. We mention [Haberman, 2006; Neishtadt & Su, 2013; Sanders *et al.*, 2007, Chapter 8] with more references there.

We also note that there is clearly a connection with the topics of Arnold-diffusion, Aubry–Mather theory and double resonances. For references on some of these topics see [Cheng, 2015]. A detailed study of double resonances, Arnold diffusion, with many references can be found in [Efthymiopoulos & Harsoula, 2013; Guzzo & Lega, 2016]. Double resonances are often connected with the intersection of two resonance manifolds producing a so-called "resonant junction". Our approach is different as we discuss cases where one resonance is dominant but where in the prominent resonance zone a secondary higher order resonance zone is embedded. This scenario is natural in many applications.

The numerical illustrations were obtained by Matcont under Matlab with ode code 78, in most cases relative tolerance and abs. tolerance e^{-15}.

2. Three Degrees-of-Freedom

Consider the three degrees-of-freedom (dof) Hamiltonian $H(p,q) = H_2(p,q) + H_3(p,q) + \cdots$ with

$$H_2 = \frac{1}{2}\omega_1(p_1^2 + q_1^2) + \frac{1}{2}\omega_2(p_2^2 + q_2^2) + \frac{1}{2}\omega_3(p_3^2 + q_3^2). \tag{1}$$

The frequencies $\omega_1, \omega_2, \omega_3$ are chosen positive; we assume that two of the frequencies, say ω_1 and ω_2, are close to a first or second order resonance of two dof, so we have that the ratios ω_1/ω_2 are $1:2$, $1:1$ or $1:3$. Often we rescale the frequencies to obtain $\omega_1 = 1$, $\omega_2 = k = 1, 2$ or 3, $\omega_3 = l$; detuning effects to allow for small frequency perturbations can be added in applications. The three frequencies are not in first or second order resonance of three dof, so for rational l we exclude neighborhoods of the natural numbers $1, 2, \ldots, 6$.

As indicated before, we scale the coordinates near the stable origin of the system by putting $p, q \to \varepsilon p, \varepsilon q$ and dividing by ε^2. This leads to the Hamiltonian

$$H(p,q) = \frac{1}{2}(p_1^2 + q_1^2) + \frac{1}{2}k(p_2^2 + q_2^2) + \frac{1}{2}l(p_3^2 + q_3^2) + \varepsilon H_3(p,q) + \varepsilon^2 \ldots. \tag{2}$$

So ε^2 is a measure for the energy with respect to stable equilibrium at the origin. We introduce action-angle coordinates I, ϕ by the transformation:

$$\begin{aligned} q_i &= \sqrt{2I_i}\sin\phi_i, \\ p_i &= \sqrt{2I_i}\cos\phi_i, \end{aligned} \quad i = 1, 2, 3, \tag{3}$$

leading with (2) to

$$H = I_1 + kI_2 + lI_3 + \varepsilon H_3 + \varepsilon^2 \ldots \quad \text{and}$$
$$\dot{I} = -\frac{\partial H}{\partial \phi}, \quad \dot{\phi} = \frac{\partial H}{\partial I}.$$

We will also use amplitude-phase coordinates r, ψ with transformations

$$\begin{aligned} q_i &= r_i\cos(\omega_i t + \psi_i), \\ \dot{q}_i &= -\omega_i r_i \sin(\omega_i t + \psi_i). \end{aligned} \tag{4}$$

2.1. *Birkhoff–Gustavson or Born-approximation*

After Birkhoff and Gustavson (earlier formulated by [Born, 1927]) we will introduce a symplectic near-identity transformation producing normal forms (see [Sanders *et al.*, 2007] for theory and literature). Prominent terms in the normal forms are produced by the resonances induced by the frequencies $1, k, l$. Introducing annihilation vectors $\mathbf{a} \in \mathbb{Z}^3$ with the property $a_1 + a_2 k + a_3 l = 0$, the normal form may contain corresponding combination angles of the form:

$$\chi = a_1\phi_1 + a_2\phi_2 + a_3\phi_3.$$

We will call $\|a\| = |a_1| + |a_2| + |a_3|$ the norm of the annihilator. The Birkhoff–Gustavson normal form to H_4 in action-angle coordinates involves the angles ϕ_1, ϕ_2; in the cases $k = 1, 2, 3$ we have:

$$\begin{cases} H_{12} = I_1 + 2I_2 + lI_3 + \varepsilon b_1 I_1 \sqrt{2I_2}\cos(\chi_1 - b_2) + \varepsilon^2 A(I_1, I_2, I_3), & k = 2, \quad \chi_1 = 2\phi_1 - \phi_2, \\ H_{11} = I_1 + I_2 + lI_3 + \varepsilon^2(A(I_1, I_2, I_3) + b_1 I_1 I_2 \cos 2(\chi_1 - b_2)), & k = 1, \quad \chi_1 = \phi_1 - \phi_2, \\ H_{13} = I_1 + 3I_2 + lI_3 + \varepsilon^2(A(I_1, I_2, I_3) + b_1 I_1^{\frac{3}{2}} I_2^{\frac{1}{2}} \cos(\chi_1 - b_2)), & k = 3, \quad \chi_1 = 3\phi_1 - \phi_2. \end{cases} \tag{5}$$

The constants b_1, b_2 are real (for potential problems $b_2 = 0$), A is a homogeneous, quadratic polynomial in I_1, I_2, I_3 (quartic in the amplitudes).

Preliminary conclusions on the Birkhoff–Gustavson normal forms (5):

(1) The three normal forms are integrable.
(2) If $k = 2$, the integrals are H_{12}, $I_1 + 2I_2$ and I_3. The flow is dominated by $H_2 + \varepsilon H_{12}$.
(3) If $k = 1$, the integrals are H_{11}, $I_1 + I_2$ and I_3.
(4) If $k = 3$, the integrals are H_{13}, $I_1 + 3I_2$ and I_3.
(5) Near stable equilibrium the energy manifolds are topologically the five-dimensional sphere S^5. They are foliated in families of tori with parametrization by the integral I_3.
(6) On the energy manifold we find families of short-periodic solutions parametrized by I_3 which is a degeneration in the sense of [Poincaré, 1892, 1893, 1899, Vol. 1].

The treatment of higher order resonance in [Sanders, 1977] is quite general for two dof, the theory will be summarized in the next section. For more than two dof the complexity of higher order resonance increases enormously. The case $k = 2$ is relatively simple as generically the normal form is dominated by H_3, see also [Verhulst, 2017]; combination angles different from χ_1 are in general timelike. Here we will study the remaining cases $k = 1$, followed by applications, for instance a low-dimensional FPU-chain.

2.2. *The notion of genericity*

In what follows we use the notion of *genericity*. This means that in a dynamical system characterized by parameters we keep track of cases producing qualitatively special phenomena that exist only for exceptional choices of the parameters. Genericity is a concept that has to be defined in the context of explicit dynamical systems. For systems in second order resonance as in Sec. 4, its use looks simple: if in Eq. (5) $b_1 \neq 0$, we have a generic case, $b_1 = 0$ which produces nongeneric dynamics.

However, it can be necessary to extend the definition in these cases, for instance if $b_1 \neq 0$ with the other parameters producing a bifurcation of periodic solutions.

We illustrate such phenomena for the $1:1:4$ resonance that is discussed in Sec. 4. Consider the $H_2 + \varepsilon^2 H_4$ part of the $1:1:4$ resonance with H_2 slightly different from (2):

$$H = \frac{1}{2}(\dot{q}_1^2 + q_1^2) + \frac{1}{2}(\dot{q}_2^2 + q_2^2) + \frac{1}{2}(\dot{q}_3^2 + 16q_3^2) - \varepsilon^2(b_1 q_1^4 + b_2 q_1^2 q_2^2 + b_3 q_2^4 + b_4 q_3^4). \tag{6}$$

The third dof is decoupled and plays no part in this illustration. It is easy to show that if $b_1 = b_3 = b$, $b_2 = 2b$, $b \neq 0$, the system has the second (angular momentum) integral $\dot{q}_1 q_2 - q_1 \dot{q}_2$, a feature that is already nongeneric. The analysis of Hamiltonian (6) as far as the $1:1$ resonance is concerned was carried out in [Verhulst, 1979]; it has been shown that for these values of the coefficients we find short-periodic solutions resulting in exceptional dynamics. This is a degenerate situation; the degeneration of this type was described by [Poincaré, 1892, 1893, 1899, Vol. 1]. Moreover I_3 is still free to choose which makes the degeneration worse. Such parameter values corresponding with nongenericity have to be studied separately.

3. Higher Order Resonance in Two Dof

We summarize the theory for two dof from [Sanders, 1977] and extend following [Tuwankotta & Verhulst, 2000], see also [Sanders *et al.*, 2007]. Consider the two dof Hamiltonian system with linear frequencies $k, l \in \mathbb{N}$. If $k + l > 4$ its Birkhoff–Gustavson normal form is in action-angle coordinates:

$$H = kI_1 + lI_2 + \varepsilon^2(AI_1^2 + 2BI_1I_2 + CI_2^2) + \cdots + \varepsilon^{k+l-2}(D_1(I_1, I_2) + D_2(I_1, I_2)\cos(\chi + b)), \tag{7}$$

where b is a constant phase-shift, the dots stand for Birkhoff normal form terms (dependent on I_1, I_2 only), $\chi = l\phi_1 - k\phi_2$. It can be shown that the actions I_1, I_2 are constant to $O(\varepsilon)$ on the timescale $1/\varepsilon^2$; with some effort the error is reduced to $O(\varepsilon^2)$ on the timescale $1/\varepsilon^2$.

The combination angle χ may vary locally in a resonance zone as follows: The *resonance manifold* N embedded in the compact energy manifold $\mathcal{E}$ is defined **using** $d\chi/dt = 0$ by:

$$N = \{I_1, I_2 \in \mathcal{E} \mid (lA - kB)I_1 + (lB - kC)I_2 = 0\}. \tag{8}$$

If N exists, small exchanges of energy will take place between the two dof in a *resonance zone* located in an $O(\varepsilon^{(k+l-4)/2})$ neighborhood of N (this is an improved estimate based on [Tuwankotta & Verhulst, 2000]). The resonance zone contains stable and unstable periodic solutions, the exchange of energy takes place on tori in the resonance zone with timescale $1/\varepsilon^{-(k+l)/2}$. In [Tuwankotta & Verhulst, 2000] it is also proved that for potential problems the phase-shift $b = 0$ in (7).

If the frequency ratio is not rational, we approximate the ratio by a suitable rational. "Suitable" means that the detuning of the irrational frequency ratio is matched by the small parameter ε. For an application of detuning see [Sanders & Verhulst, 1979].

4. Three Dof: Interaction with a Second Order Resonance

The dynamics of the $1:1:l$ and $1:3:l$ resonances (with l not in a neighborhood of $1, 2, \ldots, 6$) is different from the case $1:2:l$ discussed in [Verhulst, 2017]. To avoid too many parameters we will restrict ourselves from now on in our applications to potential problems; the results can easily be generalized. An implication is that the subsequent Hamiltonians correspond with mechanical systems. The Hamiltonian will be of the form $H(I,\phi) = H_{11} + \varepsilon^3 \ldots$ or $H(I,\phi) = H_{13} + \varepsilon^3 \ldots$ with H_{11} or H_{13} containing the combination angle $\chi_1 = \phi_1 - \phi_2$ or $\chi_1 = 3\phi_1 - \phi_2$; depending on the frequency l other combination angles will arise at $O(\varepsilon^3)$. The reasoning for $k = 3$ runs along the same lines as for $k = 1$.

4.1. *The case* $k = 1$

With system (5) the normalized equations for $k = 1$ are in a neighborhood with the normal modes excluded:

$$\begin{cases} \dot{I}_1 = 2\varepsilon^2 b_1 I_1 I_2 \sin 2(\chi_1 - b_2) + \varepsilon^3 \ldots, \\ \dot{\phi}_1 = 1 + \varepsilon^2\left(\dfrac{\partial A}{\partial I_1} + b_1 I_2 \cos 2(\chi_1 - b_2)\right) + \varepsilon^3 \ldots, \\ \dot{I}_2 = -2\varepsilon^2 b_1 I_1 I_2 \sin 2(\chi_1 - b_2) + \varepsilon^3 \ldots, \\ \dot{\phi}_2 = 1 + \varepsilon^2\left(\dfrac{\partial A}{\partial I_2} + b_1 I_1 \cos 2(\chi_1 - b_2)1\right) + \varepsilon^3 \ldots, \\ \dot{I}_3 = \varepsilon^3 \ldots, \\ \dot{\phi}_3 = l + \varepsilon^2 \dfrac{\partial A}{\partial I_3} + \varepsilon^3 \ldots. \end{cases} \tag{9}$$

$A(I)$ $(I = I_1, I_2, I_3)$ is a homogeneous quadratic polynomial in its arguments. Starting with ε^3 the dots stand for terms dependent on the actions and other resonant combination angles $\chi_2, \chi_3, \ldots$; from $O(\varepsilon^4)$ on, χ_1 may also be present.

$H_2 = I_1 + I_2 + lI_3 (= E_0)$ is conserved to $O(\varepsilon)$ for all time. In addition we have

$$\frac{d}{dt}(I_1 + I_2) = O(\varepsilon^3).$$

We have $I_1 + I_2 = E_1 + O(\varepsilon)$ on the timescale $1/\varepsilon^2$ with $E_1 \geq 0$; $\dot{I}_3 = O(\varepsilon^3)$, so I_3 is conserved with error $O(\varepsilon)$ on the same timescale. The theorem in [Nekhoroshev, 1977] cannot be applied in this case.

Consider the case with one additional combination angle arising at H_5. Cases with more angles or still higher order resonances can be treated in a similar way. A resonance at H_5 with annihilation vector (a_1, a_2, a_3) generates the combination angle χ_2. We have to order ε^2:

$$\begin{cases} \dot{\chi}_1 = \varepsilon^2\left(\dfrac{\partial A}{\partial I_1} - \dfrac{\partial A}{\partial I_2}\right. \\ \qquad\qquad \left. + b_1(I_2 - I_1)\cos 2(\chi_1 - b_2)\right) + \varepsilon^3 \ldots \\ \dot{\chi}_2 = \varepsilon^2\left(a_1 \dfrac{\partial A}{\partial I_1} + a_2 \dfrac{\partial A}{\partial I_2} + a_3 \dfrac{\partial A}{\partial I_3}\right. \\ \qquad\qquad \left. + b_1(a_1 I_2 + a_2 I_1)\cos 2(\chi_1 - b_2)\right) + \varepsilon^3 \ldots. \end{cases} \tag{10}$$

Dynamically the situation for $k = 1$ (and $k = 3$) is different from $k = 2$ as the normalization removes the terms derived from εH_3 to the normalized $\varepsilon^2 H_4$. The combination angle χ_2, is not necessarily timelike, the equation for $\dot{\chi}_2$ may contain zeros; we will call the zeros critical values of the combination angle. Periodic solutions in $1:1$ resonance can be found if $\sin 2(\chi_1 - b_2) = 0$ or $2(\chi_1 - b_2) = 0, \pi, 2\pi, 3\pi$, and when we can find solutions for I_1, I_2 from $\dot{\chi}_1 = 0$. We define a primary resonance zone M as a neighborhood of the solutions of

$$\sin 2(\chi_1 - b_2) = 0, \quad \dot{\chi}_1 = 0. \tag{11}$$

Such solutions of Eqs. (11), if they exist, are parametrized by I_3 producing to this order manifolds of periodic solutions embedded in the primary resonance zones M.

Outside M and excluding the normal mode planes, the flow is dominated to $O(\varepsilon)$ on the timescale $1/\varepsilon^2$ by the $1:1$ resonance of the first two modes. The action I_3 varies $O(\varepsilon)$ on the same timescale. Outside the resonance zones, the combination angle χ_2 is timelike, so this estimate for I_3 can be improved.

4.2. *Normal forms in the resonance zones*

Smaller, secondary resonance zones in a primary resonance zone M can possibly be found if a combination angle like χ_2 is not timelike in M. To analyze the dynamics in the resonance zones in full generality is cumbersome. We discuss the basic ideas in the case that we have one higher order combination angle χ_2 arising from H_5. If necessary, the procedure can be generalized to more angles. See also the more general formulation involving conservative and dissipative systems in [Verhulst, 1996, Chapter 11.7]. A few details regarding the asymptotics can be found in the Appendix, Sec. A.1. Consider the space-like variables $I = (I_1, I_2, I_3)$ and the angle $\chi_1 = \phi_1 - \phi_2$ determined by (11), and χ_2, a linear combination of ϕ_1, ϕ_2, ϕ_3 with annihilator norm 5. The normalized system in a primary resonance zone is:

$$\begin{cases} \dot{I}_1 = \varepsilon^3[A_1(I) + A_2(I)\sin(\chi_2 - b_3)] + \varepsilon^4 \ldots, \\ \dot{I}_2 = \varepsilon^3[B_1(I) + B_2(I)\sin(\chi_2 - b_3)] + \varepsilon^4 \ldots, \\ \dot{I}_3 = \varepsilon^3[C_1(I) + C_2(I)]\sin(\chi_2 - b_3) + \varepsilon^4 \ldots, \\ \dot{\chi}_1 = \varepsilon^3 D_1(I) + \varepsilon^4 \ldots, \\ \dot{\chi}_2 = \varepsilon^2 E_1(I) + \varepsilon^3[E_2(I) + E_3(I) \\ \qquad \times \cos(\chi_2 - b_3)] + \varepsilon^4 \ldots. \end{cases} \tag{12}$$

In the case of potential problems we have $b_2 = b_3 = 0$. In general, the angle χ_1 will arise again at H_6 ($O(\varepsilon^4)$ terms). The explicit form of the expressions $A(I) \ldots E(I)$ does not concern us at this stage; we will see examples later. Omitting the $O(\varepsilon^3)$ terms in system (9) and solving the resulting system produces an $O(\varepsilon)$ approximation of the solutions on the timescale $1/\varepsilon^2$.

