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Resonant normal form for even periodic FPU chains

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Abstract. We investigate periodic FPU chains with an even number of particles. We show that near the equilibrium point, any such chain admits a *resonant* Birkhoff normal form of order four which is *completely integrable*—an important fact which helps explain the numerical experiments of Fermi, Pasta, and Ulam. We analyze the moment map of the integrable approximation of an even FPU chain. Unlike the case of odd FPU chains these integrable systems (generically) exhibit hyperbolic dynamics. As an application we prove that any FPU chain with Dirichlet boundary conditions admits a Birkhoff normal form up to order four and show that a KAM theorem applies.

1. Introduction

In this paper we consider FPU chains with an even number *N* of particles of equal mass, normalized to be one. Such chains have been introduced by Fermi, Pasta, and Ulam [5], as models to test numerically the principle of thermalization as *N* grows larger and larger. A FPU chain consists of a string of particles moving on the line or the circle interacting only with their nearest neighbors through nonlinear springs. Its Hamiltonian is given by

$$H_V = \frac{1}{2} \sum_{n=1}^{N} p_n^2 + \sum_{n=1}^{N} V(q_n - q_{n+1}), \tag{1}$$

where $V: \mathbb{R} \to \mathbb{R}$ is a smooth potential. The corresponding Hamiltonian equations read $(1 \le n \le N)$

$$\dot{q}_n = \partial_{p_n} H_V = p_n, \quad \dot{p}_n = -\partial_{q_n} H_V = -V'(q_n - q_{n+1}) + V'(q_{n-1} - q_n).$$

Here q_n denotes the displacement of the nth particle from its equilibrium position and p_n is its momentum. If not stated otherwise, we assume periodic boundary conditions

$$(q_{i+N}, p_{i+N}) = (q_i, p_i) \quad \forall i \in \{0, 1\}.$$

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Without loss of generality, the potential $V: \mathbb{R} \to \mathbb{R}$ is assumed to have a Taylor expansion at 0 of the form

$$V(x) = \kappa \left(\frac{1}{2} x^2 - \frac{\alpha}{3!} x^3 + \frac{\beta}{4!} x^4 + \cdots \right), \tag{3}$$

where κ is the (linear) spring constant normalized to be 1 and α , $\beta \in \mathbb{R}$ are parameters measuring the strength of the nonlinear interaction. The minus sign in front of the parameter α in the expansion (3) turns out to be convenient for later computations. Substituting the expression (3) for V into (1) yields the corresponding expansion of H_V :

$$H_V = \frac{1}{2} \sum_{n=1}^{N} p_n^2 + \frac{1}{2} \sum_{n=1}^{N} (q_{n+1} - q_n)^2 + \frac{\alpha}{3!} \sum_{n=1}^{N} (q_{n+1} - q_n)^3 + \frac{\beta}{4!} \sum_{n=1}^{N} (q_{n+1} - q_n)^4 + \cdots$$
 (4)

For any FPU chain, the total momentum $P = N^{-1} \sum_{n=1}^{N} p_n$ is an integral of motion, and therefore the center of mass $Q = N^{-1} \sum_{n=1}^{N} q_n$ evolves with constant velocity. Hence any FPU chain can be viewed as a family of Hamiltonian systems of 2N - 2 degrees of freedom, parametrized by the vector of initial conditions $(Q, P) \in \mathbb{R}^2$ with Hamiltonian independent of Q. In particular, for N=2 any FPU chain is integrable, and hence we will concentrate on the case $N \geq 3$. Further, note that for any vector $(Q, P) \in \mathbb{R}^2$, the origin in \mathbb{R}^{N-2} is an equilibrium point of the corresponding system. The momentum of such an equilibrium point is given by the constant vector $(p_1, \ldots, p_N) = P(1, \ldots, 1)$.

The frequencies $(\omega_k^0)_{1 \le k \le N-1}$ of the linearization of an arbitrary FPU chain at (q, p)= (0, 0) can be easily computed to be

$$\omega_k^0 = 2\sin\frac{k\pi}{N}.$$

The corresponding resonance lattice is given by (see Appendix A of [7])

$$\left\{ l = (l_1, \dots, l_{N-1}) \in \mathbb{Z}^{N-1} \mid \sum_{k=1}^{N-1} l_k \sin \frac{k\pi}{N} = 0 \right\}$$

and generated by the vectors $l^{(k)}$, $1 \le k \le N-1$, defined by $l^{(k)} = e_k - e_{N-k}$, where e_i , $1 \le i \le N-1$, denotes the standard basis in \mathbb{R}^{N-1} . For any point $(x, y) \in \mathbb{R}^{2N-2}$ introduce the variables $I = (I_k)_{1 \le k \le N-1}$, where

$$I_k = \frac{1}{2}(x_k^2 + y_k^2),\tag{5}$$

as well as $M=(M_k)_{1\leq k\leq N-1}$, $J=(J_k)_{1\leq k\leq N-1}$, and $L=(L_k)_{1\leq k\leq N-1}$. They are defined on \mathbb{R}^{2N-2} with values in \mathbb{R}^{N-1} and given by

$$M_k = \frac{1}{2}(x_k y_{N-k} - x_{N-k} y_k), \ J_k = \frac{1}{2}(x_k x_{N-k} + y_k y_{N-k}), \ L_k = \frac{1}{2}(I_k - I_{N-k}).$$
 (6)

Note that for any $1 \le k \le N-1$, $(M_k, J_k, L_k) = (-M_{N-k}, J_{N-k}, -L_{N-k})$ and $I_k I_{N-k} = M_k^2 + J_k^2$, or

$$\left(\frac{I_k + I_{N-k}}{2}\right)^2 = M_k^2 + J_k^2 + L_k^2,$$
(7)

i.e. M_k , J_k , L_k are the Hopf variables expressed in x_k , y_k , x_{N-k} , y_{N-k} . They describe the image of the Hopf map from the three-dimensional sphere of radius $\frac{1}{2}(I_k + I_{N-k})$ centered at the orgin of \mathbb{R}^4 . Further, define the function $H_{\alpha,\beta}: \mathbb{R}^{N-1} \to \mathbb{R}$ by

$$H_{\alpha,\beta}(I) = 2\sum_{k=1}^{N-1} \sin\frac{k\pi}{N} I_k + \frac{1}{4N} \sum_{k=1}^{N-1} d_k^+ I_k^2 + \frac{\beta - \alpha^2}{2N} \sum_{\substack{l \neq m \\ 1 \le l, m \le N-1}} \sin\frac{l\pi}{N} \sin\frac{m\pi}{N} I_l I_m$$
(8)

where

$$d_k^+ \equiv d_k^+(\alpha, \beta) := \alpha^2 + (\beta - \alpha^2) \sin^2 \frac{k\pi}{N}$$
 (9)

and let

$$R_{\alpha,\beta}(J,M) := \frac{\beta - \alpha^2}{4N} (R(J,M) + R_{N/4}(J,M))$$
 (10)

where

$$R(J, M) = 4 \sum_{1 \le k < N/4} \sin \frac{2k\pi}{N} (J_k J_{N/2-k} - M_k M_{N/2-k})$$
 (11)

and

$$R_{N/4}(J, M) = \begin{cases} J_{N/4}^2 - M_{N/4}^2 & \text{if } N/4 \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases}$$
 (12)

Note that for $\alpha, \beta \in \mathbb{R}$ with $\beta = \alpha^2$, referred to as the *Toda case*, $R_{\alpha,\beta}$ vanishes.

In [7] we proved that even FPU chains admit a resonant normal form near the equilibrium point.

Theorem 1.1. If $N \ge 4$ is even, there are canonical coordinates $(x_k, y_k)_{1 \le k \le N-1}$ such that the Hamiltonian of any FPU chain, when expressed in these coordinates, takes the form $H_V^{trunc}(I, J, M) + O(|(x, y)|^5)$ where

$$H_V^{\text{trunc}} = NP^2/2 + H_{\alpha,\beta}(I) - R_{\alpha,\beta}(J,M)$$
(13)

with $\alpha, \beta \in \mathbb{R}$ as in (3) and where $H_{\alpha,\beta}(I)$ and $R_{\alpha,\beta}(J,M)$ are given by (8) and (10), respectively.

Note that in the case $\beta \neq \alpha^2$, the Hamiltonian H_V cannot be transformed into Birkhoff normal form up to order 4 due to resonances. Nevertheless, the Hamiltonian truncated at order 4, H_V^{trunc} , can be proved to be completely integrable. The form of the resonance lattice introduced above suggests that $I_k + I_{N-k}$ ($1 \leq k \leq N/2$) are integrals of H_V^{trunc} in involution. To find the remaining commuting integrals we express $H_{\alpha,\beta}(I)$ in terms of $I_k + I_{N-k}$ ($1 \leq k \leq N/2$) and a remainder term,

$$H_{\alpha,\beta}(I) = H^{(2)}(I) + H_{\alpha,\beta}^{(4)}(I) + \frac{1}{2N} \sum_{k=1}^{N/2-1} d_k^- I_k I_{N-k}$$
 (14)

where

$$\begin{split} H^{(2)}(I) &= 2 \sum_{k=1}^{N/2-1} \sin \frac{k\pi}{N} (I_k + I_{N-k}) + 2I_{N/2}, \\ H^{(4)}_{\alpha,\beta}(I) &= \frac{1}{4N} \sum_{k=1}^{N/2-1} d_k^+ (I_k + I_{N-k})^2 + \frac{\beta}{4N} I_{N/2}^2 \\ &\quad + \frac{\beta - \alpha^2}{N} I_{N/2} \sum_{k=1}^{N/2-1} \sin \frac{k\pi}{N} (I_k + I_{N-k}) \\ &\quad + \frac{\beta - \alpha^2}{2N} \sum_{\substack{1 \le k, l < N/2 \\ k \ne l}} \sin \frac{k\pi}{N} \sin \frac{l\pi}{N} (I_k + I_{N-k}) (I_l + I_{N-l}), \end{split}$$

and

$$d_k^- \equiv d_k^-(\alpha, \beta) := -\alpha^2 + (\beta - \alpha^2) \sin^2 \frac{k\pi}{N}.$$

By (7), one has $I_k I_{N-k} = J_k^2 + M_k^2$ for any $1 \le k \le N/2 - 1$ so that the remainder term $(2N)^{-1} \sum_{k=1}^{N/2-1} d_k^{-1} I_k I_{N-k}$ in (14) can be written as

$$\frac{1}{2N} \Big(\sum_{1 \le k \le N/4} (d_k^- (J_k^2 + M_k^2) + d_{\tilde{k}}^- (J_{\tilde{k}}^2 + M_{\tilde{k}}^2)) + d_{N/4}^- (J_{N/4}^2 + M_{N/4}^2) \Big),$$

where the latter term is defined to be 0 if $N/4 \notin \mathbb{Z}$, and $\tilde{k} \equiv \tilde{k}(k) = N/2 - k$. Combined with the expression (10) for $R_{\alpha,\beta}(J,M)$ the Hamiltonian H_V^{trunc} in (13) then takes the form

$$H_V^{\text{trunc}} = \frac{NP^2}{2} + H^{(2)}(I) + H_{\alpha,\beta}^{(4)}(I) + \frac{1}{2N} \sum_{1 \le k \le N/4} K_k(I, J, M)$$
 (15)

where for $1 \le k < N/4$,

$$K_k(I, J, M) = d_k^-(J_k^2 + M_k^2) + d_{\tilde{k}}^-(J_{\tilde{k}}^2 + M_{\tilde{k}}^2) - 2(\beta - \alpha^2) \sin \frac{2k\pi}{N} (J_k J_{\tilde{k}} - M_k M_{\tilde{k}})$$
 (16)

and

$$K_{N/4}(J, M) = \begin{cases} -\alpha^2 J_{N/4}^2 + (\beta - 2\alpha^2) M_{N/4}^2 & \text{if } N \equiv 0 \bmod 4, \\ 0 & \text{otherwise.} \end{cases}$$
 (17)

Theorem 1.2. Let $N \ge 4$ be an even integer. Then the truncated FPU Hamiltonian H_V^{trunc} given by (13) is completely integrable. If the expansion of V in (3) satisfies $(\alpha, \beta) \ne (0, 0)$, then the following N-1 quantities are functionally independent integrals in involution:

$$(I_k + I_{N-k})_{1 \le k \le N/2}, \quad (I_k + I_{N/2+k})_{1 \le k \le N/4}, \quad (K_k)_{1 \le k \le N/4}.$$

Remark. In the case $\beta = \alpha^2$, the integrals $K_k(I, J, M)$ only depend on the action variables I, as $M_j^2 + J_j^2 = I_j I_{N-j}$ for any $1 \le j < N/2$.

In Sections 3 and 4 we present a detailed analysis of the geometry of the moment map of the integrable system of Theorem 1.2. In particular, we show that whenever $\beta \neq \alpha^2$, then this integrable system exhibits hyperbolic dynamics.

In Section 5, we will use Theorem 1.1 to show that any FPU chain with Dirichlet boundary conditions admits a Birkhoff normal form up to order 4 by recognizing such a system as an invariant submanifold of a periodic FPU chain. Consider a chain with N' ($N' \geq 3$, not necessarily even) moving particles and Hamiltonian given by

$$H_V^D = \frac{1}{2} \sum_{n=1}^{N'} p_n^2 + \sum_{n=1}^{N'} V(q_n - q_{n+1}).$$

Assume that its endpoints are fixed, i.e.

$$q_0 = q_{N'+1} = 0. (18)$$

Theorem 1.3. Any FPU chain with $N' \geq 3$ moving particles and Dirichlet boundary conditions admits a Birkhoff normal form of order 4, i.e. there are canonical coordinates $(x_k, y_k)_{1 \leq k \leq N'}$ such that H_V^D takes the form

$$(N'+1)P^2/2 + H_{\alpha,\beta}^D(I) + O(|(x,y)|^5)$$

where $I = (I_1, ..., I_{N'})$ is given by (5), α , β are as in (3), and $H_{\alpha,\beta}^D(I)$ is of the form

$$2\sum_{k=1}^{N'} s_{k} I_{k} + \frac{1}{16(N'+1)} \sum_{k=1}^{N'} (\alpha^{2} + 3(\beta - \alpha^{2}) s_{k}^{2}) I_{k}^{2} \underbrace{+ \frac{\beta - \alpha^{2}}{32(N'+1)} I_{N/4}^{2}}_{only if N/4 \in \mathbb{N}} + \frac{\beta - \alpha^{2}}{16(N'+1)} \Big(\sum_{\substack{l \neq m \\ 1 \leq l, m \leq N'}} 4s_{l} s_{m} I_{l} I_{m} - \sum_{k=1}^{N'} s_{2k} I_{k} I_{N'+1-k} \Big).$$
 (19)

Note that in (19), the numbers $s_k = \sin \frac{k\pi}{N} = \sin \frac{k\pi}{2N'+2}$ for any $1 \le k \le N'$ are pairwise different.

