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Global Behaviour of Nonlinear Lattices

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Anton Zand BSc

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Univ.-Prof. Dipl.-Ing. Dr. Gerald Teschl

Abriss

Nichtlineare Gitter verbinden die Physik, wo sie in einer Vielzahl von Bereichen wie der Optik, Akustik und Mechanik auftreten, mit der Mathematik, wo ihre Untersuchung eine Anwendung der reichhaltigen Theorie gewöhnlicher Differentialgleichungen auf Banachräumen darstellt.

Nach dem Aufbau des analytischen Rahmens untersucht diese Arbeit das globale Verhalten unendlicher nichtlinearer Gitter. Insbesondere werden neue Resultate bewiesen, die unter bestimmten energiebasierten Bedingungen Blow-up Verhalten für das FPUT- α - und das nichtlineare Klein-Gordon-Gitter sichern. Hierfür wird ein an Levine-Glassey angelehntes Konkavitätsargument aus der Theorie der partiellen Differentialgleichungen adaptiert. Darüber hinaus wird globale Existenz für das FPUT- α -Modell bei kleinen Anfangsdaten mithilfe eines regionsbasierten Ansatzes bewiesen.

Abstract

Nonlinear lattices connect physics, where they appear in a variety of fields such as optics, acoustics and mechanics, and mathematics, where their study represents an application of the rich theory of ordinary differential equations on Banach spaces.

After establishing the analytical framework, this thesis investigates the global behaviour of infinite nonlinear lattices. In particular, we present new results proving blow-up for the FPUT- α and the nonlinear Klein-Gordon lattices under certain energy-based conditions, using a Levine-Glassey-type concavity argument from the theory of partial differential equations. Moreover, we show global existence for the FPUT- α model with small initial data via a region-based approach.

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1 Ordinary Differential Equations on Banach Spaces

In this section, we lay the analytic groundwork for our later investigations. After fixing notation, we study contractions to prove the implicit function theorem, which is in turn used to establish local uniqueness of solutions for differential equations on Banach spaces. We will follow [14] for this chapter. Other textbooks on the subject include [17].

1.1 Notation and Facts from Functional Analysis

Recall that a normed space is a vector space X equipped with a norm $\|\cdot\|_X$. If every Cauchy sequence in X has a limit, we say X is complete and call it a Banach space. For the norm, we will often write simply $|\cdot|$.

Let X, Y be Banach spaces and $U \subseteq X$ open. We denote the space of continuous operators $F : U \rightarrow Y$ by $C(U, Y)$ and the space of bounded linear operators from X to Y by $\mathcal{L}(X, Y)$. Equipped with the norm

$$\|F\|_\infty := \sup_{|e|=1} |Fe|,$$

$\mathcal{L}(X, Y)$ is a Banach space. Note that in the setting of normed spaces, an operator being bounded is equivalent to it being continuous. Since operators in $\mathcal{L}(X, Y)$ are also linear, we have $\mathcal{L}(X, Y) \subseteq C(X, Y)$.

Suppose there exists an operator $dF(x) \in \mathcal{L}(X, Y)$ such that

$$\lim_{u \rightarrow 0} \frac{|F(x+u) - F(x) - dF(x)u|}{|u|} = 0,$$

then we call F differentiable at x and $dF(x)$ the (unique) derivative of F at x . If F is differentiable at all x , we say F is differentiable and if in addition $dF : U \rightarrow \mathcal{L}(X, Y)$ is continuous we call F continuously differentiable and write $F \in C^1(U, Y)$.

In the case where $X = X_1 \times \cdots \times X_n$, we denote by $\partial_{x_i} F(x) \in \mathcal{L}(X_i, Y)$ the partial derivative of F with respect to X_i , defined as the derivative of F with all variables fixed except x_i . Then,

$$\sum_{1 \leq i \leq n} \partial_{x_i} F(x) u_i = dF(x)u, \quad u = (u_1, \dots, u_n) \in X.$$

An isomorphism between X and Y is a bijection F such that both F and also F^{-1} are continuous. If in addition both F and its inverse are differentiable, we call F a diffeomorphism.

Theorem 1.1 (Mean Value Theorem). *We discuss three versions of the mean value theorem for later use:*

(i) *Let X be a Banach space, $I \subseteq \mathbb{R}$ an interval and $f \in C^1(I, X)$. Then, for $s \leq t \in I$, we have*

$$\|f(t) - f(s)\| \leq M_1 |t - s| \quad M_1 := \sup_{\xi \in [s, t]} \|f'(\xi)\|. \quad (1.1)$$

Moreover, in the setting of real numbers, for $f \in C^1([a, b], \mathbb{R})$, there exists $\xi \in (a, b)$ with

$$f'(\xi)(b - a) = (f(b) - f(a)).$$

(ii) *Let X, Y be Banach spaces, $U \subseteq X$ open and convex, and consider a map $F \in C^1(U, Y)$. Then*

$$\|F(x_1) - F(x_2)\| \leq M_2 \|x_1 - x_2\| \quad (1.2)$$

holds for all $x_{1,2} \in U$ with

$$M_2 := \sup_{t \in [0, 1]} \|dF((1-t)x_1 + tx_2) \frac{x_1 - x_2}{\|x_1 - x_2\|}\|.$$

(iii) *Let X, Y be Banach spaces, $U \subseteq X$ open, and consider a map $F \in C^1(U, Y)$. If there exists a constant $M_3 > 0$ such that*

$$\|F(x_1) - F(x_2)\| \leq M_3 \|x_1 - x_2\|$$

for all $x_{1,2} \in U$, then

$$\sup_{x \in U, |e|=1} \|dF(x)e\| \leq M_3.$$

In particular, this holds for any partial derivative.

Proof. (i) We assume to the contrary that the claim only holds on $[s, \xi]$ with $\xi < t$. For any fixed $N > M_1$, define

$$\Delta(x) = \|f(x) - f(s)\| - N(x - s), \quad x \in [s, \xi].$$

By assumption, $\Delta(x) \leq 0$ on $[s, \xi]$, but there exists a sequence $\varepsilon_n \rightarrow 0$ with $\varepsilon_n > 0$ for all n such that

$$\begin{aligned} 0 &< \Delta(\xi + \varepsilon_n) = \|f(\xi + \varepsilon_n) - f(s)\| - N(\xi + \varepsilon_n - s) \\ &\leq \|f(\xi + \varepsilon_n) - f(\xi)\| - N\varepsilon_n + \|f(\xi) - f(s)\| - N(\xi - s) \\ &\leq \|f'(\xi)\varepsilon_n + o(\varepsilon_n)\| - N\varepsilon_n + \Delta(\xi) \leq (M_1 - N + o(1))\varepsilon_n < 0, \end{aligned}$$

which is a contradiction if we take $n \rightarrow \infty$. Therefore, $\xi = t$. The last claim is a generalization of and can be proven by Rolle's theorem.

(ii) Consider the function $f(t) = F((1-t)x_1 + tx_2)$ with $t \in [0, 1]$. Then $df(t) = dF((1-t)x_1 - tx_2)(x_2 - x_1)$ shows $\|df(t)\| \leq M_2\|x_1 - x_2\|$ by the definition of M_2 . Applying (i) to $f(t)$ yields the constant M_1 as defined in (1.1), now satisfying also $M_1 \leq M_2\|x_1 - x_2\|$. Thus we arrive at

$$\|F(x_1) - F(x_2)\| = \|f(0) - f(1)\| \leq M_1|0 - 1| \leq M_2\|x_2 - x_1\|.$$

(iii) Assume to the contrary there exist $e \in X$ and $\alpha > 0$ satisfying $\|e\| = 1$, $\|dF(x)e\| = M_3 + \alpha$ and choose $\varepsilon > 0$ small enough such that $\alpha\varepsilon - |o(\varepsilon)| > 0$. Then

$$\begin{aligned} M_3\varepsilon &= M_3|x + e\varepsilon - x| \geq |F(x + e\varepsilon) - F(x)| \\ &= |dF(x)e\varepsilon + o(\varepsilon)| \geq (M_3 + \alpha)\varepsilon - |o(\varepsilon)| > M_3\varepsilon, \end{aligned}$$

a contradiction. □

Note that in (ii) and (iii), one could only require F to be Gâteaux differentiable in U .

The following theorem will be the central argument for proving blow-up behaviour in the next chapter.

Lemma 1.2 (Concavity Argument). *Consider a function $f \in C^2(\mathbb{R}, \mathbb{R})$ satisfying $f(0) > 0$ and $f''(x) < 0$ for all x . Then either*

(i). *There exist x_1 such that $f'(x_1) < 0$ and further $f(x_0) = 0$ for some $x_0 > 0$,*
or

(ii). *$f'(x) \geq 0$ for all x and there exists a constant $c \in \mathbb{R} \cup \{\infty\}$ such that $\lim_{x \rightarrow \infty} f(x) = c$.*

If at least one of the additional conditions

$$a) f'(0) \leq 0 \quad \text{or} \quad b) f''(x) \leq \delta < 0 \quad \text{for some } \delta < 0 \tag{1.3}$$

holds, case (i) is guaranteed.

Proof. Observe first that $f'(x)$ is a strictly monotonically decreasing function due to $f''(x) < 0$, consequently, either there exist x_1 such that $f'(x_1) < 0$, or $f'(x) \geq 0$ for all x . Suppose the first case is true. By the mean value theorem 1.1, for $x > x_1$, there exists $\tilde{x} \in (x_1, x)$ with

$$f(x) - f(x_1) = f'(\tilde{x})(x - x_1).$$

Since f' is decreasing, $f'(\tilde{x}) < f'(x_1)$ and thus

$$f(x) < f(x_1) + f'(x_1)(x - x_1).$$

Now taking the limit $x \rightarrow \infty$ yields

$$\lim_{x \rightarrow \infty} f(x) < \lim_{x \rightarrow \infty} f(x_1) + f'(x_1)(x - x_1) = -\infty.$$

We infer that the function must eventually turn negative and again by the mean value theorem 1.1, there exists $x_0 \in (0, \infty)$ with $f(x_0) = 0$. In the other case, $f'(x) \geq 0$ everywhere, $f(x)$ is monotonically increasing, and therefore must converge to a limit $c \in \mathbb{R} \cup \infty$.

Now we show that either of the conditions in (1.3) leads to case (i). If $f'(0) \leq 0$, by continuity and $f''(x) < 0$, we must have $f'(x) < 0$ for all $x \in (0, \infty)$. Suppose $f''(x) \leq \delta < 0$. Then integration shows

$$f'(x) = f'(0) + \int_0^x f''(x) \leq f'(0) + \int_0^x \delta = f'(0) + \delta x,$$

and the choice $x_1 > -\frac{f'(0)}{\delta}$ confirms $f'(x_1) < 0$. □

Example 1.3. Consider the functions with derivatives

$$\begin{aligned} f(x) &:= 1 - e^{-x}, & f'(x) &= e^{-x}, & f''(x) &= -e^{-x}; \\ g(x) &:= x - e^{-x}, & g'(x) &= 1 + e^{-x}, & g''(x) &= -e^{-x}. \end{aligned}$$

Clearly, $f'' < 0$. However we see $f'(x) > 0$ for all x , and $\lim_{x \rightarrow \infty} f(x) = 1$ while f never reaches zero. Moreover, $\lim_{x \rightarrow \infty} g(x) = \infty$. Hence without additional conditions, $f(x_0) = 0$ is not guaranteed.

Lastly, we discuss discrete spaces. Let ℓ be the space of real-valued sequences $\{x_n\}_{n \in \mathbb{Z}}$. We will identify $\{x_n\}_{n \in \mathbb{Z}}$ with x . Equipped with the norm

$$\|x\|_p = \left(\sum_{n \in \mathbb{Z}} |x_n|^p \right)^{\frac{1}{p}}, \quad 1 \leq p < \infty, \quad \|x\|_\infty = \sup_{n \in \mathbb{Z}} |x_n|,$$

the space

$$\ell^p := \{x \in \ell \mid \|x\|_p < \infty\}, \quad 1 \leq p \leq \infty$$

becomes a Banach space. Of particular interest is the Hilbert space ℓ^2 with scalar product

$$\langle x, y \rangle = \sum_{n \in \mathbb{Z}} x_n y_n.$$

We prove the Cauchy-Schwarz inequality and summation by parts, two useful tools for later calculations.

Theorem 1.4 (Cauchy-Schwarz Inequality). *Let a_n, b_n be sequences. Then it holds that*

$$\left(\sum_{n \in \mathbb{Z}} a_n b_n \right)^2 \leq \left(\sum_{n \in \mathbb{Z}} a_n^2 \right) \left(\sum_{n \in \mathbb{Z}} b_n^2 \right). \quad (1.4)$$

Proof. We have

$$0 \leq \frac{1}{2} \sum_{n, m \in \mathbb{Z}} (a_n b_m - a_m b_n)^2 = \left(\sum_{n \in \mathbb{Z}} a_n^2 \right) \left(\sum_{n \in \mathbb{Z}} b_n^2 \right) - \left(\sum_{n \in \mathbb{Z}} a_n b_n \right)^2.$$

□

Theorem 1.5 (Summation by Parts). *Let a_n, b_n be sequences with*

$$\lim_{n \rightarrow \pm\infty} a_n = \lim_{n \rightarrow \pm\infty} b_n = 0.$$

Similarly to integration by parts in the continuous case, we have

$$\sum_{n \in \mathbb{Z}} (a_{n+1} - a_n) b_n = - \sum_{n \in \mathbb{Z}} a_{n+1} (b_{n+1} - b_n). \quad (1.5)$$

Proof. Observe

$$\begin{aligned} \sum_{n \in \mathbb{Z}} (a_{n+1} - a_n) b_n &= \sum_{n \in \mathbb{Z}} a_{n+1} b_n - \sum_{n \in \mathbb{Z}} a_n b_n \\ &= \sum_{n \in \mathbb{Z}} a_{n+1} b_n - \sum_{n \in \mathbb{Z}} a_{n+1} b_{n+1} = - \sum_{n \in \mathbb{Z}} a_{n+1} (b_{n+1} - b_n). \end{aligned}$$

□

1.2 Contractions and the Implicit Function Theorem

Let us define contractions, a powerful tool used to prove the implicit function theorem.

