Computer Assisted Proofs for the FPU Model

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The Fermi-Pasta-Ulam model consists of P particles whose dynamics is described by the equations

$$\ddot{q}_m = \phi'(q_{m+1} - q_m) - \phi'(q_m - q_{m-1})\,, \qquad m = 1, 2, \ldots, P\,,$$

where $\phi(x) = \frac{x^2}{2} + \alpha\frac{x^3}{3} + \beta\frac{x^4}{4}$.

We investigate time-periodic solutions with $\alpha = 0$.

By homogeneity, it suffices to consider the case $\beta = 1$. Similarly, the fundamental period T of a non-constant solution can be normalized to 2π by a rescaling of time. This leads us to consider the equation

$$\omega^2\ddot{q} = -\nabla^*\left[\nabla q + (\nabla q)^3\right],$$

where $\omega = 2\pi/T$, and where ∇ and ∇^* are defined by

$$\big(\nabla q\big)_m(t) = q_{m+1}(t) - q_m(t)\,, \qquad \big(\nabla^* q\big)_m(t) = q_{m-1}(t) - q_m(t)\,.$$

The best known periodic solutions of the β-model are near $q = 0$. In this regime, the cubic term is small compared to q, and we have $L_\omega q \approx 0$, where

$$L_\omega q = -\omega^2 \ddot{q} - \nabla^* \nabla q \, .$$

The values of $\omega > 0$ for which L_ω has an eigenvalue zero, and the corresponding nonzero solutions of $L_\omega q = 0$, will be referred to as resonant frequencies and normal modes, respectively.

Proposition 1. *A frequency $\omega_n > 0$ is resonant, that is, L_ω has an eigenvalue zero, if and only if*

$$\omega_n k = \pm 2 \sin(h\theta/2) \, ,$$

for some nonzero $k \in \mathbb{Z}$ and $h \in \mathcal{P} := \mathbb{Z}/(P\mathbb{Z})$.

For every $h \in \mathcal{P}$, let $\mathbb{P}'_h$ be the orthogonal projection on the h-th normal mode.

As a measure for the size of the h-th spatial mode of $q \in H^1_o$, we consider its "harmonic energy"

$$E_h(q) = E(\mathbb{P}'_h q)\,, \qquad E(q) = \tfrac{1}{2}\langle \dot{q}, \dot{q}\rangle + \tfrac{1}{2}\langle \nabla q, \nabla q\rangle\,.$$

These energies are not directly related to the FPU Hamiltonian (unless $\alpha = \beta = 0$), but they have the advantage of being additive, that is, the sum of $E_h(q)$ over all $h \in \mathbb{Z}/(2P\mathbb{Z})$ is equal to $E(q)$.

Theorem 1. *For $P = 32$ and $\omega = 0.1989$, the equation has a set of 11 real analytic solutions, $\{f_A, f_B, \ldots, f_K\}$, with the properties listed in the following table, where Φ_ω denotes the value of the functional, E is the harmonic energy of the given solution, and $\mathcal{E}_h = E_h/E$. The symbol ϵ stands for a real number of modulus less than 0.002, which may vary from one instance to the next.*

solution	E	$\mathcal{E}_1$	$\mathcal{E}_2$	$\mathcal{E}_{11}$	$\mathcal{E}_{14}$
f_A	$5.71\ldots$	$0.248\ldots$	$0.109\ldots$	$0.195\ldots$	$0.442\ldots$
f_B	$5.67\ldots$	$0.185\ldots$	$0.123\ldots$	$0.215\ldots$	$0.470\ldots$
f_C	$5.48\ldots$	ϵ	$0.243\ldots$	ϵ	$0.755\ldots$
f_D	$5.38\ldots$	ϵ	ϵ	$0.375\ldots$	$0.622\ldots$
f_E	$5.21\ldots$	$0.537\ldots$	ϵ	$0.458\ldots$	ϵ
f_F	$5.16\ldots$	ϵ	ϵ	ϵ	$0.999\ldots$
f_G	$5.02\ldots$	$0.814\ldots$	$0.137\ldots$	ϵ	ϵ
f_H	$4.97\ldots$	$0.974\ldots$	ϵ	ϵ	ϵ
f_I	$4.95\ldots$	$0.883\ldots$	ϵ	ϵ	$0.075\ldots$
f_J	$4.81\ldots$	ϵ	ϵ	$0.999\ldots$	ϵ
f_K	$3.65\ldots$	ϵ	$0.996\ldots$	ϵ	ϵ