Corollary 1.4. Near the equilibrium state, any FPU chain with N' moving particles and Dirichlet boundary conditions can be approximated up to order 4 by an integrable system of N' harmonic oscillators which are coupled at fourth order except if $\beta = \alpha^2$.

Denote by $Q^D_{\alpha,\beta}$ the Hessian of $H^D_{\alpha,\beta}(I)$ at I=0. Note that $Q^D_{\alpha,\beta}$ is an $N'\times N'$ -matrix which only depends on the parameters α and β .

Theorem 1.5. (i) For any given $\alpha \in \mathbb{R} \setminus \{0\}$, $\det(Q_{\alpha,\beta}^D)$ is a polynomial in β of degree N' and has N' real zeroes (counted with multiplicities). When listed in increasing order, the zeroes $\beta_k = \beta_k(\alpha)$ satisfy

$$\beta_1 \leq \cdots \leq \beta_{\lceil (N'+1)/2 \rceil} < \alpha^2 < \beta_{\lceil (N'+3)/2 \rceil} \leq \cdots \leq \beta_{N'}.$$

Moreover, index $(Q_{\alpha,\beta}^D)$, defined as the number of negative eigenvalues of $Q_{\alpha,\beta}^D$, is given by

$$\operatorname{index}(Q_{\alpha,\beta}^D) = \begin{cases} \lceil (N'+1)/2 \rceil & \text{for } \beta < \beta_1, \\ 0 & \text{for } \beta_{\lceil (N'+1)/2 \rceil} < \beta < \beta_{\lceil (N'+3)/2 \rceil}, \\ \lfloor (N'-1)/2 \rfloor & \text{for } \beta > \beta_{N'}. \end{cases}$$

(ii) For $\alpha = 0$, $\det(Q_{0,\beta}^D)$ is a polynomial in β of degree N', and $\beta = 0$ is the only zero of $\det(Q_{0,\beta}^D)$. It has multiplicity N', and the index of $Q_{0,\beta}^D$ is given by

$$\operatorname{index}(Q_{0,\beta}^D) = \begin{cases} \lceil (N'+1)/2 \rceil & \text{for } \beta < 0, \\ \lfloor (N'-1)/2 \rfloor & \text{for } \beta > 0. \end{cases}$$

Applications. Theorems 1.3 and 1.5 allow one to apply for any given $\alpha \in \mathbb{R}$ the classical KAM theorem (see e.g. [9]) near the equilibrium point to the FPU chain with Hamiltonian H_V^D and Dirichlet boundary conditions for a real analytic potential $V(x) = \frac{1}{2}x^2 - \frac{\alpha}{3!}x^3 + \frac{\beta}{4!}x^4 + \cdots$ with $\beta \in \mathbb{R} \setminus \{\beta_1(\alpha), \ldots, \beta_{N'}(\alpha)\}$. Moreover, as for any given $\alpha \in \mathbb{R} \setminus \{0\}$, $Q_{\alpha,\beta}^D$ is positive definite for $\beta_{\lfloor (N'-1)/2 \rfloor}(\alpha) < \beta < \beta_{\lfloor (N'+1)/2 \rfloor}(\alpha)$, one can apply Nekhoroshev's theorem (see e.g. [10]) near the equilibrium point to the FPU chain with Hamiltonian H_V^D for V with such β 's. These perturbation results confirm long standing conjectures—see e.g. [3].

In subsequent work we plan to compare orbits of the FPU chain with Hamiltonian H_V with the ones of its integrable approximation H_V^{trunc} , with the intention to explain the numerical experiments of Fermi, Pasta, and Ulam.

Related work. Theorems 1.2 and 1.3 improve on earlier results of Rink in [11] and [13], respectively, where the case $\alpha=0$ has been treated. Our approach has been shaped by our work on the Toda lattice [6]. The latter, introduced by Toda [14] and extensively studied, is a special FPU chain which is integrable (i.e. the original Hamiltonian H_V —not just H_V^{trunc} —is integrable). It turns out that the same canonical transformations which near the equilibrium bring the Toda lattice into Birkhoff normal form can be used for any FPU chain. If N is odd, this transformation brings H_V into Birkhoff normal form up to order 4; we have studied this case in detail in [7].

One of the most important open problems in the field of FPU chains is the investigation of the dynamics of these chains when the number of particles gets larger and larger. It is likely that our results on FPU chains with Dirichlet boundary conditions can be used for this purpose. For recent contributions in this direction see e.g. [1], [2].

2. Proof of Theorem 1.2

Denote by $\{\cdot,\cdot\}$ the standard Poisson bracket on \mathbb{R}^{2N-2} . In a straightforward way one computes the Poisson brackets between the variables $I, M, J, L \in \mathbb{R}^{N-1}$, given by (5) and (6) (cf. [4, p. 28]):

Lemma 2.1. The Poisson brackets between the variables I_k , J_k , M_k $(1 \le k \le N-1)$ are given by

$${I_l, I_k} = {J_l, J_k} = {M_l, M_k} = 0,$$
 (20)

$$\{J_l, I_k\} = -M_l(\delta_{kl} - \delta_{k+l,N}),$$
 (21)

$$\{M_l, I_k\} = J_l(\delta_{kl} - \delta_{k+l,N}), \tag{22}$$

As a consequence, one obtains the following relations between the variables M_k , J_k , and L_k , $1 \le k \le N-1$:

$$\{M_k, J_l\} = L_l(\delta_{k+l,N} - \delta_{kl}),$$

$$\{J_k, L_l\} = M_k(\delta_{k+l,N} - \delta_{kl}),$$

$$\{L_k, M_l\} = J_l(\delta_{k+l,N} - \delta_{kl}).$$

First note that the list of functions of Theorem 1.2.

$$(I_k + I_{N-k})_{1 \le k \le N/2}, \quad (I_k + I_{N/2+k})_{1 \le k \le N/4}, \quad (K_k)_{1 \le k \le N/4},$$
 (23)

contains N-1 terms whether N/4 is an integer or not. In addition, for any $1 \le k < N/4$, the terms $I_k + I_{N-k}$, $I_{N/2-k} + I_{N/2+k}$, $I_k + I_{N/2+k}$, K_k are functions of the eight variables x_k , y_k , $x_{N/2-k}$, $y_{N/2-k}$, $x_{N/2+k}$, $y_{N/2+k}$, x_{N-k} , and y_{N-k} , the term $I_{N/2}$ is a function of the two variables $x_{N/2}$, $y_{N/2}$, and, in the case $N/4 \in \mathbb{N}$, the terms $I_{N/4} + I_{3N/4}$, $K_{N/4}$ are functions of the four variables $x_{N/4}$, $y_{N/4}$, $y_{3N/4}$, $y_{3N/4}$. Hence we obtain a partition of the 2N-2 variables x_1 , y_1 , ..., x_{N-1} , y_{N-1} into $\lfloor N/4 \rfloor + 1$ pairwise disjoint sets of variables, and all Poisson brackets between variables of different sets of this partition vanish.

Lemma 2.2. The N-1 functions listed in (23) are pairwise in involution.

Proof. The functions in (23) depend on only one of the $\lfloor N/4 \rfloor + 1$ pairwise disjoint sets of variables. As the Poisson brackets between terms depending on variables of different sets vanish, it remains to check that functions of (23) with the same k are in involution with each other. In view of the definitions (16) and (17) of K_l and $K_{N/4}$, respectively, and taking into account that $(I_k)_{1 \le k \le N-1}$ are pairwise in involution, this amounts to proving that for any $1 \le l < N/4$,

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_l + I_{N-l}\} = 0, (24)$$

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_{N/2-l} + I_{N/2+l}\} = 0,$$
(25)

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_l + I_{N/2+l}\} = 0, (26)$$

$$\{J_{N/4}^2 - M_{N/4}^2, I_{N/4} + I_{3N/4}\} = 0. (27)$$

First we note that by (21) and (22) one has, for any $1 \le l < N/2$,

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_l\} = -J_{N/2-l} M_l - M_{N/2-l} J_l, \tag{28}$$

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_{N-l}\} = J_{N/2-l} M_l + M_{N/2-l} J_l.$$
(29)

Since the right hand sides of (28) and (29) are invariant under exchanging l and N/2 - l, the same must hold for the left hand sides, and we conclude that

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_{N/2-l}\} = -J_{N/2-l} M_l - M_{N/2-l} J_l, \tag{30}$$

$$\{J_l J_{N/2-l} - M_l M_{N/2-l}, I_{N/2+l}\} = J_{N/2-l} M_l + M_{N/2-l} J_l.$$
(31)

The identities (24)–(26) now follow from the appropriate combinations of (28)–(31). In the same fashion, one concludes that (27) holds.

Proof of Theorem 1.2. In view of Lemma 2.2, it remains to check that the quantities listed in (23) are functionally independent integrals. The independence is easy to verify, and the fact that they are conserved quantities follows from the formula (15), showing that H_V^{trunc} can be written as a function of them.

3. Foliation by Liouville tori

In the next two sections we describe the geometry of the moment map of the truncated resonant normal form (13) for any even periodic FPU chain H_V with potential V whose expansion (3) satisfies $(\alpha, \beta) \neq (0, 0)$. The case $\beta = \alpha^2$ is special as in this case the normal form (13) is the Birkhoff normal form of order four of the Toda chain. Its foliation is well known—it is the one of uncoupled harmonic oscillators. Hence we will concentrate on the case $\beta \neq \alpha^2$ only. The special case $\alpha = 0$ has been partially studied by Rink [12]. Surprisingly, it turns out that many of his results continue to hold in the general case. If we use the notation $\tilde{k} \equiv \tilde{k}(k) = N/2 - k$, the integrals of Theorem 1.2 can be grouped as follows:

$$(\mathcal{H}_k, \mathcal{H}_{\tilde{k}}, L_k, K_k)_{1 \le k < N/4}, \quad I_{N/2}, \quad \mathcal{H}_{N/4}, K_{N/4},$$
 (32)

where for $1 \le k < N/2$,

$$\mathfrak{H}_k := I_k + I_{N-k}, \quad L_k := I_k - I_{\tilde{k}}.$$

(Here we used the fact that $L_k = (I_k + I_{N/2+k}) - (I_{N/2-k} + I_{N/2+k})$ is the difference of two integrals listed in Theorem 1.2.)

Using the assumption $\beta - \alpha^2 \neq 0$, we rewrite the integrals $(K_l)_{1 \leq l \leq N/4}$ as follows. Introduce the bifurcation parameter

$$\gamma \equiv \gamma(\alpha, \beta) := \frac{\alpha^2}{\alpha^2 - \beta} \tag{33}$$

and note that

$$d_k^- = -\alpha^2 + (\beta - \alpha^2)s_k^2 = (\beta - \alpha^2)(\gamma + s_k^2).$$

For any $1 \le k < N/4$, one has

$$K_k = -d_k^-(J_k^2 + M_k^2) - d_{\tilde{k}}^-(J_{\tilde{k}}^2 + M_{\tilde{k}}^2) + 2(\beta - \alpha^2)s_{2k}(J_kJ_{\tilde{k}} - M_kM_{\tilde{k}}),$$

whereas for k = N/4,

$$K_k = \alpha^2 J_k^2 - (\beta - 2\alpha^2) M_k^2 = (\alpha^2 - \beta) (\gamma J_k^2 + (1 + \gamma) M_k^2).$$

Below, we will *omit* the factor $s_{2k}(\alpha^2 - \beta)$ in K_k for simplicity, since it does not influence the geometry of the level sets of the integrals $(K_k)_{1 < k < N/4}$.

Each of the $\lfloor N/4 \rfloor + 1$ groups of integrals listed in (32) depends only on a subset of the variables $\{(x_k, y_k)_{1 \le k \le N-1}\}$. These subsets form a disjoint partition of $\{(x_k, y_k)_{1 \le k \le N-1}\}$. More precisely, the following result holds.

Proposition 3.1. The phase space $T^*\mathbb{R}^{N-1}$ of the truncated resonant normal form H_V^{trunc} given by (13) is the direct sum of invariant symplectic subspaces,

$$T^*\mathbb{R}^{N-1} = \bigoplus_{0 \le k \le N/4} \mathcal{P}_k,$$

where

$$\mathcal{P}_k = \{ (x_i, y_i)_{1 \le i \le N-1} \in T^* \mathbb{R}^{N-1} \mid x_i = y_i = 0 \,\forall j \notin \{k, N-k, \tilde{k}, N-\tilde{k}\} \}.$$

The foliation of $T^*\mathbb{R}^{N-1}$ by level sets of the integrals (32) is the Cartesian product of the foliations of the \mathfrak{P}_k .

We now analyze the foliations of \mathcal{P}_0 , $\mathcal{P}_{N/4}$, and \mathcal{P}_k for 0 < k < N/4 separately. Note that \mathcal{P}_0 and \mathcal{P}_k (0 < k < N/4) can be canonically identified with $T^*\mathbb{R}$ and $T^*\mathbb{R}^4$, respectively, and $\mathcal{P}_{N/4}$ with $T^*\mathbb{R}^2$ (if $N/4 \in \mathbb{N}$) or $\{0\}$ (if $N/4 \notin \mathbb{N}$).