Definition 1.6. Let X be a Banach space with subset $A \subseteq X$ and consider map $F : X \rightarrow A$. A point $x \in A$ with $F(x) = x$ is called a fixed point (of F). If F possesses a so-called contraction constant $\theta \in [0, 1)$ such that, for any $x_1, x_2 \in A$,

$$|F(x_1) - F(x_2)| \leq \theta |x_1 - x_2|$$

holds, F is called a contraction. Clearly, any contraction is Lipschitz continuous with constant θ .

Applying a contraction iteratively to any starting point will lead to the unique fixed point of that contraction.

Theorem 1.7 (Contraction Principle). *Let A be a nonempty closed subset of a Banach space X . Each contraction $F : A \rightarrow A$ possesses a unique fixed point $\tilde{x} \in A$ such that for all $x \in A$*

$$|F^m(x) - \tilde{x}| \leq \frac{\theta^m}{1 - \theta} |F(x) - x|. \quad (1.6)$$

Proof. To show existence, we start with some point $x_0 \in A$ and iterate it via $x_n = F^n(x_0)$. Using the triangle inequality, the contraction property

$$|x_{n+1} - x_n| = |F(x_n) - F(x_{n-1})| \leq \theta |x_n - x_{n-1}| \leq \cdots \leq \theta^n |x_1 - x_0|,$$

and the formula for converging geometric series ($\theta < 1$) respectively, we get the estimate

$$\begin{aligned} |x_n - x_m| &\leq \sum_{i=m+1}^n |x_i - x_{i-1}| \leq \sum_{i=m+1}^n \theta^{i-1} |x_1 - x_0| = \theta^m \sum_{i=0}^{n-m-1} \theta^i |x_1 - x_0| \\ &\leq \theta^m \frac{1 - \theta^{n-m}}{1 - \theta} |x_1 - x_0| \leq \frac{\theta^m}{1 - \theta} |x_1 - x_0| \end{aligned} \quad (1.7)$$

for $n > m$. Now letting $m, n \rightarrow \infty$ shows that x_n is Cauchy, thus closedness of A yields a limit $\tilde{x}$. Indeed, $\tilde{x}$ is a fixed point since

$$|F(\tilde{x}) - \tilde{x}| \leq \lim_{n \rightarrow \infty} |x_{n+1} - x_n| = 0.$$

For uniqueness, assume that there are two such fixed points $x = F(x)$ and $y = F(y)$. Then $\theta < 1$ and

$$|x - y| = |F(x) - F(y)| \leq \theta |x - y|$$

shows $|x - y| = 0$. Finally, to see formula (1.6), we simply let $n \rightarrow \infty$ in equation (1.7). $\square$

The next example shows that setting $\theta < 1$ is required and we can not simply demand $|F(x_1) - F(x_2)| < |x_1 - x_2|$.

Example 1.8. Consider $F(x) = x + \frac{1}{x}$ with $X = [1, \infty)$. Then

$$|F(x) - F(y)| = |x - y + \frac{1}{x} - \frac{1}{y}| < |x - y|$$

holds true since $x > y$ implies $\frac{1}{x} < \frac{1}{y}$. However, $F(x)$ does not possess a fixed point, as applying F iteratively will always push x towards $\pm\infty$. In the proof of

existence above, the requirement $|F(x_1) - F(x_2)| < |x_1 - x_2|$ would not allow us to use the geometric series formula, while the proof of uniqueness still works in this setting. Demanding even less, $|F(x_1) - F(x_2)| \leq |x_1 - x_2|$, we also lose uniqueness. The Identity on $\mathbb{R}$ fulfills this criteria but has infinitely many fixed points.

Example 1.9. The contraction principle can be applied to prove Newton's method for finding zeroes of a function $f \in C^2(\mathbb{R}, \mathbb{R})$. The iteration function is given by

$$F(x) = x - \frac{f(x)}{f'(x)}.$$

Assume there exists a point x_0 with $f(x_0) = 0$ and $f'(x) \neq 0$. Any such zero is clearly a fixed point of F and it remains to show that $F^n(x)$ indeed converges to x_0 on some subset of $\mathbb{R}$. Differentiating F ,

$$F'(x) = 1 - \frac{(f'(x))^2 - f(x)f''(x)}{(f'(x))^2} = 1 - 1 + \frac{f(x)f''(x)}{(f'(x))^2},$$

shows $F'(x_0) = 0$. By continuity, there exists a closed interval I containing x_0 such that for all $x \in I$, both $F'(x) \leq \theta < 1$ and $f'(x) \neq 0$ holds true. For $x, y \in I$, we have

$$|F(x) - F(y)| = F'(\xi)|x - y| \leq \theta|x - y|$$

due to the mean value theorem on $\mathbb{R}$, proving that F is a contraction on I .

Definition 1.10. Consider a contraction F that also depends on an additional parameter. If the contraction constant is independent of that parameter, we call F a uniform contraction. More precisely, let X, Y be Banach spaces with open subsets U, V respectively and $F : \overline{U} \times V \rightarrow U$. For all $y \in V$, we demand

$$|F(x_1, y) - F(x_2, y)| \leq \theta|x_1 - x_2|, \quad x_{1,2} \in \overline{U}.$$

For any $y \in V$, $F(\cdot, y)$ has a unique fixed point, which we denote by $\bar{x}(y)$.

The continuity and differentiability properties of a uniform contraction $F(x, y)$ are passed on to $\bar{x}(y)$.

Theorem 1.11 (Uniform Contraction Principle). *Let X, Y, U, V and F be as in the preceding definition and $r \geq 0$. If $F \in C^r(U \times V, U)$, then $\bar{x}(\cdot) \in C^r(V, U)$. Lipschitz continuity is inherited analogously.*

Proof. We prove continuity, $r = 0$, directly by inserting the definition of $\bar{x}$ and using the contraction properties of F . The calculation

$$\begin{aligned} |\bar{x}(y + \delta) - \bar{x}(y)| &= |F(\bar{x}(y + \delta) - F(\bar{x}(y), y)| \\ &= |F(\bar{x}(y + \delta) - F(\bar{x}(y), y + \delta) + F(\bar{x}(y), y + \delta) - F(\bar{x}(y), y)| \\ &\leq \theta |\bar{x}(y + \delta) - \bar{x}(y)| + |F(\bar{x}(y), y + \delta) - F(\bar{x}(y), y)| \end{aligned}$$

shows

$$|\bar{x}(y + \delta) - \bar{x}(y)| \leq \frac{1}{1 - \theta} |F(\bar{x}(y), y + \delta) - F(\bar{x}(y), y)|. \quad (1.8)$$

Since F is continuous, the righthand side of this equation will go to zero as $\delta \rightarrow 0$, which proves continuity also for $\bar{x}$. Similarly, if F is Lipschitz with constant M , $|F(\bar{x}(y), y + \delta) - F(\bar{x}(y), y)| \leq M|\delta|$, we have

$$|\bar{x}(y + \delta) - \bar{x}(y)| \leq \frac{M}{1 - \theta} |\delta|.$$

Now we look at the case $r = 1$. Formally taking the derivative of $\bar{x}(y) = F(\bar{x}(y), y)$ with respect to y yields the fixed point equation

$$\bar{x}'(y) = \partial_x F(\bar{x}(y), y) \bar{x}'(y) + \partial_y F(\bar{x}(y), y), \quad (1.9)$$

which the derivative of $\bar{x}(y)$ must satisfy. We reformulate this equation in terms of the map $T_y : \mathcal{L}(Y, X) \rightarrow \mathcal{L}(Y, X)$ with $T_y(u(y)) = \partial_x F(\bar{x}(y), y)u(y) + \partial_y F(\bar{x}(y), y)$ and claim that T_y is a uniform contraction. Indeed,

$$\begin{aligned} |T_y(u(y)) - T_y(v(y))| &= |\partial_x F(\bar{x}(y), y)u(y) - \partial_x F(\bar{x}(y), y)v(y)| \\ &= |\partial_x F(\bar{x}(y), y)| \cdot |u(y) - v(y)| \leq \theta |u(y) - v(y)|, \end{aligned}$$

where we have used the mean value theorem 1.1 in the last step. Together with the case $r = 0$, this proves existence of a unique continuous fixed point $\bar{x}'(y)$. We now show that $\bar{x}(y + \delta) - \bar{x}(y) - \bar{x}'(y)\delta \rightarrow 0$ as $\delta \rightarrow 0$. Abbreviating $\Delta\bar{x} = \bar{x}(y + \delta) - \bar{x}(y)$, we have

$$\Delta\bar{x} - \bar{x}'(y)\delta = F(\bar{x}(y + \delta), y + \delta) - F(\bar{x}(y), y) - \bar{x}'(y)\delta,$$

and multiplying by $1 - \partial_x F(\bar{x}(y), y)$ on both sides together with (1.9), the fact that $F \in C^1(U \times V, U)$, and $o(\Delta\bar{x}) = O(\delta)$ due to (1.8), leads to

$$\begin{aligned} (1 - \partial_x F(\bar{x}(y), y))(\Delta\bar{x} - \bar{x}'(y)\delta) &= \\ F(\bar{x}(y + \delta), y + \delta) - F(\bar{x}(y), y) - \partial_x F(\bar{x}(y), y)\Delta\bar{x} - \partial_y F(\bar{x}(y), y)\delta \\ &= o(\delta) + o(\Delta\bar{x}) = o(\delta). \end{aligned}$$

Finally, taking norms and observing $\|(1 - \partial_x F(\bar{x}(y), y))^{-1}\| \leq \frac{1}{1-\theta}$ due to Theorem 1.1 proves the claim.

For the case $r > 1$, we use induction. Suppose the statement is true for $r - 1$ and $F \in C^r(U \times V, U)$. By assumption, $\bar{x}(y) \in C^{r-1}(V, U)$ and from (1.9) and the reasoning thereafter we immediately conclude $\bar{x}(y) \in C^r(V, U)$. $\square$

Theorem 1.12 (Implicit Function Theorem). *Let X, Y, Z be Banach spaces with open subsets $U \subseteq X, V \subseteq Y$ and fix $(x_0, y_0) \in U \times V$. If a map F satisfies the conditions*

(i). $F \in C^r(U \times V, Z), r \geq 1$

(ii). $\partial_x F(x_0, y_0) \in \mathcal{L}(X, Z)$ is an isomorphism,

then there exists an open neighbourhood of (x_0, y_0) , $U_1 \times V_1 \subseteq U \times V$ such that we can define a function $g \in C^r(Y, X)$ with $F(g(y), y) = F(x_0, y_0)$ for all $y \in V_1$. The differential of g is given by

$$dg(y) = -(\partial_x F(g(y), y))^{-1} \circ \partial_y F(g(y), y). \quad (1.10)$$

Proof. Considering $\tilde{F} = F - F(x_0, y_0)$ instead of F , we can assume that $F(x_0, y_0) = 0$. Now define (cf. Example 1.9)

$$G(x, y) := x - \partial_x F(x_0, y_0)^{-1} F(x, y).$$

Clearly, $G \in C^r(U \times V, Z)$ and $\partial_x G(x_0, y_0) = 0$, hence we can find balls $U_1 = B_{r_1}(x_0)$ and $V_1 = B_{r_2}(y_0)$ around x_0, y_0 , such that $\|\partial_x G(x, y)\| \leq \theta < 1$ for all $(x, y) \in U_1 \times V_1$. Since U_1 is convex, we can apply Theorem 1.1 (ii) to $G(\cdot, y)$ with $M = \theta$, showing that $G(\cdot, y)$ is a uniform contraction for $y \in V_1$. To ensure $G : U_1 \times V_1 \rightarrow U_1$, choose r_2 small enough such that $|G(x_0, y) - G(x_0, y_0)| < (1 - \theta)r_1$. Then

$$\begin{aligned} |G(x, y) - x_0| &= |G(x, y) - G(x_0, y) + G(x_0, y) - G(x_0, y_0)| \\ &< \theta|x - x_0| + (1 - \theta)r_1 < r_1 \end{aligned}$$

shows G maps into U_1 only. The uniform contraction principle Theorem 1.11 now grants the function $g(y) \in C^r(Y, X)$ with the required properties.

Finally, to see (1.10), we differentiate $F(g(y), y) = 0$ using the chain rule, showing

$$d(F(g(y), y)) = \partial_x F(g(y), y)dg(y) + \partial_y F(g(y), y).$$

$\square$

Note that in the above proof, we are only concerned with the partial derivative $\partial_x F$ and do not necessarily require F to be continuously differentiable, hence the theorem could also be stated with the weaker conditions that F is continuous and $\partial_x F(x_0, y_0)$ exists.

As an immediate consequence of the implicit function theorem, we also get the inverse function theorem.