Proof of the theorem

We rewrite equation (main) in the form $F(q) = q$, where

$$F(q) = \omega^{-2}\partial^{-2}\nabla^{*}\left(\nabla q + (\nabla q)^{3}\right) \ ,$$

where ∂^{-1} denotes the antiderivative operator on the space of continuous 2π-periodic functions with average zero and we look for fixed points of F in the space of functions $q : \mathbb{R} \longrightarrow \mathbb{R}^{P}$ which extend analytically to a strip

$$\mathcal{D}_{\rho} = \{t \in \mathbb{C} : |\mathrm{Im}(t)| < \rho\} \ .$$

To be more precise, given $\rho > 0$, denote by $\mathcal{F}_\rho$ the vector space of all 2π-periodic analytic functions $f : \mathcal{D}_\rho \to \mathbb{C}$,

$$f(t) = \sum_{k=1}^{\infty} f_k \sin(kt) + \sum_{k=0}^{\infty} f'_k \cos(kt)\,, \qquad t \in \mathcal{D}_\rho\,,$$

which take real values for real arguments and for which the norm

$$\|f\|_\rho = \sum_{k=1}^{\infty} e^{\rho k} |f_k| + \sum_{k=0}^{\infty} e^{\rho k} |f'_k|$$

is finite. When equipped with this norm, $\mathcal{F}_\rho$ is a Banach space.

On the direct sum $\mathcal{F}_\rho^P$, we define the norm

$$\|q\|_\rho = \max_{1 \le i \le P} \|q_i\|\,.$$

We note that $\mathcal{F}_\rho$ is a Banach algebra, that is, $\|fg\|_\rho \le \|f\|_\rho \|g\|_\rho$, for all f and g in $\mathcal{F}_\rho$. Furthermore, ∂^{-2} acts as a compact linear operator on $\mathcal{A}_\rho$, as well as on $\mathcal{A}_\rho^P$. This shows that the equation above defines a differentiable map F on $\mathcal{A}_\rho^P$ with compact derivatives $DF(q)$. Thus, F can be well approximated locally by its restriction to a suitable finite dimensional subspace of $\mathcal{A}_\rho$. This property makes it ideal for a computer-assisted analysis.

Our goal is to find fixed points for F by using a Newton like iteration, starting with a numerical approximation q_0 for the desired fixed point. The Newton map $\mathcal{N}$ associated with F is given by

$$\mathcal{N}(q) = F(q) - \mathcal{M}(q)[F(q) - q] \, ,$$

with

$$\mathcal{M}(q) = [DF(q) - \mathbb{I}]^{-1} + \mathbb{I} \, .$$

If the spectrum of $DF(q)$ is bounded away from 1, and q_0 is sufficiently close to a fixed point of F, then $\mathcal{N}$ is a contraction in some neighborhood of q_0 .

Due to the compactness of $DF(q)$, this contraction property is preserved if we replace $\mathcal{M}(q)$ by a fixed linear operator M close to $\mathcal{M}(q_0)$. This leads us to consider the new map $\mathcal{C}$, defined by

$$\mathcal{C}(q) = F(q) - M[F(q) - q]\,, \qquad q \in \mathcal{A}_\rho^P\,.$$

M will be chosen to be a "matrix", in the sense that $M = \mathbb{P}_\ell M \mathbb{P}_\ell$ for some $\ell > 0$, where $\mathbb{P}_\ell$ denotes the canonical projection in $\mathcal{A}_\rho^P$ onto Fourier polynomials of degree $k \leq \ell$. We also verify that $M - \mathbb{I}$ is invertible, so that $\mathcal{C}$ and F have the same set of fixed points. In order to prove that $\mathcal{C}$ is a contraction on some ball $B(q_0, r)$ in $\mathcal{A}_\rho^P$ of radius $r > 0$, centered at q_0, it suffices to verify the inequalities

$$\|\mathcal{C}(q_0) - q_0\|_\rho < \varepsilon\,, \qquad \|D\mathcal{C}(q)\| < K\,, \qquad \varepsilon + Kr < r\,,$$

for some real numbers $r, \varepsilon, K > 0$, and for arbitrary q in the ball $B(q_0, r)$. These bounds imply that $\mathcal{C}$, and thus F, has a unique fixed point in $B(q_0, r)$.