In the primary resonance zone we have that the $O(\varepsilon^2)$ terms of $\dot{\chi}_1$ in system (10) vanish. For fixed energy a few unique solutions $I_1 = I_1^0, I_2 = I_2^0$ may arise parametrized by I_3. There are now at least two possibilities:

- The equation
$$E_1(I_1^0, I_2^0, I_3) = 0, \tag{13}$$
has no positive solution $\bar{I}_3$ for I_3; in this case the angle χ_2 is timelike, we can average over χ_2 reducing the normalized system drastically.
- Equation (13) has unique positive solution $I_3 = \bar{I}_3$ with the point $P = (I_1^0, I_2^0, \bar{I}_3)$ located in the primary resonance zone.

Assume that $\bar{I}_3$ exists. We localize in the primary resonance zone M near P putting

$$\xi_1 = \frac{I_1 - I_1^0}{\delta(\varepsilon)}, \quad \xi_2 = \frac{I_2 - I_2^0}{\delta(\varepsilon)}, \quad \xi_3 = \frac{I_3 - \bar{I}_3}{\delta(\varepsilon)}$$

with $\delta(\varepsilon) \to 0$ as $\varepsilon \to 0$. For the secondary resonance zone embedded in the primary zone (a neighborhood of P) we have the lowest order of equations:

$$\begin{cases} \delta(\varepsilon)\dot{\xi}_1 = \varepsilon^3(A_1(P) + A_2(P)\sin(\chi_2 - b_3)), \\ \delta(\varepsilon)\dot{\xi}_2 = \varepsilon^3(B_1(P) + B_2(P)\sin(\chi_2 - b_3)), \\ \delta(\varepsilon)\dot{\xi}_3 = \varepsilon^3(C_1(P) + C_2(P)\sin(\chi_2 - b_3)), \\ \dot{\chi}_2 = \varepsilon^2\delta(\varepsilon)\left(\dfrac{\partial E_1}{\partial I_1}(P)\xi_1 \right. \\ \qquad \left. + \dfrac{\partial E_1}{\partial I_2}(P)\xi_2 + \dfrac{\partial E_1}{\partial I_3}(P)\xi_3\right). \end{cases} \tag{14}$$

Balancing the equations (significant degeneration) means putting $\varepsilon^3/\delta(\varepsilon) = \varepsilon^2\delta(\varepsilon)$; this produces the choice $\delta(\varepsilon) = \sqrt{\varepsilon}$ which is the size of the secondary resonance zone near P. Differentiation of $\dot{\chi}_2$ yields that the dynamics of the secondary resonance near P is to the lowest order characterized by the pendulum system:

$$\begin{cases} \ddot{\chi}_2 - \varepsilon^5 \left[\dfrac{\partial E_1(P)}{\partial I_1}(A_1(P) + A_2(P)\sin(\chi_2 - b_3)) \right. \\ \quad + \dfrac{\partial E_1(P)}{\partial I_2}(B_1(P) + B_3(P)\sin(\chi_2 - b_3)) \\ \quad \left. + \dfrac{\partial E_1(P)}{\partial I_3}(C_1(P) + C_2(P)\sin(\chi_2 - b_3)) \right] = 0. \end{cases} \tag{15}$$

The system admits a saddle and a center equilibrium; the saddle character is persistent under higher order perturbations and will produce instability. The equilibria will correspond with periodic solutions and will produce other geometric structures in the primary resonance zone. The dynamics in the secondary resonance zone is governed by the timescale $1/\varepsilon^{\frac{5}{2}}$.

The analysis of the secondary resonance and the associated timescale until now is based on the role of ε^2 and ε^3 terms. If we have the combination angles χ_1 and χ_2 with

$$\dot{I}_3 = \varepsilon^m C(I, \sin\chi_1)\sin\chi_2 + \varepsilon^{m+1}\ldots, \quad m \geq 3,$$

we find $\delta(\varepsilon) = \sqrt{\varepsilon^{m-2}}$ and timescale $\varepsilon^{-\frac{m+2}{2}}$. If we have $m > 3$, the size of the secondary resonance domain becomes smaller and the timescale changes accordingly to become larger.

Another natural possibility is that H_5 generates more independent combination angles: $\chi_1, \ldots, \chi_m$, $m \geq 2$. In such a case the dimension of system (12) will become $m+3$, in general we will have more equations to analyze. In the next section we will meet an example.

As stated in Sec. 1, the usual practice in engineering and physics is to focus on low order resonances and neglect the higher order ones. In this respect, a very important question is now: can an instability in a secondary resonance zone destabilize a primary resonance zone? Surprisingly enough, the answer is positive.

4.3. *Critical values in a resonance zone*

We will consider an application to small chains of oscillators in the next sections. Examples from physical models are usually special but interesting. It is natural in applications to have a spectrum of the linearized system such as 1, 1, 5.5 or 2, $\sqrt{2}$, $\sqrt{2}$. First we consider the case of the spectrum 1, 1, m with $m \in \mathbb{N}$, $m \geq 4$ as another typical example.

Suppose we find from Eqs. (11) a primary resonance zone M with solutions

$$I_1 = I_1^0, \quad I_2 = I_2^0, \quad \dot{\chi}_1 = 0.$$

At the level of H_{m+1}, higher order resonances involving the third dof may be found with annihilation vectors

$$(a_1, a_2, a_3) = (a_1, m - a_1, -1).$$

In M where I_1, I_2 have fixed values, such smaller, secondary resonances may be found as zeros of the right-hand side of:

$$\begin{aligned} \frac{d\chi_j}{dt} &= a_1\dot{\phi}_1 + a_2\dot{\phi}_2 + a_3\dot{\phi}_3 \\ &= a_1\dot{\phi}_1 + (m - a_1)\dot{\phi}_2 - \dot{\phi}_3 \\ &= m\dot{\phi}_2 - \dot{\phi}_3, \quad j \geq 2. \end{aligned} \tag{16}$$

This is a remarkable result as it means that for all possible annihilation vectors at H_{m+1} the critical I_3 value for zeros of Eq. (16) in M will be the same. This is a special feature of the resonance $1, 1, m$ with $m \in \mathbb{N}, m \geq 4$. Furthermore, we expect that the variation of ϕ_3 caused by the $O(\varepsilon^3)$ terms will lead to instability of these accumulated resonances in M. The example in the following section will illustrate this.

Computational Strategy

To calculate normal forms of $O(\varepsilon^3)$ or higher is not always necessary in applications. For the $1:1:\omega$ resonance of system (9) one needs the $O(\varepsilon^2)$ terms of the normal form (12). This system gives the location of primary resonance zones (if any) and from the equation for χ_2 we may find the critical values in a resonance zone. This will establish the possible presence of secondary resonances in the resonance zones.

In the subsequent applications, the details of the analysis in the resonance zones are similar. We shall give them explicitly for the $1:1:4$ resonance in the next section.

5. Example: the $1:1:4$ Resonance

We illustrate the dynamics of the $1:1:4$ resonance for the Hamiltonian:

$$\begin{cases} H = \frac{1}{2}(\dot{q}_1^2+q_1^2)+\frac{1}{2}(\dot{q}_2^2+q_2^2)+\frac{1}{2}(\dot{q}_3^2+16q_3^2)-\frac{1}{4}\varepsilon^2(\alpha_1 q_1^4+2\alpha_2 q_1^2q_2^2+\alpha_3 q_2^4+\alpha_4 q_3^4) \\ \qquad -\varepsilon^3(b_1q_1^4q_3+b_2q_2^4q_3+b_3q_1^2q_2^2q_3+b_4q_1^3q_2q_3+b_5q_1q_2^3q_3). \end{cases} \tag{17}$$

The Hamiltonian was chosen in intermediate normal form with the cubic terms transformed to higher order by Birkhoff–Gustavson normalization; we have included $\chi_1=\phi_1-\phi_2$ at H_4 and five combination angles at $H_5:\chi_2,\ldots,\chi_6$. The equations of motion induced by (17) are:

$$\begin{cases} \ddot{q}_1+q_1=\varepsilon^2(\alpha_1q_1^3+\alpha_2q_1q_2^2)+\varepsilon^3(4b_1q_1^3q_3+2b_3q_1q_2^2q_3+3b_4q_1^2q_2q_3+b_5q_2^3q_3), \\ \ddot{q}_2+q_2=\varepsilon^2(\alpha_2q_1^2q_2+\alpha_3q_2^3)+\varepsilon^3(4b_2q_2^3q_3+2b_3q_1^2q_2q_3+b_4q_1^3q_3+3b_5q_1q_2^2q_3), \\ \ddot{q}_3+16q_3=\varepsilon^2\alpha_4q_3^3+\varepsilon^3(b_1q_1^4+b_2q_2^4+b_3q_1^2q_2^2+b_4q_1^3q_2+b_5q_1q_2^3). \end{cases} \tag{18}$$

At H_5 with annihilation vector (a_1,a_2,a_3), $a_1+a_2=4, a_3=-1$, we have:

$$\chi_2=4\phi_1-\phi_3,\quad \chi_3=4\phi_2-\phi_3,\quad \chi_4=2\phi_1+2\phi_2-\phi_3,\quad \chi_5=3\phi_1+\phi_2-\phi_3,\quad \chi_6=\phi_1+3\phi_2-\phi_3.$$

We will use polar (amplitude-phase) coordinates r,ψ. Using transformation (4) we find after averaging to $O(\varepsilon^2)$:

$$\begin{cases} \dot{r}_1=-\varepsilon^2\frac{\alpha_2}{8}r_1r_2^2\sin 2\chi_1+\varepsilon^3\ldots,\quad \dot{\phi}_1=-\varepsilon^2\frac{1}{8}(3\alpha_1r_1^2+2\alpha_2r_2^2+\alpha_2r_2^2\cos 2\chi_1)+\varepsilon^3\ldots, \\ \dot{r}_2=\varepsilon^2\frac{\alpha_2}{8}r_1^2r_2\sin 2\chi_1+\varepsilon^3\ldots,\quad \dot{\phi}_2=-\varepsilon^2\frac{1}{8}(2\alpha_2r_1^2+\alpha_2r_1^2\cos 2\chi_1+3\alpha_3r_2^2)+\varepsilon^3\ldots, \\ \dot{r}_3=\varepsilon^3\ldots,\quad \dot{\phi}_3=-\varepsilon^2\frac{3\alpha_4}{32}r_3^2+\varepsilon^3\ldots. \end{cases} \tag{19}$$

This system corresponds with system (9) in amplitude-phase form. The dots represent higher order terms containing the amplitudes and the combination angles $\chi_2,\ldots,\chi_6$. For the averaging-normal form (19) we have

$$r_1^2+r_2^2-2E_1=O(\varepsilon)$$

and $r_3-r_3(0)=O(\varepsilon)$ with both estimates valid on the timescale $1/\varepsilon^2$. With the Hamiltonian as first integral this makes normal form (19) integrable to $O(\varepsilon^2)$.

As before, a primary resonance zone M is defined as a neighborhood of the solutions of $\sin 2\chi_1=0, \dot{\chi}_1=0$. We find with system (19):

$$\dot{\chi}_1=-\frac{1}{8}\varepsilon^2((3\alpha_1-2\alpha_2)r_1^2+(2\alpha_2-3\alpha_3)r_2^2 \\ +\alpha_2(r_2^2-r_1^2)\cos 2\chi_1). \tag{20}$$

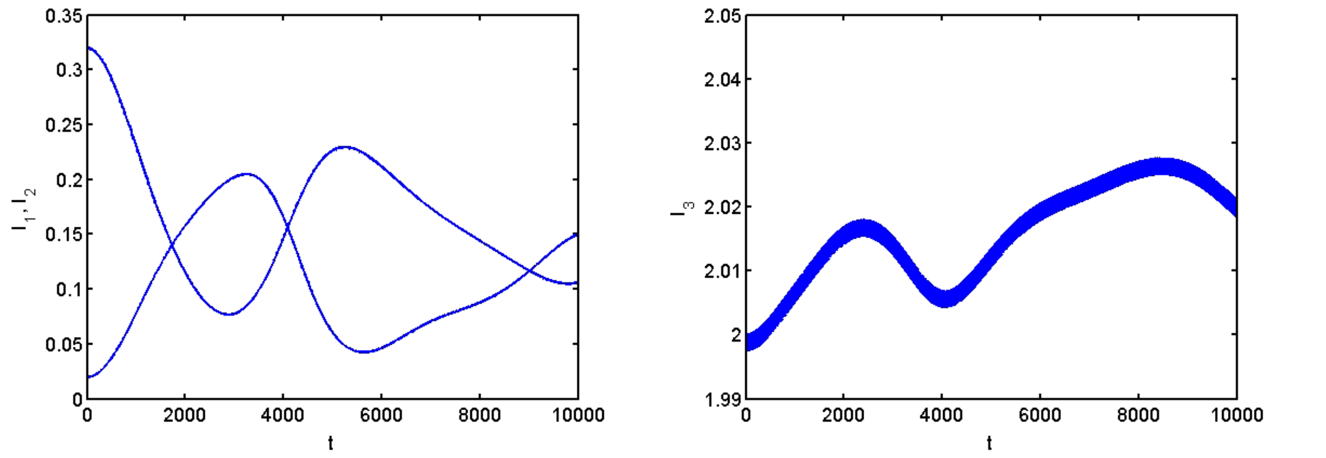
Taking the right-hand side of Eq. (20) as zero we find the primary resonance zones M_1, M_2:

$$\begin{cases} M_1: r_1^2=\dfrac{\alpha_2-\alpha_3}{\alpha_2-\alpha_1}r_2^2, \\ M_2: r_1^2=\dfrac{\alpha_2-3\alpha_3}{\alpha_2-3\alpha_1}r_2^2. \end{cases} \tag{21}$$

We require the right-hand sides of r_1^2 in (21) to be finite and positive. In Fig. 1 we present (a) the resonant actions I_1, I_2 and (b) the nearly invariant I_3 starting outside the primary resonance zones defined by (21). We find $1:1$ resonant interaction of the first two modes and small modulation of the third mode.

5.1. *Secondary resonance in the primary resonance zones*

For the five combination angles $\chi_2,\ldots,\chi_6$, $j=2,\ldots,6$, we find with annihilation vector $(a_1,a_2,a_3)=(a_1,4-a_1,-1)$ and Eq. (16) to $O(\varepsilon^2)$ in the



(a)

(b)

Fig. 1. The $1:1:4$ resonance with the actions I_1, I_2, I_3 in 10 000 timesteps for Hamiltonian (17) starting outside the primary resonance zones; initial conditions: $q_1(0) = 0.2, q_2(0) = 0.8, q_3(0) = 1$ and parameters: $\varepsilon = 0.1$, $\alpha_1 = 0.4, \alpha_2 = 1, \alpha_3 = 0.6, \alpha_4 = 4, b_1 = 1, b_2 = -1.5, b_3 = 1, b_4 = -1, b_5 = 2$. (a) I_1, I_2 showing strong energy exchanges, the q_1 and q_2 normal modes are unstable. (b) The action I_3 showing variations of order 0.01.

primary resonance zones:

$$\dot{\chi}_j = -\frac{1}{8}\varepsilon^2\left(8\alpha_2 r_1^2 + 12\alpha_3 r_2^2 + 4\alpha_2 r_1^2\cos 2\chi_1 - \frac{3}{4}\alpha_4 r_3^2\right), \quad \cos 2\chi_1 = \pm 1. \tag{22}$$

Secondary resonances involving the five combination angles in M_1 and M_2 may arise where the right-hand side of Eq. (22) vanishes; in such a case the angle χ_j is not timelike. Remarkably enough the condition is the same for the five combination angles as predicted in Sec. 4.3. To study the stability within the resonance zones we compute $\dot{\phi}_3$ to $O(\varepsilon^3)$. We find:

$$\dot{\phi}_3 = -\varepsilon^2\frac{3\alpha_4}{32}r_3^2 - \varepsilon^3\frac{69}{128^2}\alpha_4^2 r_3^4 - \frac{\varepsilon^3}{64 r_3}A(r_1, r_2, \chi_2, \ldots, \chi_6)$$

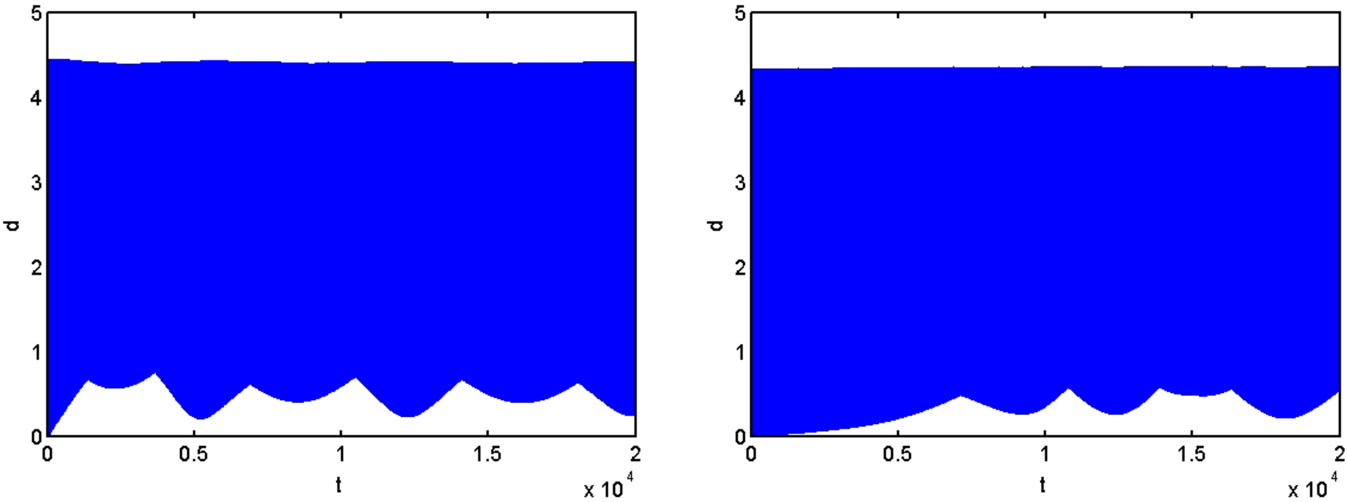
with

$$\begin{aligned} A(r_1, r_2, \chi_2, \ldots, \chi_6) &= b_1 r_1^4\cos\chi_2 + b_2 r_2^4\cos\chi_3 + b_3 r_1^2 r_2^2\cos\chi_4 \\ &\quad + b_4 r_1^3 r_2\cos\chi_5 + b_5 r_1 r_2^3\cos\chi_6. \end{aligned}$$

We conclude that unless all b_i coefficients and α_4 vanish, ϕ_3 may move out of resonance in the primary resonance zones on a timescale longer than $1/\varepsilon^2$. The higher order resonances included in M_1, M_2 may generate instabilities, see Fig. 2. From Sec. 4.2, we conclude that if secondary resonances arise from zeros of $\dot{\chi}_j, j = 2, \ldots, 6$, we find stable and unstable periodic solutions from the normal forms in the resonance zones and characteristic timescale $1/\varepsilon^{5/2}$. Consider the following analysis.