Theorem 1.13 (Inverse Function Theorem). *Let X, Y be Banach spaces with an open subset $U \subseteq X$ and fix $x_0 \in U$. Let $F \in C^r(U, Y)$, $r \geq 1$ and suppose that $dF(x_0)$ is an isomorphism. Then there is a neighbourhood $U_1 \times V_1 \subseteq U \times Y$ of $(x_0, F(x_0))$ where F is a diffeomorphism.*

Proof. The function $G(x, y) = y - F(x)$ is in $C^r(U \times Y, Y)$, $r \geq 1$, and $\partial_x G(x_0, y_0)$ is an isomorphism in $\mathcal{L}(X, Y)$ since the corresponding statements are true for F by assumption and the identity in Y , respectively. We set $y_0 = F(x_0)$ and therefore $G(x_0, y_0) = y_0 - F(x_0) = 0$. The conditions of Theorem 1.12 are met, and we obtain the function $g(y) \in C^r(V_1, U)$ with $G(g(y), y) = G(x_0, y_0)$ in some neighborhood $U_1 \times V_1$ of (x_0, y_0) . Now

$$0 = G(x_0, y_0) = G(g(y), y) = y - F(g(y))$$

shows $F(g(y)) = y$. We have thus found a differentiable inverse for F on $U_1 \times V_1$, showing that F is a diffeomorphism. $\square$

Moreover, the implicit and inverse function theorems are equivalent. For a proof of the inverse function theorem with the implicit function theorem as a corollary, see [1].

1.3 Solutions of the Cauchy Problem

We now turn to ordinary differential equations. We start with an auxiliary result.

Lemma 1.14 (Omega Lemma). *Let X, Y be Banach spaces with open subset $U \subseteq X$ and $I \subseteq \mathbb{R}$ a compact Interval. For $x \in C(I, U)$ and $f \in C^r(U, Y)$, define f_* by*

$$(f_*x)(t) := f(x(t)), \tag{1.11}$$

then $f_ \in C^r(C(I, U), C(I, Y))$.*

Proof. We start with the case $r = 0$. Let $x_0 \in C(I, U)$ and $\varepsilon > 0$ be fixed. For each $t \in I$, we may choose a radius $2\delta(t) > 0$ such that the ball remains in U , $B_{2\delta(t)}(x_0(t)) \subset U$, and $|f(x) - f(x_0(t))|$ for all $x \in \overline{B_{2\delta(t)}(x_0(t))}$. The set $\{x_0(t)\}_{t \in I}$ is covered by the balls $B_{2\delta(t)}(x_0(t))$, $t \in I$, and we can find a finite subcover $B_{2\delta(t_j)}(x_0(t_j))$ with $1 \leq j \leq N$ since I is compact. Define

$\delta := \min_{1 \leq j \leq N} \delta(t_j)$ and let $\|x - x_0\| \leq \delta$. For each $t \in I$, there exists a t_j with $|x_0(t) - x_0(t_j)| \leq \delta(t_j)$, which also shows $|x(t) - x_0(t_j)| \leq |x(t) - x_0(t)| + |x_0(t) - x_0(t_j)| \leq 2\delta(t_j)$. We arrive at

$$|f(x(t)) - f(x_0(t))| \leq |f(x(t)) - f(x_0(t_j))| + |f(x_0(t_j)) - f(x_0(t))| \leq \varepsilon.$$

For $r = 1$, we use Taylor's theorem. Recall that

$$f(x + u) = f(x) + df(x)u + R(u), \quad (1.12)$$

with the estimate for the error term

$$R(u) \leq |u| \sup_{0 \leq s \leq 1} \|df(x + su) - df(x)\|,$$

see [14], Theorems 9.13, 9.14. We claim $(df_*(x_0)x)(t) := df((x_0(t))x(t))$ and use (1.12) to see

$$\begin{aligned} |(f_*(x_0 + x))(t) - (f_*x_0)(t) - df(x_0(t))x(t)| \\ = |f(x_0(t) + x(t)) - f(x_0(t)) - df(x_0(t))x(t)| \\ \leq |x(t)| \sup_{0 \leq s \leq 1} \|df(x_0(t) + sx(t)) - df(x_0(t))\|. \end{aligned}$$

We already know that $(df)_*$ is continuous and hence for each ε , we can find δ such that $\|df(x_0(t) + sx(t)) - df(x_0(t))\| \leq \varepsilon$ for $|x_0(t) + sx(t) - x_0(t)| \leq |x(t)| \leq \delta$. This proves differentiability of f_* . To show continuity of df_* , we define the linear map

$$\begin{aligned} \lambda : C(I, \mathcal{L}(X, Y)) &\rightarrow \mathcal{L}(C(I, X), C(I, Y)), \\ T &\mapsto T_* \end{aligned}$$

with $(T_*x)(t) := T(t)x(t)$ and observe

$$\|T_*x\| = \sup_{t \in I} |T(t)x(t)| \leq \sup_{t \in I} \|T\| \cdot |x(t)| \leq \|T\| \cdot \|x\|.$$

We deduce $\|\lambda\| \leq 1$, implying λ is continuous, and $df_* = \lambda \circ (df)_*$ concludes the proof.

The case $r > 1$ follows from induction. $\square$

The following central theorem guarantees local existence and uniqueness of ordinary differential equations in Banach spaces.

Theorem 1.15 (Local Existence and Uniqueness). *Let I be an open interval in $\mathbb{R}$, U an open subset of a Banach space X and Λ an open subset of any*

other Banach space. Let further $F \in C^r(I \times U \times \Lambda, X)$ and $r \geq 1$. For any combination of $x_0 \in U, t_0 \in I$ and $\lambda \in \Lambda$, there are open subsets I_1, U_1, Λ_1 of I, U, Λ respectively, such that the initial value problem

$$\dot{x} = F(t, x, \lambda), \quad x(t_0) = x_0, \quad (t_0, x_0, \lambda) \in X \times U \times \Lambda \quad (1.13)$$

has a unique solution $x(t, t_0, x_0, \lambda) \in C^r(I_1 \times \tilde{I} \times U_1 \times \Lambda_1, U)$.

Proof. We ultimately want to invoke the implicit function theorem 1.12 to guarantee existence of solutions. To do so, we start by reformulating (1.13) into the appropriate form. Firstly, we can assume that F depends only on x . Indeed, introducing $\tau(t) = t$ and $\tilde{\lambda}(t) = \lambda$ and including them in the dependent variables yields the equivalent differential equation

$$\frac{d}{dt}(\tau, x, \tilde{\lambda}) = (1, F(\tau, x, \tilde{\lambda}), 0).$$

We write x instead of $(\tau, x, \tilde{\lambda})$. Secondly, translating t via $\tilde{t} = t - t_0$ lets us assume $t_0 = 0$.

Next, consider the scaling $y(\tau) = x(t)$ with $\varepsilon\tau = t$. We have $\frac{dt}{d\tau} = \varepsilon$ and hence

$$\frac{dy}{d\tau} = \frac{dx}{dt} \frac{dt}{d\tau} = \varepsilon F(y(\tau)).$$

With another shift, $x \rightarrow x_0 + x$, our equation turns into

$$\dot{x} = \varepsilon F(x_0 + x), \quad x \in D := \{f \in C^1([-1, 1], B_r(0)) | f(0) = 0\}, \quad (1.14)$$

where $\varepsilon \in \mathbb{R}$. This gives a relation between the case $\varepsilon = 0$, where we already know the solution, and the case $\varepsilon = 1$ which corresponds to our original problem 1.13. The implicit function theorem will guarantee solutions for ε small, and since we can rescale with $1/\varepsilon$ a solution for any $\varepsilon > 0$ will be enough to prove our theorem.

Solving this is equivalent to finding the zeroes of

$$\begin{aligned} G : D \times U_0 \times \mathbb{R} &\rightarrow C([-1, 1], X) \\ (x, x_0, \varepsilon) &\mapsto \dot{x} - \varepsilon F(x_0 + x), \end{aligned}$$

where U_0 is a neighbourhood of x_0 . In the above formulation, r needs to be small enough to ensure $U_0 + B_r(0) \subseteq U$. By the omega lemma 1.14, inserting x_0, x into F is a continuous process, making G a C^1 function. Now we fix x_0 , and define T via $(Tx)(t) = \dot{x}(t)$ with inverse $(T^{-1}x)(t) = \int_0^t x(s)ds$. Now $G(0, x_0, 0) = 0$ and $\partial_x G(0, x_0, 0) = T$, so we can apply the implicit function theorem 1.12 to find a unique solution $x(x_0, \varepsilon) \in C^1(U_1 \times (-a, a), D^1) \hookrightarrow C^1([-1, 1] \times U_1 \times (-a, a), X)$

where $a > 0$. Thus we have found the desired solution $\phi \in C^1((-\varepsilon, \varepsilon) \times U_1, X)$, given by $\phi(t, x_0) = x_0 + x(x_0, \varepsilon)(t/\varepsilon)$.

We handle $r > 0$ with induction. For $F \in C^{r+1}$, suppose $x(t, x_0)$ is a solution and C^r . We show that both partial derivatives are C^r to conclude $x(t, x_0) \in C^{r+1}$. Firstly, $\partial_t x(t, x_0) = F(x(t, x_0)) \in C^{r+1}$ is immediate. Secondly, we define $y := \partial_{x_0} x$ and calculate with Schwarz's theorem

$$\begin{aligned} \partial_t y &= \frac{\partial}{\partial t} \frac{\partial x}{\partial x_0} = \frac{\partial}{\partial x_0} \frac{\partial x}{\partial t} = \frac{\partial}{\partial x_0} F(x(x_0, t)) \\ &= \partial_x F(x(x_0, t)) \frac{\partial x}{\partial x_0}(t, x_0) = \partial_x F(x(x_0, t)) y(t, x_0), \end{aligned}$$

and we have $y \in C^r$. □

Due to the next theorem, we may also assume maximality of solutions. By joining coinciding local solutions together, we get a unique solution defined on a maximal interval of existence.

Theorem 1.16. *Consider again the Cauchy problem (1.13). Any local solution ϕ_0 defined on the interval I_0 can be extended uniquely to a maximal solution ϕ defined on $I \supseteq I_0$.*

Proof. We note that for each pair of solutions ϕ_1, ϕ_2 that coincide at some time but are defined on different intervals I_1, I_2 , the maximal interval (t_-, t_+) where these solutions coincide is equal to $I_1 \cap I_2 = (T_-, T_+)$. Otherwise, if $t_+ < T_+$, ϕ_1 and ϕ_2 would coincide at time t_+ by continuity. The Cauchy problem (1.13) with initial condition $x(t_+) = \phi_1(t_+) = \phi_2(t_+)$ together with local uniqueness yields an open interval around t_+ where ϕ_1, ϕ_2 also agree, contradicting maximality of t_+ . Therefore $t_+ = T_+$ and analogously $t_- = T_-$. We then gain the well defined solution

$$\phi(t) = \begin{cases} \phi_1 & t \in I_1, \\ \phi_2 & t \in I_2 \end{cases}$$

on $I_1 \cup I_2$. □

In general, solutions may cease to be defined within finite time, $T_+ < \infty$, which we refer to as blow up. Solutions that are defined for all $t \in \mathbb{R}$ are called global solutions.

Example 1.17. In the simple case $X = \mathbb{R}$, consider $\dot{x} = x$, $x(0) = x_0$. Dividing the equation by x , separating the variables and integrating gives the explicit solution $x = x_0 e^t$, which is defined for all t .

Example 1.18. In the same setting and by the same calculation, $\dot{x} = x^2$, $x(0) = x_0$ yields the solution $x(t) = \frac{x_0}{1 - tx_0}$. For $x_0 > 0$, $x(t)$ is now only defined on $(-\infty, \frac{1}{x_0})$ with a singularity at $\frac{1}{x_0}$. The case $x_0 < 0$ behaves similarly.

The next theorem guarantees global solutions if we can control the function F associated with our differential equation. This task will be central when discussing many examples in the next chapter.

Theorem 1.19. *Let $F \in C^1(\mathbb{R} \times X, X)$, and let $\phi(t)$ be the maximal solution of the Cauchy problem (1.13). If $|F(t, \phi(t))|$ remains bounded on finite intervals, then $\phi(t)$ is a global solution.*

Proof. Assume to the contrary that $(T_-, T_+) = I_\phi \subsetneq \mathbb{R}$, then $|F(t, \phi(t))| < C$ for $t \in I_\phi$. For any $t_0 < t_1 < t_2 < T_+$ we have

$$|\phi(t_2) - \phi(t_1)| \leq \int_{t_1}^{t_2} |\dot{\phi}(s)| ds = \int_{t_1}^{t_2} |F(s, \phi(s))| ds \leq C|t_2 - t_1|.$$

This means that, given a Cauchy sequence t_n , $\phi(t_n)$ is again Cauchy and thus $\lim_{t \rightarrow T_+} \phi(t) = \phi_+$ exists. The solution to the Cauchy problem with initial condition $\tilde{\phi}(T_+) = \phi_+$ is thus defined and can be attached to the original solution via

$$\psi(t) = \begin{cases} \phi(t) & t \in I_\phi, \\ \tilde{\phi}(t) & t \in I_{\tilde{\phi}} \cap [T_+, \infty), \end{cases}$$

which contradicts maximality of T_+ . □

2 Global Existence for nonlinear Lattices

We now investigate some examples of one-dimensional chains of particles with some interaction between them. We assign each particle $n \in \mathbb{Z}$ a function $q_n(t) \in \mathbb{R}$ dependent on time t . The dynamics of such systems are governed by laws such as the equation of motion, which reads

$$\ddot{q}_n(t)m_n = F$$

with m_n being the mass of the n -th particle and F the force acting on the chain, thus giving rise to a differential equation. A natural space to study this equation in is the Banach space ℓ^2 , which also determines the boundary condition $\lim_{n \rightarrow \infty} q_n = 0$. Typically, we can infer the existence of local solutions via the theory from chapter one. However, global solutions require more work and are not guaranteed.