Theorem 2. *In each of the 11 cases described in Theorem 1, there exists a Fourier polynomial q_0 , and real numbers $\rho, \varepsilon, r, K > 0$, such that the inequalities above hold. Furthermore, the numerical bounds given in these theorems are satisfied for all function in the corresponding ball $B(q_0, r)$.*

The proof of this theorem is based on a discretization of the problem, carried out and controlled with the aid of a computer.

At the trivial level of real numbers, the discretization is implemented by using interval arithmetics. In particular, a number $s \in \mathbb{R}$ is "represented" by an interval $S = [S^-, S^+]$ containing s, whose endpoints belong to some finite set of real numbers that are representable on the computer. Such an interval will be called a "standard sets" for $\mathbb{R}$.

The goal now is to combine these elementary bounds to obtain e.g. a bound G_1 on the norm function on $\mathcal{A}_\rho^P$, and a bound G_2 on the map $\mathcal{C}$. Then, in order to prove the first inequality, it suffices to verify that $G_1(G_2(S)) \subset U$, where S is a set in $\mathrm{std}(\mathcal{A}_\rho^P)$ containing g_0 , and U is an interval in $\mathrm{std}(\mathbb{R})$ with $U^+ < \varepsilon$.

We define the standard sets for $\mathcal{A}_\rho$. Let $n \geq \ell$ be a fixed integer. Given $U = (U_1, \ldots, U_n)$ in $\mathrm{std}(\mathbb{R}^n)$, and $V = (V_0, \ldots, V_{2n})$ in $\mathrm{std}(\mathbb{R}_+^{2n+1})$, denote by $S(U, V)$ the set of all functions f that can be represented as

$$f(t) = \sum_{k=1}^{n} u_k \sin(kt) + \sum_{m=0}^{2n} v_m(t)\,, \qquad v_m(t) = \sum_{k=m}^{\infty} v_{m,k} \sin(kt)\,,$$

with $u_k \in U_k$, and $v_m \in \mathcal{A}_\rho$ with $\|v_m\|_\rho \in V_m$, for all k and m. We now define $\mathrm{std}(\mathcal{A}_\rho)$ to be the collection of all such sets $S(U, V)$, subject to the condition that $V_m^- = 0$ for all m.

It is now straightforward to implement a bound on the norm function on $\mathcal{A}_\rho^P$, or the operator ∂^{-2}, or the sum of two functions in $\mathcal{A}_\rho^P$. In order to obtain a bound on the product of two functions in $\mathcal{A}_\rho$, we simply multiply the representations of the two factors term by term, and write the result again as an explicit Fourier polynomial of order n, plus a sum of "error terms" of orders greater than m, for $m = 0, 1, \ldots, 2n$.

The guiding principle here is to keep as much information as possible about the order of each term in the product, since the operator ∂^{-2}, which is applied last in the definition of F, contracts higher order terms more than lower order ones. This principle also motivated our choice of standard sets for $\mathcal{A}_\rho$.

For a bound on the linear operator M, we can compute explicitly its restriction to standard sets whose components $S(U_i, V_i)$ have $V_{i,m} = [0,0]$ whenever $m \leq \ell$. The remaining terms are estimated by using that $\|Mq\|_\rho \leq \|M\| \|q\|_\rho$. The operator norm $\|L\|$ of a continuous linear operator L on $\mathcal{A}_\rho^P$ is given by the following formula. Denote by $h^{j,m}$ the function $(i,k) \mapsto \delta_{ij} e^{-k\rho} \sin(kt)$. Then

$$\|L\| = \max_{1 \leq i \leq P} \sum_{j=1}^{P} \sup_{m \geq 1} \left\| \left(L h^{j,m} \right)_i \right\|_\rho \ .$$

In the case where L is the “matrix” M, the right hand side of this equation is trivial to estimate. The bounds discussed so far can be combined to yield a bound on the the map $\mathcal{C}$, suitable for proving the first and the last inequality.

In order to prove the second inequality

$$\|D\mathcal{C}(q)\| < K\ ,$$

we also need a bound on the map $q \mapsto \|D(q)\|$. Its domain only needs to include balls $B(\rho_0, r)$ with positive representable radii, and these balls are in fact standard sets of $\mathcal{A}_\rho^P$. The technique used for this estimate is similar, up to some technical details.