The recurrency properties of the phase-flow are strongly dependent on the initial conditions. To study the structure of the resonance zones we consider the normal form to $O(\varepsilon^3)$ in M_1. To make the expressions more transparent we keep only b_3 and combination angle χ_4. With $\cos 2\chi_1 = 1$ and Eq. (22) we find in M_1 the following normal form:

$$\begin{cases} \dot{r}_1 = -\varepsilon^3\dfrac{b_3}{8}r_1 r_2^2 r_3\sin\chi_4, & \dot{\phi}_1 = -\varepsilon^2\dfrac{3}{8}(\alpha_1 r_1^2 + \alpha_2 r_2^2) - \varepsilon^3\dfrac{b_3}{8}r_2^2 r_3\cos\chi_4, \\ \dot{r}_2 = -\varepsilon^3\dfrac{b_3}{8}r_1^2 r_2 r_3\sin\chi_4, & \dot{\phi}_2 = -\varepsilon^2\dfrac{3}{8}(\alpha_2 r_1^2 + \alpha_3 r_2^2) - \varepsilon^3\dfrac{b_3}{8}r_1^2 r_3\cos\chi_4, \\ \dot{r}_3 = \varepsilon^3\dfrac{b_3}{64}r_1^2 r_2^2\sin\chi_4, & \dot{\phi}_3 = -\varepsilon^2\dfrac{3\alpha_4}{32}r_3^2 - \varepsilon^3\dfrac{b_3}{64}\dfrac{r_1^2 r_2^2}{r_3}\cos\chi_4, \\ \dot{\chi}_4 = -\varepsilon^2\dfrac{3}{2}\left(\alpha_2 r_1^2 + \alpha_3 r_2^2 - \dfrac{1}{16}\alpha_3 r_3^2\right) - \varepsilon^3\dfrac{b_3 r_1^2}{64 r_3}(32 r_3^2 - r_2^2)\cos\chi_4. & \end{cases} \tag{23}$$



(a) (b)

Fig. 2. The $1:1:4$ resonance in 20 000 timesteps. (a) The Euclidean distance d of the orbits to their initial conditions in the case of initial conditions (outside M_1) and parameters of Fig. 1; recurrence takes many more timesteps; computing with higher precision than relative tolerance e^{-15}, abs. tolerance e^{-15} does not change the picture. (b) The Euclidean distance d for the same Hamiltonian (17) but inside primary resonance zone M_1, starting at a location of higher order resonances $q_1(0) = 0.3674, q_2(0) = 0.45, q_3(0) = 1.0129$ ($\cos 2\chi_1 = 1$). The recurrence is stronger until the orbit drifts further than around 2000 timesteps outside the higher order resonance location in M_1. I_3 (and r_3) experiences 0.01 variation downwards.

The normal form (23) in M_1 has the integral

$$r_1^2 + r_2^2 + 16r_3^2 = 2E_2, \tag{24}$$

with E_2 a positive constant. The integral corresponds with H_2 of the Hamiltonian and is valid for all time. The combination angle χ_4 is not timelike if in M_1:

$$\alpha_2 r_1^2 + \alpha_3 r_2^2 - \frac{1}{16}\alpha_4 r_3^2 = 0. \tag{25}$$

From Eq. (21) we have the relation between r_1 and r_2 in M_1, with the first integral (24) we determine r_3 in the primary resonance zone. In system (23) the motion of χ_4 dominates the dynamics. Differentiation of $\dot{\chi}_4$ produces the equation:

$$\begin{aligned} &\ddot{\chi}_4 - \varepsilon^5 F(r_1, r_2, r_3)\sin\chi_4 = O(\varepsilon^6), \\ &F(r_1, r_2, r_3) = \frac{3}{8}\left(\alpha_2 + \alpha_3 + \frac{1}{128}\alpha_4\right) b_3 r_1^2 r_2^2 r_3. \end{aligned} \tag{26}$$

The amplitudes are constant to this order of approximation, the timescale for $\chi_4(t)$ is $1/\varepsilon^{5/2}$. The equilibria, center and saddle, produce the stable and unstable resonances in M_1. In the terminology of papers on double resonances, a neighborhood of the center and saddle in M_1 will be called a resonant junction. Note that chaos will in general be present in the resonance zones, but as we see from system (23) it will be of small scale, the normal form is integrable to this high order.

The unstable manifolds of the unstable periodic solutions will be guiding the solutions that leave the resonance zone or are passing through it.

For illustrations we postponed the choice of the constants $\alpha_1, \ldots, \alpha_4$ to be able to exclude nongeneric cases like $\alpha_1 = \alpha_3$. We choose

$$\alpha_1 = 0.4, \quad \alpha_2 = 1, \quad \alpha_3 = 0.6, \quad \alpha_4 = 4. \tag{27}$$

This choice results in

$$\dot{\chi}_1 = -\frac{1}{8}\varepsilon^2(-0.8r_1^2 + 0.2r_2^2 + (r_2^2 - r_1^2)\cos 2\chi_1). \tag{28}$$

Equation (28) results in resonance zones generated by χ_1, i.e. small neighborhoods of

$$\begin{aligned} &M_1\colon\ 3r_1^2 - 2r_2^2 = 0, \quad (2\chi_1 = 0, 2\pi), \\ &M_2\colon\ \ r_1^2 - 4r_2^2 = 0, \quad (2\chi_1 = \pi, 3\pi). \end{aligned} \tag{29}$$

In Fig. 2 we show the Euclidean distance to the initial conditions in two cases. On the left we start away from stable periodic solutions (outside M_1), the orbits have a recurrence delayed by quasi-trapping in M_1; this is related to the invariant manifolds described above. On the right we start with the same Hamiltonian in the resonance zone M_1 but near a location where the higher order combination angles are not timelike; the recurrence is stronger but then the variation of ϕ_3 produces a drift-off of the solutions in M_1 and worse recurrence.

In Fig. 3 we show the recurrence in M_1 when we start with initial conditions for the third mode in the stable regime. The three projections of the corresponding orbits illustrate the regular recurrence.

The combination angle $\chi_j, j = 2, 3, \ldots$ from Eq. (22) is not timelike in a subset of M_1 if we can find values of the amplitudes (or actions) such that:

$$4r_1^2 + 2.4r_2^2 = r_3^2. \tag{30}$$

In M_2 we find:

$$4r_1^2 + 7.2r_2^2 = 3r_3^2. \tag{31}$$

To illustrate the stable and unstable behaviors of the solutions starting in M_1 we present in Fig. 4, the case where $q_3(0) = 0.3$ (χ_j is timelike) on the left and the unstable case $q_3(0) = 1.0129$ on the

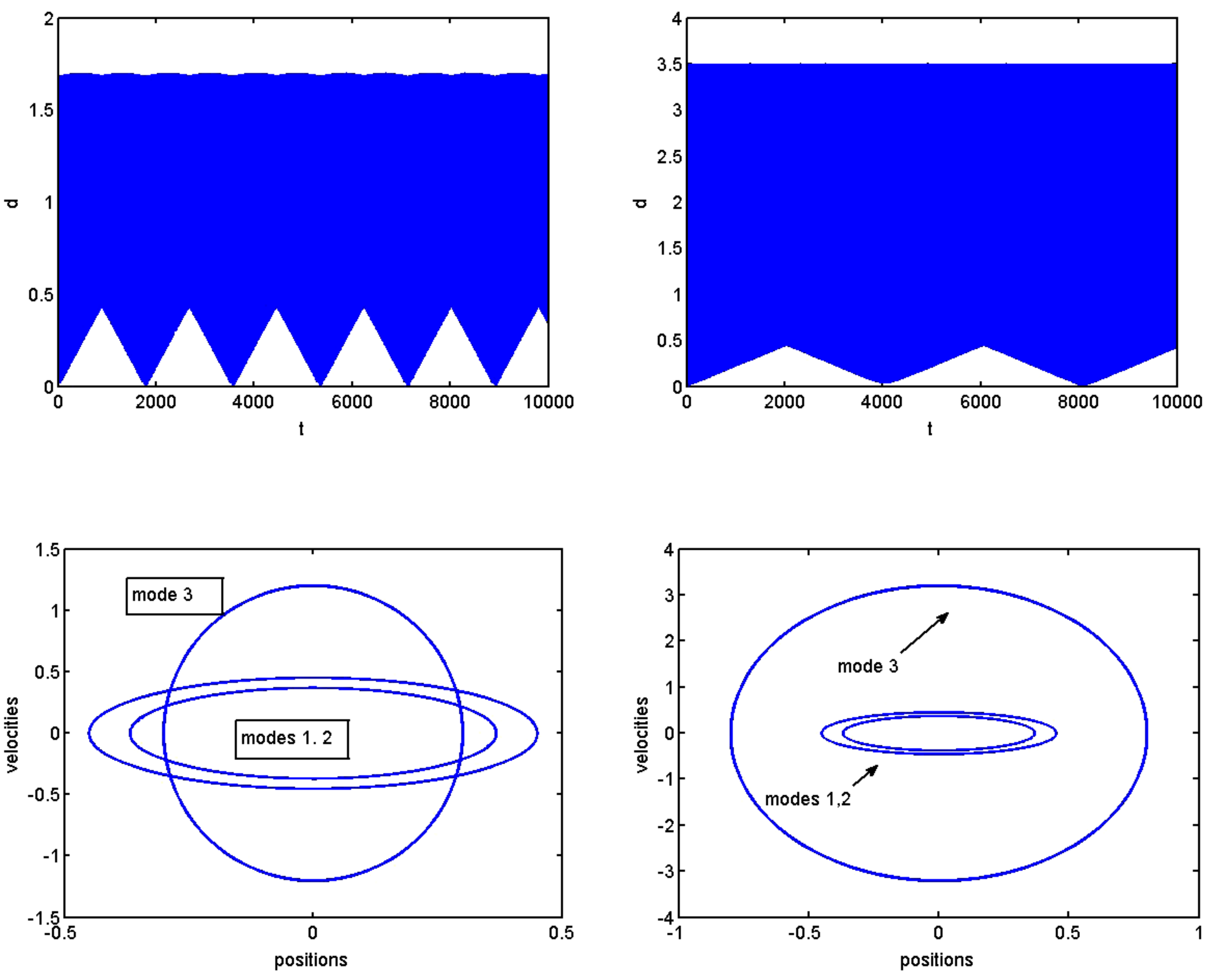


Fig. 3. (Top) Recurrence in the primary resonance zone M_1 measured by the Euclidean distance d in 10 000 timesteps of the orbits to their initial conditions. The initial conditions and parameters are as in Fig. 2 except that we considered different regions of M_1 by choosing (left) $q_3(0) = 0.3$ and (right) $q_3(0) = 0.8$. The recurrence is in both cases much faster but different as we are removed from the small higher order resonance zones in M_1. The orbits are caught in the resonance zone M_1. (Bottom) Projections of the corresponding orbits in M_1.

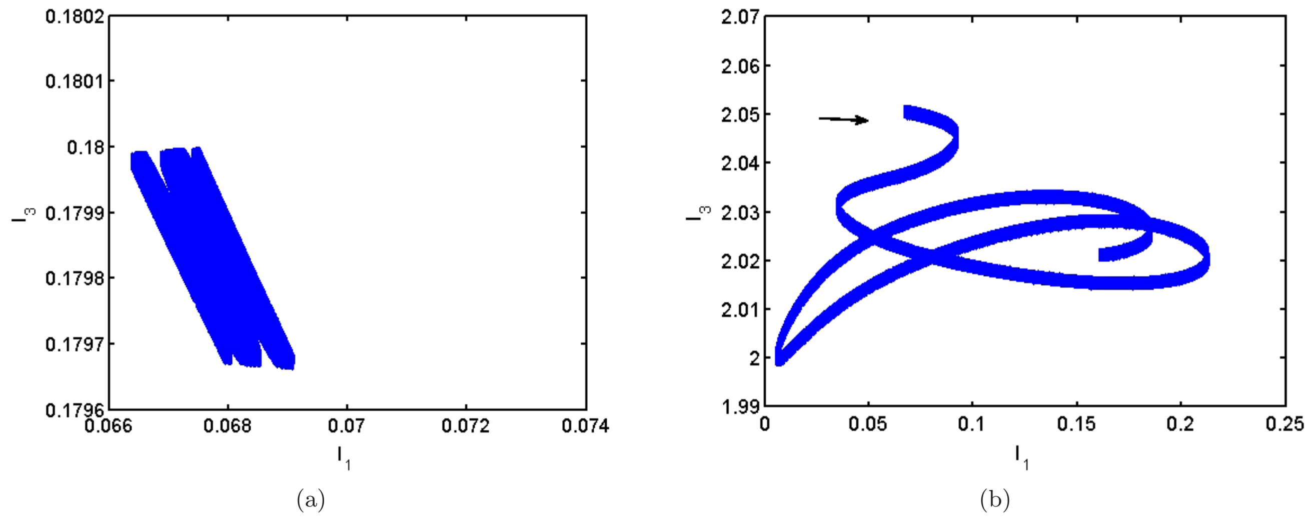


Fig. 4. Dynamics in the primary resonance zone M_1 by the diagrams (I_1, I_3) for 20 000 timesteps. (a) The case $q_3(0) = 0.3$ of Fig. 3 where $I_1(t)$ and $I_3(t)$ are close to constant (variations of order 10^{-3} and 10^{-4}). (b) The unstable case of $q_3(0) = 1.0129$ in Fig. 2; the variations of $I_1(t)$ are considerable, in this case, the orbits leave the primary resonance zone (the arrow indicates the start).

right. The scales have been adjusted to the variations of $I_1(t), I_3(t)$.

6. Application to a FPU-Chain with Four Particles

The original motivation for this paper came from the spatially periodic Fermi–Pasta–Ulam problem with alternating masses (see [Bruggeman & Verhulst, 2018]), and from studying nonlinear wave equations with Galerkin projection. The Hamiltonian in [Bruggeman & Verhulst, 2018] is more general than the classical FPU case and is of the form:

$$H(p,q) = \sum_{j=1}^{n} \left(\frac{1}{2m_j} p_j^2 + V(q_{j+1} - q_j) \right)$$

$$\text{with } V(z) = \frac{1}{2}z^2 + \frac{\alpha}{3}z^3 + \frac{\beta}{4}z^4. \quad (32)$$

For odd index j we have $m_j = 1$, for even j, $m_j = m > 0$. If $m = 1$ we have the classical FPU-chain. If $\alpha \neq 0, \beta = 0$ we will call this an α-chain, if $\alpha = 0, \beta \neq 0$, a β-chain. In the case $\alpha\beta \neq 0$, we keep α and β as free parameters as the dynamics depends on their ratio.

