Symmetric invariant manifolds in the Fermi Pasta Ulam chain

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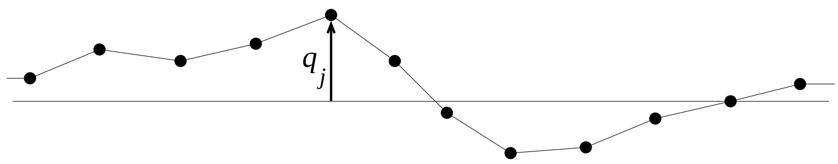
Abstract

The Fermi Pasta Ulam oscillator chain with periodic boundary conditions and n particles admits a large group of discrete symmetries. The fixed point sets of these symmetries naturally form invariant manifolds that are investigated in this short note. For each k dividing n we find invariant k degree of freedom symplectic manifolds. They represent short wavelength solutions composed of k Fourier-modes and can be interpreted as embedded chains with periodic boundary conditions and only k particles. Inside these invariant symplectic manifolds other invariant structures and exact solutions are found which represent for instance periodic and quasiperiodic solutions and standing and traveling waves. Some of these results have been found previously by other authors via a study of mode coupling coefficients. But we arrive at our results in a more systematic way and without any calculations. We show that the same invariant manifolds exist in the Klein-Gordon lattice and in the continuum limit.

1 Introduction

The Fermi Pasta Ulam chain or FPU chain is a discrete model for a continuous nonlinear string, introduced by E. Fermi, J. Pasta and S. Ulam [4]. This string is modeled by a finite number of point masses which represent the material elements of the string. Each of the point masses interacts with its nearest neighbors only.



Assume that the chain consists of a finite number $n \in \mathbb{N}$ particles. Define $q_j \in \mathbb{R}$ the vertical position of the j-th particle. We distinguish two different types of boundary

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conditions. We speak of fixed boundary conditions if the first and the last particle do not move, meaning that we have $q_0 = q_n = 0$ for all time. The FPU chain with fixed boundary conditions models a string with Dirichlet boundary conditions. It is also possible to choose periodic boundary conditions, in which case the first and the last particle are identified, that is $q_0 = q_n$ for all time. The FPU chain with periodic boundary conditions models a circular string. Both types of boundary conditions occur very often in the literature. In this paper we shall only consider chains with periodic boundary conditions, as it will become clear that each chain with fixed boundary conditions is naturally embedded as an invariant manifold of an appropriate periodic chain. The particles of the periodic chain are labeled by elements of the cyclic group $\mathbb{Z}/_{n\mathbb{Z}}$. The Hamiltonian equations of motion for the FPU chain are derived as follows.

The space of positions $q = (q_1, \ldots, q_n)$ of the particles in the chain is $\mathbb{R}^n$. The space of positions and conjugate momenta is the cotangent bundle $T^*\mathbb{R}^n$ of $\mathbb{R}^n$, the elements of which are denoted $(q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n)$. $T^*\mathbb{R}^n$ is a symplectic manifold, endowed with the symplectic form $dq \wedge dp = \sum_{j=1}^{n} dq_j \wedge dp_j$. Any smooth function $H : T^*\mathbb{R}^n \to \mathbb{R}$ now induces the Hamiltonian vector field X_H given by the defining relation $(dq \wedge dp)(X_H, \cdot) = dH$. In other words, we have the system of ordinary differential equations $\dot{q}_j = \frac{\partial H}{\partial p_j}$, $\dot{p}_j = -\frac{\partial H}{\partial q_j}$.

The Hamiltonian function for the FPU chain with periodic boundary conditions and n particles consists of a kinetic energy and a potential energy. The potential energy is assumed to depend only on the vertical distance between pairs of neighboring particles. Hence the Hamiltonian is

$$H = \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 + W(q_{j+1} - q_j) \ , \tag{1.1}$$

in which $W : \mathbb{R} \to \mathbb{R}$ is a Lennard-Jones potential energy density function of the form

$$W(x) = \frac{1}{2!} x^2 + \frac{\alpha}{3!} x^3 + \frac{\beta}{4!} x^4 \quad . \tag{1.2}$$

The α, β are real parameters measuring the nonlinearity in the forces between the particles in the chain. We also write

$$H = \left(\sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 \right) + H_2(q) + \alpha H_3(q) + \beta H_4(q) \ .$$

In which

$$H_m(q) = \frac{1}{m!} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} (q_{j+1} - q_j)^m$$

is a polynomial in q of degree m.

Fermi, Pasta and Ulam expected that for $\alpha, \beta \neq 0$, a many particle system such as the FPU chain would be ergodic, meaning that almost all orbits densely fill up an energy level set of the Hamiltonian. Ergodicity would lead to 'thermalisation' or equipartition of energy between the various Fourier modes of the system. FPU's nowadays famous numerical experiment was intended to investigate how thermalisation would take place. The result was astonishing: it turned out that there was no sign of thermalisation at all. Putting initially all the energy in one Fourier mode, they observed that this energy was shared by only a few other modes, the remaining modes were hardly excited. Within a rather short time the system returned close to its initial state.

