# Approximations of the lattice dynamics

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# Overview

# Introduction

The Fermi-Pasta-Ulam (PFU) lattice is written in the form

$$\ddot{u}_n = V'(u_{n+1}) - 2V'(u_n) + V'(u_{n-1}), \quad n \in \mathbb{Z}. \tag{1}$$

We consider $V(u)$ in the form

$$V(u) = \frac{1}{2}u^2 + \frac{\epsilon^2}{p+1}u^{p+1}, \tag{2}$$

where $p \geq 2,\ p \in \mathbb{N}$. The equation (1) can be re-written as

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1} + \epsilon^2(u_{n+1}^p - 2u_n^p + u_{n-1}^p), \quad n \in \mathbb{Z}. \tag{3}$$

# Introduction [Cont.]

Using the leading order solution

$$u_n(t) = W\left(\epsilon(n-t), \epsilon^3 t\right) = W\left(\xi, \tau\right), \ \xi = \epsilon(n-t), \quad \text{and} \quad \tau = \epsilon^3 t,$$

FPU lattice equation can be written as a gKDV equation (4)

$$2\,W_\tau + \frac{1}{12} W_{\xi\xi\xi} + (W^p)_\xi = 0. \tag{4}$$

where $p \geq 2, \ p \in \mathbb{N}$.

- Subcritical if $p = 2, 3, 4$
- Critical if $p = 5$
- Supercritical if $p \geq 6$.

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# Outline

1. Introduction
   - Motivation
2. Properties of the gKDV equation
3. Approximations of the Fermi-Pasta-Ulam lattice dynamics
4. Extension of time scale
5. Conclusion

# Motivation

The approximation of the traveling waves in the FPU lattice by the KDV type equation leads to a popular belief that *The nonlinear stability of the FPU traveling waves resembles the orbital stability of the KDV solitary waves*.

- There are some nonlinear potentials which may lead to the KDV type equations whose traveling waves are not stable for all amplitudes.
- If we consider the nonlinear potential (2) we arrive at the generalized KDV equation (4), which is known to have orbitally stable traveling waves for $p = 2, 3, 4$ (subcritical case) and orbitally unstable traveling waves for $p \geq 5$ (critical and supercritical case).
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# Motivation [Cont.]

- *Are the traveling waves of the FPU lattice* (3) *stable, if the traveling waves of the gKDV equation* (4) *are orbitally stable?*

# Properties of the gKDV equation

The gKDV equation admits the solitary wave solution

$$W = (c(p+1))^{\frac{1}{p-1}} \operatorname{sech}^{\frac{2}{p-1}} \left( \sqrt{6c}(p-1)(\eta + B) \right). \tag{5}$$

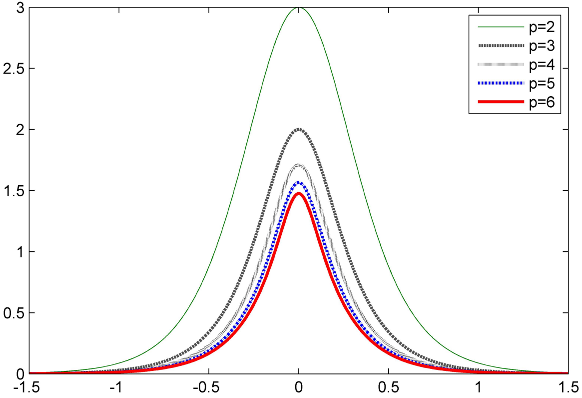


Figure : The solitary wave $W$ for $p = 2, 3, 4, 5, 6$ and $B = 0$.