To consider four particles only, is less restrictive than it appears. It was shown in [Bruggeman & Verhulst, 2018] that a system of four particles with its dynamics can be identified as a submanifold of a periodic FPU-chain with $4n$ particles (n an arbitrary natural number). There exist in this system *bushes* (in the terminology of [Chechin *et al.*, 2002]) of submanifolds with this dynamics.

The equations of motion have the momentum integral

$$m_1\dot{q}_1 + m_2\dot{q}_2 + \cdots + m_n\dot{q}_n = P_0. \quad (33)$$

P_0 is a constant. We will consider the case of four particles. The second integral (33) enables us to reduce the system by one dof. In the case of four particles we find with the usual scaling near stable equilibrium:

$$\begin{cases} \ddot{x}_1 + 2(1+a)x_1 = \varepsilon\alpha(\gamma x_2 x_3) + \varepsilon^2\beta(-(1+a)^2 x_1^3 \\ \qquad\qquad - 3(1+a)x_1(x_2^2 + a x_3^2)), \\ \ddot{x}_2 + 2x_2 = \varepsilon\alpha(\gamma x_1 x_3) + \varepsilon^2\beta(-x_2^3 - 3a x_2 x_3^2 \\ \qquad\qquad - 3(1+a)x_1^2 x_2), \\ \ddot{x}_3 + 2a x_3 = \varepsilon\alpha(\gamma x_1 x_2) + \varepsilon^2\beta(-3a x_2^2 x_3 - a^2 x_3^3 \\ \qquad\qquad - 3a(1+a)x_1^2 x_3). \end{cases} \quad (34)$$

In this system $a = 1/m$, $\gamma = 2\sqrt{2a(1+a)}$. Three exact families of periodic solutions are the normal modes associated with the eigenvalues $2(1+a)$, 2 and $2a$. The exact solutions are harmonic for an α-chain. In the classical case $a = 1$ we find in addition for the β-chain exact periodic solutions with $x_2(t) = \pm x_3(t)$. The solutions satisfy $x_1 = \dot{x}_1 = 0$ and

$$\ddot{x}_2 + 2x_2 = -4\varepsilon^2\beta x_2^3.$$

Important sets of special (exact) solutions of system (34) are found if $a = 1$ and for arbitrary α, β on putting $x_2(t) = \pm x_3(t)$. The variable x_1 is still free, so we have with these assumptions two manifolds of solutions of system (34) satisfying for $a = 1$ the system:

$$\begin{cases} \ddot{x}_1 + 4x_1 = \pm 4\varepsilon\alpha x_2^2 + 4\varepsilon^2\beta(-x_1^3 - 3x_1x_2^2), \\ \ddot{x}_2 + 2x_2 = \pm 4\varepsilon\alpha x_1x_2 + 2\varepsilon^2\beta(-2x_2^3 - 3x_1^2x_2), \\ x_2(t) = \pm x_3(t). \end{cases} \tag{35}$$

Near-Identity Transformation

To obtain normal forms for the equations of motion one uses near-identity transformations following Birkhoff–Gustavson or equivalently averaging, see [Sanders *et al.*, 2007]. We will use both.

For all choices of a the first order averaging terms of system (34) vanish (although two first order resonances are present: $a = \frac{1}{4}$ and $a = \frac{1}{3}$). Using polar coordinates as before, the implication is that the three amplitudes and phases are constant with error $O(\varepsilon)$ on the timescale $1/\varepsilon$. Interesting phenomena happen on a longer timescale; for the actions we have of course the same result.

The estimate of [Nekhoroshev, 1977] for near and long-time conservation of the actions cannot be applied in the classical case $m = 1$ because of the $1 : 1$ resonance. For arbitrary m, this also holds if $m \gg 1$ $(0 < a \ll 1)$ as we find detuned $1 : 1$ resonances. With four particles, we will focus in the sequel on the classical case $a = 1$.

6.1. *Normalizing the classical FPU-chain* $(a = 1)$

The normalization to second order was carried out by [Rink & Verhulst, 2000], we will add results regarding passage through resonance zones to the analysis. The normalized Hamiltonian $\overline{H}$ to quartic terms, quadratic in the actions, is:

$$\begin{cases} \overline{H} = 2I_1 + \sqrt{2}I_2 + \sqrt{2}I_3 - \varepsilon^2 \left[\left(\frac{1}{2}\alpha^2 - \frac{3}{8}\beta\right) I_2I_3\cos 2(\phi_2 - \phi_3) \right. \\ \qquad \left. - \frac{3}{8}\beta I_2I_3 - \frac{3}{16}\beta(I_2 + I_3)^2 - \frac{3}{8}\beta I_1^2 + \sqrt{2}\left(\frac{1}{2}\alpha^2 - \frac{3}{4}\beta\right) I_1(I_2 + I_3) \right]. \end{cases} \tag{36}$$

For the mode with frequency ω we have $q = \sqrt{2I/\omega}\sin\phi$, $p = \sqrt{2\omega I}\cos\phi$. We will consider the α- and β-chain in the case that the two normal modes x_2, x_3 of the $1 : 1$ resonance are unstable, producing passage through resonance zones and strong exchanges of energy between the two modes; the x_1 mode acts as a perturbation on the $1 : 1$ resonance. In both cases, we have, in general, the position of four periodic solutions of the normalized Hamiltonian with $\chi = \phi_2 - \phi_3$, $\sin 2\chi = 0$ located in a primary resonance zone M. Starting near an unstable normal mode will induce passage through M. The quantity

$$\sqrt{2}(I_2 + I_3) = E_1 \tag{37}$$

with constant $E_1 \geq 0$ is conserved to $O(\varepsilon)$ on the timescale $1/\varepsilon^2$, $\dot{I}_1 = O(\varepsilon^3)$. In addition, we have $2I_1 + \sqrt{2}I_2 + \sqrt{2}I_3 = E_0 + O(\varepsilon)$ for all time (E_0, E_1 positive constants).

6.2. *The α-chain*

Consider the α-chain $(\alpha = 1, \beta = 0)$. We note that the nondegeneracy condition of the KAM theorem is not satisfied for the normal form Hamiltonian (36) if $\beta = 0$ as the nonresonant frequency of x_1 removes the twist character of the $\dot{x}_1, x_1$-flow. As we will see, this has consequences for the analysis.

From [Rink & Verhulst, 2000] we know that the x_2, x_3 normal modes are unstable, the x_1 normal mode is spectrally stable. From the normal form (36) we have for the actions and the combination angle $\chi = \phi_2 - \phi_3$ omitting terms $O(\varepsilon^3)$:

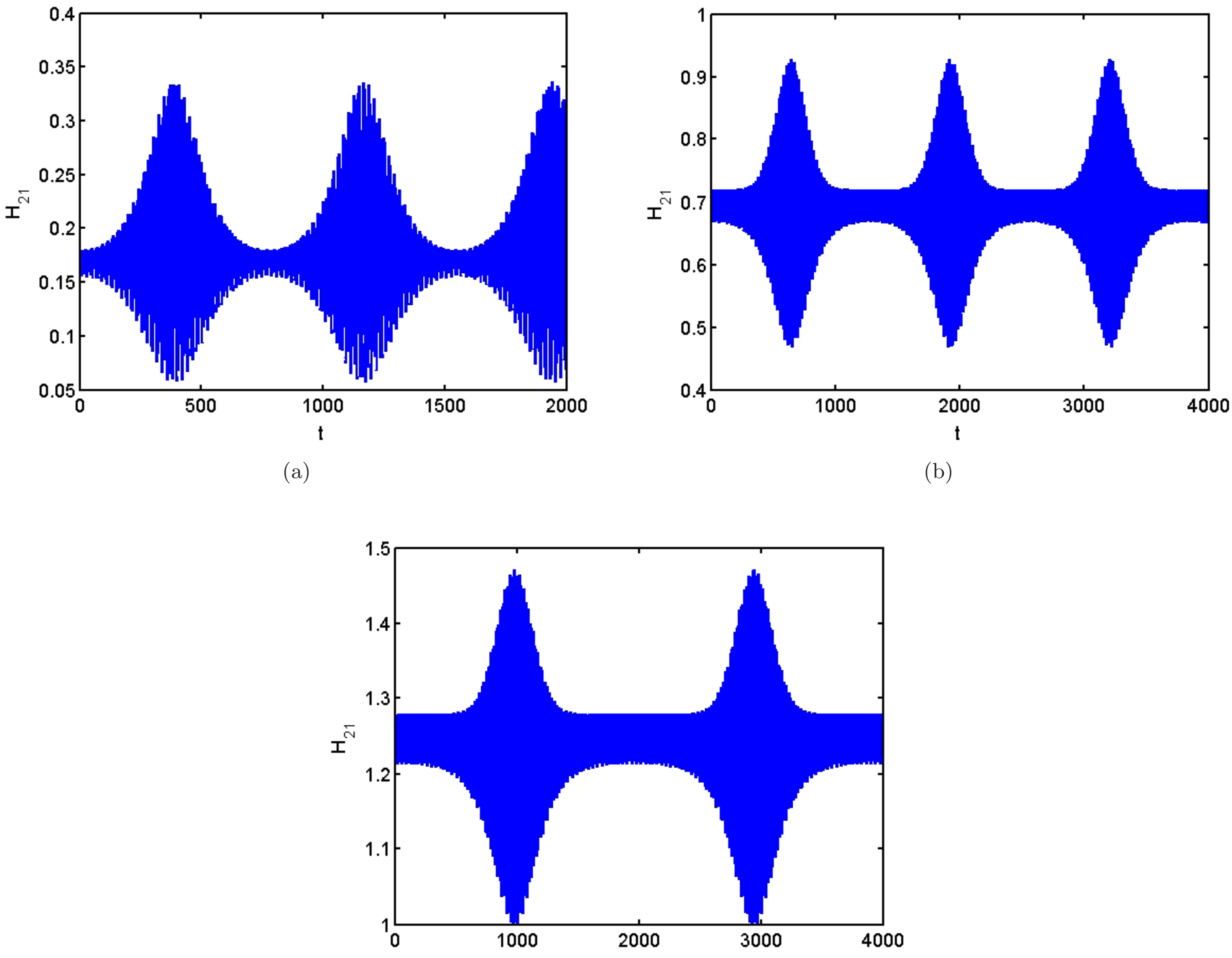
$$\begin{cases} \dot{I}_1 = 0, \quad \dot{I}_2 = -\varepsilon^2 I_2I_3\sin 2\chi, \\ \dot{I}_3 = \varepsilon^2 I_2I_3\sin 2\chi, \\ \dot{\phi}_1 = 2 - \frac{\varepsilon^2}{2}\sqrt{2}(I_2 + I_3), \\ \dot{\phi}_2 = \sqrt{2} - \frac{\varepsilon^2}{2}(I_3\cos 2\chi + \sqrt{2}I_1), \\ \dot{\phi}_3 = \sqrt{2} - \frac{\varepsilon^2}{2}(I_2\cos 2\chi + \sqrt{2}I_1), \\ 2\dot{\chi} = \varepsilon^2(I_2 - I_3)\cos 2\chi. \end{cases} \tag{38}$$

General positions of periodic solutions are found from the normal form for $I_2 = I_3 = \frac{1}{4}\sqrt{2}E_1$, $\chi = 0, \pi$ producing resonance zone M_1, or $\pi/2$, $3\pi/2$ producing resonance zone M_2; they are spectrally stable. As $I_1(0)$ is still free to choose, these periodic solutions correspond in the normal form system with manifolds located in each of the primary resonance zones M_1, M_2 on a fixed energy manifold; we have parametrization of the periodic solutions for $0 \leq I_1(0) \leq \frac{1}{2}E_0$. The primary resonance zones are small neighborhoods of the solutions given by $I_2 = I_3$, $\chi = 0, \pi$ (M_1) and $I_2 = I_3$, $\chi = \pi/2, 3\pi/2$ (M_2).

From system (34) for $a = 1$ we have the special (exact) solutions $x_2(t) = \pm x_3(t)$ satisfying:

$$\begin{cases} \ddot{x}_1 + 4x_1 = \pm 4\varepsilon x_2^2, \\ \ddot{x}_2 + 2x_2 = \pm 4\varepsilon x_1 x_2. \end{cases} \tag{39}$$

So $x_1(t)$ experiences when passing through $M_{1,2}$ a small nonresonant excitation, see Fig. 5. The periodic solutions in general position obtained from the normal form (38) do not persist in the original system as periodic solutions; we conjecture that they can be continued as quasi- or almost-periodic solutions. We offer the following



(a)

(b)

(c)

Fig. 5. The classical α-chain, passage through a primary resonance zone. The actions H_{21} for system (34) (case $a = 1$) with $\alpha = 1, \beta = 0$ in three cases with $H_2(0) = 3.01$. Initial conditions: $(x_1(0) = 0.3, x_2(0) = 1.6793, x_3(0) = 0.1)$, $(x_1(0) = 0.6, x_2(0) = 1.50997, x_3(0) = 0.1)$ and $(x_1(0) = 0.8, x_2(0) = 1.3115, x_3(0) = 0.1)$, initial velocities zero and $\varepsilon = 0.1$. The action H_{21} shows variations of magnitude 0.02 outside the resonance zone and significant excitation, magnitude 0.2, in the zone.

evidence:

From the normal form system (38) we have for these solutions in M_1 the $O(\varepsilon)$ approximations on the timescale $1/\varepsilon^2$:

$$\begin{cases} x_1(t) = \sqrt{2I_1(0)}\sin\left(2t - \dfrac{1}{2}\varepsilon^2 t\sqrt{2}(I_2(0) + I_3(0)) + \dfrac{\pi}{2}\right), \\ x_2(t) = \sqrt{2I_2(0)}\sin\left(\sqrt{2}t - \dfrac{1}{2}\varepsilon^2 t I_2(0) - \dfrac{1}{2}\varepsilon^2 t\sqrt{2}I_1(0) + \dfrac{\pi}{2}\right), \\ x_3(t) = x_2(t). \end{cases} \tag{40}$$

A similar result holds for M_2. The approximate solutions are quasi-periodic with, for fixed energy, periods dependent on the initial values of the nonresonant mode x_1 and x_2, x_3. In the resonance zones, the excitation of x_1 is during the passage $O(\varepsilon)$.

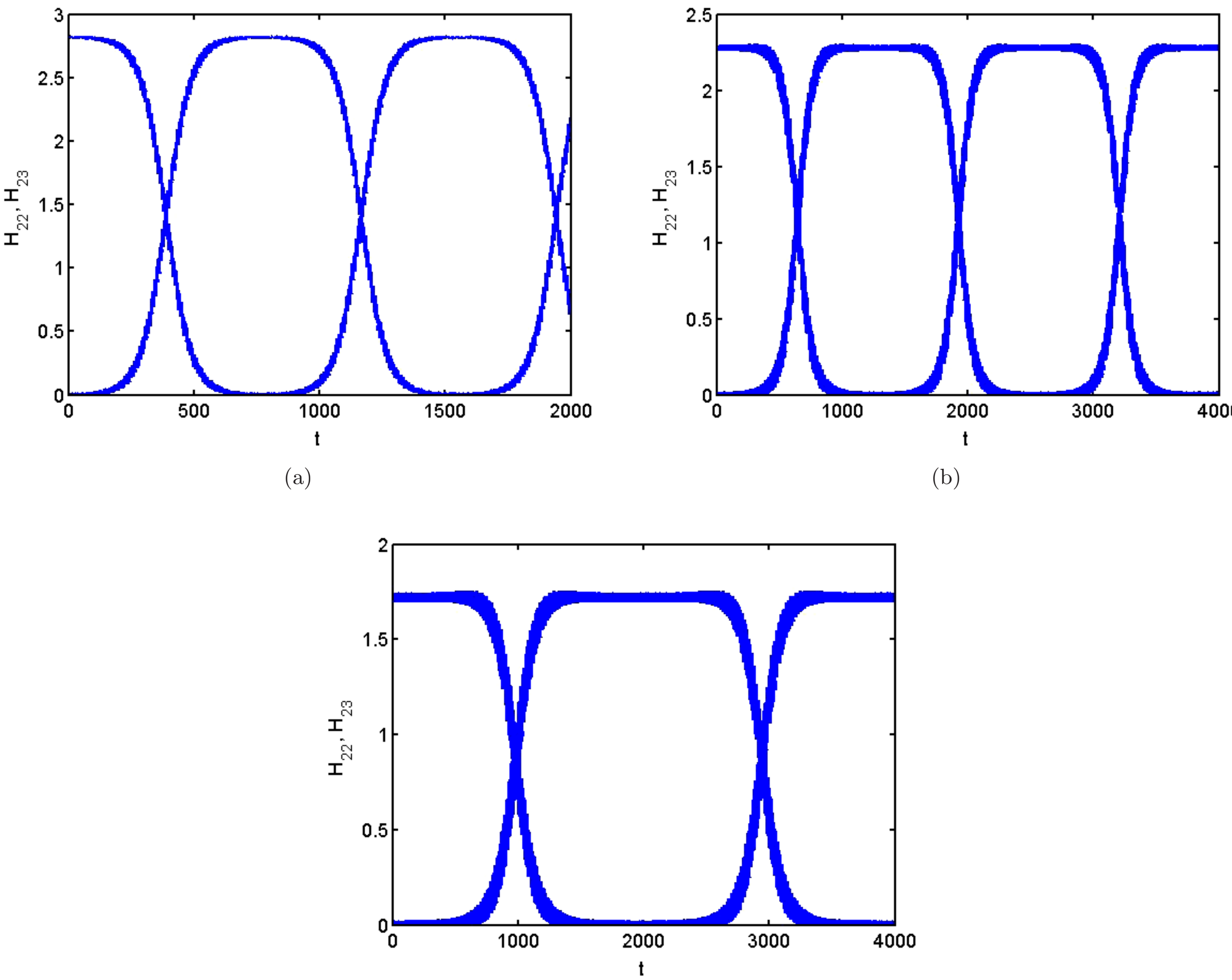


Fig. 6. The classical α-chain, passage through a primary resonance zone showing the actions H_{22}, H_{23} corresponding with x_2, x_3 of system (34) (case $a = 1$) with $\alpha = 1, \beta = 0$. The three cases have the initial conditions of the three cases in Fig. 5 with $H_2(0) = 3.01$. Whenever $H_{22} = H_{23}$ we observe excitation of the x_1 mode in the resonance zone. The time of passage increases with $x_1(0)$.