For this chapter, we will mostly follow [10], see also [4] for an overview from a physics perspective. For notational simplicity, we will often omit the dependency on t of various objects throughout.

2.1 Fermi-Pasta-Ulam-Tsingou Lattices

In this section, we discuss models of particle chains with nearest neighbor interaction. We assume the particles to have unitary mass and that the interaction is given by some potential $V \in C^2(\mathbb{R})$. Such a system is given by

$$\ddot{q}_n(t) = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}). \quad (2.1)$$

In order to reduce this to a first-order system, we introduce $p = \dot{q}$, which yields

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

Moreover, we will sometimes abbreviate $r_n = q_{n+1} - q_n$ for readability.

The (total) energy of such a system is given by the Hamiltonian

$$\mathcal{H}(p, q) := \sum_{n \in \mathbb{Z}} \left(\frac{p_n^2}{2} + V(q_{n+1} - q_n) \right). \quad (2.2)$$

Following physical nomenclature, we sometimes refer to the first component of the sum featuring the momentum p as the kinetic energy and the second part involving the potential as potential energy. We will abbreviate

$$E_k := \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2}, \quad E_p := \sum_{n \in \mathbb{Z}} V(q_{n+1} - q_n).$$

Formally, taking the derivative of $\mathcal{H}(p, q)$ yields a telescope sum:

$$\begin{aligned} \frac{d}{dt}\mathcal{H}(p, q) &= \sum_{n \in \mathbb{Z}} p_n \dot{p}_n + V'(r_n)(\dot{q}_{n+1} - \dot{q}_n) \\ &= \sum_{n \in \mathbb{Z}} p_n (V'(r_n) - V'(r_{n-1})) + V'(r_n)(p_{n+1} - p_n) \\ &= \sum_{n \in \mathbb{Z}} -p_n V'(r_{n-1}) + p_{n+1} V'(r_n) = 0, \end{aligned}$$

meaning $\mathcal{H}_0 := \mathcal{H}(p(0), q(0)) = \mathcal{H}(p(t), q(t))$ if $\mathcal{H}(p, q)$ is differentiable, making it a conserved quantity. We will hence slightly abuse notation sometimes and just write $\mathcal{H}$.

Theorem 2.1. *Consider the Cauchy problem (2.1) with potential such that $V(r) \geq 0$ for all r and $\mathcal{H} \in C^1(\ell^2 \times \ell^2, \mathbb{R})$ for all t . Then solutions exist for all times t .*

Proof. We can use $\mathcal{H}_0$ as a bound for the solution, which yields global existence by Theorem 1.19. If $0 \leq V$ and due to $q_n(t) = q_n(0) + \int_0^t p_n(s) ds$ respectively, we have

$$\|p(t)\|_2^2 \leq 2\mathcal{H}(p(t), q(t)) = 2\mathcal{H}_0$$

and further

$$\|q(t)\|_2 = \|q(0)\|_2 + \int_0^t \|p(s)\|_2 ds \leq \|q(0)\|_2 + \sqrt{2\mathcal{H}_0} t$$

as required. $\square$

In practice, all components of $\mathcal{H}$ will have some amount of regularity, which $\mathcal{H}$ inherits. However, it is not necessarily clear whether $\mathcal{H}(p, q) < \infty$ and thus whether $\mathcal{H} \in C^1(X, \mathbb{R})$. Consequently, to show global existence, it suffices to bound the energy.

For a simple quadratic potential of the form $V(r) = \frac{cr^2}{2}$, $\mathcal{H}$ can be easily bounded by

$$0 < \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2} + V(q_{n+1} - q_n) = \frac{\|p\|_2^2}{2} + \frac{c\|q^+ - q\|_2^2}{2} \leq \frac{\|p\|_2^2 + 4c\|q\|_2^2}{2},$$

where the shift q^+ is defined via $(q^+)_n = q_{n+1}$. Since solutions are in ℓ^2 for as long as they exist, the righthandside of this equation is finite. The same is possible if $V(0) = 0$ (which we can always assume since $V(0)$ does not interact with the differential equation), $V(r) > 0$ for all $r \in \mathbb{R} \setminus \{0\}$ and $V(r) < C_R r^2$ for $|r| < R$.

Intuitively, the problem that may occur is that even though the energy remains constant for as long as a given solution exists, it does so only due to

the (strictly positive) kinetic and (at some point necessarily negative) potential parts canceling each other out. At the same time as a non-global solution ceases to exist, $\mathcal{H}(p, q)$ suddenly becomes undefined as $E_k \rightarrow \infty$ and $E_p \rightarrow -\infty$. The perspective of $\mathcal{H}$ being constant forcing the lattice to behave a certain way is justified further by taking the partial derivatives of the Hamiltonian with respect to p, q and considering the set of resulting differential equations

$$\begin{aligned} -\frac{\partial \mathcal{H}(p, q)}{\partial q_n(t)} &= V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}) = \dot{p}_n(t) \\ \frac{\partial \mathcal{H}(p, q)}{\partial p_n(t)} &= p_n(t) = \dot{q}_n(t). \end{aligned}$$

Note that this holds due to the derivative being taken with regard to a specific position n in the lattice and all other summands disappearing.

Let us look at some concrete equations.

Example 2.2 (DW). The discrete wave equation

$$\dot{p}_n = a(\Delta_d q)_n \tag{2.3}$$

results from setting

$$V_{DW}(r) = \frac{a}{2}r^2.$$

Here,

$$\Delta_d q_n(t) = q_{n+1}(t) + q_{n-1}(t) - 2q_n(t)$$

is the discrete Laplacian. We will omit the subscript d from here on. The DW directly fulfills the criteria above and solutions are therefore global. Notice that the linear interaction based on the operator $a\Delta$ in (2.3) renders the DW a so-called harmonic lattice. We will revisit harmonic lattices in Chapter 2.2.

Example 2.3 (TL). The Toda-lattice, where we set

$$V_T(r) = e^{-r} + r - 1,$$

also has global solutions, since we can bound $V_T(r)$ by a quadratic function for $|r| < R$.

The Toda lattice is of interest due to its soliton solutions, meaning localized waves which travel in space but do not change their shape. It was first discovered by M. Toda, see [15], but is also treated rigorously in [12]. The following two examples are so-called Fermi-Pasta-Ulam-Tsingou lattices (FPUT), named after E. Fermi, J. Pasta, S. Ulam and M. Tsingou who studied these models numerically in [6]. For a review of the subject from a physics point of view, see also [11]. Stability for the case of periodic lattices, meaning we consider $n \in \{0, \dots, N\}$ and

set $q_i = q_{i+N}$, is treated in [2] by D. Bambusi and A. Ponno, while [3] provides a more recent result on the time of existence. Soliton solutions are also possible in the FPUT lattices under certain conditions, as has been proven by G. Friesecke and J. Wattis in [7].

Example 2.4 (FPUT- β). The FPUT- β model with

$$V_\beta(r) = \frac{1}{2}r^2 + \frac{\beta}{4}r^4, \quad \text{where } \beta > 0,$$

has global solutions by Theorem 2.1.

Example 2.5 (FPUT- α). The FPUT- α model arises from setting

$$V_\alpha(r) = \frac{1}{2}r^2 + \frac{\alpha}{3}r^3.$$

Since V can not be bounded from below by 0, $\mathcal{H}$ may now be unbounded and therefore not differentiable. However, for small initial data, we still have global existence. We define

$$\mathfrak{D}(t) := \|q^+(t) - q(t)\|_\infty, \quad \mathfrak{D}_0 := \mathfrak{D}(0).$$

As we will see, this quantity is a deciding factor for the stability of solutions.

Theorem 2.6. *Let $A, B \in \mathbb{R}$ be such that $0 < A < \frac{3}{2}$ and $\frac{1}{B} = \frac{1}{2} - \frac{A}{3}$. Solutions of the FPUT- α equation satisfying*

$$\mathfrak{D}_0 < \frac{A}{|\alpha|} \quad \text{and} \quad 0 < \mathcal{H}_0 < \frac{A^2}{B\alpha^2}$$

are global. Moreover, we have

$$\mathfrak{D}(t) < \frac{A}{|\alpha|} \tag{2.4}$$

for all t .

Proof. A and B are chosen such that

$$0 \leq \frac{r^2}{B} \leq V_\alpha(r) \leq r^2$$

holds for as long as $|r| \leq \frac{A}{|\alpha|}$. Thus

$$\infty > \|p\|_2^2 + 2\|q\|_2^2 \geq \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2} + V(q_{n+1} - q_n) = \mathcal{H}(p, q)$$

for as long as the solution exists and q does not leave the required region. This

shows $\mathcal{H} \in C^1(X, \mathbb{R})$ and we have $\frac{d}{dt}\mathcal{H}(p, q) = 0$ as in the consideration above. On the other hand,

$$\begin{aligned} \frac{A^2}{B\alpha^2} &> \mathcal{H}_0 = \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2} + V(q_{n+1} - q_n) \\ &\geq \frac{\|q^+ - q\|_2^2}{B} \geq \frac{\|q^+ - q\|_\infty^2}{B} = \frac{\mathfrak{D}(t)^2}{B} \end{aligned} \quad (2.5)$$

shows that the solution can not leave the interval. $\square$

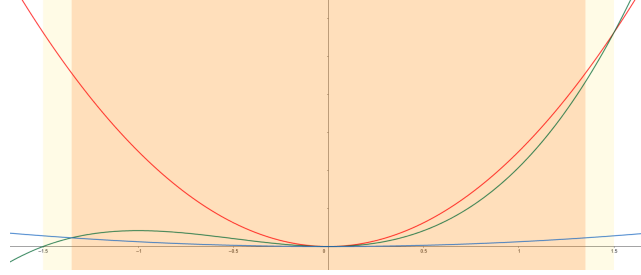


Figure 1: An illustration of the above proof for $\alpha = 1$. In the lighter shaded area $(-1.5, 1.5)$, we have $r^2 \geq V(r)$, hence solutions are global if they remain in this region. The darker shaded region $(-1.35, 1.35)$ can not be left, because we can estimate $V(r)$ from below with $r^2/20$.

Note that choosing A arbitrarily close to $\frac{3}{2}$ means $\frac{1}{B} \approx 0$, allowing only energy marginally larger than 0. As can be seen from maximizing $\frac{A^2}{B\alpha^2}$ for $0 < A < \frac{3}{2}$, the maximal allowed energy $\frac{1}{6\alpha^2}$ is attained at $A = 1$, which corresponds to the local maximum of V at $r = -\frac{1}{\alpha}$. If we choose A smaller, we get additional control in the sense of (2.4) over the solution in exchange.

However, it should be mentioned that this result is not optimal. For instance, considering initial data with only one particle displaced from its initial position, a factor of $\sqrt{2}$ is lost when passing from the 2- to the ∞ -norm in (2.5), which would allow for a larger initial energy than the theorem requires.

Let us look at an example of a global solution. Set $A = 1$ and consider the initial conditions

$$q_n(0) = \begin{cases} s & n = 0 \\ 0 & n \neq 0 \end{cases} \quad \text{and} \quad p(0) \equiv 0. \quad (2.6)$$

Then, we have initial energy

$$\mathcal{H}_0 = 0 + \frac{1}{2}s^2 + \frac{\alpha}{3}s^2 + \frac{1}{2}(-s)^2 + \frac{\alpha}{3}(-s)^2 = s^2.$$

To guarantee global solutions with Theorem 2.6, we must satisfy $\mathcal{H}_0 < \frac{\sqrt{2}}{6\alpha^2}$. Therefore, with the choice $|s| < \frac{\sqrt[4]{2}}{\sqrt{6}|\alpha|} < \frac{1}{|\alpha|}$, the data (2.6) yields a global solution.

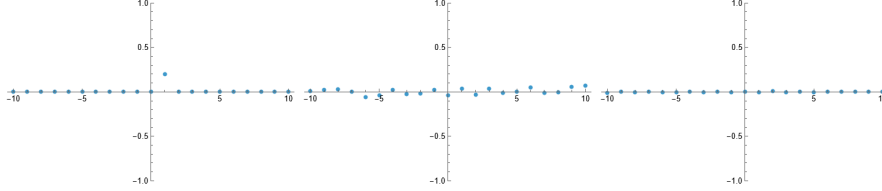


Figure 2: A solution of the FPUT- α model with $\alpha = 1$ and a small initial displacement of $q_1 = 0.2$ and no initial momentum, $p(0) = 0$, at times $t_1 = 0$, $t_2 = 10$ and $t_3 = 100$. At $t_3 = 100$, the initial spike seems to have dissipated completely. See the Appendix: Mathematica Code for the code used to produce the images shown.

On the other hand, the FPUT- α possesses solutions that only exist for finite times. To show this, we adapt the Levine concavity method introduced by Levine in [9] for parabolic PDEs, although the proof hereafter is more similar to an idea by Glassey, see [8]. A straightforward application of the ansatz by Levine to the (continuous) nonlinear Schrödinger equation can be found in [13], Chapter 14. The central identity (2.7) in the following lemma is sometimes referred to as a virial identity.