The observations of Fermi, Pasta and Ulam greatly stimulated work on nonlinear dynamical systems. Nowadays people tend to explain the FPU experiment in two ways. In 1965 Zabuski and Kruskal [16] considered the Korteweg-de Vries equation as a continuum limit of the FPU chain and numerically found the first indications for the stable behaviour of solitary waves. We now know that the Korteweg-de Vries equation is integrable [10]. This clearly suggests an explanation for FPU's observations, although the relation between the FPU chain and its infinite dimensional limits has never been completely understood.

Another, possibly correct explanation for the quasiperiodic behaviour of the FPU system, is based on the Kolmogorov-Arnol'd-Moser theorem. As is well-known [1], the solutions of an n degree of freedom Liouville integrable Hamiltonian system are constrained to move on n-dimensional tori and are not at all ergodic but periodic and quasiperiodic. The KAM theorem states that most invariant tori of such an integrable system persist under small Hamiltonian perturbations, if the unperturbed integrable system satisfies the Kolmogorov nondegeneracy condition. Although several authors, starting with Izrailev and Chirikov [6], have stated that the KAM theorem explains the observations of the FPU experiment, it has for a long time been completely unclear how the FPU system can be viewed as a perturbation of a nondegenerate integrable system. This gap in the theory was recently mentioned again in the review article of Ford [5] and the book of Weissert [15]. The only results in this direction that are known to me were obtained by Nishida [9] and Rink [12]. Although the results in Nishida [9] are unfortunately incomplete, in Rink [12] the Birkhoff normal form for the FPU chain is calculated and it is proven to be nondegenerately integrable. This explains why the FPU chain at low energy can not be ergodic. On the other hand, there are many numerical studies indicating that above a certain energy threshold the chain indeed thermalises. Reference [11] contains a rather complete overview of these results.

Contrary to these more or less global results, several authors have been trying to find lower dimensional invariant manifolds for the FPU chain. First of all because they represent interesting classes of solutions such as periodic and quasiperiodic solutions and standing and traveling waves. But also because it is believed by some authors, see for instance [3], that the destabilisation of invariant manifolds can lead to chaos and hence maybe to ergodicity.

Most of the invariant manifolds that are known in the FPU chain were discovered more or less emperically. In their original paper Fermi, Pasta and Ulam [4] already remarked that if the nonlinearity coefficient α in (1.2) vanishes and initially only waves with an odd wave number are excited, then waves with an even wave number will never gain energy. Later on other invariant manifolds were discovered by studying mode coupling coefficients in detail, see for instance [2] and [11]. In these papers it is shown that certain sets of normal modes will not be excited if they initially have no energy.

In this paper, it will be shown that the same results and more can be obtained without introducing Fourier modes or studying mode coupling coefficients. The idea is to exploit the discrete symmetries that are naturally present in the FPU chain. The fixed point sets of these symmetries form invariant manifolds for the equations of motion. Although the idea behind this approach is quite simple, I am not aware of any systematic study of the dynamical implications of these symmetries. Nevertheless, symmetries seem to be the basic object to investigate if one wants to discover invariant manifolds. We find all the invariant manifolds that were already known in the literature and many more, without having to calculate mode coupling coefficients or to restrict ourselves to the case $\alpha = 0$. The results are obtained in a systematic way and they are not only valid for the FPU chain, but for any lattice with the same symmetries, such as the Klein-Gordon lattice [8]. Moreover, our results apply in the continuum limit as we can also point out several infinite dimensional invariant manifolds for a rather broad class of nonlinear homogeneous partial differential equations.

2 Quasiparticles

Since we want to be able to compare our results with previous work, we introduce Fourier modes in this section. It is natural to view the solutions of the FPU chain as a superposition of waves and to make the following Fourier transformation:

$$q_j = \frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{\frac{2\pi i jk}{n}} \bar{q}_k \tag{2.1}$$

$$p_j = \frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{-\frac{2\pi i jk}{n}} \bar{p}_k \tag{2.2}$$

Using that

$$\frac{1}{n} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} e^{\frac{2\pi i jk}{n}} = \begin{cases} 1 & \text{if } j = 0 \text{ mod } n \\ 0 & \text{if } j \neq 0 \text{ mod } n \end{cases}$$

one easily calculates that $\{\bar{q}_j, \bar{q}_k\} = \{\bar{p}_j, \bar{p}_k\} = 0$ and $\{\bar{q}_j, \bar{p}_k\} = \delta_{jk}$, the Kronecker delta. Hence, $(\bar{q}, \bar{p})$ are canonical coordinates. They are traditionally called *phonons* or *quasiparticles*. Written out in phonons, the FPU Hamiltonian (1.1) reads as follows. The kinetic energy becomes:

$$\sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2} p_j^2 = \frac{1}{2} \bar{p}_{\frac{n}{2}}^2 + \sum_{1 \leq j < \frac{n}{2}} \bar{p}_j \bar{p}_{n-j} \ ,$$

where it is understood that the term $\frac{1}{2}\bar{p}_{\frac{n}{2}}^2$ occurs only if n is even. The potential energies H_m become