Foliation of \mathcal{P}_0 . One easily sees that $I_{N/2}$ foliates $T^*\mathbb{R}$ by circles, centered at the origin.

Foliation of $\mathfrak{P}_{N/4}$ for $N/4 \in \mathbb{Z}$. Let us study the geometry of the moment map $\mathfrak{M}: T^*\mathbb{R}^2 \to \mathbb{R}^2$ defined by the integrable system with commuting integrals $H \equiv H_{N/4}$ and $K \equiv K_{N/4}$. It is convenient to introduce the following notation. Denote the standard coordinates of $T^*\mathbb{R}^2$ by $(x,y)=(x_1,x_2,y_1,y_2)$ and introduce the action variables $I_j=\frac{1}{2}(x_i^2+y_j^2)$ (j=1,2), as well as the Hopf variables M,J,L given as in (6),

$$(M, J, L) = \frac{1}{2}(x_1y_2 - x_2y_1, x_1x_2 + y_1y_2, I_1 - I_2).$$

Then the moment map $\mathcal{M} = (H, K)$ takes the form

$$H = \frac{1}{2}(I_1 + I_2)$$
 and $K = (1 + \gamma)M^2 + \gamma J^2$.

As already remarked in (7) one has

$$M^2 + J^2 + L^2 = H^2$$

Further, we may replace K by K_{γ} given by

$$K_{\gamma} := \begin{cases} (1+\gamma)M^2 + \gamma J^2, & \gamma \notin \{0, 1\}, \\ M, & \gamma = 0, \\ J, & \gamma = 1. \end{cases}$$

First observe that the origin (x, y) = (0, 0) of $T^*\mathbb{R}^2$ is the only critical point of M with rank $(d_{(x,y)}M) = 0$. Moreover,

$$\mathcal{M}^{-1}\{(0,0)\} = \{(0,0)\}.$$

The critical points $(x, y) \in T^*\mathbb{R}^2 \setminus \{(0, 0)\}$ with $\mathrm{rank}(d_{(x, y)}\mathcal{M}) = 1$ are analyzed by symplectic reduction via the Hamiltonian vector field of H. On the sphere $\mathbb{S}^3_\rho = \{H = \rho^2/4\}$ of radius $\rho > 0$ in $T^*\mathbb{R}^2$ define the Hopf map

$$\mathfrak{F}: \mathbb{S}^3_\rho \to \mathbb{S}^2_r, \quad (x, y) \mapsto (M, J, L),$$

where $r = \sqrt{M^2 + J^2 + L^2}|_{\mathbb{S}^3_\rho} = H|_{\mathbb{S}^3_\rho} = \rho^2/4$. The fibers of \mathcal{F} are circles obtained by the \mathbb{S}^1 -action of H. The reduced system is then given by $(\mathbb{S}^2_r, X_\gamma)$ where X_γ denotes the reduced Hamiltonian vector field induced by K_γ . To compute X_γ , note that the equations of motion in the reduced system corresponding to the Hamiltonian K_γ are given by

$$\frac{d}{dt} \begin{pmatrix} M \\ J \\ L \end{pmatrix} = \begin{pmatrix} M \\ J \\ L \end{pmatrix} \times \begin{pmatrix} \partial_M K_{\gamma} \\ \partial_J K_{\gamma} \\ \partial_L K_{\gamma} \end{pmatrix}. \tag{34}$$

Indeed, according to the procedure of reduction in Section I.5 of [4], formula (34) follows from

$$\dot{w}_j = \{w_j, K_\gamma\} = \sum_{i=1}^3 \partial_{w_i} K_\gamma \{w_j, w_i\} \quad (1 \le j \le 3)$$

and the commutation relations of the variables $(w_1, w_2, w_3) = (M, J, L)$ given by Lemma 2.1. We then obtain

$$X_{\gamma} = \begin{cases} (-2\gamma JL, 2(1+\gamma)ML, -2MJ), & \gamma \notin \{-1, 0\}, \\ (0, L, -J), & \gamma = 0, \\ (-L, 0, M), & \gamma = -1. \end{cases}$$

It turns out that the foliation of \mathbb{S}^2_r by level sets of K_γ depends on the bifurcation parameter γ . If $\gamma=0$, then $(\pm r,0,0)$ are the only two fixed points of X_0 . They are both elliptic and the level sets of K_0 in $\mathbb{S}^2_r \setminus \{(\pm r,0,0)\}$ are circles. Similarly, for $\gamma=-1$, $(0,\pm r,0)$ are the only two fixed points of X_{-1} . They are both elliptic and the level sets of K_{-1} in $\mathbb{S}^2_r \setminus \{(0,\pm r,0)\}$ are circles. Now let us consider the case $\gamma \in \mathbb{R} \setminus \{0,-1\}$. Then X_γ admits six fixed points,

$$(\pm r, 0, 0), (0, \pm r, 0), (0, 0, \pm r),$$

two of which are hyperbolic and the remaining four elliptic. Note that the corresponding values of K_{γ} are $(1 + \gamma)r^2$, γr^2 , and 0, respectively, and the two hyperbolic fixed points are contained in the same connected component of the inverse image of K_{γ} in \mathbb{S}_r^2 . This component consists of two great circles where each of the four half circles is a heteroclinic X_{γ} -orbit connecting the two hyperbolic fixed points.

	hyperbolic fixed points	critical value
$\gamma < -1$	$(\pm r, 0, 0)$	$(1+\gamma)r^2$
$-1 < \gamma < 0$	$(0,0,\pm r)$	0
$\gamma > 0$	$(0,\pm r,0)$	γr^2

Let us verify the claimed classification of the two fixed points $(0, 0, \varepsilon r)$ with $\varepsilon \in \{\pm\}$. The other four fixed points are treated in a similar fashion. Near $(0, 0, \varepsilon r)$ we choose M, J as coordinates of \mathbb{S}^2_r . The equations of motion induced by X_γ on \mathbb{S}^2_r in these coordinates read

$$\dot{M} = -\varepsilon 2\gamma J\sqrt{r^2 - M^2 - J^2}, \quad \dot{J} = \varepsilon 2(1+\gamma)M\sqrt{r^2 - M^2 - J^2}.$$

If linearized at $(0, 0, \varepsilon r)$, the corresponding linear system is given by the 2×2 -matrix εA where

$$A = 2r \begin{pmatrix} 0 & -\gamma \\ 1+\gamma & 0 \end{pmatrix}.$$

The eigenvalues of A are given by

$$\lambda^2 + 4\gamma(1+\gamma)r^2 = 0$$
, i.e. $\lambda_{1,2} = \pm 2r\sqrt{-\gamma(1+\gamma)}$.

As $-\gamma(1+\gamma) > 0$ iff $-1 < \gamma < 0$ it follows that $\lambda_{1,2}$ are in $\mathbb{R} \setminus \{0\}$ and hence $(0,0,\pm r)$ are both hyperbolic fixed points for $-1 < \gamma < 0$, whereas they are both elliptic if $\gamma < -1$ or $\gamma > 0$. For $-1 < \gamma < 0$, the inverse image $K_{\nu}^{-1}(\{0\})$ is given by

$$\begin{split} K_{\gamma}^{-1}(\{0\}) &= \{(M,J,L) \mid (1+\gamma)M^2 + \gamma J^2 = 0; M^2 + J^2 + L^2 = r^2\} \\ &= \left\{ (M,J,L) \mid M = \pm \left| \frac{\gamma}{1+\gamma} \right|^{1/2} J, \ M^2 + J^2 + L^2 = r^2 \right\}, \end{split}$$

whereas for $\gamma < -1$ or $\gamma > 0$, $K_{\gamma}^{-1}(\{0\}) = \{(0, 0, \pm r)\}.$

Foliation of \mathcal{P}_k for 0 < k < N/4. The foliation of \mathcal{P}_k for 0 < k < N/4 is more complicated than in the case k = N/4. We describe it in detail in the subsequent section.

4. Integrable system $(\mathcal{H}_k, \mathcal{H}_{\tilde{k}}, G_k, K_k)$

In this section we present a detailed study of the geometry of the moment map $\mathcal{M}: T^*\mathbb{R}^4 \to \mathbb{R}^4$ defined by the integrable system \mathcal{P}_k with commuting integrals \mathcal{H}_k , $\mathcal{H}_{\tilde{k}}$, G_k , K_k for $1 \leq k < N/4$. As in Section 3 we restrict to FPU chains with potential V whose expansion (3) satisfies $\beta \neq \alpha^2$. We show that in this case the vector field induced by K_k

exhibits hyperbolic dynamics. It is convenient to introduce the following notation. Denote the standard coordinates of $T^*\mathbb{R}^4$ by (x, y) with $x = (x_i)_{1 \le i \le 4}$ and $y = (y_i)_{1 \le i \le 4}$, and introduce the action variables $I_j = \frac{1}{2}(x_j^2 + y_j^2)$ $(1 \le j \le 4)$, as well as the Hopf variables $(M_i, J_i, L_i)_{1 \le i \le 2}$ given by

$$(M_1, J_1, L_1) = \frac{1}{2}(x_1y_2 - x_2y_1, x_1x_2 + y_1y_2, I_1 - I_2),$$

$$(M_2, J_2, L_2) = \frac{1}{2}(x_3y_4 - x_4y_3, x_3x_4 + y_3y_4, I_3 - I_4).$$

By Lemma 2.1, the Poisson brackets between the variables $(M_i, J_i, L_i)_{1 \le i \le 2}$ are given by

$$\{M_i, J_i\} = -L_i, \quad \{J_i, L_i\} = -M_i, \quad \{L_i, M_i\} = -J_i,$$

whereas all other brackets vanish.

The moment map $\mathfrak M$ then takes the form

$$\mathcal{M}: T^*\mathbb{R}^4 \to \mathbb{R}^4, \quad (x, y) \mapsto (H_1, H_2, G, K_{\gamma}),$$

where

$$H_1 = \frac{1}{2}(I_1 + I_2), \quad H_2 = \frac{1}{2}(I_3 + I_4), \quad G = L_1 - L_2$$

and where K_{γ} is a scalar multiple of K_k , given by

$$K_{\gamma} = \sum_{i=1}^{2} \frac{1}{2} d_{i,\gamma} (M_i^2 + J_i^2) + (M_1 M_2 - J_1 J_2)$$

with the coefficients $d_{1,\gamma}$, $d_{2,\gamma}$ defined by

$$d_{1,\gamma} = \frac{\gamma + s_k^2}{s_{2k}}, \quad d_{2,\gamma} = \frac{\gamma + c_k^2}{s_{2k}}$$

and $s_k = \sin\frac{k\pi}{N}$, $c_k = \cos\frac{k\pi}{N}$. (The definition of the integral G above differs from the one given earlier by a multiple of the integral $H_1 - H_2$ as $I_1 - I_3 = L_1 - L_2 + H_1 - H_2$.) First note that the origin (0,0) in $T^*\mathbb{R}^4$ is the only critical point of \mathfrak{M} with rank $(d\mathfrak{M}) = 0$. Moreover, $\mathfrak{M}^{-1}\{(0,0)\} = \{(0,0)\}$. Next observe that upon restriction to $T^*\mathbb{R}^2 \times \{0\}$, one has $G = \frac{1}{2}(I_1 - I_2)$ and $K_{\gamma} = d_{1,\gamma}(H_1^2 - L_1^2)$, hence they are functions of I_1 , I_2 alone and $\mathfrak{M}|_{T^*\mathbb{R}^2 \times \{0\}}$ may be replaced by the map $(x,y) \mapsto (I_1,I_2,0,0)$. The geometry of the latter map is the one of two uncoupled harmonic oscillators. The subspace $\{0\} \times T^*\mathbb{R}^2$ is treated similarly. It remains to study the restriction of \mathfrak{M} to $T^*\mathbb{R}^4 \setminus ((T^*\mathbb{R}^2 \times \{0\}) \cup \{\{0\} \times T^*\mathbb{R}^2\})$. The Hamiltonian vector fields of H_1 and H_2 induce a torus action on $T^*\mathbb{R}^2$. The corresponding symplectic reduction is given by the product of two Hopf maps,

$$\mathcal{F}: \mathbb{S}^3_{\rho_1} \times \mathbb{S}^3_{\rho_2} \to \mathbb{S}^2_{r_1} \times \mathbb{S}^2_{r_2}, \quad (x,y) \mapsto (M_i,J_i,L_i)_{1 \leq i \leq 2},$$

where for i=1,2, $\mathbb{S}^3_{\rho_i}=\{H_i=\rho_i^2/4\}$ is a sphere in $T^*\mathbb{R}^2$ and $r_i=\rho_i^2/4=\sqrt{M_i^2+J_i^2+L_i^2}|_{\mathbb{S}^3_{\rho_i}}=H_i|_{\mathbb{S}^3_{\rho_i}}$. The fibers of \mathcal{F} are 2-dimensional tori, obtained by the $\mathbb{S}^1\times\mathbb{S}^1$ -action of $H_1\cdot H_2$. The reduced system is then given by $(\mathbb{S}^2_{r_1}\times\mathbb{S}^2_{r_2},Y,X_\gamma)$, where

Y and X_{γ} denote the reduced Hamiltonian vector fields induced by G and K_{γ} , respectively. To compute Y and X_{γ} , note that the equations of motion in the reduced system, corresponding to a Hamiltonian H, are given by

$$\frac{d}{dt} \begin{pmatrix} M_i \\ J_i \\ L_i \end{pmatrix} = \begin{pmatrix} M_i \\ J_i \\ L_i \end{pmatrix} \times \begin{pmatrix} \partial_{M_i} H \\ \partial_{J_i} H \\ \partial_{L_i} H \end{pmatrix}, \quad i = 1, 2$$
 (36)

-see Section 3 for details. We then obtain

$$Y = \begin{pmatrix} J_1 \\ -M_1 \\ 0 \\ -J_2 \\ M_2 \\ 0 \end{pmatrix}, \quad X_{\gamma} = \begin{pmatrix} (J_2 - d_{1,\gamma} J_1) L_1 \\ (d_{1,\gamma} M_1 + M_2) L_1 \\ -(M_1 J_2 + M_2 J_1) \\ (J_1 - d_{2,\gamma} J_2) L_2 \\ (d_{2,\gamma} M_2 + M_1) L_2 \\ -(M_1 J_2 + M_2 J_1) \end{pmatrix}.$$
(37)

Further, introduce the reduced moment map

$$\mathcal{M}_{\gamma}: \mathbb{S}^2_{r_1} \times \mathbb{S}^2_{r_2} \to \mathbb{R}^2, \quad (M_i, J_i, L_i)_{1 \leq i \leq 2} \mapsto (G, K_{\gamma}).$$

We now study the critical points of \mathfrak{M}_{γ} with $\operatorname{rank}(d\mathfrak{M}_{\gamma})=0$, i.e. points of $\mathbb{S}^2_{r_1}\times\mathbb{S}^2_{r_2}$ which are fixed points of both Y and X_{γ} . From the expressions for Y and X_{γ} derived above, one easily sees that there are only four such critical points,

$$(M_i, J_i, L_i)_{1 \le i \le 2} = \varepsilon(0, 0, r_1, 0, 0, \pm r_2),$$

where $\varepsilon \in \{\pm\}$. The value of \mathcal{M}_{γ} at the critical point $\varepsilon(0,0,r_1,0,0,-r_2)$ is $(\varepsilon(r_1+r_2),0)$ and

$$\mathcal{M}_{\gamma}^{-1}\{(\varepsilon(r_1+r_2),0)\} = \{\varepsilon(0,0,r_1,0,0,-r_2)\}.$$

Computing the Jacobian of the reduced vector field X_{γ} at the critical points one sees that they are elliptic fixed points of X_{γ} . The values of \mathfrak{M}_{γ} at the other two critical points $\varepsilon(0,0,r_1,0,0,r_2)$ are $(\varepsilon(r_1-r_2),0)$. The inverse image of $(\varepsilon(r_1-r_2),0)$ might have several connected components, depending on the values of γ and the additional bifurcation parameter

$$r := r_1/r_2 > 0.$$

Our main results concerning the critical points $\varepsilon(0,0,r_1,0,0,r_2)$ are collected in the following theorem.