Lemma 2.7. *Consider the FPUT- α model, that is the Cauchy problem 2.1 with $V_\alpha(r) = \frac{1}{2}r^2 + \frac{\alpha}{3}r^3$, suppose $\mathcal{H}_0 < 0$ and define*

$$M(t) := \frac{1}{2} \sum_{n \in \mathbb{Z}} q_n(t)^2.$$

There exist constants $\varepsilon > 0 > \delta$ such that for all t , $M(t) \geq \varepsilon > 0$ and

$$(1 + \gamma)\dot{M}^2 - M\ddot{M} \leq \delta < 0, \quad \gamma := \frac{1}{4}. \quad (2.7)$$

Proof. To see the first claim, observe $E_p \leq \mathcal{H} < 0$, since $E_k \geq 0$ and $\mathcal{H} < 0$. To achieve $E_p < 0$, at least one n with $V_\alpha(r_n) < 0$ is required. Looking at the potential

$$V_\alpha(r) = \frac{1}{2}r^2 + \frac{\alpha}{3}r^3 = r^2\left(\frac{1}{2} + \frac{\alpha}{3}r\right),$$

this is the case if and only if $r_n < -\frac{3}{2\alpha}$, i.e. $\mathfrak{D}_0 > \frac{3}{2\alpha}$. The triangle inequality shows

$$|q_{n+1}| + |q_n| \geq |q_{n+1} - q_n| = |r_n| > \frac{3}{2\alpha},$$

and minimizing

$$q_{n+1}^2 + q_n^2 \quad \text{with constraints} \quad |q_{n+1}| + |q_n| = \frac{3}{2\alpha}$$

with the Cauchy-Schwarz inequality 1.4 implies $|q_{n+1}| = |q_n| = \frac{3}{4\alpha}$. We arrive at

$$q_{n+1}^2 + q_n^2 \geq 2\left(\frac{3}{4\alpha}\right)^2 = \frac{9}{8\alpha^2}$$

and finally

$$M(t) = \frac{1}{2} \sum_{n \in \mathbb{Z}} q_n(t)^2 \geq \frac{q_{n+1}(t)^2 + q_n(t)^2}{2} \geq \frac{9}{16\alpha^2} > 0.$$

For the second claim, we begin by differentiating M twice:

$$\begin{aligned} \dot{M} &= \sum_{n \in \mathbb{Z}} q_n \dot{q}_n \\ \ddot{M} &= \sum_{n \in \mathbb{Z}} \dot{q}_n^2 + \sum_{n \in \mathbb{Z}} q_n \ddot{q}_n. \end{aligned}$$

Next, inserting the differential equation (2.1) for $\ddot{q}_n$ and applying the summation by parts formula Theorem 1.5 yields

$$\begin{aligned} \ddot{M} &= 2E_k + \sum_{n \in \mathbb{Z}} q_n (V'_\alpha(r_n) - V'_\alpha(r_{n-1})) \\ &= 2E_k - \sum_{n \in \mathbb{Z}} (q_{n+1} - q_n) V'_\alpha(r_n) = 2E_k - \sum_{n \in \mathbb{Z}} r_n V'_\alpha(r_n). \end{aligned} \quad (2.8)$$

Note that we can apply the summation by parts formula due to $V'(0) = 0$ and $q_n \in \ell^2$ forcing $\lim_{n \rightarrow \infty} V(r_n) = 0$. Observe further

$$r V'_\alpha(r) = r^2 + \alpha r^3 = 3\left(\frac{1}{2}r^2 + \frac{\alpha}{3}r^3\right) - \frac{1}{2}r^2 = 3V_\alpha(r) - \frac{1}{2}r^2$$

and express $\sum_{n \in \mathbb{Z}} V_\alpha(r)$ in terms of the Hamiltonian (2.2),

$$\sum_{n \in \mathbb{Z}} V_\alpha(r_n) = \mathcal{H} - \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2}.$$

Substituting into (2.8), we have

$$\ddot{M} = 2E_k - 3\mathcal{H} + 3E_k + \sum_{n \in \mathbb{Z}} \frac{1}{2}r_n^2, \quad (2.9)$$

and due to $\sum_{n \in \mathbb{Z}} \frac{1}{2} r_n^2 \geq 0$, we arrive at

$$\ddot{M} > 5E_k - 3\mathcal{H}. \quad (2.10)$$

Now the Cauchy-Schwarz inequality Theorem 1.4 shows

$$\dot{M}^2 = \left(\sum_{n \in \mathbb{Z}} q_n \dot{q}_n \right)^2 \leq \left(\sum_{n \in \mathbb{Z}} q_n^2 \right) \left(\sum_{n \in \mathbb{Z}} \dot{q}_n^2 \right) = 2M2E_k, \quad (2.11)$$

hence

$$E_k \geq \frac{\dot{M}^2}{4M}.$$

Finally, substituting into (2.10) yields

$$\ddot{M} > \frac{5\dot{M}^2}{4M} - 3\mathcal{H} = (1 + \gamma) \frac{\dot{M}^2}{M} - 3\mathcal{H},$$

thus with $\mathcal{H}$ a negative constant and $M \geq \varepsilon > 0$ we arrive at

$$(1 + \gamma)\dot{M}^2 - M\ddot{M} \leq 3\mathcal{H}M < 0.$$

□

Theorem 2.8 (Concavity Method). *Solutions of the FPUT- α model with $\mathcal{H}_0 < 0$ are not global in time.*

Proof. Define

$$N(t) := M(t)^{-\gamma}, \quad \gamma = \frac{1}{4}. \quad (2.12)$$

Differentiating twice yields

$$\begin{aligned} \dot{N} &= -\gamma M^{-\gamma-1} \dot{M}, \\ \ddot{N} &= -\gamma M^{-\gamma-1} \ddot{M} - \gamma(-\gamma-1) M^{-\gamma-2} \dot{M}^2 \\ &= -\gamma M^{-\gamma-2} \left(M \ddot{M} + (-\gamma-1) \dot{M}^2 \right) \\ &= \gamma M^{-\gamma-2} \left((\gamma+1) \dot{M}^2 - M \ddot{M} \right), \end{aligned} \quad (2.13)$$

and since $M \geq \varepsilon > 0$ and the bracket is negative and bounded away from zero due to Lemma 2.7, $N(t)$ is concave with $N(0) \geq 0$ and $\ddot{N} \leq \zeta < 0$. We invoke Lemma 1.2 to deduce that there exists $T_+ < \infty$ such that

$$\lim_{t \rightarrow T_+} N(t) = \lim_{t \rightarrow T_+} M(t)^{-\gamma} = 0,$$

which is equivalent to

$$\lim_{t \rightarrow T_+} M(t) = \infty.$$

Hence $q(T_+) \notin \ell^2$, proving the claim. $\square$

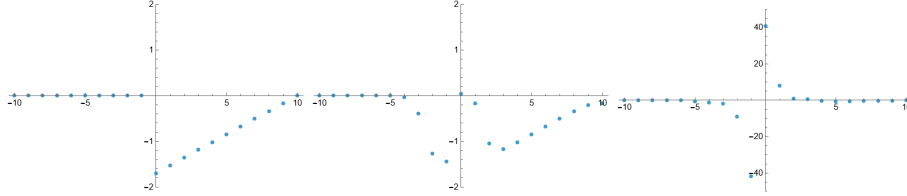


Figure 3: A solution of the FPUT- α model with $\alpha = 1$ and initial displacement as in (2.14) with $s = 1.7$ and $a = 10$, at times $t_1 = 0$, $t_2 = 2$ and $t_3 = 3.93$. After $t = 3$, we see a large rift forming at the position of the initial spike. Around $t_+ \approx 4.14$, the numerical calculation leads to a singularity, indicating blow up.

Solutions of the FPUT- α model with $\mathcal{H}_0 < 0$ indeed exist. Choose $s > \frac{3}{2\alpha}$ and $a \in \mathbb{N}_+$, and set

$$q_n(0) = \begin{cases} 0 & n > a \\ -\frac{(a-n)}{a}s & 0 \leq n \leq a \\ 0 & n < 0 \end{cases} \quad \text{and} \quad p(0) \equiv 0. \quad (2.14)$$

Then $r_{-1} = -s$ and $r_n = \frac{1}{a}s$ for $0 \leq n \leq a$, therefore we have for the initial energy

$$\begin{aligned} \mathcal{H}_0 &= 0 + \sum_{n \in \mathbb{Z}} V_\alpha(r_n) = \frac{1}{2}(-s)^2 + \frac{\alpha}{3}(-s)^3 + \sum_{n=0}^{a-1} \left(\frac{1}{2} \left(\frac{1}{a}s \right)^2 + \frac{\alpha}{3} \left(\frac{1}{a}s \right)^3 \right) \\ &= \frac{1}{2}s^2 - \frac{\alpha}{3}s^3 + \frac{1}{2a}s^2 + \frac{\alpha}{3a^2}s^3. \end{aligned}$$

Now formally letting $a \rightarrow \infty$ and

$$\frac{1}{2}s^2 - \frac{\alpha}{3}s^3 = s^2 \left(\frac{1}{2} - \frac{\alpha}{3}s \right) < 0$$

for $s > \frac{3}{2\alpha}$ would show that $\mathcal{H}_0 < 0$. Of course, if $a \rightarrow \infty$ we would leave ℓ^2 , but $\mathcal{H}_0 < 0$ still holds true for any a with the stronger condition $s > \frac{3}{2\alpha} + \delta$ for a suitable δ . For example, $s > \frac{3}{\alpha}$ for $a = 2$ blows up in finite time.

Solutions may blow up even if the energy is positive, which we prove for sufficiently large initial momentum using an integration ruse.

Theorem 2.9. *Solutions of the FPUT- α model with $\mathcal{H}_0 > 0$ satisfying*

$$\dot{M}(0) > 0 \quad \text{and} \quad \dot{M}(0)^2 > 4\mathcal{H}M(0) \quad (2.15)$$

are not global in time.

Proof. Considering equation (2.9), we manipulate

$$\begin{aligned} \ddot{M} &= 2E_k - 3\mathcal{H} + 3E_k + \sum_{n \in \mathbb{Z}} \frac{1}{2} r^2. \\ \ddot{M}M &\geq 5E_k M - 3M\mathcal{H}. \end{aligned}$$

As in (2.11), we use Cauchy-Schwarz to get the estimate $5ME_k \geq (1 + \gamma)\dot{M}^2$, leading to

$$(1 + \gamma)\dot{M}^2 - \ddot{M}M \leq 3M\mathcal{H}.$$

Inserting this into the equation for $\ddot{N}$, (2.13), shows

$$\begin{aligned} \ddot{N} &\leq (\gamma M^{-\gamma-2})(3M\mathcal{H}) \\ &= 3\gamma M^{-\gamma-1}\mathcal{H} \\ &= 3\gamma(M^{-\gamma})^5 \mathcal{H}(p, q) = 3\gamma N^5 \mathcal{H}. \end{aligned}$$

Since $\dot{M}(0) > 0$ and $N = M^{-\gamma}$, there exists an interval $I := [0, s)$ such that $\dot{N}(t) < 0$ for $t \in I$ (and where the solution exists by Theorem 1.15). Hence we may multiply both sides with $2\dot{N}$ without ambiguity over the direction of the estimate as long as we stay in I . Integrating the resulting equation

$$2\ddot{N}\dot{N} \geq 6\gamma N^5 \dot{N}\mathcal{H} \quad (2.16)$$

from zero to t yields

$$\begin{aligned} \dot{N}(t)^2 - \dot{N}(0)^2 &\geq 6\gamma\mathcal{H} \left(\frac{N(t)^6 - N(0)^6}{6} \right) \\ \dot{N}(t)^2 &\geq \gamma\mathcal{H}N(t)^6 - \gamma\mathcal{H}N(0)^6 + \dot{N}(0)^2. \end{aligned} \quad (2.17)$$

We claim that the right-hand side of this equation is always positive. For the first component $\gamma\mathcal{H}N(t)^6$, this is the case trivially. For the rest, we insert the

definition of N and γ , and finally use condition (2.15),

$$\begin{aligned}\zeta &:= \dot{N}(0)^2 - \gamma \mathcal{H} N(0)^6 = \left(-\gamma M(0)^{-\gamma-1} \dot{M}(0) \right)^2 - \gamma \mathcal{H} M(0)^{-6\gamma} \\ &= \frac{1}{16} M(0)^{-\frac{10}{4}} \dot{M}(0)^2 - \frac{1}{4} \mathcal{H} M(0)^{-\frac{6}{4}} \\ &> \frac{1}{16} M(0)^{-\frac{10}{4}} 4 \mathcal{H} M(0) - \frac{1}{4} \mathcal{H} M(0)^{-\frac{6}{4}} = 0.\end{aligned}$$