$$H_m = \frac{1}{m!} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} (q_{j+1} - q_j)^m = \frac{1}{m!} \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \left(\frac{1}{\sqrt{n}} \sum_{k \in \mathbb{Z}/_{n\mathbb{Z}}} (e^{\frac{2\pi i (j+1)k}{n}} - e^{\frac{2\pi i jk}{n}}) \bar{q}_k \right)^m =$$

$$\frac{1}{m! n^{\frac{m}{2}}} \sum_{\substack{j \in \\ \mathbb{Z}/_{n\mathbb{Z}}}} \sum_{\theta : |\theta| = m} \binom{m}{\theta} e^{\frac{2\pi i j (\sum_k k\theta_k)}{n}} \prod_{k \in \mathbb{Z}/_{n\mathbb{Z}}} (e^{\frac{2\pi i k}{n}} - 1)^{\theta_k} \bar{q}_k^{\theta_k} = n^{\frac{2-m}{2}} \sum_{\substack{\theta : |\theta| = m \\ \sum_k k\theta_k = 0 \text{ mod } n}} \prod_{k \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{\theta_k!} (e^{\frac{2\pi i k}{n}} - 1)^{\theta_k} \bar{q}_k^{\theta_k}$$

in which the sum is taken over multi-indices $\theta \in \mathbb{Z}^n$ for which $|\theta| := \sum_k |\theta_k| = m$. We also used the multinomial coefficient $\binom{m}{\theta} := \frac{m!}{\prod_k \theta_k!}$. We have obtained a rather compact and tractible formula for the Hamiltonian in phonon-coordinates.

Let us also introduce real-valued phonons. For $1 \le k < \frac{n}{2}$ define

$$Q_k = (\bar{q}_k + \bar{q}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \cos(\frac{2jk\pi}{n}) q_j \ , \ Q_{n-k} = i(\bar{q}_k - \bar{q}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \sin(\frac{2jk\pi}{n}) q_j$$

$$P_k = (\bar{p}_k + \bar{p}_{n-k})/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \cos(\frac{2jk\pi}{n}) p_j \ , \ P_{n-k} = i(\bar{p}_{n-k} - \bar{p}_k)/\sqrt{2} = \sqrt{\frac{2}{n}} \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \sin(\frac{2jk\pi}{n}) p_j$$

and

$$Q_{\frac{n}{2}} = \bar{q}_{\frac{n}{2}} \ , \ P_{\frac{n}{2}} = \bar{p}_{\frac{n}{2}} \ , \ Q_n = \bar{q}_n \ , \ P_n = \bar{p}_n$$

The transformation $(\bar{q}, \bar{p}) \mapsto (Q, P)$ is again symplectic and one can express the Hamiltonian in terms of Q and P. In the case that $\alpha = \beta = 0$, that is for the harmonic FPU chain, one gets

$$H = \sum_{j\in\mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2}p_j^2 + \frac{1}{2}(q_{j+1} - q_j)^2 = \sum_{j=1}^{n} \frac{1}{2}(P_j^2 + \omega_j^2 Q_j^2)$$

in which for $j = 1, \ldots, n$ the numbers ω_j are the well-known normal mode frequencies of the periodic FPU chain:

$$\omega_j := 2\sin(\frac{j\pi}{n})$$

Note that written down in real-valued phonon coordinates, the equations of motion of the harmonic chain are simply the equations for $n-1$ uncoupled harmonic oscillators and one free particle. The situation is not so simple anymore if $\alpha, \beta \neq 0$, when the normal modes interact in a complicated manner that is governed by the Hamiltonians

$$H_m = \sum_{\theta:|\theta|=m} c_\theta \prod_{k=1}^{n-1} Q_k^{\theta_k}$$

in which the c_θ are certain coefficients. An expression for the c_θ with $|\theta| = 4$ can be found in [11], although the explicit calculation is not given there.

Note that H is independent of $Q_n = \bar{q}_n = \frac{1}{\sqrt{n}}\sum_j q_j$. Hence the total momentum $P_n = \bar{p}_n = \frac{1}{\sqrt{n}}\sum_j p_j$ is a constant of motion and the equations for the remaining variables are completely independent of $(Q_n, P_n) = (\bar{p}_n, \bar{q}_n)$. It is common to set the latter coordinates equal to zero, or to neglect them completely.

Although the other normal modes interact in a complicated manner, not every possible coupling term occurs. Only those monomials $\bar{q}^\theta = \prod_k \bar{q}_k^{\theta_k}$ are present in $H_m(\bar{q})$ for which $\sum_k k\theta_k = 0 \bmod n$, whereas $H_m(Q)$ contains only the monomials $Q^\theta = \prod_k Q_k^{\theta_k}$ for which $c_\theta \neq 0$. In the next section we will see that this is a consequence of discrete symmetries in the system.