Theorem 4.1. Assume that $1 \le k < N/4$, $0 < r \le 1$, $\varepsilon \in \{\pm\}$, and $\gamma \in \mathbb{R}$. The critical point $\varepsilon(0, 0, r_1, 0, 0, r_2)$ of \mathfrak{M}_{γ} is a hyperbolic fixed point of the vector field X_{γ} if and only if

$$\left| (\gamma + s_k^2)\sqrt{r} + (\gamma + c_k^2) \frac{1}{\sqrt{r}} \right| < 2s_{2k}.$$
 (38)

Otherwise it is an elliptic fixed point of X_{γ} . If (38) is satisfied, the stable and unstable manifolds of $\varepsilon(0,0,r_1,0,0,r_2)$ both have dimension two. In the case r<1, the connected component of $\mathcal{M}_{\nu}^{-1}\{\varepsilon(r_1-r_2,0)\}$ containing $\varepsilon(0,0,r_1,0,0,r_2)$ is a 2-dimensional torus

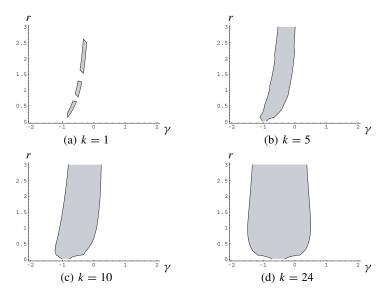


Fig. 1. Subsets of parameters (γ, r) with hyperbolic dynamics of X_{γ} (N = 100).

pinched at $\varepsilon(0,0,r_1,0,0,r_2)$ and consists of homoclinic X_{γ} -orbits. In the case r=1, $\mathcal{M}_{\gamma}^{-1}\{(0,0)\}$ is a 2-dimensional torus pinched at the two points $\pm(0,0,r_1,0,0,r_1)$, and $\mathcal{M}_{\gamma}^{-1}\{(0,0)\}\setminus\{\pm(0,0,r_1,0,0,r_1)\}$ consists of heteroclinic X_{γ} -orbits.

To prove Theorem 4.1 we separately treat for any given $1 \le k < N/4$ three subsets of the domain of the parameters γ and r. The results for these three cases are stated in detail in Propositions 4.2–4.4 below.

Note that the inverse image $\mathcal{M}_{\gamma}^{-1}\{(\varepsilon(r_1-r_2),0)\}$ is invariant under the action of the vector field Y. The orbits of this action can be easily described,

$$\{(R_{-\phi}(M_1, J_1), L_1, R_{\phi}(M_2, J_2), L_2) \mid |\phi| \le \pi\},\tag{39}$$

where $R_{\phi}(u, v)$ denotes the image of $(u, v) \in \mathbb{R}^2$ under the counterclockwise rotation R_{ϕ} by the angle ϕ . Hence given L_1 and L_2 with $|L_i| < r_i$ for i = 1, 2 there exists a unique point $(\hat{M}_i, \hat{J}_i, L_i)_{1 \le i \le 2}$ on such an orbit with the property that

$$(\hat{M}_1, \hat{J}_1) = (\sqrt{r_1^2 - L_1^2}, 0)$$
 and $(\hat{M}_2, \hat{J}_2) = \sqrt{r_2^2 - L_2^2} (\cos \alpha, \sin \alpha)$

for some $0 \le \alpha < 2\pi$. We denote the corresponding *Y*-orbit by $\mathcal{L}(L_1, L_2, \alpha)$, i.e.

$$\mathcal{L}(L_1, L_2, \alpha) = \{ (R_{-\phi}(\sqrt{r_1^2 - L_1^2}, 0), L_1, R_{\alpha + \phi}(\sqrt{r_2^2 - L_2^2}, 0), L_2) \mid |\phi| \le \pi \}.$$
 (40)

As G and K_{γ} commute, K_{γ} is invariant along any orbit of the vector field Y and we conclude that

$$K_{\gamma}((M_i, J_i, L_i)_{1 \le i \le 2}) = \frac{1}{2} \sum_{i=1}^{2} d_{i,\gamma}(r_i^2 - L_i^2) + \sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)} \cos \alpha. \tag{41}$$

Let us now determine $\mathcal{M}_{\gamma}^{-1}\{(\varepsilon(r_1-r_2),0)\}$ for $\varepsilon=1$ and $r\leq 1$. (The case where r>1 and/or $\varepsilon=-1$ is treated in a similar fashion.) Let $(M_i,J_i,L_i)_{1\leq i\leq 2}$ be an element of $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}\setminus\{(0,0,r_1,0,0,r_2)\}$. Then $r_2-L_2=r_1-L_1$ and $K_{\gamma}((M_i,J_i,L_i)_{1\leq i\leq 2})=0$. First note that $L_1< r_1$. Indeed, if $L_1=r_1$, then $L_2=r_2$ and $(M_i,J_i)=(0,0)$ for i=1,2, contradicting our assumption on the point considered. Hence in the expression for K_{γ} displayed above we can factor out r_1-L_1 and the equation $K_{\gamma}=0$ reads

$$0 = d_{1,\gamma}(r_1 + L_1) + d_{2,\gamma}(r_2 + L_2) + 2\sqrt{(r_1 + L_1)(r_2 + L_2)}\cos\alpha. \tag{42}$$

Next let us consider the case where $L_1=-r_1$. Then $(M_1,J_1,L_1)=-(0,0,r_1)$ and (42) reads $(\gamma+c_k^2)(r_2+L_2)=0$. Hence either $L_2=-r_2$ or $\gamma=-c_k^2$. In the case $L_2=-r_2$ it follows from $r_2-L_2=r_1-L_1=2r_1$ that $r_2=r_1$ and $L_2=L_1$. As a consequence, $(M_2,J_2,L_2)=-(0,0,r_1)$. On the other hand, if $\gamma=-c_k^2$ and $r_1< r_2$, then

$$-r_2 < r_2 - 2r_1 = L_2 < r_2$$
 and $M_2^2 + J_2^2 = r_2^2 - L_2^2 = 4r_1(r_2 - r_1)$.

If $L_1 \neq -r_1$ (and hence $L_2 \neq -r_2$ as $r_1 \leq r_2$) we set, for $-r_1 < L_1 < r_1$,

$$Q(L_1) := \begin{cases} \sqrt{\frac{r_1 + L_1}{2r_2 + L_1 - r_1}} & \text{if } r_1 < r_2, \\ 1 & \text{if } r_1 = r_2. \end{cases}$$

$$(43)$$

Then $0 < Q < \sqrt{r}$ and for r < 1, Q is increasing on $-r_1 < L_1 < r_1$. After division by $\frac{1}{s_{7k}}\sqrt{(r_1+L_1)(r_2+L_2)}$ equation (42) reads

$$(\gamma + s_k^2)Q + (\gamma + c_k^2)\frac{1}{Q} + 2s_{2k}\cos\alpha = 0.$$
 (44)

To investigate the solutions of (44) we distinguish between three cases: r=1, $[\gamma+c_k^2=0]$ and r<1, and $[\gamma+c_k^2\neq0]$ and r<1.

Let us first treat the case r = 1. Then $Q \equiv 1$ and equation (44) takes the form

$$2\gamma + 1 = -2s_{2k}\cos\alpha,\tag{45}$$

which is independent of L_1 .

Proposition 4.2. Let $\gamma \in \mathbb{R}$ be arbitrary and assume $1 \le k < N/4$ and r = 1. Then the following statements hold:

(i) If $|2\gamma + 1| > 2s_{2k}$, then

$$\mathcal{M}_{\gamma}^{-1}\{(0,0)\} = \{\varepsilon(0,0,r_1,0,0,r_1) \mid \varepsilon = \pm\},\$$

and $\pm (0, 0, r_1, 0, 0, r_1)$ are both elliptic fixed points of the vector field X_{γ} .

(ii) If $|2\gamma + 1| < 2s_{2k}$, then $\mathcal{M}_{\gamma}^{-1}\{(0,0)\} = \mathcal{N}_{\alpha} \cup \mathcal{N}_{-\alpha}$, where α is the unique angle satisfying $0 < \alpha < \pi$ and $2\gamma + 1 = -2s_{2k}\cos\alpha$, and where for any $-\pi \le \beta \le \pi$,

$$\mathcal{N}_{\beta} = \bigcup_{\substack{|L_1| \le r_1 \\ L_2 = L_1}} \mathcal{L}(L_1, L_2, \beta)$$

with $\mathcal{L}(L_1, L_2, \beta)$ given by (40). Both points, $\pm (0, 0, r_1, 0, 0, r_1)$, are hyperbolic fixed points of X_γ , and their stable and unstable manifolds each have dimension two. The set $\mathcal{N}_\alpha \setminus \{\pm (0, 0, r_1, 0, 0, r_1)\}$ consists of heteroclinic X_γ -orbits from $(0, 0, r_1, 0, 0, r_1)$ to $-(0, 0, r_1, 0, 0, r_1)$, whereas $\mathcal{N}_{-\alpha} \setminus \{\pm (0, 0, r_1, 0, 0, r_1)\}$ consists of heteroclinic X_γ -orbits with opposite direction. Topologically, $\mathcal{M}_\gamma^{-1}\{(0, 0)\}$ is a 2-dimensional torus, pinched at each of the two fixed points $\pm (0, 0, r_1, 0, 0, r_1)$.

- (iii) If $2\gamma + 1 = -2s_{2k}$, then $\alpha = 0$ and $\mathcal{M}_{\gamma}^{-1}\{(0,0)\} = \mathcal{N}_0$, whereas if $2\gamma + 1 = 2s_{2k}$, then $\alpha = \pi$ and $\mathcal{M}_{\gamma}^{-1}\{(0,0)\} = \mathcal{N}_{\pi}$. In both cases, $\pm (0,0,r_1,0,0,r_1)$ are elliptic fixed points of X_{γ} . On $\mathcal{N}_0 \cup \mathcal{N}_{\pi}$, any X_{γ} -orbit is periodic and coincides with the corresponding Y-orbit at least up to orientation.
- *Proof.* (i) By a straightforward computation one shows that under the given assumptions, both points $\pm (0, 0, r_1, 0, 0, r_1)$ are elliptic fixed points of X_{γ} . In view of equation (45), item (i) then easily follows.
- (ii) By the discussion preceding Proposition 4.2 it follows that the inverse image $\mathcal{M}_{\gamma}^{-1}\{(0,0)\}$ is as claimed. Again by a straightforward computation one shows that both fixed points $\pm(0,0,r_1,0,0,r_1)$ are hyperbolic. To see that $\mathcal{N}_{\alpha}\setminus\{\pm(0,0,r_1,0,0,r_1)\}$ consists of heteroclinic orbits of the vector field X_{γ} , consider the third component $(X_{\gamma})_3$ of X_{γ} (cf. (37)). Any element $(M_i,J_i,L_i)_{1\leq i\leq 2}$ in \mathcal{N}_{α} is of the form

$$(M_1, J_1) = \sqrt{r_1^2 - L_1^2} (\cos \phi, -\sin \phi), \quad (M_2, J_2) = \sqrt{r_1^2 - L_1^2} (\cos(\alpha + \phi), \sin(\alpha + \phi)). \tag{46}$$

Thus

$$(X_{\gamma})_3 = -(M_1 J_2 + M_2 J_1) = -(r_1^2 - L_1^2)(\cos\phi\sin(\alpha + \phi) - \cos(\alpha + \phi)\sin\phi). \tag{47}$$

Hence $(X_{\gamma})_3 = -(r_1^2 - L_1^2) \sin \alpha < 0$ for any point in $\mathcal{N}_{\alpha} \setminus \{\pm(0,0,r_1,0,0,r_1)\}$. As the last component of X_{γ} coincides with the third one, it follows that any X_{γ} -orbit on $\mathcal{N}_{\alpha} \setminus \{\pm(0,0,r_1,0,0,r_1)\}$ originates from $(0,0,r_1,0,0,r_1)$ and ends at $-(0,0,r_1,0,0,r_1)$. The orbits on $\mathcal{N}_{-\alpha}$ are analyzed in a similar way.