We have thus shown

$$\dot{N}(t)^2 \geq \zeta > 0 \quad \text{for } t \in I. \quad (2.18)$$

Now suppose s were finite and maximal, then by continuity we would have $\dot{N}(s) = 0$. On the other hand, $\dot{N}(t) \leq -\sqrt{\zeta} < 0$ follows from (2.18) and together with continuity this implies $\dot{N}(s) < 0$. This is a contradiction, therefore there can not be a finite and maximal s and we must have $I = \mathbb{R}_+$. Finally, since $\dot{N}(t) \leq -\sqrt{\zeta} < 0$ for all t , there exists T_+ with $\lim_{t \rightarrow t_+} N(T_+) = 0$ and

$$\lim_{t \rightarrow t_+} M(T_+) = \infty.$$

□

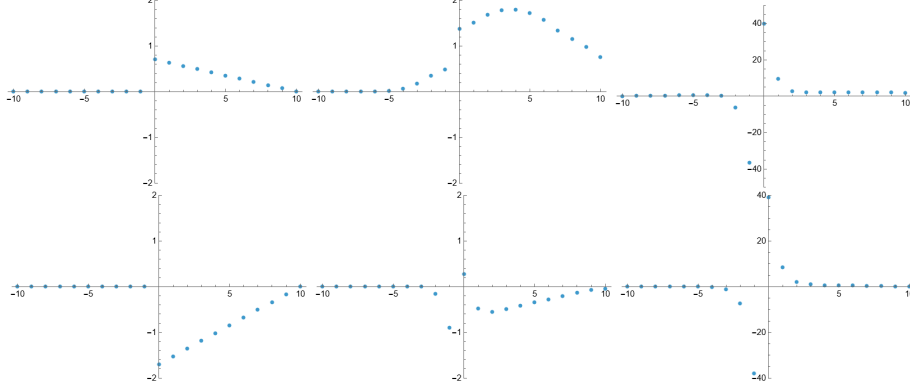


Figure 4: The first row displays the Lattice with initial data similar to (2.14), with $s = -0.7$, but $p_n(0) = 0.35$ for all $n \in \{0, \dots, 9\}$ and 0 elsewhere at $t_1 = 0$, $t_2 = 4$ and $t_3 = 8.5$. Computing the relevant quantities $\mathcal{H} = 1.45$, $M(0) = 1.89$, $4\mathcal{H}M(0) = 10.96$ and $\dot{M}(0)^2 = 12.25$ shows that the conditions of Theorem 2.9 are fulfilled and numerics indeed suggest blow up around $t_+ \approx 8.72$. The second row shows the behaviour of (2.19) with $s = 1.7 > 3/2$ at $t_1 = 0$, $t_2 = 1$ and $t_3 = 2.7$. Blow up happens at $t_+ \approx 2.912$.

To construct solutions that satisfy the conditions of Theorem 2.9, we modify (2.14) to

$$q_n(0) = \begin{cases} 0 & n > a \\ -\frac{(a-n)}{a}s & 0 \leq n \leq a \\ 0 & n < 0 \end{cases} \quad \text{and} \quad p(0) = \lambda q(0) \quad (2.19)$$

for $\lambda \in \mathbb{R}$ and calculate the relevant quantities, (see solution (2.14)),

$$\mathcal{H} = \frac{1}{2} \sum_{n \in \mathbb{Z}} (\lambda q_n(0))^2 + E_p = \lambda^2 M(0) + E_p$$

$$\dot{M}(0) = \sum_{n \in \mathbb{Z}} (\lambda q_n(0)) q_n(0) = 2\lambda M(0).$$

Observe now

$$\dot{M}(0)^2 - 4\mathcal{H}M(0) = 4\lambda^2 M(0)^2 - 4\lambda^2 M(0)^2 - 4E_p M(0) = -4E_p M(0).$$

As established before, E_p is negative for suitable s , thus

$$\dot{M}(0)^2 - 4\mathcal{H}M(0) > 0,$$

and we conclude that solutions of this form have no global solutions for s large enough.

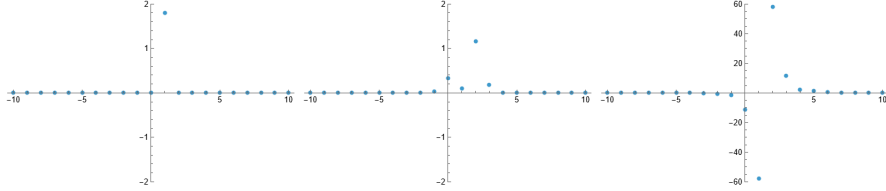


Figure 5: FPUT- α with $\alpha = 1$, $q_1 = 1.8 > \frac{3}{2\alpha}$, $p(0) = 0$, at times $t_1 = 0$, $t_2 = 1$ and $t_3 = 3.4$. Blow up appears to happen around $t \approx 3.7$ for this constellation, despite not fulfilling the conditions of Theorems 2.8 or 2.9.

Together with Theorems 2.6, 2.8, and the examples thereafter this seems to indicate a division of initial states into two regions. Whereas for $\mathfrak{D}_0 < \frac{3}{2\alpha}$, we have seen that global solutions exist for small energy, the examples (2.14) and (2.19) above show solutions with $\mathfrak{D}_0 > \frac{3}{2\alpha}$ exhibiting blow-up behaviour. This is consistent with intuition, as the point $r = -\frac{3}{2\alpha}$ represents a zero of $V_\alpha(r)$, and for r smaller, the potential is negative and therefore uncontrollable by 2-norms, leading to the following conjecture.

Conjecture 2.10. *Consider initial conditions satisfying $\mathfrak{D}_0 > \frac{3}{2|\alpha|}$. Then solutions blow up in finite time.*

It remains unclear whether this or something similar is true or how to attempt a proof.

2.2 Harmonic Lattices

In this section, we briefly discuss harmonic lattices. We will not prove statements, but instead refer to [5], Chapter 6 and [10], Chapter 1.3 for details. A rigorous treatment of Jacobi operators can be found in [12], with an application to harmonic lattices in Chapter 1.5. See also [14], Chapter 5 for a review of spectral theory.

Let us assume linear nearest neighbour interaction given by a sequence a_n and an autonomous linear oscillation of each particle given by some potential $U_n(r)$. This leads to the equation

$$\ddot{q}_n(t) = -U'_n(q_n(t)) + a_{n-1}(q_{n-1}(t) - q_n(t)) - a_n(q_n(t) - q_{n+1}(t)).$$

Imposing the condition that the oscillation is of the form $U_n(r) = -\frac{c_n}{2}r^2$ allows for the simplification

$$\ddot{q}_n(t) = a_n q_{n+1}(t) + a_{n-1} q_{n-1}(t) + b_n q_n(t), \quad (2.20)$$

where $b_n = c_n - a_n - a_{n-1}$. From here on, we assume that the sequences a_n, c_n are bounded. We also implicitly assume unitary mass, as m_n can be absorbed by a_n, b_n after a transformation. Now we introduce the Jacobi operator A with

$$-(Aq)_n := a_n q_{n+1} + a_{n-1} q_{n-1} + b_n q_n, \quad (2.21)$$

which is a symmetric linear operator on ℓ^2 . Our equation then becomes

$$\ddot{q}_n = -Aq. \quad (2.22)$$

The dynamics of this system are well-understood. Since a_n, b_n are bounded, A is Lipschitz and we can apply the global existence and uniqueness theorem, see e.g. [1] Lemma 4.1.6, hence solutions are global. It is readily verified that solutions are given by

$$q_n(t) = \cos(tA^{\frac{1}{2}})q_n(0) + A^{-\frac{1}{2}} \sin(tA^{\frac{1}{2}})p_n(0), \quad (2.23)$$

where $\cos$ and $\sin$ are defined via their expansion series

$$\begin{aligned}\cos(A) &:= \sum_{k=0}^{\infty} \frac{(-1)^k}{2k!} A^{2k}, \\ \sin(A) &:= \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} A^{2k+1}.\end{aligned}$$

The ansatz $q_n(t) = \exp(i\omega t)x_n$, where x_n is a sequence, describes standing waves if $\omega \in \mathbb{R}$. Inserting this into (2.22) yields the eigenvalue problem

$$Ax - \lambda x = 0$$

with $\lambda := \omega^2$. The operator A is bounded due to $|a_n| < \infty$ and $|b_n| < \infty$ and hence must have bounded spectrum. Moreover, it holds that

$$\sigma(A) \subseteq [c_-, c_+], \quad \text{where} \quad c_{\pm} = \sup_{n \in \mathbb{Z}} (b_n \pm |a_n| + |a_{n-1}|),$$

and if $c_n > 0$ for all n , we even have

$$\sigma(A) \subseteq [0, 4\|c\|_{\infty}].$$

Regarding examples, we have already seen that such systems arise naturally from nearest neighbour interaction as in Chapter 2.1 with potential $V_n(r) = \frac{c_n}{2}r^2$ via

$$\ddot{q}_n = V'_{n+1}(q_{n+1} - q_n) - V'_n(q_n - q_{n-1}) = c_{n+1}q_{n+1} - (c_{n+1} + c_n)q_n + c_nq_{n-1}, \quad (2.24)$$

as is the case for the DW (2.3) with $c_n \equiv a$. In the next chapter, we will investigate similar lattices with added nonlinearity.

2.3 Nonlinear Klein-Gordon and Wave Equation

In this section, we consider a system of coupled nonlinear oscillators. We assume unitary mass and linear interaction between nearest neighbors as in Chapter 2.2, but combine them with nonlinear oscillation in each particle. Setting $U_n(r) = -\frac{c(n)}{2}r^2 + V_n(r)$ yields, analogously to (2.20),

$$\ddot{q}_n(t) = a_n q_{n+1}(t) + a_{n-1} q_{n-1}(t) + b_n q_n(t) - V'_n(q_n(t)), \quad (2.25)$$

or, using the Jacobi operator,

$$\ddot{q}_n = (Aq)_n - V'(q_n). \quad (2.26)$$

To ensure that 0 is the resting point for each particle, assuming $V(0) = V'(0) = 0$ is natural, as is setting $\lim_{n \rightarrow \pm\infty} q_n(0) = 0$. The case $V = 0$ is already covered and we will assume otherwise. Again, we may introduce $p = \dot{q}$ to reduce (2.20) to a first order system.

The Hamiltonian of this system reads

$$\mathcal{H}(p, q) := \sum_{n \in \mathbb{Z}} \left(\frac{p_n^2}{2} - \frac{(Aq)_n q_n}{2} + V(q_n) \right). \quad (2.27)$$

We will again abbreviate

$$E_k := \frac{1}{2} \sum_{n \in \mathbb{Z}} p_n^2, \quad E_l := -\frac{1}{2} \sum_{n \in \mathbb{Z}} (Aq)_n q_n, \quad E_p := \sum_{n \in \mathbb{Z}} V(q_n). \quad (2.28)$$

From a physics point of view, E_k corresponds to the kinetic energy while E_l is the linear and E_p the nonlinear part of the potential energy. A calculation similar to that in Chapter 2.1 shows that $\mathcal{H}(p, q)$ is again a conserved quantity, given that it is differentiable. Observe

$$\begin{aligned} \sum_{n \in \mathbb{Z}} (A\dot{q})_n q_n &= \sum_{n \in \mathbb{Z}} a_n \dot{q}_{n+1} q_n + \sum_{n \in \mathbb{Z}} a_{n-1} \dot{q}_{n-1} q_n + \sum_{n \in \mathbb{Z}} b_n \dot{q}_n q_n \\ &= \sum_{n \in \mathbb{Z}} a_{n-1} \dot{q}_n + q_{n-1} + \sum_{n \in \mathbb{Z}} a_n \dot{q}_n q_{n+1} + \sum_{n \in \mathbb{Z}} b_n \dot{q}_n q_n = \sum_{n \in \mathbb{Z}} (Aq)_n \dot{q}_n, \end{aligned}$$

thus taking the derivative of $\mathcal{H}(p, q)$ yields

$$\begin{aligned} \frac{d}{dt} \mathcal{H}(p, q) &= \sum_{n \in \mathbb{Z}} \left(p_n \dot{p}_n - \frac{(A\dot{q})_n q_n + (Aq)_n \dot{q}_n}{2} + V'(q_n) \dot{q}_n \right) \\ &= \sum_{n \in \mathbb{Z}} \left(\dot{q}_n ((Aq)_n - V'(q_n)) - (Aq)_n \dot{q}_n + V'(q_n) \dot{q}_n \right) = 0. \end{aligned}$$

Theorem 2.11. *Consider the Cauchy problem (2.25). If $\mathcal{H} \in C^1(\ell^2 \times \ell^2, \mathbb{R})$, $V(r) \geq 0$ for all $r \in \mathbb{R}$ and A is a non-positive operator, that is $\sum_{n \in \mathbb{Z}} (Aq)_n q_n = \langle Aq, q \rangle \leq 0$, then solutions of the Cauchy problem are global.*

Proof. The proof is analogous to the one for Theorem 2.1. The additional condition $\langle Aq, q \rangle \leq 0$ is needed to ensure

$$\|p(t)\|_2^2 \leq 2\mathcal{H}(p(t), q(t)).$$

□

Example 2.12 (FK). The Frenkel-Kontorova Model

$$\ddot{q}_n(t) = a(\Delta q)_n(t) - \sin q_n(t) \quad (2.29)$$

results from setting $a_n = a > 0$, $c_n = 0$, and

$$A_{FK} = a\Delta, \quad V_{FK}(r) = 1 - \cos(r).$$

This is a discretized version of the sin-Gordon equation

$$q_{tt} - aq_{xx} + \sin q = 0.$$

Global solutions follow from Theorem 2.11. We have $V_{FK}(r) \geq 0$ and $A_{FK} = a\Delta$ is a non positive operator, as will be shown in Lemma 2.16.

Example 2.13 (DNKG). The discrete nonlinear Klein-Gordon equation

$$\ddot{q}_n(t) = a(\Delta q)_n(t) - m^2 q_n(t) + \lambda q_n^k(t) \quad (2.30)$$

arises from $a_n = a > 0$, $c_n = -m^2 < 0$ and

$$A_{KG} = a\Delta - m^2, \quad V_{KG}(r) = -\frac{\lambda}{k+1} r^{k+1},$$

where k is a positive integer.