It is exactly the fact that not every coupling term occurs which accounts for the existence of various invariant manifolds, see [2] and [11]. Let $\mathcal{A} \subset \mathbb{Z}/_{n\mathbb{Z}}$. Then the manifold spanned by modes in $\mathcal{A}$ is

$$M_n^{\mathcal{A}} = \{(Q, P) \in T^*\mathbb{R}^n | Q_j = P_j = 0 \ \forall j \notin \mathcal{A}\} \ .$$

$M_n^{\mathcal{A}}$ is an invariant manifold if and only if $c_\theta = 0$ for all θ with the property that $\theta_j = 1$ for some $j \notin \mathcal{A}$ and $\theta_k = 0$ for all $k \notin \mathcal{A} \cup \{j\}$. Making use of this fact, several invariant manifolds have been discovered. If n is even, one can for instance choose $\mathcal{A} = \{\frac{n}{2}\}$. It is then obvious that $\mathcal{A}$ satisfied the required property since $j + (m-1)\frac{n}{2} \neq 0 \mod n$. The solutions in the invariant manifold $M_n^{\{\frac{n}{2}\}}$ are of the form $q_j(t) = \frac{(-1)^j}{\sqrt{n}} Q_{\frac{n}{2}}(t)$. This type of periodic solutions in which neighbouring particles are exactly out of phase, is well-known. In [11] a linear stability analysis is given for it.

Studying mode coupling coefficients in this way, several invariant manifolds have been discovered. In [2] it is shown that if $\alpha = 0$ and n is even, $M_n^{\{2,4,\ldots,n\}}$ and $M_n^{\{1,3,\ldots,n-1\}}$ are invariant. Poggi and Ruffo [11] show that $M_n^{\{\frac{n}{3},\frac{2n}{3}\}}$ and $M_n^{\{\frac{n}{4},\frac{3n}{4}\}}$ are invariant.

The above method is rather simple but has the following limitations:

1. An explicit expression for the c_θ is required.
2. The method becomes more elaborate if one wants to find invariant manifolds of higher dimensions.
3. There is no a priori ‘physical’ reason why a certain $M_n^{\mathcal{A}}$ will be invariant.
4. Invariant manifolds might exist that are not of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A} \subset \mathbb{Z}/_{n\mathbb{Z}}$.
5. It is not clear whether the discovered invariant manifolds will also be present in the continuum limit or in other one-dimensional lattice systems.

For these reasons, studying mode coupling coefficients is rather unsatisfactory. But with the method presented in the following sections of this paper it is possible to detect easily many more invariant manifolds. They arise in a natural way as fixed point sets of symmetries.

3 Symmetry

The Hamiltonian function (1.1) of the periodic FPU chain has some discrete symmetries. They have some important dynamical consequences. Define the linear mappings $R, S, T : \mathbb{R}^n \to \mathbb{R}^n$ by

$$
\begin{aligned}
R &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (q_2, q_3, \ldots, q_n, q_1) \ , \\
S &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (-q_{n-1}, -q_{n-2}, \ldots, -q_1, -q_n) \quad \text{and} \\
T &: (q_1, q_2, \ldots, q_{n-1}, q_n) \mapsto (-q_1, -q_2, \ldots, -q_{n-1}, -q_n) \ ,
\end{aligned}
$$

The mappings $(q,p) \mapsto (Rq, Rp)$, $(q,p) \mapsto (Sq, Sp)$ and $(q,p) \mapsto (Tq, Tp)$ from $T^*\mathbb{R}^n$ to $T^*\mathbb{R}^n$ are also denoted R, S and T respectively. R and S satisfy the multiplication relations $R^n = S^2 = \mathrm{Id}$ and $RS = SR^{-1}$ and hence the discrete group $\langle R, S\rangle := \{\mathrm{Id}, R, R^2, \ldots, R^{n-1}, S, RS, \ldots, R^{n-1}S\}$ is a representation of the n-th dihedral group D_n, the symmetry group of the n-gon. Moreover, $T^2 = \mathrm{Id}$ and T commutes with R and S and therefore the group $\langle R, S, T\rangle$ generated by R, S and T is a representation of $D_n \times \mathbb{Z}/_{2\mathbb{Z}}$.

R, S and T are symplectic maps: $R^*(dq \wedge dp) = S^*(dq \wedge dp) = T^*(dq \wedge dp) = dq \wedge dp$. Furthermore, note that R and S leave the Hamiltonian H invariant: $R^*H := H \circ R = H$ and $S^*H := H \circ S = H$. We find that $T^*H = H \circ T = H$ if and only if the potential energy density function W is an even function, in other words if $\alpha = 0$. The group $\langle R, S\rangle$ is called a symmetry group of H, its elements symmetries. The same is true for $\langle R, S, T\rangle$ if W is even.

For any symmetry P we have $P^*(dq \wedge dp) = dq \wedge dp$ and $P^*H = H$ so the Hamiltonian vector field X_H induced by H is equivariant under P: $P^*X_H = X_{P^*H} = X_H$. In other words: if $\gamma : \mathbb{R} \to T^*\mathbb{R}^n$ is an integral curve of X_H, then $P \circ \gamma : \mathbb{R} \to T^*\mathbb{R}^n$ is also an integral curve of X_H. This implies that P commutes with the flow of X_H, that is $e^{tX_H} \circ P = P \circ e^{tX_H}$.