(iii) Clearly, if $2\gamma + 1 = -2s_{2k}$, one has $\mathcal{M}_{\gamma}^{-1}\{(0,0)\} = \mathcal{N}_0$ and one verifies in a straightforward way that $\pm(0,0,r_1,0,0,r_1)$ are elliptic fixed points of X_{γ} . According to (47), $(X_{\gamma})_3$ vanishes identically on \mathcal{N}_0 . Further, $2\gamma + 1 = -2s_{2k}$ implies that $1 + d_{2,\gamma} = -1 - d_{1,\gamma}$. In view of (46) it then follows that

$$X_{\gamma} = (1 + d_{2,\gamma})L_2 \cdot Y.$$

The claimed statements for the case $2\gamma + 1 = 2s_{2k}$ are proved in a similar fashion. \Box

Next we consider the case where r < 1 and $\gamma + c_k^2 = 0$. Then $\gamma + s_k^2 = -c_{2k}$ and hence

$$d_{1,\gamma} = -c_{2k}/s_{2k}$$
 and $d_{2,\gamma} = 0$.

Thus equation (44) takes the form

$$c_{2k}Q(L_1) = 2s_{2k}\cos\alpha. \tag{48}$$

Note that $0 < c_{2k} < 1$ as $1 \le k < N/4$.

Proposition 4.3. Assume that $1 \le k < N/4$, 0 < r < 1, and $\gamma + c_k^2 = 0$. Then the following statements hold:

- (i) If $\sqrt{r} > 2s_{2k}/c_{2k}$, then the connected component of $\mathcal{M}_{\gamma}^{-1}\{(r_1 r_2, 0)\}$ containing the critical point $(0, 0, r_1, 0, 0, r_2)$ consists of this point alone. It is an elliptic fixed point of X_{γ} .

$$\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\} = \bigcup_{\substack{|L_1| \leq r_1 \\ L_2 = L_1 + r_2 - r_1}} \mathcal{L}(L_1,L_2,\alpha_{L_1}) \cup \mathcal{L}(L_1,L_2,-\alpha_{L_1})$$

where for any $|L_1| \le r_1$, α_{L_1} is the unique angle satisfying

$$c_{2k}Q(L_1) = 2s_{2k}\cos\alpha_{L_1}$$
 and $0 \le \alpha_{L_1} \le \pi/2$

and $Q(L_1)$ denotes the function defined by (43), continuously extended to the closed interval $[-L_1, L_1]$. Furthermore, the connected component of $\mathcal{M}_{\gamma}^{-1}\{(r_1 - r_2, 0)\}$ containing $(0, 0, r_1, 0, 0, r_2)$ consists of homoclinic X_{γ} -orbits which originate and end at $(0, 0, r_1, 0, 0, r_2)$. Topologically, it is a 2-dimensional torus, pinched at $(0, 0, r_1, 0, 0, r_2)$.

If $\sqrt{r} < 2s_{2k}/c_{2k}$, then $(0,0,r_1,0,0,r_2)$ is a hyperbolic fixed point of X_{γ} and its stable and unstable manifolds each have dimension two. If $\sqrt{r} = 2s_{2k}/c_{2k}$, $(0,0,r_1,0,0,r_2)$ is an elliptic fixed point of X_{γ} .

Proof. (i) By a straightforward computation one shows that under the given assumptions, $(0, 0, r_1, 0, 0, r_2)$ is an elliptic fixed point of X_{γ} . In view of (48) and the discussion of the case $L_1 = \pm r_1$ item (i) then follows easily.

(ii) Again by the discussion preceding Proposition 4.2 it follows that $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}$ is as claimed. Again by a straightforward computation one sees that $(0,0,r_1,0,0,r_2)$ is a hyperbolic fixed point of X_{γ} if $\sqrt{r} < 2s_{2k}/c_{2k}$, and an elliptic one if $\sqrt{r} = 2s_{2k}/c_{2k}$. Next consider a point $(M_i, J_i, L_i)_{1 \le i \le 2}$ in $\mathcal{M}_{\gamma}^{-1}\{(r_1 - r_2, 0)\}$ with

$$(M_1, J_1) = \sqrt{r_1^2 - L_1^2} (\cos \phi, -\sin \phi),$$

$$(M_2, J_2) = \sqrt{r_2^2 - L_2^2} (\cos(\alpha_{L_1} + \phi), \sin(\alpha_{L_1} + \phi))$$

where $|L_1| < r_1$. Then the third component of X_{γ} is given by (cf. (47))

$$(X_{\gamma})_3 = -\sqrt{r_1^2 - L_1^2}\sqrt{r_2^2 - L_2^2} \sin \alpha_{L_1}.$$

Hence $(X_{\gamma})_3 = (X_{\gamma})_6 < 0$. It follows that the X_{γ} -orbit passing through such a point originates at $(0,0,r_1,0,0,r_2)$ and then reaches a point of the form $(0,0,-r_1,M_2,J_2,L_2)$ with

$$L_2 = r_2 - 2r_1 > -r_2$$
 and $(M_2, J_2) = \sqrt{r_2^2 - L_2^2} (\cos(\pi + \tilde{\phi}), \sin(\pi + \tilde{\phi})).$ (49)

At this point the vector field X_{γ} is given by

$$(-r_1J_2, -r_1M_2, 0, 0, 0, 0)$$
.

Note that this vector does not vanish as $M_2^2 + J_2^2 = r_2^2 - L_2^2 > 0$. Similarly, at a point $(M_i, J_i, L_i)_{1 \le i \le 2}$ in $\mathcal{M}_{\nu}^{-1}\{(r_1 - r_2, 0)\}$ satisfying

$$\begin{split} (M_1, J_1) &= \sqrt{r_1^2 - L_1^2} \; (\cos \phi, -\sin \phi), \\ (M_2, J_2) &= \sqrt{r_2^2 - L_2^2} \; (\cos(-\alpha_{L_1} + \phi), \sin(-\alpha_{L_1} + \phi)) \end{split}$$

and $|L_1| < r_1$ one has

$$(X_{\gamma})_3 = \sqrt{r_1^2 - L_1^2} \sqrt{r_2^2 - L_2^2} \sin \alpha_{L_1}.$$

Hence $(X_{\gamma})_3 = (X_{\gamma})_6 > 0$. It follows that the X_{γ} -orbit passing through such a point ends up at $(0, 0, r_1, 0, 0, r_2)$ and passes through a point of the form $(0, 0, -r_1, M_2, J_2, L_2)$ with (M_2, J_2, L_2) as in (49). We conclude that the connected component of $\mathcal{M}_{\gamma}^{-1}\{(r_1 - r_2, 0)\}$ containing $(0, 0, r_1, 0, 0, r_2)$ consists of homoclinic X_{γ} -orbits originating and ending at $(0, 0, r_1, 0, 0, r_2)$.

Finally, let us treat the case r<1 and $\gamma+c_k^2\neq 0$. Denote by $Q(L_1)$ the function defined by (43), extended continuously to the closed interval $[-r_1,r_1]$. Further, introduce the function

$$f:(0,\sqrt{r})\to\mathbb{R}, \quad q\mapsto (\gamma+s_k^2)q+(\gamma+c_k^2)\frac{1}{q}.$$
 (50)

Note that $\lim_{q \searrow 0} |f(q)| = \infty$.

Proposition 4.4. Assume that $1 \le k < N/4$, 0 < r < 1, and $\gamma + c_k^2 \ne 0$. Then the following statements hold:

(i) If $|f(\sqrt{r})| \ge 2s_{2k}$, then the connected component of $\mathcal{M}_{\gamma}^{-1}\{(r_1 - r_2, 0)\}$ containing the critical point $(0, 0, r_1, 0, 0, r_2)$ consists of this point alone. It is an elliptic fixed point of X_{γ} .

(ii) If $|f(\sqrt{r})| < 2s_{2k}$, then there exists $-r_1 < l_{\gamma,r} < r_1$ such that the connected component of $\mathcal{M}_{\nu}^{-1}\{(r_1-r_2,0)\}$ containing $(0,0,r_1,0,0,r_2)$ is given by

$$\bigcup_{\substack{l_{\gamma,r} \leq L_1 \leq r_1 \\ L_2 = L_1 + r_2 - r_1}} \mathcal{L}(L_1, L_2, \alpha_{L_1}) \cup \mathcal{L}(L_1, L_2, -\alpha_{L_1})$$

where for any $l_{\gamma,r} \leq L_1 \leq r_1$, α_{L_1} is the unique angle satisfying $0 \leq \alpha_{L_1} \leq \pi$ and

$$f(Q(L_1)) = -2s_{2k}\cos\alpha_{L_1}.$$

The point $(0,0,r_1,0,0,r_2)$ is a hyperbolic fixed point of X_γ and its stable and unstable manifolds each have dimension two. The connected component of the set $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}$ containing $(0,0,r_1,0,0,r_2)$ consists of homoclinic X_{γ} -orbits which originate and end at $(0,0,r_1,0,0,r_2)$. Topologically, it is a 2-dimensional torus, pinched at $(0,0,r_1,0,0,r_2)$.

- *Proof.* (i) By a straightforward computation one shows that under the given assumptions, $(0,0,r_1,0,0,r_2)$ is a (possibly degenerate) elliptic fixed point of X_γ . We have already seen that under the given assumption, $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}\setminus\{(0,0,r_1,0,0,r_2)\}$ is the set of points $(M_i,J_i,L_i)_{1\leq i\leq 2}$ satisfying $L_2=L_1+r_2-r_1$ and (44). Note that equation (44) admits a solution α for $Q=\sqrt{r}$ iff $|f(\sqrt{r})|\leq s_{2k}$. In the case $|f(\sqrt{r})|>2s_{2k}$ it follows immediately that $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}=\{(0,0,r_1,0,0,r_2)\}$. If $|f(\sqrt{r})|=2s_{2k}$, then an analysis of the graph of f near $(\sqrt{r},f(\sqrt{r}))$ leads to the claimed result.
- (ii) As $\lim_{q\searrow 0} |f(q)| = \infty$ it follows that there exists $-r_1 < l_{\gamma,r} < r_1$ such that the interval $[l_{\gamma,r},r_1]$ is a connected component of $(f\circ Q)^{-1}([-2s_{2k},2s_{2k}])$. It follows that for any $l_{\gamma,r}\leq L_1\leq r_1$ there exists a unique angle $0\leq \alpha_{L_1}\leq \pi$ such that

$$f(Q(L_1)) = -2s_{2k}\cos\alpha_{L_1}.$$

The connected component of $\mathcal{M}_{\gamma}^{-1}\{(r_1-r_2,0)\}$ containing $(0,0,r_1,0,0,r_2)$ is then as claimed. Again by a straightforward computation $(0,0,r_1,0,0,r_2)$ is a hyperbolic fixed point of X_{γ} . One can then argue as in the proof of Proposition 4.3(ii) to show the remaining claims.

Proof of Theorem 4.1. Theorem 4.1 follows from Propositions 4.2–4.4. □

It remains to study the critical points of \mathcal{M}_{γ} with $\mathrm{rank}(d\mathcal{M}_{\gamma})=1$, i.e. the points of $(\mathbb{S}^2_{r_1}\times\mathbb{S}^2_{r_2})\setminus\{\pm(0,0,r_1,0,0,\pm r_2)\}$ where the vector fields Y and X_{γ} are collinear. In view of the formulas (37) for Y and X_{γ} , points $(M_i,J_i,L_i)\in S^2_{r_i}$, i=1,2, of this type have the property that the determinant of any 2×2 -submatrix of the 2×4 -matrix formed by Y and X_{γ} vanishes. This leads to the following system of equations:

$$M_1 J_2 + M_2 J_1 = 0, (51)$$

$$J_1^2 L_2 + L_1 J_2^2 - J_1 J_2 (d_{1,\gamma} L_1 + d_{2,\gamma} L_2) = 0,$$
(52)

$$M_1^2 L_2 + L_1 M_2^2 + M_1 M_2 (d_{1,\gamma} L_1 + d_{2,\gamma} L_2) = 0,$$
(53)

$$M_1 J_1 L_2 - L_1 M_2 J_2 + J_1 M_2 (d_{1,\nu} L_1 + d_{2,\nu} L_2) = 0.$$
 (54)

Theorem 4.5. Assume that $1 \le k < N/4$, $0 < r \le 1$, and $\gamma \in \mathbb{R}$. If a point $(M_i, J_i, L_i)_{1 \le i \le 2} \in \mathbb{S}^2_{r_1} \times \mathbb{S}^2_{r_2} \setminus \{\pm(0, 0, r_1, 0, 0, \pm r_2)\}$ is a critical point of \mathcal{M}_{γ} with $\operatorname{rank}(d\mathcal{M}_{\gamma}) = 1$ then $(M_2, L_2) = \lambda(M_1, -J_1)$ for some $\lambda \in \mathbb{R}$, and

$$(r_1^2 - L_1^2)^2 L_2^2 + (r_2^2 - L_2^2)^2 L_1^2 + 2(r_1^2 - L_1^2)(r_2^2 - L_2^2)(2L_1L_2 - (d_{1,\gamma}L_1 + d_{2,\gamma}L_2)^2) = 0.$$

Given any point $(M_1, J_1, L_1) \in \mathbb{S}^2_{r_1} \setminus \{\pm(0, 0, r_1)\}$ there exist at most eight points $(M_2, J_2, L_2) \in \mathbb{S}^2_{r_2} \setminus \{\pm(0, 0, r_2)\}$ such that $(M_i, J_i, L_i)_{1 \le i \le 2}$ is a critical point of \mathcal{M}_{γ} with $\operatorname{rank}(d\mathcal{M}_{\gamma}) = 1$.