Example 2.14 (DNW). The discrete nonlinear wave equation

$$\ddot{q}_n(t) = a(\Delta q)_n(t) + \lambda q_n^k(t) \quad (2.31)$$

is the extreme case of the DNKG where we set $m^2 = 0$, thus

$$A_W = a\Delta, \quad V_W(r) = -\frac{\lambda}{k+1} r^{k+1}$$

In applications, the quadratic and cubic case $k = 2, k = 3$ respectively, are of particular interest for both the DNKG and DNW.

Example 2.15 (ϕ^4). The discrete ϕ^4 -equation

$$\ddot{q}_n(t) = a(\Delta q)_n(t) + m^2 q_n(t) - \lambda q_n^3 \quad (2.32)$$

results from $a_n = a$, $c_n = m^2 > 0$, $\lambda > 0$ and

$$A_\phi = a\Delta + m^2, \quad V_\phi(r) = \frac{\lambda}{4} r^4.$$

Lemma 2.16. *The discrete Laplacian Δ , A_W and A_{KG} are non-positive operators on ℓ^2 . The operator A_{KG} is negative definite, meaning there exists $\alpha > 0$ such that*

$$\langle Aq, q \rangle \leq -\alpha \|q\|_2^2$$

for all $q \in \ell^2$. Moreover, $\rho(q) := \sqrt{-\langle A_{KG}q, q \rangle}$ is an equivalent norm on ℓ^2 .

Proof. For A_W and Δ (set $a = 1$), use $q_n^2 + q_{n+1}^2 \geq 2q_n q_{n+1}$ (square of difference), to conclude

$$\langle A_W q, q \rangle = a \sum_{n \in \mathbb{Z}} q_n (q_{n-1} + q_{n+1} - 2q_n) = a \sum_{n \in \mathbb{Z}} (2q_n q_{n+1} - (q_n^2 + q_{n+1}^2)) \leq 0,$$

and also for later use

$$\langle A_W q, q \rangle \geq -2a \sum_{n \in \mathbb{Z}} (q_n^2 + q_{n+1}^2) = -4a \|q\|_2^2.$$

Regarding A_{KG} , observe

$$\begin{aligned} \langle A_{KG} q, q \rangle &= \langle (A_W - m^2)q, q \rangle = \langle A_W q, q \rangle - m^2 \langle q, q \rangle \leq -m^2 \|q\|_2^2. \\ \langle A_W q, q \rangle - m^2 \langle q, q \rangle &\geq -(4a + m^2) \|q\|_2^2 \end{aligned}$$

which yields

$$m \|q\|_2 \leq \rho(q) \leq \sqrt{4a + m^2} \|q\|_2. \quad (2.33)$$

□

Theorem 2.17. *If $\lambda < 0$ and k is odd, solutions are global for both the DNKG (2.30) and the DNW (2.31).*

Proof. In the given case, $V(r) \geq 0$, and A_W, A_{KG} are non-positive by Lemma 2.16, therefore we can apply Theorem 2.11. □

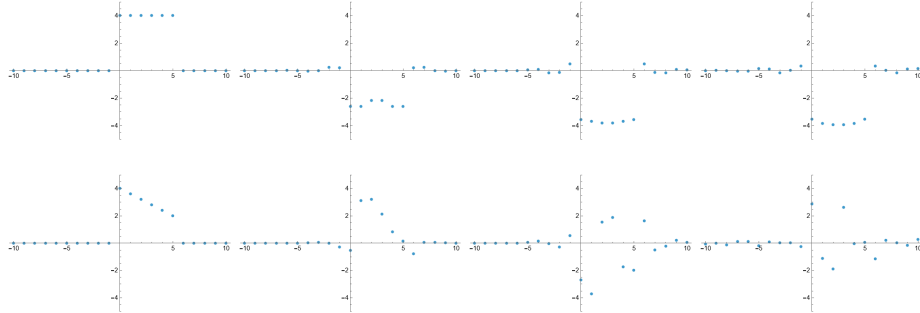


Figure 6: The Klein-Gordon Lattice in the case $\lambda = -1$, $k = 3$, $m^2 = 2$ with a flat initial spike and $4q(0) = p(0)$, at times $t_1 = 0$, $t_2 = 4$, $t_3 = 6$ and $t_4 = 9.2$ in the first row. As Theorem 2.17 suggests, solutions are stable and this data even exhibits periodic behaviour. Slightly modified $q_n(0)$ with $p(0) = 0$ at $t_1 = 0$, $t_2 = 2$, $t_3 = 6$ and $t_4 = 25$ can be seen in the second row. Even at later times, the mass mostly remains localized in $\{0, \dots, 5\}$.

Additionally, we can show global existence for the quadratic DNKG with any $\lambda \neq 0$ as long as we start with small initial data. This result is due to Pankov, see [10]. The idea is, similarly to Theorem 2.6, to trap $q(t)$ within a bounded set which it can not escape. To construct this set, we establish some technical results first.

Lemma 2.18. (i) *We may view the components of the Hamiltonian $E_k(p)$, $E_{l,p}(q)$, see (2.28), as functionals depending on p, q , turning $\sqrt{2E_l}$ into an equivalent norm.*

(ii) *There exists a constant $\mu > 0$ such that equivalently*

$$\frac{1}{\mu^6} \leq \frac{(2E_l)^3}{(3E_p)^2} \quad \text{and} \quad |E_p| \leq \frac{\mu^3}{3} (\sqrt{2E_l})^3. \quad (2.34)$$

We set $\mu = \frac{\sqrt[3]{\lambda}}{m}$.

(iii) *Let $\varphi(q) := E_l(q) + E_p(q)$ and*

$$\gamma := \inf \left\{ \sup_{\tau \geq 0} \varphi(\tau q) \mid q \in \ell^2, q \neq 0 \right\}.$$

It holds that

$$\gamma \geq \frac{1}{6\mu^6}. \quad (2.35)$$

(iv) *Define*

$$W := \{q \in \ell^2 \mid \forall \tau \in [0, 1] : 0 \leq \varphi(\tau q) < \gamma\}.$$

The set W is nonempty and star-shaped with respect to the origin, meaning if $q \in W$, then $\theta q \in W$ for all $\theta \in [0, 1]$.

(v) *For each $\nu > 0$ with*

$$\nu \leq \frac{9}{4\mu^6}, \quad \frac{\nu}{2} + \frac{\mu^3}{3} \sqrt{\nu^3} < \gamma, \quad (2.36)$$

define

$$V := \{q \in \ell^2 \mid 2E_l < \nu\}.$$

The set V is open and $V \subseteq W$.

(vi) *Define*

$$U := \{q \in \ell^2 \mid 0 < 2E_l(q) + 3E_p(q), \varphi(q) < \gamma\}.$$

The set U is open and $W = U \cup V$.

(vii) The set W is open and bounded.

Proof. (i) The last claim holds due to $\rho(q) = \sqrt{2E_l}$ and Lemma 2.16.

(ii) Observe

$$|3E_p| \leq \lambda \|q\|_3^3 \leq \lambda \|q\|_2^3,$$

and (i) guarantees a constant $\mu > 0$ such that

$$\begin{aligned} \sqrt[3]{|3E_p|} &\leq \sqrt[3]{\lambda} \|q\|_2 \leq \mu \rho(q) = \mu \sqrt{2E_l}, \\ \frac{1}{\mu} &\leq \frac{\sqrt{2E_l}}{\sqrt[3]{|3E_p|}}. \end{aligned}$$

The choice for μ is justified by (2.33).

(iii) We have the cubic polynomial

$$\varphi(\tau q) = E_l \tau^2 + E_p \tau^3. \quad (2.37)$$

If $E_p(q) \geq 0$, due to $E_l(q) \geq 0$,

$$\sup_{\tau \geq 0} \varphi(\tau q) = +\infty.$$

If $E_p(q) < 0$, maximizing $\varphi(\tau q)$ gives the extremum $\tau_0 = -\frac{2E_l}{3E_p}$, showing

$$\sup_{\tau \geq 0} \varphi(\tau q) = \varphi\left(-\frac{2E_l}{3E_p} q\right) = \frac{1}{6} \frac{(2E_l)^3}{(3E_p)^2}.$$

Together with (2.34), we conclude

$$\gamma \geq \frac{1}{6\mu^6}.$$

(iv) Note that W is well defined due to (2.35). Trivially, $q \equiv 0 \in W$. If $q \in W$, $0 \leq \varphi(\tau q) < \gamma$ ensures also

$$0 \leq \theta^2 \tau^2 E_l + \theta^3 \tau^3 E_p = \varphi(\tau \theta q) \leq \gamma$$

for $\theta \in [0, 1]$.

(v) Assume $q \in V$ and consider (2.37). We calculate using (2.34)

$$\tau^2 E_l - \frac{\mu^3 \tau^3}{3} (\sqrt{2E_l})^3 \leq \varphi(\tau q) = \tau^2 E_l + \tau^3 E_p \leq \tau^2 E_l + \frac{\mu^3 \tau^3}{3} (\sqrt{2E_l})^3.$$

Regarding the lefthand side of the equation, the first condition in (2.36) ensures for any $\tau \in [0, 1]$

$$\varphi(\tau q) \geq \tau^2 E_l \left(1 - \frac{2\mu^3 \tau}{3} \sqrt{2E_l} \right) \geq \tau^2 E_l \left(1 - \frac{2\mu^3 \tau}{3} \frac{3}{2\mu^3} \right) \geq 0.$$

On the other hand, the second condition in (2.36) shows

$$\varphi(\tau q) \leq \tau^2 E_l + \frac{\mu^3 \tau^3}{3} (\sqrt{2E_l})^3 \leq \frac{\nu}{2} + \frac{\mu^3}{3} \sqrt{\nu^3} < \gamma.$$

Thus $q \in W$ also and we have shown $V \subseteq W$.

(vi) By continuity of the functionals E_l, E_p, φ , the set U is open. From (v), we know $V \subseteq W$, hence it suffices to show $W = U \cup \{0\}$. Furthermore, the case $q = 0$ is trivial, so we consider only $q \neq 0$ in the following. Assume $q \in W$, then either $E_p \geq 0$ or $E_p < 0$. If $E_p \geq 0$,

$$0 \leq E_l + E_p \leq 2E_l + 3E_p < \gamma.$$

Conversely, if $E_p < 0$, we have

$$\sup_{\tau \geq 0} \varphi(\tau q) = \varphi \left(-\frac{2E_l}{3E_p} q \right) \geq \gamma.$$

Since $q \in W$, we have $\sup_{\tau \in [0, 1]} \varphi(\tau q) < \gamma$, thus

$$-\frac{2E_l}{3E_p} > 1, \tag{2.38}$$

which is equivalent to $3E_p + 2E_l > 0$. In both cases, $\varphi(q) < \gamma$, hence $q \in U$ holds.

On the other hand, let $q \in U$. If $E_p \geq 0$, then

$$\sup_{\tau \in [0, 1]} \varphi(\tau q) = \varphi(q) < \gamma.$$

If $E_p < 0$, then (2.38) implies the same. In both cases, $q \in W$.

(vii) The union of two open sets is open, therefore W is open by (vi). To see that W is bounded, we prove $W \subseteq T$, where

$$T := \{q \in \ell^2 \mid E_l(q) < 3\gamma\}$$

is a bounded set.

Let $q \in W$. If $E_p \geq 0$,

$$E_l \leq \varphi(q) < \gamma$$

is immediate. If $E_p < 0$, we have $3E_p > -2E_l$ by (2.38), which yields

$$\gamma > \varphi(q) = E_p + E_l > \frac{1}{3}E_l.$$

We conclude $W \subseteq T$ and the proof is finished. $\square$

Now we are ready to prove the anticipated result.

Theorem 2.19. *Consider the quadratic case of the DNKG 2.30, i.e.*

$$V(r) = -\frac{\lambda}{3}r^3$$

with $\lambda \neq 0$ and suppose the initial values $q_0 \in W$, $p_0 \in \ell^2$ satisfy

$$\mathcal{H}_0 = \frac{\|p_0\|_2^2}{2} + \varphi(q_0) < \gamma.$$

Then solutions to the Cauchy problem are global.

Proof. We prove that $q(t) \in W$ for all t , and hence, since W is bounded, $q(t)$ remains bounded. Theorem 1.19 then finishes the proof.

Assume to the contrary that $q(t) \notin W$ for some t and let t_1 be the smallest value where this is true. Then, since W open and star-shaped, $q(t_1) \in \partial W$, where ∂W is the boundary of W , but $\theta q(t_1) \in W$ for $\theta \in [0, 1)$. Therefore, $\varphi(\theta q(t_1)) < \gamma$ for $\theta \in [0, 1)$, and by continuity and letting $\theta \rightarrow 1$, we obtain $\varphi(q(t_1)) \leq \gamma$. Now $\varphi(q(t_1)) < \gamma$ leads to the immediate contradiction $q(t_1) \in W$, thus $\varphi(q(t_1)) = \gamma$ must be true. Finally, energy conservation yields the contradiction

$$\begin{aligned} \gamma &= \varphi(q(t_1)) \leq E_k(p(t_1)) + \varphi(q(t_1)) = \mathcal{H}(p(t_1), q(t_1)) \\ &= \mathcal{H}_0 = E_k(p_0) + \varphi(q_0) \\ &< \gamma, \end{aligned}$$

hence $q(t) \in W$ for all t . $\square$

One can generalize this theorem in two ways. Firstly, the proof works for any negative definite operator A . Secondly, one can consider a bounded sequence λ_n instead of λ , however some concrete constants in Lemma 2.18 will have to be exchanged for more general ones.