In the illustrations, we use quantities that, apart from a scaling factor, are equal to the actions:

$$H_{21} = \frac{1}{2}(\dot{x}_1^2 + 4x_1^2),$$
$$H_{22} = \frac{1}{2}(\dot{x}_2^2 + 2x_2^2), \quad (41)$$
$$H_{23} = \frac{1}{2}(\dot{x}_3^2 + 2x_3^2).$$

We keep $H_2(0)$ constant in the pictures as H_2 is an integral of the normal form. Figure 5 shows, as expected, small variations of the first mode except for the excitation when passing a resonance zone, see system (39). The fluctuations of $x_1, \dot{x}_1$ in Fig. 5 are clearly larger when passing the primary resonance zone where $H_{22} = H_{23}$. We demonstrate this in the corresponding figures of the exchanges of energy in Fig. 6. As we start near the unstable x_2 normal mode, we find rather strong exchanges of energy; this suggests that we will have quasi-trapping near the tori surrounding the solutions in the resonance zones where x_1 also plays a part.

The recurrence times T_r of the phase-flow can be deduced from the behavior of the actions in Figs. 5 and 6. The mechanism of quasi-trapping is illustrated by the recurrence displayed in Fig. 7. The Euclidean distance d to the initial conditions corresponding with the three cases of Fig. 5 shows large gaps in the recurrence behavior.

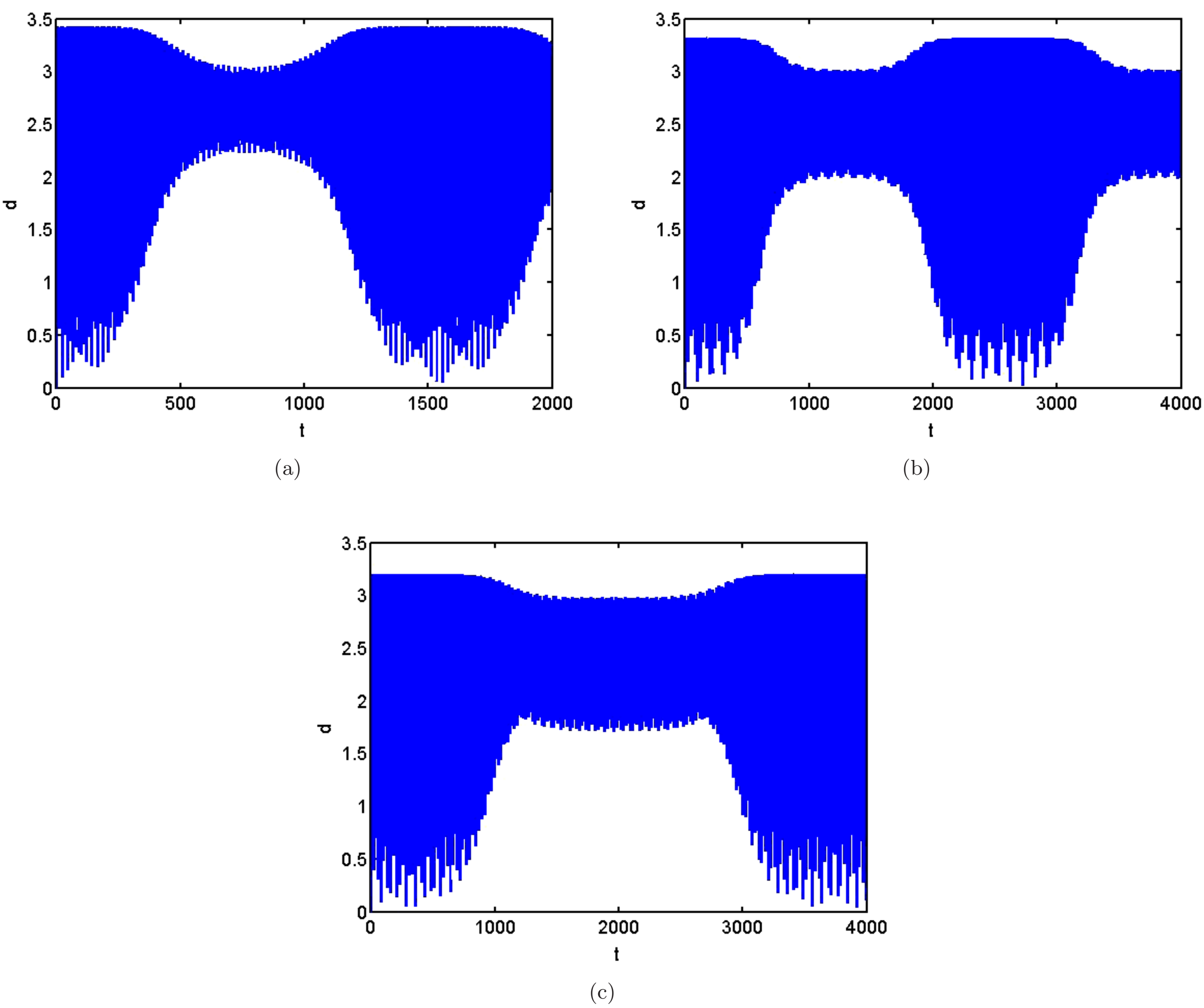


Fig. 7. The classical α-chain, passage through resonance, showing the Euclidean distance d to the initial conditions in the cases of Fig. 5, keeping $H_2(0) = 3.01$ fixed. The recurrence times increase with $x_1(0)$, see also Fig. 8.

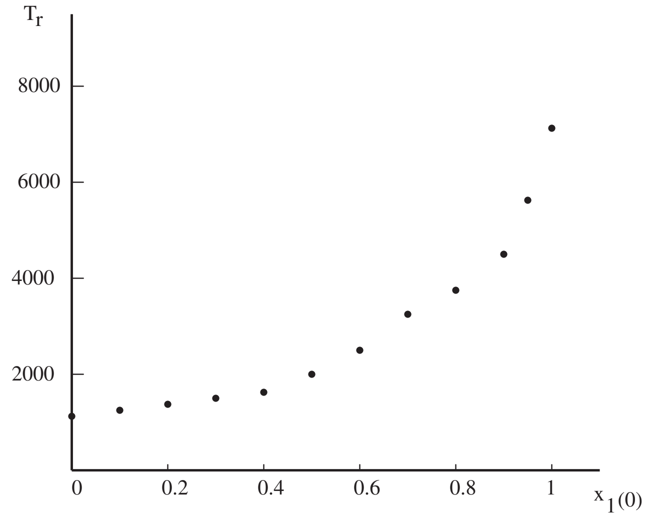


Fig. 8. The classical α-chain, recurrence times T_r after passage through a primary resonance zone from numerical integration of system (34) (case $a = 1$) with $\alpha = 1, \beta = 0$. We consider 12 cases with $H_2(0) = 3.01, x_3(0) = 0.1$ fixed; initial velocities of the components are zero and $\varepsilon = 0.1$. Starting near the unstable x_2 normal mode, the recurrence time increases strongly when the nonresonant x_1 mode starts at a higher energy level.

A systematic integration of system (34) for $x_1(0)$ ranging from values 0 to 1 and fixed $H_2(0) = 3.01$ shows the increase of recurrence times T_r if $x_1(0)$ increases. The excitation of x_1 in the resonance zones produces clearly a quasi-trapping obstruction to the passage of the phase-flow through the resonance zone, see Fig. 8. The recurrence times will depend polynomially on $x_1(0)$ as T_r is bounded for a neighborhood of the initial conditions with positive measure. The form of the dependence is sensitive to the six initial conditions.

A *detuned* higher order resonance of any dynamical importance in the primary resonance zones cannot be expected in the classical FPU-chain with four particles. Expressing $\sqrt{2}$ by the rational $1.4 + \delta(\varepsilon), \delta(\varepsilon) = 0.0142\ldots$ we can study the combination angle

$$\chi_{755} = 7\phi_1 - 5\phi_2 - 5\phi_3.$$

If this angle is active it will be at very small size and at very long timescales. We find in the primary resonance zones M_1, M_2 that the three actions and χ_1 are varying in $O(\varepsilon^3)$ whereas:

$$\dot{\chi}_{755} = -\frac{\varepsilon^2}{2}\left(7E_1 - \frac{5}{\sqrt{2}}E_1\cos 2\chi_1 - 10\sqrt{2}I_1\right) - 10\delta(\varepsilon) + O(\varepsilon^3). \tag{42}$$

If $\delta(\varepsilon)/\varepsilon^2$ is not small, the right-hand side has no zeros, χ_{755} will be timelike and we can average over the angle to remove the $O(\varepsilon^2)$ terms of Eq. (42). But even if $\delta(\varepsilon)/\varepsilon^2$ is small, we need not have a term of the form $x_1^7 x_2^5 x_3^5$ in the higher order normal form. Extensive numerical experiments suggest that this resonance plays no part. The same holds for resonances like 7 : 10.

We conclude, see Figs. 5–7, that because of nonresonant excitation, passage through a resonance zone can produce a considerable delay of recurrence. Starting in a resonance zone the choice of $H_{21}(0)$ has a strong influence on the recurrence properties.

6.3. *The β-chain*

The β-chain ($\alpha = 0, \beta = 1$) shows dynamics that is different. From [Rink & Verhulst, 2000], we know that the x_2, x_3 normal modes are unstable; the resonance zone M_1: $I_2 = I_3 = \frac{1}{2}E_1$ contains two stable periodic solutions for $\chi = 0, \pi$; we have M_2 with two unstable periodic solutions for $\chi = \pi/2, 3\pi/2$ (parametrized by $I_1(0)$ as for the α-chain). One of the motivations to study also the β-chain is that the nearest-neighbor interaction in this case is symmetric. We will find that this results in different dynamics.

From system (35) we find the exact solutions of the β-chain:

$$\begin{cases} \ddot{x}_1 + 4x_1 = 4\varepsilon^2\beta(-x_1^3 - 3x_1x_2^2), \\ \ddot{x}_2 + 2x_2 = 2\varepsilon^2\beta(-2x_2^3 - 3x_1^2x_2), \\ x_2(t) = \pm x_3(t). \end{cases} \tag{43}$$

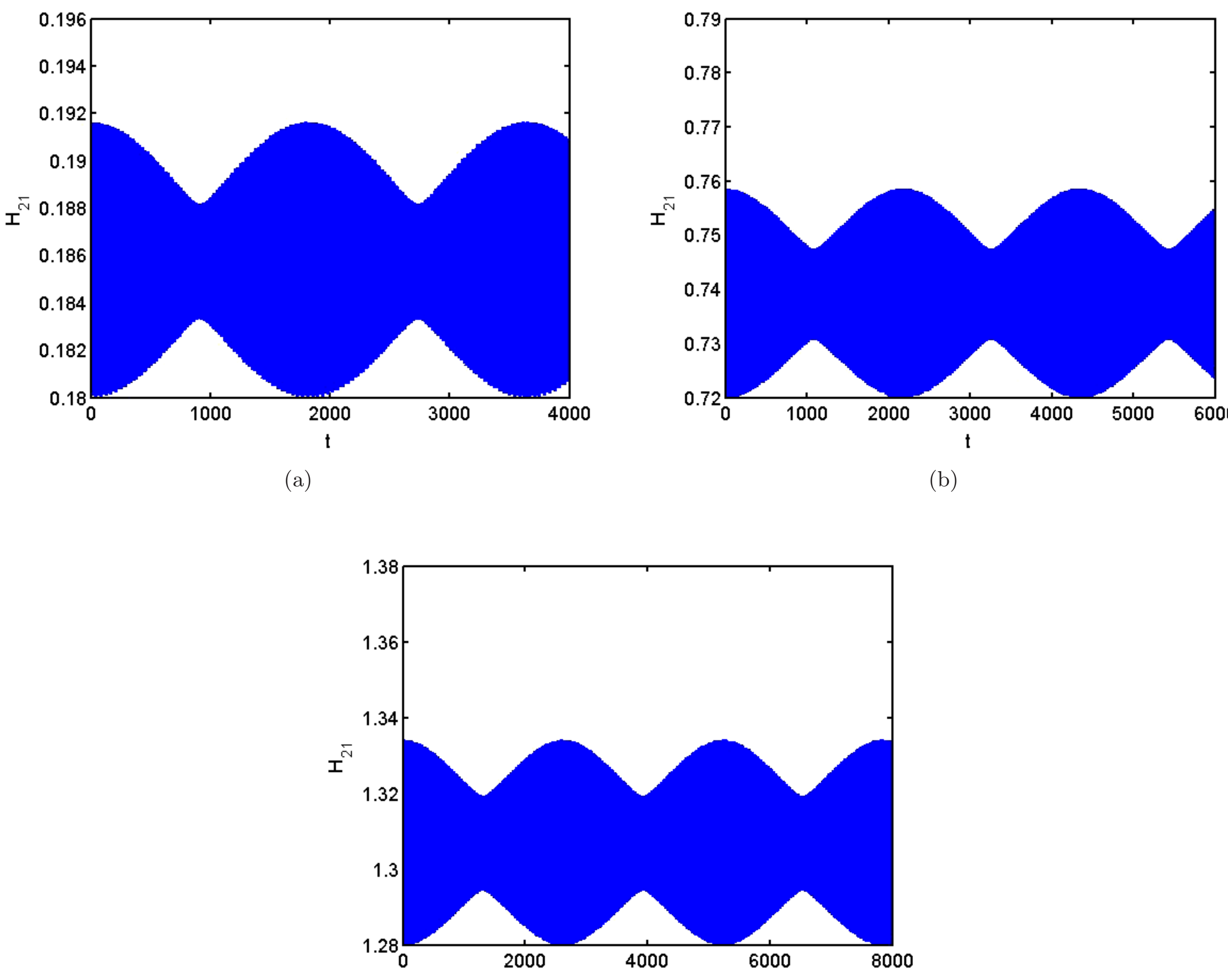
From the normal form (36) we have for the actions and the combination angle χ when omitting terms $O(\varepsilon^3)$:

$$\begin{cases} \dot{I}_1 = 0, \quad \dot{I}_2 = -\dfrac{3}{4}\varepsilon^2 I_2 I_3 \sin 2\chi, \quad \dot{I}_3 = \dfrac{3}{4}\varepsilon^2 I_2 I_3 \sin 2\chi, \\ \dot{\phi}_1 = 2 + \dfrac{3}{4}\varepsilon^2[I_1 + \sqrt{2}(I_2 + I_3)], \\ \dot{\phi}_2 = \sqrt{2} + \dfrac{3}{8}\varepsilon^2(I_3\cos 2\chi + I_2 + 2I_3 + 2\sqrt{2}I_1), \\ \dot{\phi}_3 = \sqrt{2} + \dfrac{3}{8}\varepsilon^2(I_2\cos 2\chi + 2I_2 + I_3 + 2\sqrt{2}I_1), \\ 2\dot{\chi} = -\dfrac{3}{4}\varepsilon^2(I_2 - I_3)(\cos 2\chi + 1). \end{cases} \tag{44}$$

The $1:1$ resonance zone is with the integral (37): $\sqrt{2}(I_2 + I_3) = E_1$ again determined by $I_2 = I_3 = \frac{1}{4}\sqrt{2}E_1$. The analysis runs along the same lines as for the α-chain. The transitions through the resonance zone are shown in Figs. 9–11. We observe a few differences and, because of the two unstable periodic solutions in the resonance zone, we consider the dynamics in the resonance zones.

We consider again the possibility of higher order resonance. As before, we consider the combination angle $\chi_{755} = 7\phi_1 - 5\phi_2 - 5\phi_3$. However, it is easy to show that $d\chi_{755}/dt$ is sign-definite, so higher order resonance of this type cannot be expected to exist. Also the $7:10$ resonance is not present in the classical β-chain with four particles.

Passage through a primary resonance zone of the β-chain produces considerable delay of recurrence. Figure 11 shows that increasing $x_1(0)$ while keeping $H_2(0) = 3.01$ fixed, the recurrence time increases. The increase is caused by the increasing amplitude of the x_1-oscillations resulting in a larger geometric obstruction in the resonance zone. If $x_1(0) = 0.3$, H_{21} varies by 0.004 around value 0.186, if $x_1(0) = 0.6$, H_{21} varies by 0.02 around



(a)

(b)

(c)

Fig. 9. The classical β-chain, passage through a primary resonance zone. The actions H_{21} for system (34) (case $a = 1$) with $\alpha = 0, \beta = 1$ in three cases with $H_2(0) = 3.01$. Initial conditions: $(x_1(0) = 0.3, x_2(0) = 1.6793, x_3(0) = 0.1)$, $(x_1(0) = 0.6, x_2(0) = 1.50997, x_3(0) = 0.1)$ and $(x_1(0) = 0.8, x_2(0) = 1.3115, x_3(0) = 0.1)$, initial velocities are zero and $\varepsilon = 0.1$. The nonresonant action H_{21} shows small variations outside the resonance zone and smaller ones in the zone.