Proof. First assume that $L_1 \in \{\pm r_1\}$. Then $J_1 = M_1 = 0$. Hence (51) is automatically satisfied and equations (52) and (53) read $J_2 = 0$ and $M_2 = 0$, respectively. As a consequence, $(M_1, J_1, L_1) = (0, 0, \pm r_1)$ and $(M_2, J_2, L_2) = (0, 0, \pm r_2)$. In view of Theorem 4.1 we may thus assume that $|L_1| < r_1$. Then $(M_1, J_1) \neq (0, 0)$. Hence the first equation (51) says that there exists $\lambda \in \mathbb{R}$ such that

$$(M_2, J_2) = \lambda(M_1, -J_1). \tag{55}$$

The conditions $(M_i, J_i, L_i) \in \mathbb{S}_{r_i}^2$, i = 1, 2, then imply that λ satisfies

$$\lambda^2 = \frac{r_2^2 - L_2^2}{r_1^2 - L_1^2}. (56)$$

Substituting (55) into (52)–(54) one sees, again using $(M_1, J_1) \neq (0, 0)$, that (52)–(54) is equivalent to

$$L_2 + \lambda^2 L_1 + \lambda (d_{1,\gamma} L_1 + d_{2,\gamma} L_2) = 0, \tag{57}$$

or, taking squares, $(L_2 + \lambda^2 L_1)^2 - \lambda^2 (d_{1,\gamma} L_1 + d_{2,\gamma} L_2)^2 = 0$. By (56), the latter equation reads

$$(r_1^2 - L_1^2)^2 L_2^2 + (r_2^2 - L_2^2)^2 L_1^2 + 2(r_1^2 - L_1^2)(r_2^2 - L_2^2)(2L_1L_2 - (d_{1,\gamma}L_1 + d_{2,\gamma}L_2)^2) = 0,$$

or, after dividing by $r_1^2 r_2^4$ and using the bifurcation parameter r and the normalized variables $l_i := L_i/r_i \in (0, 1)$ (i = 1, 2),

$$r^{2}(1-l_{1}^{2})^{2}l_{2}^{2} + (1-l_{2}^{2})^{2}l_{1}^{2} + 2r(1-l_{1}^{2})(1-l_{2}^{2})\left(2l_{1}l_{2} - \left(\sqrt{r}d_{1,\gamma}l_{1} + \frac{1}{\sqrt{r}}d_{2,\gamma}l_{2}\right)^{2}\right) = 0.$$
(58)

Note that for given r and $0 < l_1 < 1$, the left hand side of (58) is a polynomial in l_2 of degree four, $(l_1^2 + d_{2,\nu}^2(1 - l_1^2))l_2^4 + O(l_2^3)$.

Summarizing, we have shown that for any given point $(M_1, J_1, L_1) \in \mathbb{S}^2_{r_1} \setminus \{(0, 0, \pm r_1)\}$, there exist at most eight points $(M_2, J_2, L_2) \in \mathbb{S}^2_{r_2} \setminus \{(0, 0, \pm r_2)\}$ such that Y and X_{γ} are collinear. Indeed, for any $(M_1, J_1, L_1) \in \mathbb{S}^2_{r_1} \setminus \{(0, 0, \pm r_1)\}$ a solution $(M_2, J_2, L_2) \in \mathbb{S}^2_{r_2} \setminus \{(0, 0, \pm r_2)\}$ of (51)–(54) is given by $(M_2, J_2) = \lambda(M_1, J_1)$ and $L_2 = r_2 l_2$ with λ and l_2 satisfying (56), respectively (58). As a consequence, the set of solutions of (51)–(54) is an algebraic subset of $\mathbb{S}^2_{r_1} \times \mathbb{S}^2_{r_2}$ of dimension at most two. \square

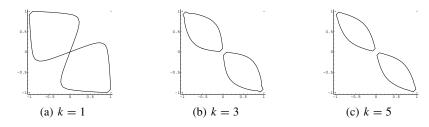


Fig. 2. Sets of solutions (l_1, l_2) of (58) for N = 24, r = 1, $\gamma = -0.5$.

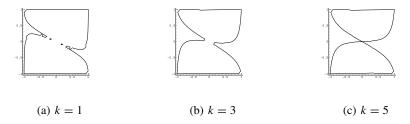


Fig. 3. Sets of solutions (l_1, l_2) of (58) for N = 24, r = 0.3, $\gamma = -2.5$.

In order to analyze the critical points of \mathcal{M}_{γ} with $\mathrm{rank}(d\mathcal{M}_{\gamma})=1$, we perform another symplectic reduction. First we pass to the orbit space of the flow of Y on $\mathbb{S}^2_{r_1}\times\mathbb{S}^2_{r_2}$ and then to the level sets of G.

In view of (39), the Y-flow is an \mathbb{S}^1 -action. Note that besides L_1 and L_2 , the quantities σ and τ are invariant under this \mathbb{S}^1 -action, where

$$\sigma := M_1 M_2 - J_1 J_2, \quad \tau := M_1 J_2 + M_2 J_1.$$

They are related by the identity

$$\sigma^2 + \tau^2 = \prod_{i=1}^2 (r_i^2 - L_i^2). \tag{59}$$

Define

$$\mathcal{F}^{(3)}: \dot{\mathbb{S}}^2_{r_1} \times \dot{\mathbb{S}}^2_{r_2} \to \mathbb{R}^4, \quad (M_1, J_1, L_1, M_2, J_2, L_2) \mapsto (L_1, L_2, \sigma, \tau),$$

where $\dot{\mathbb{S}}_{r_i}^2:=\mathbb{S}_{r_i}^2\setminus\{(0,0,\pm r_i)\}$. Let \mathbb{O}_r denote the image of $\mathfrak{F}^{(3)}$. For any element $(L_1,L_2,s,t)\in \mathbb{O}_r$ we have

$$s^2 + t^2 = \prod_{i=1}^{2} (r_i^2 - L_i^2)$$
 and $|L_i| \le r_i \ (i = 1, 2)$. (60)

The fibers of $\mathcal{F}^{(3)}$ are the orbits of the Y-action on $\dot{\mathbb{S}}^2_{r_1} \times \dot{\mathbb{S}}^2_{r_2}$, i.e. \mathcal{O}_r coincides with the orbit space of the Y-action on $\dot{\mathbb{S}}^2_{r_1} \times \dot{\mathbb{S}}^2_{r_2}$. As a consequence, any function on $\dot{\mathbb{S}}^2_{r_1} \times \dot{\mathbb{S}}^2_{r_2}$ which Poisson commutes with G factors through \mathcal{O}_r .

In particular, K_{γ} and G factor through O_r . In fact, K_{γ} and G, when expressed in the variables L_1, L_2, σ, τ , are polynomials, given by

$$K_{\gamma} = \sum_{i=1}^{2} \frac{1}{2} d_{i,\gamma} (r_i^2 - L_i^2) + \sigma, \quad G = L_1 - L_2.$$

By reducing the system (G, K_{γ}) by the *Y*-action one obtains a family of integrable systems with one degree of freedom parametrized by the value c of G. Denote by $X_{\gamma,c}$ the Hamiltonian vector field induced by K_{γ} . The fixed points of $X_{\gamma,c}$ can then be characterized in terms of the bifurcation parameters γ , r, and k.

Note that by (51), the rank-1-points of the reduced moment map \mathcal{M}_{γ} satisfy $\tau=0$, and by (55)–(56), $\sigma^2=(r_2^2-L_2^2)(r_1^2-L_1^2)$. Hence the image of the set of the rank-1-points under $\mathcal{F}^{(3)}$ is an algebraic subset of \mathcal{O}_r of dimension at most one—see (58).

By (59), σ and τ are located on a circle of radius $\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)}$,

$$(\sigma, \tau) = \sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)} (\cos \phi, \sin \phi), \tag{61}$$

where $\phi \in \mathbb{R}/2\pi\mathbb{Z}$. The phase spaces, reduced by the *Y*-action, are now obtained by taking subsets of \mathbb{O}_r corresponding to level sets of *G*, i.e. by replacing L_2 by L_1-c , where c is the value of *G*. The restriction $K_{\gamma,c}$ of K_{γ} to the reduced phase space corresponding to the value c of *G* is then given by

$$K_{\gamma,c}(L_1,\phi) = \frac{1}{2} (d_{1,\gamma}(r_1^2 - L_1^2) + d_{2,\gamma}(r_2^2 - (L_1 - c)^2)) + \sqrt{(r_1^2 - L_1^2)(r_2^2 - (L_1 - c)^2)} \cos \phi$$
(62)

with $L_1 \in (-r_1, r_1) \cap (c - r_2, c + r_2)$ and $\phi \in \mathbb{R}/2\pi\mathbb{Z}$.

The reduced Hamiltonian vector field induced by $K_{\gamma,c}$ is given by

$$X_{\gamma,c}(L_1,\phi) = \frac{d}{dt} \begin{pmatrix} L_1 \\ \phi \end{pmatrix} = \{L_1,\phi\} \begin{pmatrix} \partial K_{\gamma,c}/\partial \phi \\ -\partial K_{\gamma,c}/\partial L_1 \end{pmatrix}. \tag{63}$$

Note that

$$\begin{split} \{L_1,\phi\} &= \left\{L_1, \arctan\frac{\tau}{\sigma}\right\} = \frac{1}{1+(\tau/\sigma)^2} \left\{L_1, \frac{\tau}{\sigma}\right\} \\ &= \frac{1}{1+(\tau/\sigma)^2} \cdot \frac{\sigma\{L_1,\tau\} - \tau\{L_1,\sigma\}}{\sigma^2} = \frac{1}{1+(\tau/\sigma)^2} \cdot \frac{\sigma^2 + \tau^2}{\sigma^2} = 1, \end{split}$$

since $\{L_1, \tau\} = \sigma$ and $\{L_1, \sigma\} = -\tau$. Furthermore, with $L_2 = L_1 - c$,

$$\begin{split} \frac{\partial K_{\gamma,c}}{\partial \phi} &= -\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)} \, \sin \phi, \\ \frac{\partial K_{\gamma,c}}{\partial L_1} &= -(d_{1,\gamma}L_1 + d_{2,\gamma}L_2) - \frac{L_1(r_2^2 - L_2^2) + L_2(r_1^2 - L_1^2)}{\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)}} \cos \phi. \end{split}$$

Hence (63) reads

$$X_{\gamma,c}(L_1,\phi) = \begin{pmatrix} -\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)} & \sin\phi \\ (d_{1,\gamma}L_1 + d_{2,\gamma}L_2) + \frac{L_1(r_2^2 - L_2^2) + L_2(r_1^2 - L_1^2)}{\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)}} & \cos\phi \end{pmatrix}, \quad (64)$$

where we treat $L_2 = L_1 - c$ as a dependent variable.

By (64), the fixed points of the vector field $X_{\gamma,c}$ with $|L_1| < r_1$ are given by (L_1, ϕ) satisfying

$$\phi \in \pi \mathbb{Z} \tag{65}$$

and

$$(d_{1,\gamma}L_1 + d_{2,\gamma}L_2) + \frac{L_1(r_2^2 - L_2^2) + L_2(r_1^2 - L_1^2)}{\sqrt{(r_1^2 - L_1^2)(r_2^2 - L_2^2)}}\cos\phi = 0.$$
 (66)

Note that (65) and the square of (66) are equivalent to the system of equations (51)–(58) derived above.

In order to determine the type of the fixed points (L_1, ϕ) , i.e. points satisfying (65)–(66) for a given value c of G, one computes the Jacobian of $X_{\gamma,c}$, $H \equiv H_{\gamma,c}(L_1, \phi) = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}$ at these points. Note that at such points $h_{11} = 0$ and $h_{22} = 0$ and thus $\det(H) = -h_{12}h_{21}$. Hence such a fixed point is an elliptic or hyperbolic fixed point of $X_{\gamma,c}$ if $h_{12}h_{21}$ is positive, respectively negative. We omit a more detailed analysis of these points.

5. Chains with Dirichlet boundary conditions

In this section we consider a FPU chain with N' ($N' \ge 3$, not necessarily even) moving particles and fixed endpoints, i.e. with boundary conditions (18).

It has been observed that such a chain can be treated as an invariant subsystem of a periodic lattice with N=2N'+2 particles—see [13]: Let $T^*\mathbb{R}^N$ be endowed with the canonical symplectic structure and consider the linear map $S: T^*\mathbb{R}^N \to T^*\mathbb{R}^N$ sending $(q_i)_{1 \le i \le N}$, $(p_i)_{1 \le i \le N}$ to

$$-(q_{N-1},\ldots,q_1,q_N),-(p_{N-1},\ldots,p_1,p_N).$$

Then *S* is a canonical linear involution satisfying $H_V \circ S = H_V$. Denote by Fix(*S*) the fixed point set of *S*. Then Fix(*S*) is the subset of all elements (q, p) in $T^*\mathbb{R}^N$ satisfying

$$(q_n, p_n) = -(q_{N-n}, p_{N-n}) \quad \forall 1 \le n \le N-1 \quad \text{and} \quad q_N = p_N = 0.$$
 (67)

In particular, on Fix(S), $q_N = q_{N'+1} = 0$ and $p_N = p_{N'+1} = 0$. Note that on Fix(S), both the center of mass coordinate $Q = N^{-1} \sum_{i=1}^{N} q_i$ and its momentum $P = N^{-1} \sum_{i=1}^{N} p_i$ are identically 0. Hence $Fix(S) \subseteq \mathcal{M}$, where

$$\mathcal{M} := \{ (q, p) \in T^* \mathbb{R}^N \mid Q = 0, \ P = 0 \}.$$

We endow \mathfrak{M} with the symplectic structure induced from $T^*\mathbb{R}^N$.

The phase space of an FPU chain with N' moving particles satisfying Dirichlet boundary conditions is $T^*\mathbb{R}^{N'}$, endowed with the canonical symplectic structure $\sum_{i=1}^{N'} dq_i \wedge dp_i$. It can be embedded into $\mathfrak M$ by the map $\Theta: T^*\mathbb{R}^{N'} \to \mathfrak M$ defined by

$$(q_i, p_i)_{1 \le i \le N'} \mapsto \frac{1}{\sqrt{2}}((q_i, p_i)_{1 \le i \le N'}, (0, 0), -(q_{N'-i}, p_{N'-i})_{0 \le i \le N'-1}, (0, 0)).$$

Note that $\Theta(T^*\mathbb{R}^{N'})=\operatorname{Fix}(S)$, i.e. Θ is a parametrization of $\operatorname{Fix}(S)$ and the pullback of the canonical symplectic form on \mathbb{M} by Θ is $\sum_{i=1}^{N'}dq_i\wedge dp_i$, which means that Θ is canonical. It then follows that $\operatorname{Fix}(S)$ is a symplectic submanifold of \mathbb{M} .