Indeed, global solutions satisfying the conditions of 2.19 exist. By Lemma 2.18 (ii), (iii),

$$\gamma \geq \frac{1}{6\mu^6} = \frac{m^6}{6\lambda^2},$$

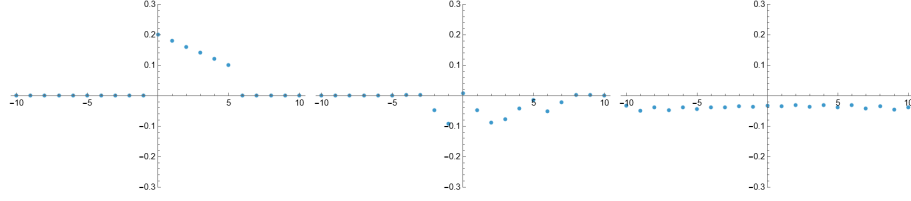


Figure 7: Initial data for $\lambda = -1$, $k = 2$ and $m^2 = 2$ fulfilling the conditions of Theorem 2.19 with $p(0) = 0$ and $\varphi(q_0) < 1/6$ at times $t_1 = 0$, $t_2 = 3$ and $t_3 = 100$. Spikes seem to dissipate.

so ensuring $\mathcal{H}_0 < \frac{m^6}{6\lambda^2}$ is enough. Consider again

$$q_n(0) = \begin{cases} s & n = 0 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad p(0) \equiv 0,$$

then

$$\mathcal{H}_0 = -(\Delta q)_0 q_0 - \frac{\lambda}{3} q_0^3 = 2s^2 - \frac{\lambda}{3} s^3 < \frac{m^6}{6\lambda^2}$$

is easily satisfied for a suitable s , but dependence on m makes concrete values cumbersome. However, let $s = \frac{6}{\lambda}$, then certainly $2s^2 - \frac{\lambda}{3} s^3 = 0 < \frac{m^6}{6\lambda^2}$. By continuity, there exists an interval $I := (\frac{6}{\lambda} - \varepsilon, \frac{6}{\lambda} + \varepsilon)$ such that $q(t)$ is global for $s \in I$.

To show blow-up of solutions, we again use the Concavity Method. An application of the concavity method to the continuous Klein-Gordon equation can be found in [16].

Lemma 2.20. *Consider the DNKG (2.30) or DNW (2.31) with $\lambda > 0$, $k \geq 1$ even and assume $\mathcal{H}_0 < 0$. Define*

$$M(t) := \frac{1}{2} \sum_{n \in \mathbb{Z}} q_n(t)^2.$$

There exist constants $\varepsilon > 0 > \delta$ such that for all t , $M(t) \geq \varepsilon > 0$ and

$$(\gamma + 1)\dot{M}^2 - M\ddot{M} \leq \delta < 0, \quad \gamma := \frac{k-1}{4}. \quad (2.39)$$

Proof. Similarly to Lemma 2.7, the claim $M(t) \geq \varepsilon > 0$ follows from the assumption $\mathcal{H}_0 < 0$. Both E_k and E_l are non-negative, thus $E_p \leq \mathcal{H} < 0$, meaning

$$\frac{-\lambda}{k+1} \sum_{n \in \mathbb{Z}} q^{k+1} = \frac{-\lambda}{k+1} \|q\|_{k+1}^{k+1} \leq \mathcal{H}.$$

Now we use the fact that the 2-norm dominates any other p -norm to see

$$-\frac{k+1}{\lambda}\mathcal{H} \leq \|q\|_{k+1}^{k+1} \leq \|q\|_2^{k+1} = (2M)^{\frac{k+1}{2}},$$

$$M \geq \frac{1}{2} \left(-\frac{k+1}{\lambda}\mathcal{H} \right)^{\frac{2}{k+1}} > 0.$$

Next, taking the first and second derivative of M yields

$$\dot{M} = \sum_{n \in \mathbb{Z}} q_n \dot{q}_n$$

$$\ddot{M} = \sum_{n \in \mathbb{Z}} \dot{q}_n^2 + \sum_{n \in \mathbb{Z}} q_n \ddot{q}_n$$

and inserting the differential equation (2.30) or (2.31), respectively, leads to

$$\ddot{M} = 2E_k - 2E_l + \lambda \sum_{n \in \mathbb{Z}} q_n^{k+1}. \quad (2.40)$$

We infer from the definition of the Hamiltonian and energy conservation

$$\frac{-\lambda}{k+1} \sum_{n \in \mathbb{Z}} q_n^{k+1} = \mathcal{H}_0 - E_k - E_l$$

$$\lambda \sum_{n \in \mathbb{Z}} q_n^{k+1} = (k+1)(E_k + E_l - \mathcal{H}_0)$$

and inserting into (2.40) yields

$$\ddot{M} = 2E_k - 2E_l + (k+1)(E_k + E_l - \mathcal{H}_0)$$

$$= (k+3)E_k + (k-1)E_l - (k+1)\mathcal{H}_0.$$

From $k-1 \geq 0$ and $E_l \geq 0$ by Lemma 2.16, we deduce

$$\ddot{M} \geq (k+3)E_k - (k+1)\mathcal{H}_0. \quad (2.41)$$

The Cauchy-Schwarz inequality Theorem 1.4 applied to $\dot{M} = \sum_{n \in \mathbb{Z}} q_n \dot{q}_n$ shows as in Lemma 2.7

$$E_k \geq \frac{\dot{M}^2}{4M}$$

$$(k+3)E_k \geq \frac{k+3}{4} \frac{\dot{M}^2}{M} = (\gamma+1) \frac{\dot{M}^2}{M}.$$

We insert into (2.41) and from

$$\ddot{M} \geq (\gamma+1) \frac{\dot{M}^2}{M} - (k+1)\mathcal{H}_0$$

and the fact that $M \geq \varepsilon$ and $\mathcal{H}_0 < 0$ we finally conclude

$$(\gamma + 1)\dot{M}^2 - \ddot{M}M \leq (k + 1)\mathcal{H}_0M \leq \delta < 0.$$

□

Theorem 2.21 (Concavity Method). *Solutions of the DNKG (2.30) or the DNW (2.31) with $\lambda > 0$, $k \geq 1$ even and $\mathcal{H}_0 < 0$ are not global in time.*

Proof. The proof is analogous to Theorem 2.8. Set

$$N(t) := M^{-\gamma}, \quad \gamma := \frac{k-1}{4}. \quad (2.42)$$

Then by the same calculation as in (2.13) we have

$$\begin{aligned} \dot{N} &= -\gamma M^{-\gamma-1} \dot{M} \\ \ddot{N} &= \gamma M^{-\gamma-2} \left((\gamma + 1)\dot{M}^2 - M\ddot{M} \right). \end{aligned}$$

Due to Lemma 2.20, $M \geq \varepsilon > 0$ and the bracket is negative and bounded away from zero, therefore we conclude that N concave, $N(0) > 0$ and $\ddot{N} \leq \zeta < 0$ and apply Lemma 1.2. We have proven, with the same reasoning as in Theorem 2.8,

$$\lim_{t \rightarrow T_+} M(t) = \infty$$

for some $T_+ < \infty$.

□

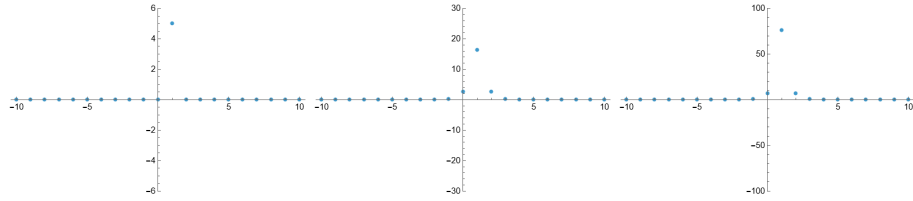


Figure 8: Initial data similar to (2.43) in the setting $m = a = \lambda = 1$ and $k = 2$, fulfilling the conditions of Theorem 2.21, at times $t_1 = 0$, $t_2 = 1$ and $t_3 = 1.35$. Blow up happens at $t \approx 1.5$.

The conditions of Theorem 2.21 are easily fulfilled by initial data of the form

$$q_n(0) = \begin{cases} s & n = 0 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad p(0) \equiv 0 \quad (2.43)$$

for s large enough. We have, using $\sum_{n \in \mathbb{Z}} (\Delta q(0))_n q_n(0) = -2s^2$,

$$E_k = 0, \quad E_l = \frac{2+m^2}{2}s^2, \quad E_p = -\frac{\lambda}{k+1}s^{k+1},$$

thus

$$\mathcal{H} = \frac{2+m^2}{2}s^2 - \frac{\lambda}{k+1}s^{k+1} < 0$$

if and only if $\frac{\lambda}{k+1}s^{k+1} > \frac{2+m^2}{2}s^2$, which is achieved with the choice

$$s > \left(\frac{(2+m^2)(k+1)}{2\lambda} \right)^{\frac{1}{k-1}}.$$

Appendix: Mathematica Code

We present the Mathematica code used to produce the images shown in this thesis, with the exemplary case of the FPUT- α model (see Image 2). We define the Potential ($\alpha = 1$).

```
In[1]:= V[r_] := r^2 / 2 - r^3 / 3;
```

Next, we establish the t and n ranges for our computation.

```
In[2]:= max = 100;
        tmax = 700;
```

We set $q(0)$ and $p(0)$. For any n , we may assign an arbitrary value to $q_n(0)$ with the Piecewise function.

```
In[3]:= q0[n_] := Piecewise[{{0, n == 0}, {0.2, n == 1},
                           {0, n == 2}, ...,}, 0];
        p0[n_] := Piecewise[...]
```

Now we set up the specific, in this case FPUT, differential equation, define the solution space and the Cauchy problem.

```
In[4]:= ode = Flatten[Table[{D[q[n, t], t] == p[n, t], D[p[n, t], t] ==
                           -(V'[q[n, t] - q[n-1, t]] - V'[q[n+1, t] - q[n, t]]},
                           {n, -max, max}] /. {q[-max-1, t] -> q[max, t],
                           q[max+1, t] -> q[-max, t]}];

In[5]:= vars = Flatten[Table[{q[n, t], p[n, t]}, {n, -max, max}]];

In[6]:= eqs = Flatten[{ode, Table[p[n, 0] == p0[n],
                           {n, -max, max}], Table[q[n, 0] == q0[n],
                           {n, -max, max}]}];
```

We solve the system numerically and finally plot the result, choosing appropriate time and range.

```
In[7]:= sol = NDSolve[eqs, vars, {t, 0, tmax}];

In[8]:= ListPlot[Table[{n, q[n, t]}, {n, -10, 10}] /. sol /.
        t -> 100, PlotRange -> {-1, 1}]
```

References

- [1] R. Abraham, J.E. Marsden, and T. Ratiu. *Manifolds, Tensor Analysis, and Applications*. Springer Science Business Media, 1993.
- [2] D. Bambusi and A. Ponno. On metastability in fpu. *Commun.Math. Phys.*, 264:539–561, 2006.
- [3] A. Carati and A. Ponno. Chopping time of the fpu α -model. *Stat Phys*, 170:883–894, 2018.
- [4] R. Carretero-González, D. Frantzeskakis, and P. Kevrekidis. *Nonlinear Waves Hamiltonian Systems: From One To Many Degrees of Freedom, From Discrete To Continuum*. Oxford University Press, 2024.
- [5] K. Deimling. *Ordinary Differential Equations in Banach Spaces*. Springer Berlin, Heidelberg, 1977.
- [6] E. Fermi, J. Pasta, and S. Ulam. *Studies of nonlinear problems*. Los Alamos Sci. Lab. Rept LA-1940, 1955.
- [7] Wattis J.A.D. Friesecke, G. Existence theorem for solitary waves on lattices. *Commun.Math. Phys.*, 161:391–418, 1994.
- [8] R.T. Glassey. Blow-up theorems for nonlinear wave equations. *Math Z*, 132:183–203, 1973.
- [9] H.A. Levine. Some nonexistence and instability theorems for solutions of formally parabolic equations of the form $Pu_t = Au + F(u)$. *Arch. Rational Mech. Anal*, 51:371–386, 1973.
- [10] A. Pankov. *Travelling Waves and Periodic Oscillations in Fermi-Pasta-Ulam Lattices*. The College of William and Mary, 2005.
- [11] P. Poggi and S. Ruffo. Exact solutions in the fpu oscillator chain. *Physica D: Nonlinear Phenomena*, 103:251–272, 1997.
- [12] G. Teschl. *Jacobi Operators and Completely Integrable Nonlinear Lattices*. American Mathematical Society, 2000.
- [13] G. Teschl. *Partial Differential Equations*. American Mathematical Society, in press.
- [14] G. Teschl. *Topics in Linear and Nonlinear Functional Analysis*. American Mathematical Society, in press.
- [15] M. Toda. *Theory of Nonlinear Lattices*. Springer Berlin, Heidelberg, 1989.

- [16] Y. Yang and R. Xu. Finite time blowup for nonlinear klein-gordon equations with arbitrarily positive initial energy. *Applied Mathematics Letters*, 77, 2017.
- [17] E. Zeidler. *Applied Functional Analysis*. Springer New York, NY, 1995.