Of particular dynamical interest is the fixed point set of a symmetry P,

$$\text{Fix } P = \{(q,p) \in T^*\mathbb{R}^n | (Pq, Pp) = (q,p)\} \tag{3.1}$$

Let $x \in \text{Fix } P$, then $P(e^{tX_H}(x)) = e^{tX_H}(P(x)) = e^{tX_H}(x)$ so Fix P is an invariant manifold for the flow of X_H. In the next sections we investigate the various invariant manifolds Fix P. We shall describe them in terms of the original coordinates (q,p), but also in phonon-coordinates $(\bar{q}, \bar{p})$ and (Q, P). Therefore it is interesting to write down the action of R, S and T in phonon coordinates:

$$\begin{aligned}
R :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (e^{2\pi i/n}\bar{q}_1, e^{4\pi i/n}\bar{q}_2, \ldots, e^{2\pi i(n-1)/n}\bar{q}_{n-1}, e^{2\pi i n/n}\bar{q}_n)\ ,\\
&(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (e^{-2\pi i/n}\bar{p}_1, e^{-4\pi i/n}\bar{p}_2, \ldots, e^{-2\pi i(n-1)/n}\bar{p}_{n-1}, e^{-2\pi i n/n}\bar{p}_n)\ .\\
S :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (-\bar{q}_{n-1}, -\bar{q}_{n-2}, \ldots, -\bar{q}_1, -\bar{q}_n)\ ,\\
&(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (-\bar{p}_{n-1}, -\bar{p}_{n-2}, \ldots, -\bar{p}_1, -\bar{p}_n)\ .\\
T :&(\bar{q}_1, \bar{q}_2, \ldots, \bar{q}_{n-1}, \bar{q}_n) \mapsto (-\bar{q}_1, -\bar{q}_2, \ldots, -\bar{q}_{n-1}, -\bar{q}_n)\ ,\\
&(\bar{p}_1, \bar{p}_2, \ldots, \bar{p}_{n-1}, \bar{p}_n) \mapsto (-\bar{p}_1, -\bar{p}_2, \ldots, -\bar{p}_{n-1}, -\bar{p}_n)\ .
\end{aligned}$$

Note that by performing the transformation to phonons, the action of R on the coordinate functions has been diagonalised. The actions of S and T however have not at all changed. R acts on a monomial q^θ as follows:

$$R^*\left(\prod_k q_k^{\theta_k}\right) = e^{2\pi i \sum_k k\theta_k/n} \prod_k q_k^{\theta_k}$$

In other words, the monomial q^θ is R-symmetric if and only if $\sum_k k\theta_k = 0 \bmod n$. So R-symmetry is the reason why only these monomials occur in the FPU Hamiltonian.

4 Invariant manifolds for arbitrary potentials

In this section we study the invariant manifolds that are formed by the fixed point sets of elements of $\langle R, S\rangle$. So it is not yet assumed that the potential energy density function W is even.

For integers n and k, let $\gcd(n,k)$ be the greatest common divisor of n and k. For $k \in \mathbb{Z}$,

$$\text{Fix } R^k = \{q_j = q_{j+\gcd(n,k)}, p_j = p_{j+\gcd(n,k)}\ \forall j\}$$

is an invariant $\gcd(n,k)$ degree of freedom symplectic submanifold of $T^*\mathbb{R}^n$. The Hamiltonian function $H|_{\text{Fix } R^k}$ on the symplectic submanifold Fix R^k obviously simply models the periodic FPU chain with $\gcd(n,k)$ particles. In this way, the periodic chain with k particles is naturally embedded in the chain with n particles if k divides n. In phonon coordinates,

$$\text{Fix } R^k = \{\bar{q}_j = \bar{p}_j = 0\ \forall j \neq 0 \bmod \frac{n}{\gcd(n,k)}\} = \{Q_j = P_j = 0\ \forall j \neq 0 \bmod \frac{n}{\gcd(n,k)}\}$$

So if k divides n, then Fix $R^k = M_n^{\{\frac{n}{k},\frac{2n}{k},\ldots,\frac{(k-1)n}{k},n\}}$ and is hence spanned by modes which represent a repeating spatial pattern with period k.

If for instance n is even, then Fix $R^2 = M_n^{\{\frac{n}{2},n\}}$ is the two degree of freedom invariant manifold spanned by the $\frac{n}{2}$-th and the n-th normal modes. If we as usual neglect the n-th mode, which moves independently of all other modes, we find that Fix R^2 consists of all solutions of the form $q_j(t) = \frac{(-1)^j}{\sqrt{n}} Q_{\frac{n}{2}}(t)$. These are the previously mentioned periodic solutions in which neighboring particles are exactly out of phase. On the other hand one has for even n that Fix $R^{\frac{n}{2}} = M_n^{\{2,4,\ldots,n\}}$. It consists of all even modes.