We now express the equations defining Fix(S) locally near 0 as a subset of $\mathfrak M$ in terms of the canonical coordinates $(x_k,y_k)_{1\leq k\leq N-1}$ provided by Theorem 1.1, or even more conveniently, in terms of the associated complex coordinates $(\zeta_k)_{1\leq |k|\leq N-1}$, defined for $1\leq k\leq N-1$ by

$$\zeta_k = \frac{1}{\sqrt{2}}(x_k - iy_k), \quad \zeta_{-k} = \overline{\zeta_k} = \frac{1}{\sqrt{2}}(x_k + iy_k).$$

Denote by \mathcal{Z} the linear subspace of \mathbb{C}^{2N-2} consisting of such vectors $(\zeta_k)_{1 \leq |k| \leq N-1}$. Below we also write $(\zeta_k)_{1 \leq k \leq N-1}$ for the element $(\zeta_k)_{1 \leq |k| \leq N-1} \in \mathcal{Z}$ and use the notations $(n \in \mathbb{Z})$

$$c_n := \cos \frac{n\pi}{N}, \quad s_n := \sin \frac{n\pi}{N}.$$

Define the map $S_{\mathcal{Z}}: \mathcal{Z} \to \mathcal{Z}$ by

$$(\zeta_k)_{1 \le k \le N-1} \mapsto (-e^{4\pi i k/N} \zeta_{N-k})_{1 \le k \le N-1}.$$
 (68)

Like the map $S: \mathcal{M} \to \mathcal{M}$, $S_{\mathcal{Z}}$ is a canonical linear involution. In fact, the maps S and $S_{\mathcal{Z}}$ are conjugate to each other under the coordinate change of Theorem 1.1. Before making this statement more precise, let us introduce a parametrization of the fixed point set $Fix(S_{\mathcal{Z}})$. Introduce

$$\mathcal{Z}_{\text{Dir}} := \{ (\zeta_k)_{1 < |k| < N'} \in \mathbb{C}^{2N'} \mid \overline{\zeta_k} = \zeta_{-k} \ \forall 1 \le k \le N' \},$$

endowed with the *canonical* symplectic structure induced from $\mathbb{C}^{2N'}$, and the embedding $\Theta_{\mathcal{Z}}: \mathcal{Z}_{\mathrm{Dir}} \to \mathcal{Z}$ mapping $(\zeta_k)_{1 \leq |k| \leq N'}$ to the element $(\tilde{\zeta}_k)_{1 \leq k \leq N-1} \in \mathcal{Z}$ given by

$$\frac{1}{\sqrt{2}} ((\zeta_k)_{1 \le k \le N'}, 0, (-e^{4\pi i k/N} \zeta_{N'+1-k})_{1 \le k \le N'}).$$

Note that $\Theta_{\mathcal{Z}}(\mathcal{Z}_{\text{Dir}}) = \text{Fix}(S_{\mathcal{Z}})$, i.e. $\Theta_{\mathcal{Z}}$ is a parametrization of Fix $(S_{\mathcal{Z}})$.

Using the explicit construction in [7] of the canonical transformation Ψ of Theorem 1.1 one verifies the following lemma.

Lemma 5.1. In terms of the complex variables $(\zeta_k)_{1 \le |k| \le N-1}$ defined by Theorem 1.1, near 0, the map S is given by $S_{\mathcal{Z}}$. More precisely, if Ψ , defined near $0 \in \mathcal{Z}$, is the coordinate transformation given by Theorem 1.1, then $S \circ \Psi = \Psi \circ S_{\mathcal{Z}}$. In particular, locally near 0, the set $\operatorname{Fix}(S_{\mathcal{Z}}) \subseteq \mathcal{Z}$, described by the equations

$$e^{-2\pi ik/N}\zeta_k + e^{2\pi ik/N}\zeta_{N-k} = 0 \quad (1 \le k \le N-1), \tag{69}$$

is the image of Fix(S) under Ψ^{-1} . Expressed in terms of the real variables $(x_k, y_k)_{1 \le k \le N-1}$, the conditions (69) are given by

$$\begin{pmatrix} c_{2k} & -s_{2k} \\ s_{2k} & c_{2k} \end{pmatrix} \begin{pmatrix} x_k \\ y_k \end{pmatrix} + \begin{pmatrix} c_{2k} & s_{2k} \\ -s_{2k} & c_{2k} \end{pmatrix} \begin{pmatrix} x_{N-k} \\ y_{N-k} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{70}$$

In particular, for k = N' + 1 (= N/2) we get $\zeta_{N'+1} = 0$ and therefore

$$(x_{N'+1}, y_{N'+1}) = (0, 0).$$

Corollary 5.2. On Fix(S_7), for any 1 < k < N/2,

$$I_k = I_{N-k} \tag{71}$$

and

$$J_k J_{N/2-k} - M_k M_{N/2-k} = I_k I_{N/2-k}. (72)$$

Moreover,

$$I_{N/2} = 0.$$
 (73)

Proof. In terms of the complex variables $(\zeta_k)_{1 \le |k| \le N-1}$, $I_k = \zeta_k \zeta_{-k}$ for any $1 \le k \le N-1$. Hence on Fix $(S_{\mathcal{Z}})$,

$$I_k = \zeta_k \zeta_{-k} = (-e^{4\pi i k/N} \zeta_{N-k})(-e^{-4\pi i k/N} \zeta_{-(N-k)}) = \zeta_{N-k} \zeta_{-(N-k)} = I_{N-k},$$

showing (71). The identity (73) follows from $\zeta_{N/2}|_{\text{Fix}(S_{\mathbb{Z}})}=0$. To prove (72), we first conclude from (69) that on Fix($S_{\mathbb{Z}}$), for any $1 \le k \le N-1$,

$$J_k = -c_{4k}I_k, \quad M_k = -s_{4k}I_k.$$

Hence on $Fix(S_{\mathcal{Z}})$,

$$J_k J_{N/2-k} - M_k M_{N/2-k} = I_k I_{N/2-k} (c_{4k} c_{4(N/2-k)} - s_{4k} s_{4(N/2-k)})$$

$$= I_k I_{N/2-k} (c_{4k}^2 + s_{4k}^2) = I_k I_{N/2-k}.$$

From the definitions (6), (11), and (12) of the variables I_k , J_k , M_k , and of the expressions R and $R_{N/4}$ one then obtains the following

Corollary 5.3. *On* $Fix(S_2)$,

$$R = 4 \sum_{1 \le k < N/4} s_{2k} I_k I_{N/2-k} \quad and \quad R_{N/4} = \begin{cases} I_{N/4}^2 & \text{if } N/4 \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases}$$

It follows from Corollary 5.3 that on $Fix(S_Z)$, the expression (13) is in Birkhoff normal form up to order 4. This allows us to prove Theorem 1.3.

Proof of Theorem 1.3. We start with the resonant normal form (13) for even chains, $NP^2/2 + H_{\alpha,\beta}(I) - R_{\alpha,\beta}(J,M) + O(|(x,y)|^5)$, where $H_{\alpha,\beta}(I)$ and $R_{\alpha,\beta}(J,M)$ are given by (8) and (10), respectively. In view of the identity $I_k = I_{N-k}$, the terms in the decomposition (14) of $H_{\alpha,\beta}$, when restricted to Fix($S_{\mathcal{Z}}$), are given by

$$H^{(2)}(I) = 4\sum_{k=1}^{N'} s_k I_k, \tag{74}$$

$$H_{\alpha,\beta}^{(4)}(I) = \frac{1}{N} \sum_{k=1}^{N'} d_k^+ I_k^2 + \frac{4(\beta - \alpha^2)}{2N} \sum_{\substack{1 \le k,l \le N' \\ k \ne l}} s_k s_l I_k I_l, \tag{75}$$

and

$$\frac{1}{2N} \sum_{k=1}^{N/2-1} d_k^- I_k I_{N-k} = \frac{1}{2N} \sum_{k=1}^{N'} d_k^- I_k^2.$$
 (76)

From Corollary 5.3, we conclude that on $Fix(S_2)$,

$$-R_{\alpha,\beta}(J,M) = -\frac{\beta - \alpha^2}{4N} (R(J,M) + R_{N/4}(J,M))$$

$$= -\frac{\beta - \alpha^2}{4N} \left(4 \sum_{1 \le k < N/4} s_{2k} I_k I_{N/2-k} + I_{N/4}^2 \right). \tag{77}$$

Formula (19) is then obtained by adding up (74)–(77), noting that $d_k^+ + d_k^-/2 = \frac{1}{2}(\alpha^2 + 3(\beta - \alpha^2)s_k^2)$, and replacing I_k by its pullback $\frac{1}{2}I_k$ with respect to the parametrization $\Theta_{\mathcal{Z}}$ of Fix($S_{\mathcal{Z}}$) introduced above.

It remains to prove Theorem 1.5. We first consider the case $\alpha = 0$.

Proposition 5.4. Assume that $\alpha = 0$ in (3). Then the following holds:

(i) The Birkhoff normal form of H_V with Dirichlet boundary conditions up to order 4 is given by $(N'+1)P^2/2 + H_{0,\beta}^D(I)$ where

$$H_{0,\beta}^{D}(I) = 2\sum_{k=1}^{N'} s_{k} I_{k} + \frac{\beta}{16(N'+1)} \left(\sum_{k=1}^{N'} 3s_{k}^{2} I_{k}^{2} \underbrace{+\frac{1}{2} I_{(N'+1)/2}^{2}}_{only if \frac{N'+1}{2} \in \mathbb{N}} + 4 \sum_{\substack{l \neq m \\ 1 \leq l, m \leq N'}} s_{l} s_{m} I_{l} I_{m} - \sum_{k=1}^{N'} s_{2k} I_{k} I_{N'+1-k} \right).$$
 (78)

(ii) For any $\beta \neq 0$, $H_{0,\beta}^D(I)$ is nondegenerate at I=0.

Proof. The Birkhoff normal form (78) of H_V with Dirichlet boundary conditions is given by the formula (19) evaluated at $\alpha = 0$. To investigate the Hessian of $Q_{0,\beta}^D$ of $H_{0,\beta}^D(I)$ at I = 0, we write

$$Q_{0,\beta}^{D} = \frac{2\beta}{16(N'+1)} \Delta^{N'} P^{D} \Delta^{N'}, \tag{79}$$

where $\Delta^{N'}=\mathrm{diag}(\sin\frac{k\pi}{2N'+2})_{1\leq k\leq N'}$ and P^D is the $N'\times N'$ -matrix which for N' even resp. odd is of the form

$$\begin{pmatrix}
3 & 4 & \dots & & & \dots & 4 & 2 \\
4 & 3 & 4 & \dots & & \dots & 4 & 2 & 4 \\
\vdots & \ddots & & & & \ddots & \vdots \\
& & 3 & 4 & 4 & 2 & & & \\
& & 4 & 3 & 2 & 4 & & & \\
& & 4 & 2 & 3 & 4 & & & \\
& & 2 & 4 & 4 & 3 & & \\
\vdots & & \ddots & & & & \ddots & \vdots \\
4 & 2 & 4 & \dots & & \dots & 4 & 3 & 4 \\
2 & 4 & \dots & & \dots & 4 & 3 & 4 \\
& & & & & & & & \ddots & \vdots \\
& & & 3 & 4 & 2 & & & \\
& & & 4 & 2 & 4 & & & \\
& & & 2 & 4 & 3 & & \\
\vdots & & \ddots & & & \ddots & \vdots \\
4 & 2 & 4 & \dots & \dots & 4 & 3 & 4 \\
2 & 4 & \dots & \dots & 4 & 3 & 4 \\
2 & 4 & \dots & \dots & 4 & 3 & 4
\end{pmatrix},$$

$$\begin{pmatrix}
3 & 4 & \dots & & \dots & 4 & 2 & 4 \\
\vdots & \ddots & & & \ddots & \vdots \\
4 & 2 & 4 & \dots & \dots & 4 & 3 & 4 \\
2 & 4 & \dots & \dots & 4 & 3 & 4 \\
2 & 4 & \dots & \dots & 4 & 3
\end{pmatrix},$$

$$\begin{pmatrix}
(N' \text{ even}) & & & & & & & \\
(N' \text{ odd}) & & & & & \\
(N' \text{ odd}) & & & & & \\
\end{pmatrix},$$

where we have used the fact that $s_{2k} = 2s_k c_k = 2s_k s_{N'+1-k}$ and, if $(N'+1)/2 \in \mathbb{N}$, $s_{(N'+1)/2}^2 = 1/2$. It follows that

$$\det(Q_{0,\beta}^D) = \left(\frac{2\beta}{16(N'+1)}\right)^{N-1} \cdot \det(P^D) \cdot \prod_{k=1}^{N'} \sin^2 \frac{k\pi}{2N'+2}.$$

In order to see that P^D is nonsingular, observe that $\det(P^D) \in \mathbb{Z}$. For N' even we show that $\det(P^D) \equiv 1 \mod 2$. Note that in this case the diagonal of P^D consists of 3's only. Therefore $\det(P^D) \equiv 3^{N'} \mod 2 \equiv 1 \mod 2$. If N' is odd, the same argument shows that $\det(P^D) \equiv 2 \mod 4$. Hence, if $\beta \neq 0$, then $\det(Q^D_{0,\beta}) \neq 0$, and the nondegeneracy of the Hessian of $H^D_{0,\beta}(I)$ at I=0 follows.

Lemma 5.5. If $\beta < 0$, then $Q_{0,\beta}^D$ has $\lceil (N'+1)/2 \rceil$ negative eigenvalues, whereas if $\beta > 0$, then $Q_{0,\beta}^D$ has $\lfloor (N'-1)/2 \rfloor$ negative eigenvalues. In particular, for any $\beta \neq 0$, $Q_{0,\beta}^D$ is indefinite (and $H_{0,\beta}^D$ is therefore not convex).