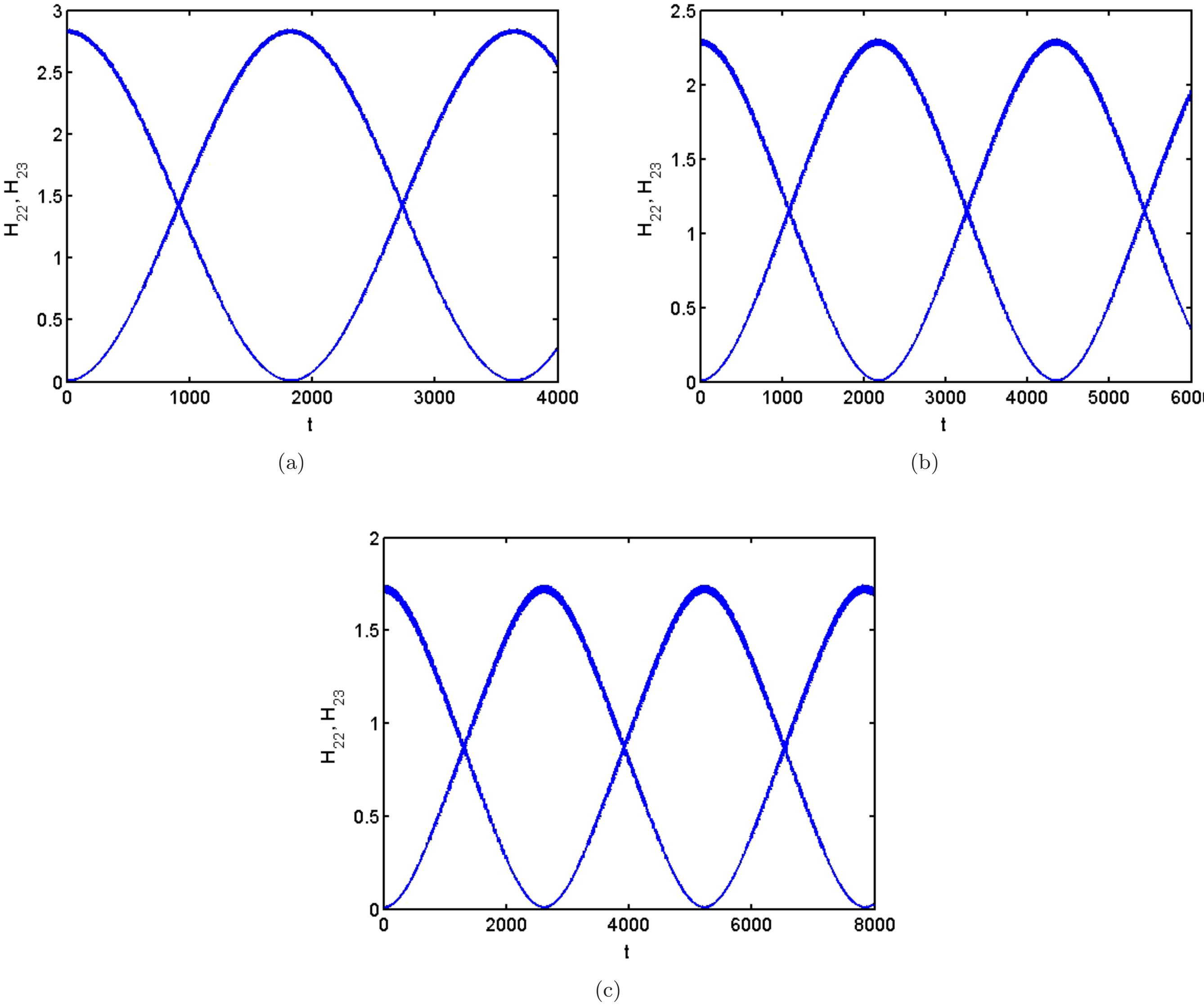


Fig. 10. The classical β-chain, passage through a primary resonance zone showing the actions H_{22}, H_{23} corresponding with x_2, x_3 of system (34) (case $a = 1$) with $\alpha = 0, \beta = 1$. The three cases have the initial conditions of the three cases in Fig. 9 with $H_2(0) = 3.01$ fixed. Whenever $H_{22} = H_{23}$ we observe *smaller* excitation of the x_1 mode in the resonance zone. The time of passage and the recurrence times increase with $x_1(0)$.

value 0.74, if $x_1(0) = 0.8$, H_{21} varies by 0.03 around value 1.31.

Starting in the resonance zone, M_1 yields fairly good recurrence because of the stability of the periodic solutions; see Fig. 12(a). In Fig. 12(b) we show the recurrence when starting near an unstable quasi-periodic solution in M_2. Whereas in M_1 recurrence times are typically around 500 timesteps, starting in M_2 with $x_1(0) = 0.6$, this is nearly 30 000 timesteps. In the second case the variations of H_{22} and H_{23} are near 2, H_{21} shows variations of size 0.02 on the time-interval 0–30 000.

The recurrence time varies with $x_1(0)$. In Fig. 13 we have for $x_1(0) = 0.1$ a recurrence time of more than 130 000 timesteps, for $x_1(0) = 0.8$ at least 30 000 timesteps, for $x_1(0) = 1$ the recurrence time is more than 40 000 timesteps. As we have noted, the $1 : 1$ quasi-periodic solutions in M_2 are unstable with corresponding unstable manifolds dominating the expansion if $x_1(0)$ is small. The x_1-oscillations are spectrally stable. Increasing $x_1(0)$ will reduce the size of the unstable manifolds resulting in reduced expansion and so relatively shorter recurrence times. However, increasing $x_1(0)$ even

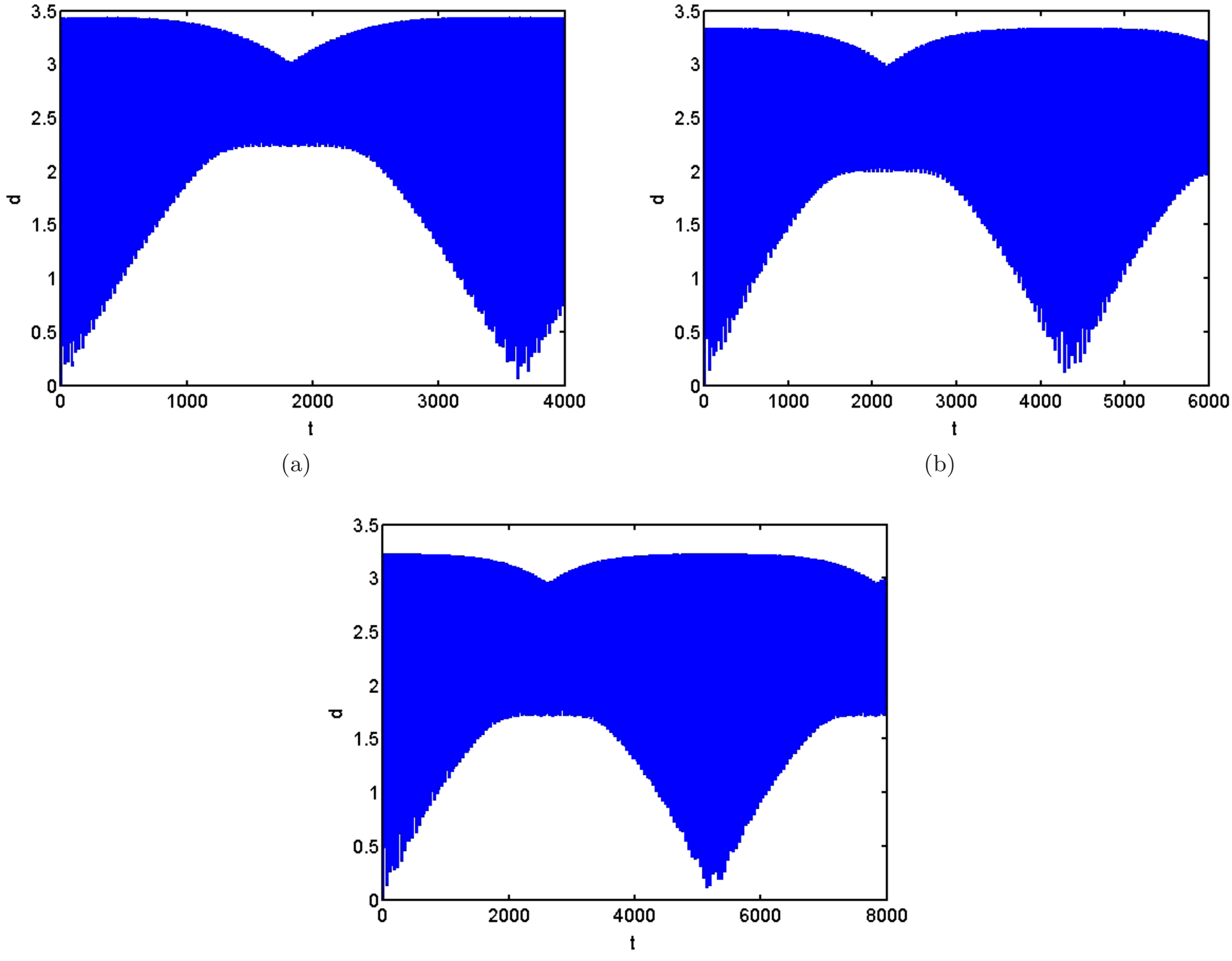


Fig. 11. The classical β-chain, passage through resonance, showing the Euclidean distance d to the initial conditions in the cases of Fig. 9 with $H_2(0) = 3.01$ fixed. The recurrence times increase with $x_1(0)$.

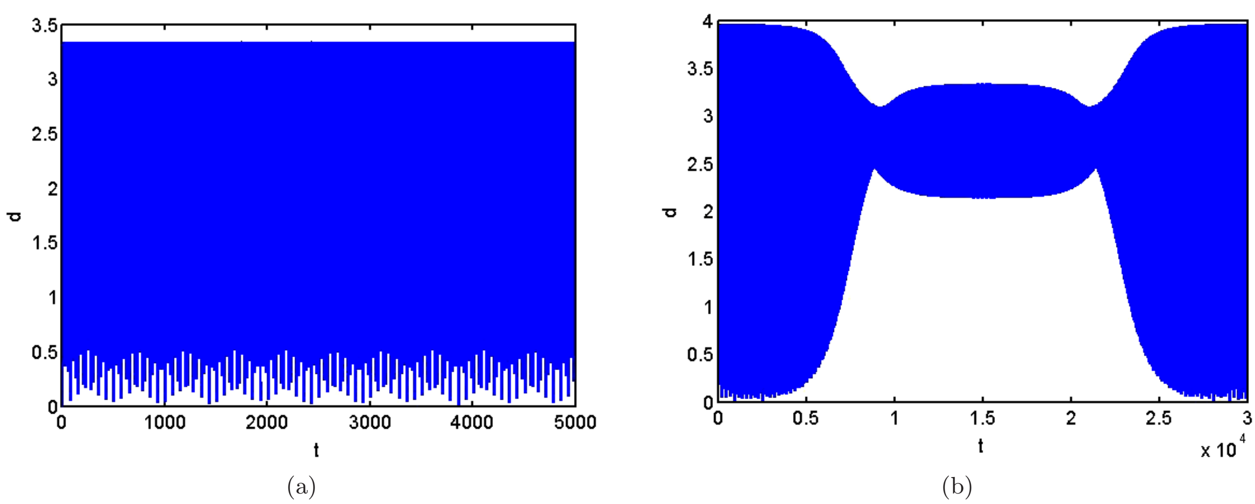
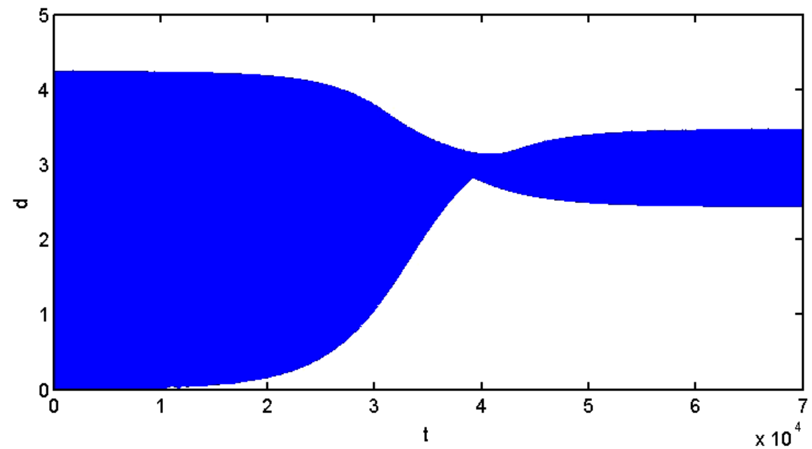
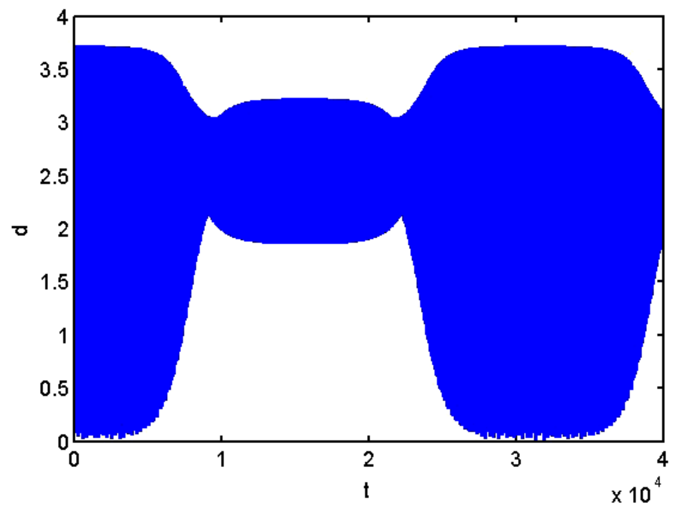


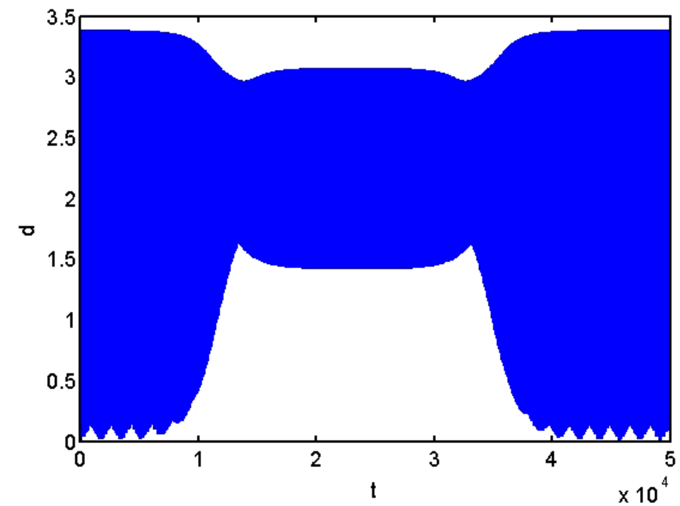
Fig. 12. (a) The classical β-chain, dynamics in the resonance zone M_1, showing relative fast recurrence d with initial conditions $x_1(0) = 0.6, x_2(0) = 1.2356, x_3(0) = 1.2356$ and initial velocities zero, starting near a stable quasi-periodic solution. (b) We start near an unstable quasi-periodic solution in resonance zone M_2, initial conditions $x_1(0) = 0.6, \dot{x}_1(0) = 0, x_2(0) = 1.0700, \dot{x}_2(0) = 0, x_3(0) = 0, \dot{x}_3(0) = -1.5132$. Starting in M_2 the recurrence time increases strongly, in this case to around 30 000 timesteps.



(a)



(b)



(c)

Fig. 13. (a) The classical β-chain with four particles, dynamics in the resonance zone M_2, showing recurrence d with initial conditions for various initial conditions near an unstable quasi-periodic solution with $H_2(0) = 3.01$ fixed. (a)–(c) Initial conditions $x_1(0) = 0.1, \dot{x}_1(0) = 0, x_2(0) = 1.2227, \dot{x}_2(0) = 0, x_3(0) = 0, \dot{x}_3(0) = -1.7292$, $x_1(0) = 0.8, \dot{x}_1(0) = 0, x_2(0) = 0.93005, \dot{x}_2(0) = 0, x_3(0) = 0, \dot{x}_3(0) = -1.3153$, $x_1(0) = 1, \dot{x}_1(0) = 0, x_2(0) = 0.7106, \dot{x}_2(0) = 0, x_3(0) = 0, \dot{x}_3(0) = -1.00499$. Starting in M_2 the recurrence time varies considerably with $x_1(0)$ of the nonresonant mode.

more, the x_1-oscillations clearly pose a separate obstruction to recurrence as in Fig. 11 for M_1.