If 3 divides n, then Fix $R^3 = M_n^{\{\frac{n}{3},\frac{2n}{3},n\}}$, whereas Fix $R^{\frac{n}{3}} = M_n^{\{3,6,\ldots,n-3,n\}}$. Etcetera.

Let us now for arbitrary $l \in \mathbb{Z}$ study

$$\begin{aligned}
&\text{Fix } R^l S = \{q_j = -q_{l-j}, p_j = -p_{l-j}\ \forall j\} = \{\bar{q}_j = -e^{-\frac{2\pi i j l}{n}} \bar{q}_{n-j}\ ,\ \bar{p}_j = -e^{\frac{2\pi i j l}{n}} \bar{p}_{n-j}\ \forall j\} = \\
&\{Q_j \cos(\frac{lj\pi}{n}) + Q_{n-j}\sin(\frac{lj\pi}{n}) = P_j\cos(\frac{lj\pi}{n}) + P_{n-j}\sin(\frac{lj\pi}{n}) = 0\ \forall\ 1 \le j < \frac{n}{2}\ , \\
&Q_{\frac{n}{2}} = (-1)^{l+1} Q_{\frac{n}{2}}\ ,\ P_{\frac{n}{2}} = (-1)^{l+1} P_{\frac{n}{2}}\ ,\ Q_n = P_n = 0\}
\end{aligned}$$

It is a $(2n-2-(-1)^l-(-1)^{n+l})/4$ degree of freedom symplectic subspace of $T^*\mathbb{R}^n$.

Note that Fix $R^l S$ is not always of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A}$. On the other hand, Fix $S = M_n^{\{j|\frac{n}{2}<j<n\}}$ and if n is even, then Fix $R^{\frac{n}{2}} S = M_n^{\{1,n-2,3,n-4,\ldots\}} = M_n^{\{j|2\le j\le \frac{n}{2},\ j=1 \bmod 2\}\cup\{j|\frac{n}{2}<j<n,\ j=0 \bmod 2\}}$. So for instance for $n=8$ these are $M_8^{\{5,6,7\}}$ and $M_8^{\{1,3,6\}}$.

If both n and l are even, then Fix $R^l S$ has dimension $n/2-1$ and in Fix $R^l S$ we have $q_{\frac{l}{2}} = q_{\frac{n+l}{2}} = 0$. In other words, if n is even, then for every even l the Hamiltonian function $H|_{\text{Fix } R^l S}$ on the symplectic subspace Fix $R^l S$ models the FPU chain with fixed boundary conditions and $n/2-1$ moving particles. Hence, the FPU chain with fixed boundary conditions and $n/2-1$ moving particles is naturally embedded in the periodic FPU chain with n particles. This is the reason why we do not study FPU chains with fixed boundary conditions separately.

5 Invariant manifolds for even potentials

If the potential energy density function W is even, then also T is a symmetry and the full symmetry group of the FPU Hamiltonian is $\langle R, S, T\rangle \cong D_n \times \mathbb{Z}/_{2\mathbb{Z}}$. Let us study the fixed point sets of the symmetries $R^k T$ and $R^l S T$ which have not yet been discussed in the previous section.

For $k \in \mathbb{Z}$,

$$\text{Fix } R^k T = \{q_j = -q_{j+\gcd(n,k)}, p_j = -p_{j+\gcd(n,k)}\ \forall j\}$$

which is nontrivial only if $n/\gcd(n,k)$ is even -and hence n must be even. In this case it is a $\gcd(n,k)$ degree of freedom invariant symplectic manifold. In phonons,

$$\begin{aligned}\text{Fix } R^kT =&\{\bar{q}_j = \bar{p}_j = 0\ \forall j \neq \frac{n}{2\gcd(n,k)} \bmod \frac{n}{\gcd(n,k)}\} \\ = \{Q_j =& P_j = 0\ \forall j \neq \frac{n}{2\gcd(n,k)} \bmod \frac{n}{\gcd(n,k)}\}\ .\end{aligned}$$

So if $2k$ divides n, then Fix $R^kT = M_n^{\{\frac{n}{2k},\frac{3n}{2k},\ldots,\frac{(2k-1)n}{2k}\}}$.

The special choice $k = \frac{n}{2}$ gives us the invariant manifold Fix $R^{\frac{n}{2}}T = M_n^{\{1,3,5,\ldots,n-1\}}$ of all odd normal modes that was already discovered by Fermi, Pasta and Ulam [4]. The choice $k = 1$ gives us Fix $RT = M_n^{\{\frac{n}{2}\}}$, the well known $\frac{n}{2}$-th mode.

If n is divisible by 4, then Fix $R^{\frac{n}{4}}T = M_n^{\{2,6,10,\ldots,n-2\}}$ is invariant. This is a new result. The invariant manifold Fix $R^2T = M_n^{\{\frac{n}{4},\frac{3n}{4}\}}$ is discussed in [11]. It contains quasiperiodic solutions.

For an n divisible by 6 we find the invariant manifolds $M_n^{\{3,9,15,\ldots,n-3\}}$ and $M_n^{\{\frac{n}{6},\frac{n}{2},\frac{5n}{6}\}}$. Etcetera.