Proof. We want to use the decomposition (79) of $Q_{0,\beta}^D$ to show that $Q_{0,\beta}^D$ can be deformed continuously to $\frac{2\beta}{16(N'+1)}P^D$: Consider, for $0 \le t \le 1$,

$$Q_{0,\beta}^{D}(t) := \frac{2\beta}{16(N'+1)} (t\Delta^{N'} + (1-t)\operatorname{Id}) P^{D}(t\Delta^{N'} + (1-t)\operatorname{Id}).$$

As $t\Delta^{N'}+(1-t)$ Id is positive definite for any $0\leq t\leq 1$ and P^D is regular and symmetric, $Q^D_{0,\beta}(t)$ is a symmetric regular $N'\times N'$ -matrix for any $0\leq t\leq 1$. For t=0, $Q^D_{0,\beta}(0)=\frac{2\beta}{16(N'+1)}P^D$, whereas for t=1, $Q^D_{0,\beta}(1)=Q^D_{0,\beta}$. Therefore, index $(Q^D_{0,\beta})$ (i.e. the number of negative eigenvalues of $Q^D_{0,\beta}$) coincides with index $\left(\frac{2\beta}{16(N'+1)}P^D\right)$. To describe the spectrum of P^D , we distinguish between N' even and odd.

If N' is even, the eigenvalues of P^D are 4N'-3 (with multiplicity one), 1 (with multiplicity N'/2), and -3 (with multiplicity N'/2-1), hence P^D has N'/2-1 negative eigenvalues. If N' is odd, the eigenvalues of P^D are 1 (with multiplicity (N'-1)/2), -3 (with multiplicity (N'-3)/2), and $\frac{1}{2}(4N'-5)\left(1\pm\sqrt{1+\frac{8(4N'-1)}{(4N'-5)^2}}\right)$ (each with multiplicity one), hence P^D has (N'-1)/2 negative eigenvalues. These facts are verified in Appendix A. The claim of the lemma now follows.

We now turn to the case $\alpha \neq 0$.

Proposition 5.6. Assume that $\alpha \neq 0$ in (3). Then, for α fixed, $\det(Q_{\alpha,\beta}^D)$ is a polynomial in β of degree N' and has N' real zeroes (counted with multiplicities). When denoted by $\beta_k = \beta_k(\alpha)$ ($1 \leq k \leq N'$) and listed in increasing order, they satisfy

$$\beta_1 \leq \cdots \leq \beta_{\lceil (N'+1)/2 \rceil} < \alpha^2 < \beta_{\lceil (N'+3)/2 \rceil} \leq \cdots \leq \beta_{N'}.$$

Moreover,

$$\mathrm{index}(Q^D_{\alpha,\beta}) = \begin{cases} \lceil (N'+1)/2 \rceil & \textit{for } \beta < \beta_1, \\ 0 & \textit{for } \beta_{\lceil (N'+1)/2 \rceil} < \beta < \beta_{\lceil (N'+3)/2 \rceil}, \\ \lfloor (N'-1)/2 \rfloor & \textit{for } \beta > \beta_{N'}, \end{cases}$$

Proof. Fix $\alpha \in \mathbb{R} \setminus \{0\}$ and consider the map $\beta \mapsto \det(Q_{\alpha,\beta}^D)$. It follows from (19) that $\det(Q_{\alpha,\beta}^D)$ is a polynomial in β of degree at most N',

$$\det(Q_{\alpha,\beta}^D) = \sum_{j=0}^{N'} r_j \beta^j,$$

where $r_0=\det(Q^D_{\alpha,0})$ and $r_{N'}=\det(Q^D_{0,1})$. By Proposition 5.4, $\det(Q^D_{0,1})\neq 0$, hence the degree of the polynomial $\det(Q^D_{\alpha,\beta})$ is N'. We claim that $\det(Q^D_{\alpha,\beta})$ has N' real zeroes (counted with multiplicities). For $|\beta|$ large enough, $\operatorname{index}(Q^D_{\alpha,\beta})$ is equal to $\operatorname{index}(Q^D_{0,\beta})$. By Lemma 5.5, $\operatorname{index}(Q^D_{0,\beta})$ is $\lfloor (N'-1)/2 \rfloor$ for $\beta>0$ and $\lceil (N'+1)/2 \rceil$ for $\beta<0$. Hence there exists R>0 such that $\operatorname{index}(Q^D_{\alpha,\beta})=\lfloor (N'-1)/2 \rfloor$ for any $\beta>R$ and $\operatorname{index}(Q^D_{\alpha,\beta})=\lceil (N'+1)/2 \rceil$ for any $\beta<-R$. For $\beta=\alpha^2$, Q^D_{α,α^2} is a positive multiple of the identity matrix, hence $\operatorname{index}(Q^D_{\alpha,\alpha^2})=0$. It then follows that, when counted with multiplicities, $\operatorname{index}(Q^D_{\alpha,\beta})$ must change at least $\lceil (N'+1)/2 \rceil$ times in the open interval $(-\infty,\alpha^2)$ and at least $\lfloor (N'-1)/2 \rfloor$ times in (α^2,∞) . Since a change of $\operatorname{index}(Q^D_{\alpha,\beta})$ induces a real zero of $\det(Q^D_{\alpha,\beta})$, our considerations show that $\beta\mapsto \det(Q^D_{\alpha,\beta})$ has N'

real zeroes. Further, we have $\beta_{\lceil (N'+1)/2 \rceil}(\alpha) < \alpha^2 < \beta_{\lceil (N'+3)/2 \rceil}(\alpha)$. This proves the proposition.

Proof of Theorem 1.5. Part (i) is proved by Proposition 5.6, whereas (ii) follows from Proposition 5.4 and Lemma 5.5. □

A. Spectrum of the matrix P^D

Here we compute for any integer $N' \ge 3$ the eigenvalues of the $N' \times N'$ -matrix P^D appearing in the proof of Proposition 5.4.

Lemma A.1. If N' is even, the eigenvalues of P^D are 4N'-3 (with multiplicity one), 1 (with multiplicity N'/2), and -3 (with multiplicity N'/2-1). If N' is odd, the eigenvalues of P^D are 1 (with multiplicity (N'-1)/2), -3 (with multiplicity (N'-3)/2), and $\frac{1}{2}(4N'-5)\left(1\pm\sqrt{1+\frac{8(4N'-1)}{(4N'-5)^2}}\right)$ (each with multiplicity one).

Proof. Throughout this proof, antidiag $(a_1, \ldots, a_{N'})$ denotes the "antidiagonal" $N' \times N'$ -matrix M with $M_{kl} = a_l$ if k + l = N' + 1 and $M_{kl} = 0$ otherwise.

First consider the case where N' is even. We write P^D in the form

$$P^D = \operatorname{diag}(-1, \dots, -1) + \operatorname{antidiag}(-2, \dots, -2) + 4 \cdot 1_{N' \times N'}$$

and, with $\mu := -1 - \lambda$,

$$P^{D} - \lambda \operatorname{Id} = \underbrace{\operatorname{diag}(\mu, \dots, \mu) + \operatorname{antidiag}(-2, \dots, -2)}_{=:L^{(N')}} + 4 \cdot 1_{N' \times N'}.$$

Here $1_{N'\times N'}$ denotes the $N'\times N'$ -matrix whose entries are all equal to 1.

We compute $\det(P^D - \lambda \operatorname{Id}) = \det(L^{(N')} + 4 \cdot 1_{N' \times N'})$ by column expansion. Note that in the column expansion of the determinant only those terms contribute which are determinants of matrices containing at most one column consisting of entries all equal to four. We obtain

$$\det(P^{D} - \lambda \operatorname{Id}) = \det(L^{(N')}) + \sum_{j=1}^{N'} \det(L_{j}^{(N')}), \tag{80}$$

where $L_j^{(N')}$ is defined as the matrix $L^{(N')}$ with the jth column replaced by the column $4 \cdot 1_{N' \times 1}$. By expansion with respect to the first column and then the last column, the determinant of $L^{(N')}$ can be computed recursively,

$$\det(L^{(N')}) = (\mu^2 - 2^2) \det(L^{(N'-2)}).$$

Since $det(L^{(2)}) = \mu^2 - 4$, it follows by induction that

$$\det(L^{(N')}) = (\mu^2 - 4)^{N'/2}.$$
(81)

To compute $\det(L_1^{(N')})$, we expand the determinant in the same way and obtain the identity $\det(L_1^{(N')}) = 4(\mu + 2) \det(L^{(N'-2)})$, from which it follows that

$$\det(L_1^{(N')}) = 4(\mu + 2)(\mu^2 - 4)^{N'/2 - 1}.$$
(82)

Similarly one gets $\det(L_2^{(N')}) = (\mu^2 - 4) \det(L_1^{(N'-2)})$, and thus

$$\det(L_2^{(N')}) = \det(L_1^{(N')}) = 4(\mu + 2)(\mu^2 - 4)^{N'/2 - 1}.$$
 (83)

For any 1 < j < N'/2, this procedure leads to $\det(L_j^{(N')}) = (\mu^2 - 4) \det(L_{j-1}^{(N'-2)})$ and hence

$$\det(L_i^{(N')}) = \det(L_1^{(N')}) = 4(\mu + 2)(\mu^2 - 4)^{N'/2 - 1}.$$
 (84)

For j>N'/2, note that $\det(L_j^{(N')})=\det(L_{N-j}^{(N')})$, since $L_j^{(N')}$ and $L_{N-j}^{(N')}$ can be transformed into each other by exchanging the jth and the (N-j+1)th columns and then the jth and the (N-j+1)th rows. By (81)–(84), we obtain

$$\det(P^D - \lambda \operatorname{Id}) = (\mu^2 - 4)^{N'/2 - 1} \cdot ((\mu^2 - 4) + N' \cdot 4(\mu + 2))$$
$$= (\mu^2 - 4)^{N'/2 - 1} (\mu + 2)(\mu - 2 + 4N').$$

Hence, if N' is even, the zeroes of $\det(P^D - \lambda \operatorname{Id})$ are $\mu = 2$ (with multiplicity N'/2 - 1), $\mu = -2$ (with multiplicity N'/2), and $\mu = -4N' + 2$ (with multiplicity 1). Transforming back to $\lambda = -1 - \mu$, we obtain the claimed eigenvalues.

It remains to consider the case where N' is *odd*. Again, we write

$$P^{D} = \text{diag}(-1, \dots, -1, \overbrace{0}^{((N'+1)/2)}, -1, \dots, -1) + \text{antidiag}(-2, \dots, -2) + 4 \cdot 1_{N' \times N'}.$$

With $\mu = -1 - \lambda$ we get

$$P^D - \lambda \operatorname{Id} = L^{(N')} + 4 \cdot 1_{N' \times N'}$$

with

$$L^{(N')} = \begin{pmatrix} \mu & 0 & \dots & 0 & -2 \\ 0 & \ddots & & \ddots & 0 \\ \vdots & & \mu - 1 & & \vdots \\ 0 & \ddots & & \ddots & 0 \\ -2 & 0 & \dots & 0 & \mu \end{pmatrix}.$$

As above, we obtain the expansion (80) for the determinant of $P^D - \lambda$ Id. We expand $\det(L^{(N')})$ with respect to the first column and then the last column, obtaining the recursion formula

$$\det(L^{(N')}) = (\mu^2 - 4) \det(L^{(N'-2)}).$$

which together with $det(L^{(1)}) = \mu - 1$ leads to

$$\det(L^{(N')}) = (\mu^2 - 4)^{(N'-1)/2}(\mu - 1). \tag{85}$$

For $\det(L_1^{(N')})$, we obtain the identity $\det(L_1^{(N')}) = 4(\mu+2)\det(L^{(N'-2)})$ and hence

$$\det(L_1^{(N')}) = 4(\mu + 2)(\mu^2 - 4)^{(N'-3)/2}(\mu - 1). \tag{86}$$

More generally, for any 1 < j < N'/2, we have

$$\det(L_{N-j}^{(N')}) = \det(L_j^{(N')}) = \det(L_1^{(N')}). \tag{87}$$

It remains to compute $\det(L_{(N'+1)/2}^{(N')})$. Expanding $\det(L_{(N'+1)/2}^{(N')})$ by the first column and then the last column, we obtain the recursion relation

$$\det(L_{(N'+1)/2}^{(N')}) = (\mu^2 - 4) \det(L_{((N'-2)+1)/2}^{(N'-2)}).$$

Together with $\det(L_2^{(3)}) = \det\begin{pmatrix} \mu & 4 & -2 \\ 0 & 4 & 0 \\ -2 & 4 & \mu \end{pmatrix} = 4(\mu^2 - 4)$, this implies

$$\det(L_{(N'+1)/2}^{(N')}) = 4(\mu^2 - 4)^{(N'-1)/2}.$$
(88)

Hence, combining (85)–(88) we obtain

$$\det(P^D - \lambda \operatorname{Id}) = (\mu^2 - 4)^{(N'-3)/2}$$

$$\cdot ((\mu^2 - 4)(\mu - 1) + (N' - 1) \cdot 4(\mu + 2)(\mu - 1) + 4(\mu^2 - 4))$$

$$= (\mu^2 - 4)^{(N'-3)/2}(\mu + 2)(\mu^2 + (4N' - 3)\mu - (4N' + 2)).$$

Hence, if N' is odd, the zeroes of $\det(P^D - \lambda \operatorname{Id})$ are $\mu = 2$ (with multiplicity (N' - 3)/2), $\mu = -2$ (with multiplicity (N' - 1)/2), and

$$\mu = -\frac{1}{2}(4N' - 3) \pm \frac{1}{2}\sqrt{16N'^2 - 8N' + 17}$$

(each with multiplicity 1). Transforming back to $\lambda = -1 - \mu$, we obtain the claimed formulas for the eigenvalues in the case where N' is odd. This completes the proof of Lemma A.1.

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