6.4. *Comparison between Toda chain and FPU α-chains*

An interesting question was raised in [Ferguson *et al.*, 1982]. Considering chains of unit masses connected by identical springs, they analyzed the cases of harmonic forces, the Toda chain which is integrable and the FPU α-chain. In the case of the FPU α-chain the force field derived from Hamiltonian (32) is

$$F_{\mathrm{FPU}}(z) = -z - \alpha z^2, \tag{45}$$

whereas we have for the Toda chain with constant B:

$$\begin{aligned} F_{\mathrm{Toda}}(z) &= \frac{1}{B}(e^{-Bz} - 1) \\ &= -z + \frac{1}{2}Bz^2 - \frac{1}{6}B^2z^3 + \cdots. \end{aligned} \tag{46}$$

With the choice $\alpha = 1/4, B = -1/2$ and so making the first two terms of the forces equal, regarding the well-known recurrence phenomena of the α-chain and a numerical computation, Ferguson *et al.* [1982, Figs. 25–26] conjecture that both chains show, at least at low energy level, the same qualitative and nearly the same quantitative behaviors.

We will show that in the case of four particles this conjecture is correct at low energy level for a small range of α, B values but not in general. For the force fields to be equal to quadratic terms we require $-\alpha = B/2$. It was shown by [Rink & Verhulst, 2000] that for a FPU-chain with four particles and both α and β terms, the qualitative behavior is governed by the bifurcation parameter:

$$\gamma = \frac{3\beta}{3\beta - 4\alpha^2}. \tag{47}$$

The bifurcations involve existence and stability of periodic solutions. For the α-chain we find $\gamma = 0$. With $B = -2\alpha$ we have for the Toda chain $\gamma = -B^4/4$, so positive bifurcation values are excluded. According to [Rink & Verhulst, 2000], a bifurcation involving exchanges of stability takes place for $\gamma = \pm 1$ or $B = \sqrt{2}$. Note that the choice of Ferguson *et al.* [1982] was $B = -1/2$ so that $\gamma = -1/64$, close to the value of the α-chain. The zones M_1, M_2 found in Sec. 6.2 will for these values also be found in the Toda chain.

Recently it was shown by Bruggeman and Verhulst [2018] that for the FPU-chain with $4n$ particles the system with four particles is recovered in an invariant manifold. This settles the question of qualitative inequality of Toda chain and FPU-chain in more generality.

7. Application to the Classical FPU β-Chain with Eight Particles

A β-chain with four particles shows different dynamics as compared with an α-chain. This difference persists in a system with eight particles, in general, in a system with $4n$ particles. In addition, as indicated in Sec. 6 and [Bruggeman & Verhulst, 2018], a FPU-system with eight particles is found again as a submanifold in FPU-chains with $16, 24, \ldots,$ or $8n$ particles. This is in itself is a motivation to study low-dimensional FPU-chains.

Consider the FPU-chain (32) in the classical case with equal masses, eight particles and $\alpha = 0$, $\beta = 1$. We have for the eigenvalues $\lambda_i = \omega_i^2$ of the linearized system:

$$\omega_i^2 : 4, 2 + \sqrt{2}\ (\text{twice}), 2, 2, 2 - \sqrt{2}\ (\text{twice}), 0.$$

We have $\omega_1 = 2, \omega_{2,3} = 1.848\ldots, \omega_{4,5} = 1.414\ldots$, $\omega_{6,7} = 0.765\ldots$. Using the momentum integral we can reduce the system from eight dof to seven dof. The symplectic transformation $(p, q) \to (y, x)$ produces a quartic Hamiltonian with 49 terms, see Sec. A.2 where we list the coefficients.

7.1. *Two invariant manifolds*

Inspection of the equations of motion produces the following invariant manifolds:

- IM_{145} (six-dimensional) defined by $x_2(t) = x_3(t) = x_6(t) = x_7(t) = 0$.

  The equations of motion describing the dynamics in IM_{145} are:

$$\begin{cases} \ddot{x}_1 + 4x_1 \\ \quad = -\varepsilon^2(4e_{1111}x_1^3 + 2e_{1144}x_1x_4^2 + 2e_{1155}x_1x_5^2), \\ \ddot{x}_4 + 2x_4 \\ \quad = -\varepsilon^2(2e_{1144}x_1^2x_4 + 4e_{4444}x_4^3 + 2e_{4455}x_4x_5^2), \\ \ddot{x}_5 + 2x_5 \\ \quad = -\varepsilon^2(2e_{1155}x_1^2x_5 + 2e_{4455}x_4^2x_5 + 4e_{5555}x_5^3). \end{cases} \tag{48}$$

As predicted by the theorem in [Bruggeman & Verhulst, 2018], this invariant manifold corresponds with the six-dimensional phase-space of the FPU-chain with four particles discussed in Sec. 6.

- IM_{2367} (eight-dimensional) defined by $x_1(t) = x_4(t) = x_5(t) = 0$.
  We will analyze the dynamics in IM_{2367} separately.

One of the conclusions of [Bruggeman & Verhulst, 2018] is that in a system with eight particles the submanifolds are spectrally stable except if $a = 0.75$ ($m = 4/3$). However, we will find instability in the classical case. Using the list in Sec. A.2 we find the equations of motion in IM_2:

$$\begin{cases} \ddot{x}_2 + \omega_2^2 x_2 = -\varepsilon^2(4e_{2222}x_2^3 + 3e_{2226}x_2^2x_6 + 2e_{2233}x_2x_3^2 + 2e_{2237}x_2x_3x_7 + 2e_{2266}x_2x_6^2 \\ \qquad\qquad + 2e_{2277}x_2x_7^2 + e_{2336}x_3^2x_6 + e_{2367}x_3x_6x_7 + e_{2666}x_6^3 + e_{2677}x_6x_7^2), \\ \ddot{x}_3 + \omega_3^2 x_3 = -\varepsilon^2(2e_{2233}x_2^2x_3 + e_{2237}x_2^2x_7 + 2e_{2336}x_2x_3x_6 + e_{2367}x_2x_6x_7 + 4e_{3333}x_3^3 \\ \qquad\qquad + 3e_{3337}x_3^2x_7 + 2e_{3366}x_3x_6^2 + 2e_{3377}x_3x_7^2 + e_{3667}x_6^2x_7 + e_{3777}x_7^3), \\ \ddot{x}_6 + \omega_6^2 x_6 = -\varepsilon^2(e_{2226}x_2^3 + 2e_{2266}x_2^2x_6 + e_{2336}x_2x_3^2 + e_{2367}x_2x_3x_7 + 3e_{2666}x_2x_6^2 + e_{2677}x_2x_7^2 \\ \qquad\qquad + 2e_{3366}x_3^2x_6 + 2e_{3667}x_3x_6x_7 + 4e_{6666}x_6^3 + 2e_{6677}x_6x_7^2), \\ \ddot{x}_7 + \omega_7^2 x_7 = -\varepsilon^2(e_{2237}x_2^2x_3 + 2e_{2277}x_2^2x_7 + e_{2367}x_2x_3x_6 + 2e_{2677}x_2x_6x_7 + e_{3337}x_3^3 \\ \qquad\qquad + 2e_{3377}x_3^2x_7 + e_{3667}x_3x_6^2 + 3e_{3777}x_3x_7^2 + 2e_{6677}x_6^2x_7 + 4e_{7777}x_7^3). \end{cases} \tag{49}$$

The dynamics in IM_{2367} is interesting as it involves two $1:1$ resonances ($\omega_2 = \omega_3, \omega_6 = \omega_7$) that are mutually nonresonant. The IM_{2367} Hamiltonian contains 19 terms; after normalization, 11 quartic terms remain.

We are interested in the phase-flow in IM_{2367}, the stability of the two invariant manifolds and their interaction. From the preceding section we conclude that IM_{2367} will be unstable as we can start in a neighborhood of the manifold in the unstable resonance zone M_2 of manifold IM_{145}. This is illustrated in Fig. 14.

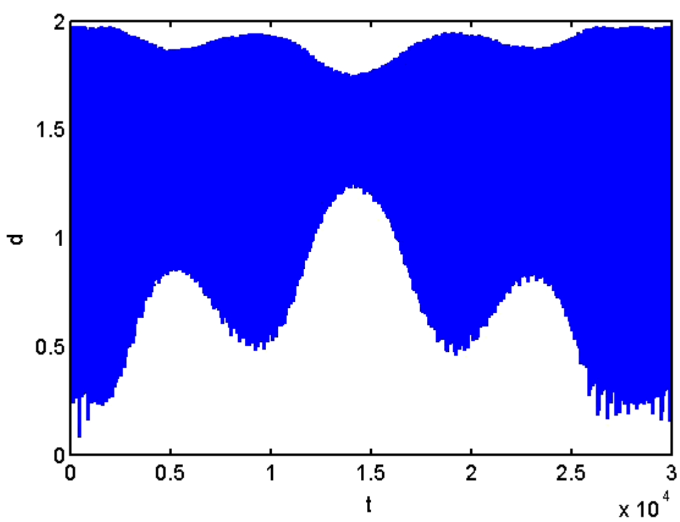


Fig. 14. The classical β-chain with eight particles, recurrence given by the Euclidean distance d when starting near IM_{2367} in the resonance zone M_2 of IM_{145}. This illustrates the instability of invariant manifold IM_{2367}. We choose in IM_{2367} the case $x_2(0) = x_3(0) = 0.5, x_6(0) = x_7(0) = 0.4$ with $(\chi_{23}, \chi_{67}) = (0, 0)$. For modes 1, 4 and 5 we took $x_1(0) = 0.1, \dot{x}_1(0) = 0, x_4(0) = 0.1, \dot{x}_4(0) = 0, x_5(0) = 0, \dot{x}_5(0) = -0.1414$. The integration was carried out for the original system induced by (32) with $\varepsilon^2 = 0.1$ (to speed up the dynamics).

7.2. *The normalized amplitudes in seven dof*

We normalize the full system of seven dof equations using transformation (4). The Hamiltonian of the β-chain in y, x-coordinates contains 49 quartic terms. We find after transformation and normalization, using Sec. A.2, combination angles:

$$\chi_{23} = \phi_2 - \phi_3, \quad \chi_{45} = \phi_4 - \phi_5, \quad \chi_{67} = \phi_6 - \phi_7,$$

$$\begin{cases} \dot{r}_1 = 0, \quad \dot{r}_2 = \dfrac{\varepsilon^2}{4\omega_2}\left(\dfrac{3}{16}(3+2\sqrt{2})r_2 r_3^2 \sin 2\chi_{23} + \dfrac{3}{4} r_3 r_6 r_7 \sin\chi_{23}\cos\chi_{67}\right), \\ \dot{r}_3 = -\dfrac{\varepsilon^2}{4\omega_3}\left(\dfrac{3}{16}(3+2\sqrt{2})r_2^2 r_3 \sin 2\chi_{23} + \dfrac{3}{4} r_2 r_6 r_7 \sin\chi_{23}\cos\chi_{67}\right), \\ \dot{r}_4 = \dfrac{3\varepsilon^2}{16\sqrt{2}} r_4 r_5^2 \sin\chi_{45}, \quad \dot{r}_5 = -\dfrac{3\varepsilon^2}{16\sqrt{2}} r_4^2 r_5 \sin\chi_{45}, \\ \dot{r}_6 = \dfrac{\varepsilon^2}{4\omega_6}\left(\dfrac{3}{4} r_2 r_3 r_7 \cos\chi_{23}\sin\chi_{67} + \dfrac{3}{16}(3-2\sqrt{2}) r_6 r_7^2 \sin 2\chi_{67}\right), \\ \dot{r}_7 = -\dfrac{\varepsilon^2}{4\omega_7}\left(\dfrac{3}{4} r_2 r_3 r_6 \cos\chi_{23}\sin\chi_{67} + \dfrac{3}{16}(3-2\sqrt{2}) r_6^2 r_7 \sin 2\chi_{67}\right). \end{cases} \tag{50}$$

The use of transformation (4) assumes that the amplitudes do not vanish, but it has been checked by using co-moving coordinates that, as system (50) suggests, the normal modes are solutions of the normalized system. We find four integrals of the amplitude normal form:

$$r_1 = r_1(0), \quad r_2^2 + r_3^2 = 2E_1, \quad r_4^2 + r_5^2 = 2E_2, \quad r_6^2 + r_7^2 = 2E_3 \quad (E_1, E_2, E_3 \geq 0).$$

To this order of normalization, interaction between the two invariant manifolds does not take place by the amplitudes, but as we shall see, by the angle ϕ_1. Although the first mode, x_1, is nonresonant, we have seen in Sec. 6.3 that the choice of $x_1(0)$ influences the dynamics and the recurrence.

7.3. *The normalized phases in seven dof*

$$\begin{cases} \dot{\phi}_1 = \dfrac{3\varepsilon^2}{8}(r_1^2(0) + (2+\sqrt{2})E_1 + 2E_2 + (2-\sqrt{2})E_3), \\ \dot{\chi}_{23} = \dfrac{\varepsilon^2}{\omega_2}\left(\dfrac{9}{64}(3+2\sqrt{2})(r_2^2 - r_3^2) + \dfrac{3}{32}(3+2\sqrt{2})(r_3^2 - r_2^2)\left(1 + \dfrac{1}{2}\cos 2\chi_{23}\right)\right. \\ \qquad \left. + \dfrac{3}{16}(r_7^2 - r_6^2) + \dfrac{3}{16}\left(\dfrac{r_3}{r_2} - \dfrac{r_2}{r_3}\right) r_6 r_7 \cos\chi_{23}\cos\chi_{67}\right), \\ \dot{\chi}_{45} = \dfrac{3\varepsilon^2}{16}(r_5^2 - r_4^2)\left(1 + \dfrac{1}{2}\cos 2\chi_{45}\right), \\ \dot{\chi}_{67} = \dfrac{\varepsilon^2}{\omega_6}\left(\dfrac{3}{16}(r_3^2 - r_2^2) + \dfrac{3}{16} r_2 r_3 \cos\chi_{23}\cos\chi_{67}\left(\dfrac{r_7}{r_6} - \dfrac{r_6}{r_7}\right)\right. \\ \qquad \left. + \dfrac{3}{32}(3-2\sqrt{2})(r_6^2 - r_7^2) + \dfrac{1}{4}(r_7^2 - r_6^2)\cos 2\chi_{67}\right). \end{cases} \tag{51}$$

We find from Eqs. (50) and (51) in IM_{145}:

(1) The three normal mode periodic solutions x_1, x_4, x_5.
(2) Periodic solutions in the primary resonance zones $r_1(0) = 0$, $r_4 = r_5$, $\sin 2\chi_{45} = 0$.

We find in IM_{2367}:

(1) Two periodic solutions:

$r_6 = r_7 = 0,\ \sin 2\chi_{23} = 0,\ r_2 = r_3.$

$r_2 = r_3 = 0,\ \sin 2\chi_{67} = 0,\ r_6 = r_7.$

(2) Eight quasi-periodic solutions if $r_2r_3r_6r_7 \neq 0$:

$\sin\chi_{23} = \sin\chi_{67} = 0, r_2 = r_3, r_6 = r_7$ producing $(\chi_{23}, \chi_{67}) = (0, 0), (0, \pi), (\pi, 0), (\pi, \pi)$.

$\cos\chi_{23} = \cos\chi_{67} = 0$, $r_2 = r_3$, $r_6 = r_7$ producing $(\chi_{23}, \chi_{67}) = (\frac{\pi}{2}, \frac{\pi}{2}), (\frac{\pi}{2}, 3\frac{\pi}{2}), (3\frac{\pi}{2}, \frac{\pi}{2}), (3\frac{\pi}{2}, 3\frac{\pi}{2})$.

7.4. *Interaction of the two invariant manifolds*

We consider perturbations of the solutions starting in a primary resonance zone of invariant manifold IM_{2367} by small values of $x_1(0), x_4(0), x_5(0)$ in the unstable resonance zone M_2 of IM_{145}. In Fig. 14 we show the instability of IM_{2367} by plotting the Euclidean distance d to the initial conditions in 30 000 timesteps. The normal form Eqs. (50) and (51) show interaction of the angle of mode x_1 with the other six modes but not vice versa. As we have shown earlier, the $O(\varepsilon^3)$ terms of the normal form equations induce the instability on a long timescale; we took $\varepsilon^2 = 0.1$ to speed up the dynamics.

Conclusion

As stated before, we will find invariant manifold IM_{145} in the classical FPU-chain with $4n$ particles. An important consequence of our analysis is that any other invariant manifold present in the classical FPU-chain with $4n$ particles will be unstable.

8. Note on the FPU-Chain with Eight Particles and Alternating Masses

It has been shown in [Bruggeman & Verhulst, 2018] that also in the case of alternating masses, the dynamics of a FPU-chain with eight particles will be found again in submanifolds of periodic FPU-chains with $8n$ particles. In the classical case ($m = 1$) we have found in a chain with four particles instability phenomena in a resonance zone of the β-chain. In the case of four alternating masses, low order resonances arise if $m = 3, 4, 8, 9$. However, the normal forms in these cases degenerate so that we would have to consider high order normal forms in these cases.

We will make some remarks on the α-chain, the β-chain with eight alternating masses is left as an open problem.