For $l \in \mathbb{Z}$,

$$\begin{aligned}&\text{Fix } R^lST = \{q_j = q_{l-j}, p_j = p_{l-j}\ \forall j\} = \{\bar{q}_j = e^{-\frac{2\pi ijl}{n}}\bar{q}_{n-j}\ ,\ \bar{p}_j = e^{\frac{2\pi ijl}{n}}\bar{p}_{n-j}\ \forall j\} = \\ &\{Q_j \sin(\frac{lj\pi}{n}) - Q_{n-j}\cos(\frac{lj\pi}{n}) = P_j\sin(\frac{lj\pi}{n}) - P_{n-j}\cos(\frac{lj\pi}{n}) = 0\ \forall\ 1 \leq j < \frac{n}{2}\ , \\ &Q_{\frac{n}{2}} = (-1)^l Q_{\frac{n}{2}}\ ,\ P_{\frac{n}{2}} = (-1)^l P_{\frac{n}{2}}\}\end{aligned}$$

is an $(2n-2+(-1)^l+(-1)^{n+l})/4$ degree of freedom invariant symplectic manifold.

Note that again Fix R^lST is not always of the form $M_n^{\mathcal{A}}$, but that on the other hand Fix $ST = M_n^{\{j|0\leq j\leq\frac{n}{2}\}}$ and if n is even, Fix $R^{\frac{n}{2}}ST = M_n^{\{0,n-1,2,n-3,4,\ldots\}} = M_n^{\{j|0\leq j\leq\frac{n}{2},\ j=0 \bmod 2\}\cup\{j|\frac{n}{2}<j<n,\ j=1 \bmod 2\}}$. So for instance for $n = 8$ these are $M_8^{\{1,2,3,4\}}$ and $M_8^{\{2,4,5,7\}}$.

6 Examples of intersections

We have studied all fixed point sets of the elements of the symmetry groups $\langle R, S\rangle$ and $\langle R, S, T\rangle$. More invariant manifolds are formed by taking intersections of these fixed point sets. We will give just a few examples here.

If 3 divides n, then Fix $R^3 \cap$ Fix $S = M_n^{\{\frac{2n}{3}\}}$, whereas Fix $R^3 \cap$ Fix $ST = M_n^{\{\frac{n}{3}\}}$. The latter is only invariant if the potential W is even.

If 4 divides n, then Fix $R^4 \cap$ Fix $S = M_n^{\{\frac{3n}{4}\}}$, Fix $R^4 \cap$ Fix $ST = M_n^{\{\frac{n}{4},\frac{n}{2}\}}$ and Fix $R^2T \cap$ Fix $ST = M_n^{\{\frac{n}{4}\}}$.

If 5 divides n, then Fix $R^5\cap$Fix $S = M_n^{\{\frac{3n}{5},\frac{4n}{5}\}}$, whereas Fix $R^5\cap$Fix $ST = M_n^{\{\frac{n}{5},\frac{2n}{5}\}}$.

If 6 divides n, then Fix $R^6 \cap$ Fix $S = M_n^{\{\frac{2n}{3},\frac{5n}{6}\}}$ and Fix $R^6 \cap$ Fix $ST = M_n^{\{\frac{n}{6},\frac{n}{3},\frac{n}{2}\}}$. And we find that Fix $R^3T = M_n^{\{\frac{n}{6},\frac{n}{2},\frac{5n}{6}\}}$ can be split into Fix $R^3T \cap$ Fix $S = M_n^{\{\frac{5n}{6}\}}$ and Fix $R^3T \cap$ Fix $ST = M_n^{\{\frac{n}{6},\frac{n}{2}\}}$. The normal mode solutions in $M_n^{\{\frac{5n}{6}\}}$ have as far as I know not been discussed previously in the literature.

One can proceed and compute, if k divides n, the intersections of the various fixed point sets of $R^k, S, R^{\frac{n}{2}}S, R^kT, ST$ and $R^{\frac{n}{2}}ST$. We choose not to make a systematic classification of the results, since most invariant manifolds in the FPU chain are not even of the form $M_n^{\mathcal{A}}$ for some $\mathcal{A}$.

7 Other lattices and the continuum limit

A major advantage of our method is that fixed point sets of symmetries are invariant manifolds in any Hamiltonian system admitting these symmetries. Hence we expect to find the invariant manifolds that we discovered in the FPU chain with periodic boundary conditions also in other one-dimensional spatially homogeneous lattices, such as the Klein-Gordon lattice [8]. The Klein-Gordon lattice with periodic boundary conditions has the Hamiltonian

$$H = \sum_{j \in \mathbb{Z}/_{n\mathbb{Z}}} \frac{1}{2}p_j^2 + \frac{1}{2}(q_{j+1} - q_j)^2 + W(q_j) \ ,$$

in which W is a potential energy density function. The Klein-Gordon lattice models a one dimensional mono-atomic structure with small coupling between the atoms. It is clear that the mappings R and ST, see formulas (3.1), again leave this Hamiltonian invariant, whereas R, S and T separately have this property if W is an even function. Thus we have again found symmetries and their fixed point sets are invariant manifolds. In particular, the invariant manifolds that we discovered in the FPU chain with even potential are also present in the Klein-Gordon lattice with even potential.