The α-chain

The analysis for eight particles in [Bruggeman & Verhulst, 2018] shows that for the α-chain we have from the equations of motion, three invariant manifolds: M_{145} (as expected), M_{256} and M_{357}.

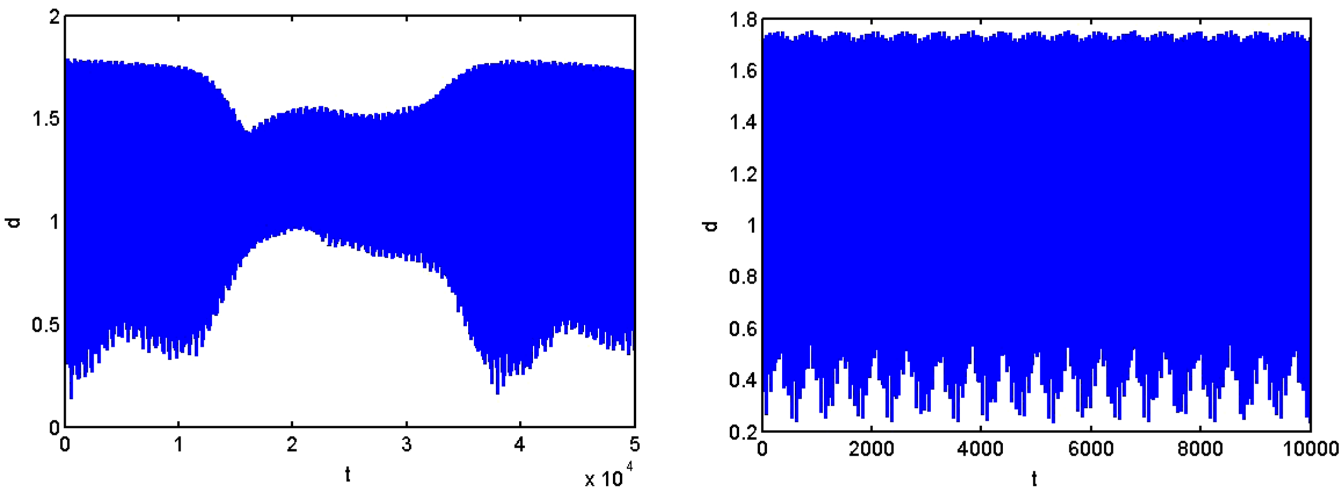
The first order normal forms are degenerate except in the cases $a = 0.5$ and 0.75. Spectral stability analysis in [Bruggeman & Verhulst, 2018] shows that only for $a = 0.75$ we find from the normal forms instability of the invariant manifolds. This instability persists in alternating periodic FPU-chains with $a = 0.75$ and $8n$ particles.

The remaining problem at this order of normalization is to show whether the spectral stability of the three manifolds persists as stability in the case $a = 0.5$. We are inspired by the fact that mode x_5 plays a pivotal role in the three manifolds. Consider the invariant manifold M_{256} in the case of eight particles, $a = 0.5$. According to [Bruggeman & Verhulst, 2018, system (12)], the dynamics in the manifold for the x_2, x_5 and x_6 modes is governed by:

$$\begin{cases} \ddot{x}_2 + \lambda_2 x_2 = -\varepsilon(2x_2x_5d_{225} + x_5x_6d_{256}), \\ \ddot{x}_5 + x_5 = -\varepsilon(x_2^2d_{225} + x_6x_2d_{256} + x_6^2d_{665}), \\ \ddot{x}_6 + \lambda_6 x_6 = -\varepsilon(x_2x_5d_{256} + 2x_5x_6d_{665}). \end{cases} \tag{52}$$

Here $\lambda_2 = \frac{1}{2}(3 + \sqrt{5}), \lambda_6 = \frac{1}{2}(3 - \sqrt{5})$, the d-coefficients are given in [Bruggeman & Verhulst, 2018] with $d_{225} < 0, d_{256} = \sqrt{10}/10, d_{665} > 0$. Restricting to IM_{256} only, d_{256} plays a part in the intermediate normal form of system (52). The $x_5, \dot{x}_5$ coordinate plane contains harmonic solutions of the form $r_0\cos(t + \phi_0)$ that produce by linearization a Floquet system of the form:

$$\begin{aligned} \ddot{x}_2 + \lambda_2 x_2 &= -\varepsilon d_{256} r_0 \cos(t + \phi_0)x_6, \\ \ddot{x}_6 + \lambda_6 x_6 &= -\varepsilon d_{256} r_0 \cos(t + \phi_0)x_2. \end{aligned} \tag{53}$$



(a) (b)

Fig. 15. The instability of manifold IM_{357} in the eight particle α-chain with $a = 0.5, \varepsilon = 0.1$. (a) The recurrence d with initial conditions $x(0) = 0, -0.1, 0.5, 0, 0.2, 0.1, 0.4$ and initial velocities $\dot{x}(0) = 0, -0.1, 0, 0, 0.2, 0.1, 0.4$. (b) The distance to the initial conditions of the modes 3, 5, 7 in the manifold IM_{357} without the perturbing modes 1, 2, 4, 6, $x_3(0) = 0.5, x_5(0) = 0.2, x_7(0) = 0.4$, velocities $\dot{x}_3(0) = 0, \dot{x}_5(0) = 0.2, \dot{x}_7(0) = 0.4$. For the integration we used the original system derived from Hamiltonian (32) with corresponding initial conditions (a) $q(0) = 0.1, -0.0646447, -0.45, 0.135355, -0.1, 0.135355, 0.45, 0.0646447$ and initial velocities $\dot{q}(0) = 0.1, -0.241421, -0.2, -0.0414214, -0.1, 0.0414214, 0.2, 0.241421$.

The resonance $\sqrt{\lambda_2} = 1 + \sqrt{\lambda_6}$ destabilizes the normal mode; this is confirmed by averaging of the linearized system (53) and numerical simulations of system (52). We conjecture now that the instability of the x_5 normal mode in IM_{256} will affect the stability of manifold IM_{357}. Figure 15 shows the instability; in the manifold we start with $x(0) = 0.5, 0.2, 0.4$, $\dot{x}(0) = 0, 0.2, 0.4$ and add small perturbations to the other modes. Inverting the symplectic transformation we integrate numerically for the original α-chain generated by Hamiltonian (32). On the left we show the Euclidean distance d to the initial conditions for the eight modes of the chain; the interval of time, 50 000 timesteps, in this unstable case is not enough for recurrence. On the right we show the Euclidean distance for the modes starting in IM_{357} without other perturbing modes. The recurrence is relatively fast.

9. Discussion and Conclusions

(1) The main purpose of this paper is to show how in Hamiltonian systems low and high order resonances may interact to produce delay of recurrence and instability of invariant manifolds. The dynamics involves a special type of double resonance. This has been demonstrated for three dof systems with as an example, the $1:1:4$ resonance. In addition this has been applied for the periodic FPU-chain with four and eight particles (and so for $4n$ and $8n$ particles).

(2) In [Ferguson *et al.*, 1982] it was shown that for certain parameter values the FPU α-chain and the Toda chain have the same qualitative and nearly the same quantitative behavior. We have shown in Sec. 6.4 that this is not a general feature, it is correct for a range of parameters involving small values of the parameter γ in Eq. (47).

(3) Delay of recurrence takes different forms. An important one is caused by quasi-trapping in resonance zones where the higher order resonance may become effective. This involves an extension of the theory of higher order resonance as described by [Sanders, 1977; Sanders *et al.*, 2007; Tuwankotta & Verhulst, 2000]. The presence of tori and other invariant manifolds in the resonance zones is a well-known explanation of delay of recurrence.

An unexpected other effect resulting in delay occurs in the classical periodic α-chain with $4n$ particles. It is shown in Sec. 6.2 that nonresonant excitation may take place in a resonance zone.

(4) Normalization helps to describe in detail the phase-flow in primary zones with double resonance. We have noted that the normal form of the $1:1:4$ resonance is integrable, this

also holds in the primary resonance zone and near the resonant junction. In this sense the embedded double resonance is different from the general double resonance as described in [Efthymiopoulos & Harsoula, 2013]. In this case chaos does not play an important part at low energy level.

(5) Hamiltonian systems contain in general an infinite number of periodic solutions that are close (detuned) to the main resonances producing the so-called short-periodic orbits. This implies that the picture we have developed corresponds with the dominant aspects of the phase-flow in three dof. Our picture is not complete but this becomes apparent only when going beyond the low energy level where the normal forms are valid. Detuned resonances will arise in normal forms that contain terms of size $\varepsilon^{c\|a\|}$ with c positive and $\|a\|$ the annihilator norm of the detuned resonance. The domains where they are found are extremely small or even nonexistent at low energy level.

(6) In a number of cases we find that spectral stability of a periodic solution or a manifold does not persist in the nonlinear setting. For Hamiltonian systems this a known phenomenon, but explicit examples in the case of three or more dof are rare. For instance in Sec. 8, we have spectral stability of an invariant manifold that does not persist in an FPU-chain with alternating mass.

(7) We mention a number of open problems.

The periodic FPU-chain with six particles was studied in [Rink & Verhulst, 2000]. In this system we find a degenerate $1 : 2 : 1$ resonance which may cause quasi-trapping phenomena. In itself, this system, which is typical for the classical periodic FPU-chain with $6n$ particles would be useful to study in more detail.

Another interesting open problem is the dynamics of the β FPU-chain with alternating masses indicated in Sec. 8.

A basic approximation problem is that the exponential estimates in [Nekhoroshev, 1977] cannot be applied in the case of interacting low and higher resonances; new mathematical estimates are necessary here.

Finally, a natural problem would be to use the present theory for FPU cell-chains as described in [Verhulst, 2016].

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Appendix A

A.1. *On normalization*

Our results on normalization and error estimates are based on [Sanders *et al.*, 2007] with slight modifications. We assume existence and uniqueness of solutions of initial value problems, sufficient smoothness and T-periodicity of vector fields. To study the dynamics of secondary resonance in three dof, we have to normalize at least to $O(\varepsilon^3)$, in a Hamiltonian formulation to H_5. We start with putting system (5) with $k = 1, 3$ in the standard form for averaging-normalization using transformation (4):

$$\dot{x} = \varepsilon^2 f(t, x) + \varepsilon^3 g(t, x) + \varepsilon^4 \ldots, x(0) = x_0. \tag{A.1}$$

Consider the averaged vector field

$$f^0(x) = \frac{1}{T}\int_0^T f(s, x)ds$$

and the initial value problem

$$\dot{y} = \varepsilon^2 f^0(y), \quad y(0) = x_0,$$

then $x(t) - y(t) = O(\varepsilon)$ on the timescale $1/\varepsilon^2$. Suppose that we need a higher order approximation. We will use the near-identity transformation:

$$x = z + \varepsilon^2 u^1(t, z), \tag{A.2}$$

with

$$u^1(t, z) = \int_0^t (f(s, z) - f^0(z))ds.$$

Introduce the vector field

$$f_1(t, z) = \bigtriangledown f(t, z)u^1(t, z)$$

with f_1^0 the average of f_1, then the next approximation arising from the $O(\varepsilon^2)$ terms in Eq. (A.1) are shifted to $O(\varepsilon^4)$. To $O(\varepsilon^3)$, the averaging normal form of Eq. (A.1) is

$$\dot{x} = \varepsilon^2 f^0(x) + \varepsilon^3 g^0(x).$$

We can obtain an $O(\varepsilon^2)$ approximation on the timescale $1/\varepsilon^2$. The analysis of primary and secondary resonances is too complicated to present here in full generality.

A.2. *Transformation to eigenmodes by* Mathematica

Here we document the Mathematica computations in the case of a classical periodic FPU α- and β-chain (equal masses) with eight particles. We follow the reasoning as in [Bruggeman & Verhulst, 2018, Sec. 3]. The Hamiltonian is

$$H(p, q) = H_2(p, q) + \varepsilon\alpha H_3(q) + \varepsilon^2\beta H_4(q), \tag{A.3}$$

with $H_3(q) = \frac{1}{3}\sum_{j=1}^{8}(q_{j+1} - q_j)^3$, $H_4(q) = \frac{1}{4} \times \sum_{j=1}^{8}(q_{j+1} - q_j)^4$. The vector $p = (p_1, p_2, \ldots, p_8) \in \mathbb{R}^8$ gives the impulses of the eight particles, and the vector $q \in \mathbb{R}^8$, the positions with convention $q_{m+8} = q_m$. The symplectic transformation $p = Ky$, $q = Lx$ transforms the Hamiltonian in coordinate vectors with respect to a basis of eigenvectors of the linearized system ($\varepsilon = 0$). With the coordinate vectors $y, x \in \mathbb{R}^8$ we find the expression $\frac{1}{2}\sum_{j=1}^{8} y_j^2 + \frac{1}{2}\sum_{j=1}^{7} \lambda_j\, x_j^2$ for H_2, as the eighth eigenvalue equals zero.

For the sake of reference we add the result for the cubic terms (the α-chain). We find expressions $H_3 = \sum_{ijk} d_{ijk}x_ix_jx_k$ and $H_4 = \sum_{ijkl} e_{ijkl}x_ix_jx_kx_l$ with the range of indices and coefficients in the following lists:

$$
\begin{array}{lllll}
d_{225} = -\dfrac{1}{2}(1+\sqrt{2}) & d_{335} = \dfrac{1}{2}(1+\sqrt{2}) & d_{665} = \dfrac{1}{2}(\sqrt{2}-1) & d_{775} = -\dfrac{1}{2}(\sqrt{2}-1) & d_{127} = -2 \\
d_{136} = -2 & d_{234} = 1+\sqrt{2} & d_{145} = -2\sqrt{2} & d_{346} = 1 & d_{256} = 1 \\
d_{247} = -1 & d_{357} = 1 & d_{467} = -1+\sqrt{2} & &
\end{array}
\tag{A.4}
$$

and

$$
\begin{array}{llll}
e_{1111} = \dfrac{1}{2} & e_{1122} = \dfrac{3}{4}(2+\sqrt{2}) & e_{1133} = \dfrac{3}{4}(2+\sqrt{2}) & e_{1144} = \dfrac{3}{2} \\
e_{1155} = \dfrac{3}{2} & e_{1166} = \dfrac{3}{4}(2-\sqrt{2}) & e_{1177} = \dfrac{3}{4}(2-\sqrt{2}) & e_{1224} = \dfrac{3}{4}(2+\sqrt{2}) \\
e_{1235} = -\dfrac{3}{2}(2+\sqrt{2}) & e_{1246} = -\dfrac{3}{2}\sqrt{2} & e_{1257} = \dfrac{3}{2}\sqrt{2} & e_{1334} = -\dfrac{3}{4}(2+\sqrt{2}) \\
e_{1347} = -\dfrac{3}{2}\sqrt{2} & e_{1356} = -\dfrac{3}{2}\sqrt{2} & e_{1466} = -\dfrac{3}{4}(2-\sqrt{2}) & e_{1477} = \dfrac{3}{4}(2-\sqrt{2}) \\
e_{1567} = -\dfrac{3}{2}(2-\sqrt{2}) & e_{2222} = \dfrac{3}{32}(3+2\sqrt{2}) & e_{2226} = -\dfrac{1}{8}(1+\sqrt{2}) & e_{2233} = \dfrac{3}{16}(3+2\sqrt{2}) \\
e_{2237} = -\dfrac{3}{8}(1+\sqrt{2}) & e_{2244} = \dfrac{3}{8}(2+\sqrt{2}) & e_{2255} = \dfrac{3}{8}(2+\sqrt{2}) & e_{2266} = \dfrac{3}{16} \\
e_{2277} = \dfrac{9}{16} & e_{2336} = \dfrac{3}{8}(1+\sqrt{2}) & e_{2367} = \dfrac{3}{4} & e_{2457} = \dfrac{3}{2}\sqrt{2} \\
e_{2666} = \dfrac{1}{8}(\sqrt{2}-1) & e_{2677} = -\dfrac{3}{8}(\sqrt{2}-1) & e_{3333} = \dfrac{3}{32}(3+2\sqrt{2}) & e_{3337} = \dfrac{1}{8}(1+\sqrt{2}) \\
e_{3344} = \dfrac{3}{8}(2+\sqrt{2}) & e_{3355} = \dfrac{3}{8}(2+\sqrt{2}) & e_{3366} = \dfrac{9}{16} & e_{3377} = \dfrac{3}{16} \\
e_{3456} = \dfrac{3}{2}\sqrt{2} & e_{3667} = \dfrac{3}{8}(\sqrt{2}-1) & e_{3777} = -\dfrac{1}{8}(\sqrt{2}-1) & e_{4444} = \dfrac{1}{8} \\
e_{4455} = \dfrac{3}{4} & e_{4466} = \dfrac{3}{8}(2-\sqrt{2}) & e_{4477} = \dfrac{3}{8}(2-\sqrt{2}) & e_{5555} = \dfrac{1}{8} \\
e_{5566} = \dfrac{3}{8}(2-\sqrt{2}) & e_{5577} = \dfrac{3}{8}(2-\sqrt{2}) & e_{6666} = \dfrac{3}{32}(3-2\sqrt{2}) & e_{6677} = \dfrac{3}{16}(3-2\sqrt{2}) \\
e_{7777} = \dfrac{3}{32}(3-2\sqrt{2}) & & &
\end{array}
\tag{A.5}
$$