Our results are also valid in the continuum limit, when the discrete lattice equations are replaced by a homogeneous partial differential equation. Consider for example for $x \in \mathbb{R}/_{\mathbb{Z}}$ the equation

$$u_{tt} = u_{xx} + f(u) \ ,$$

for $f : \mathbb{R} \to \mathbb{R}$. This equation can also be written as the system of equations

$$u_t = v \ , \ v_t = u_{xx} + f(u) \ ,$$

which have the Hamiltonian

$$H = \int_{\mathbb{R}/_{\mathbb{Z}}} \frac{1}{2}v(x)^2 + \frac{1}{2}u_x(x)^2 - F(u(x)) \ dx$$

in which $F' = f$. Define the symplectic operators

$$\begin{aligned} \mathcal{R}^a \quad &: u(\cdot) \mapsto u(a+\cdot), \quad v(\cdot) \mapsto v(a+\cdot) \\ \mathcal{S} \quad &: u(\cdot) \mapsto -u(-\cdot), \quad v(\cdot) \mapsto -v(-\cdot) \\ \mathcal{T} \quad &: u(\cdot) \mapsto -u(\cdot), \quad v(\cdot) \mapsto -v(\cdot) \ . \end{aligned}$$

The constant $a \in \mathbb{R}/_{\mathbb{Z}}$ is arbitrary. Clearly, H is invariant under $\mathcal{R}^a$ and $\mathcal{ST}$. H is invariant under $\mathcal{R}^a$, $\mathcal{S}$ and $\mathcal{T}$ separately if and only if F is even, that is if and only if

f is odd.

The fixed point sets of these symmetries are invariant manifolds, possibly of infinite dimension. If $a \notin \mathbb{Q}$, then Fix $\mathcal{R}^a$ consists of constant solutions only, but if $a = \frac{p}{q}$ is rational and $\gcd(p,q) = 1$, then Fix $\mathcal{R}^{\frac{p}{q}}$ represents the solutions with $u(t,x) = u(t, x+\frac{1}{q})$. Fix $\mathcal{R}^{\frac{1}{q}}\mathcal{T}$ consists of solutions with $u(x) = -u(x+\frac{1}{q})$. The latter is nontrivial only if q is even. For arbitrary a, Fix $\mathcal{R}^a\mathcal{S}$ contains solutions with $u(x) = -u(a-x)$ and Fix $\mathcal{R}^a\mathcal{S}\mathcal{T}$ represents solutions with $u(x) = u(a-x)$.

It is natural to use the Fourier transformation

$$u(x,t) = \sum_{k\in\mathbb{Z}} u_k(t)e^{ik\pi x} \ , \ v(x,t) = \sum_{k\in\mathbb{Z}} v_k(t)e^{ik\pi x}$$

and to express the fixed point sets in terms of the Fourier variables $(u_k, v_k)_{k\in\mathbb{Z}}$. We then find for instance the following invariant manifolds

$$\text{Fix } \mathcal{R}^{\frac{p}{q}} = \{u_k = v_k = 0 \ \forall k \neq 0 \mod q\} = M^{\{\cdots,-2q,-q,0,q,2q,\ldots\}}$$

$$\text{Fix } \mathcal{R}^{\frac{p}{q}}\mathcal{T} = \{u_k = v_k = 0 \ \forall k \neq q \mod 2q\} = M^{\{\cdots,-3q,-q,q,3q,\ldots\}}$$

Etcetera.

[7], [13] and [14] study the equation $u_{tt} = u_{xx} + u^3$ by the Galerkin-averaging method. By an analysis of mode coupling coefficients they discover that the manifolds $M^{\{\cdots,-2q,-q,0,q,2q,\ldots\}}$ and $M^{\{\cdots,-3q,-q,q,3q,\ldots\}}$ are invariant in a certain finite dimensional system of differential equations, the Galerkin-averaging approximation, which approximates the original partial differential equation. We arrive here at the much stronger result that their conclusions hold for any odd nonlinearity f and in the *original* partial differential equation.

8 Discussion

In a systematic way we found various invariant manifolds for the Fermi Pasta Ulam oscillator chain with periodic boundary conditions. These invariant manifolds represent interesting classes of solutions such as periodic and quasiperiodic solutions, standing and traveling waves and embedded lower dimensional FPU chains with periodic or fixed boundary conditions. They are moreover interesting since it is believed by some authors [3] that destabilisation of these invariant manifolds can lead to chaos. Some of the invariant structures that we found have previously been discovered by other authors by an analysis of mode coupling coefficients. Our method on the contrary looks for fixed point sets of symmetries which are natural invariant manifolds. We can derive our results without computing the mode coupling coefficients explicitly. The same invariant manifolds are present in other homogeneous Hamiltonian lattices such as the Klein-Gordon lattice. In the continuum limit, when the lattice equations are replaced by a homogeneous partial differential equation, we point out analogous infinite dimensional invariant structures.

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