# Properties of the gKDV equation [Cont.]

The gKDV equation (4) was proved to well posed by

- (locally) T. Kato (1981) in $H^s(\mathbb{R})$ for any $p \geq 2$ and $s > \frac{3}{2}$.
- (locally) C. Kenig, G. Ponce and L. Vega (1991,1993) in $H^s(\mathbb{R})$ with $s \geq \frac{3}{4}$ for $p = 2$, $s \geq \frac{1}{4}$ for $p = 3$, $s \geq \frac{1}{12}$ for $p = 4$, and $s \geq \frac{p-5}{2(p-1)}$ for $p \geq 5$.
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# Outline

# Properties of the gKDV equation [Cont.]

**Theorem 1**

*The Cauchy problem related to the generalized KDV equation* (4) *is globally well posed in* $H^1(\mathbb{R})$, *for* $2 \leq p \leq 4$. *Further more for* $p = 5$ *the gKDV equation* (4) *is well posed in* $H^1(\mathbb{R})$, *with small* $L^2(\mathbb{R})$ *initial data.*

# Outline

# Properties of the gKDV equation [Cont.]

The generalized KDV equation (4) reduces to

- The integrable KDV equation and mKDV equation for $p = 2, 3$ respectively.
- The integrable KDV and mKDV equations possess an infinite number of conserved quantities [R.M. Miura, C.S. Gardner, and M.D. Kruskal(1968), J. Bona, Y. Liu and N. V. Nguyen(2004)].

**Theorem 2**

*There exists a unique global solution to the KDV equation and mKDV equation in $H^s(\mathbb{R})$ for every $s \in \mathbb{N}$. In particular, there exists a constant $C_s$ such that for every $t \in \mathbb{R}$,*

$$||W||_{H^s(\mathbb{R})} \leq C_s.$$

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# Properties of the gKDV equation [Cont.]

- V. Martel, F. Merle and P. Raphaël (2000, 2001, 2002, 2004) showed in a series of papers blow up in the solution $W$ to the critical gKDV equation (4) with $p = 5$ in finite time.
- Theorem 1 excludes blow up for $p = 5$ if the initial data is small in the $L^2(\mathbb{R})$ norm.
- C. Kenig, G. Ponce, and L. Vega (1993) proved a better result for small-norm initial data.

# Properties of the gKDV equation [Cont.]

## Theorem 3

*Let* $p = 5$. *There exists* $\delta > 0$ *such that for any initial* $W_0 \in L^2(\mathbb{R})$ *with*

$$||W_0||_{L^2} < \delta,$$

*there exists a unique strong solution* $W$ *of the Cauchy problem related to the gKDV equation* (4) *satisfying*

$$W \in C(\mathbb{R}; L^2(\mathbb{R})) \cap L^\infty(\mathbb{R}; L^2(\mathbb{R})),$$

*and*

$$\sup_{\xi} \left|\left| \frac{\partial W}{\partial \xi} \right|\right|_{L^2_\tau} \le D < \infty. \tag{6}$$

# Properties of the gKDV equation [Cont.]

**Theorem 4**

*For $p = 5$, the upper bound for the $H^s(\mathbb{R})$ norm of the solution $W$ of the gKDV equation (4) is given by*

$$||W||_{H^s(\mathbb{R})} \leq c_s e^{k_s \int_0^\tau ||W_\xi||_{L^\infty} d\tau}, \tag{7}$$

*where $c_s > 0$ and $k_s > 0$ are constants.*

# Approximations of the Fermi-Pasta-Ulam lattice dynamics

The FPU equation (3) can be written as the FPU system,

$$\begin{cases} \dot{u}_n = q_{n+1} - q_n, \\ \dot{q}_n = u_n - u_{n-1} + \epsilon^2 \left( u_n^p - u_{n-1}^p \right), \end{cases} n \in \mathbb{Z}. \tag{8}$$

Any solution $(u, q) \in C^1(\mathbb{R}, l^2(\mathbb{Z}))$ to the FPU system (8) provides a $C^2(\mathbb{R}, l^2(\mathbb{Z}))$ solution $u$ to the FPU equation (3). The FPU lattice system (8) admit the conserved energy

$$H := \frac{1}{2} \sum_{n \in \mathbb{Z}} \left( q_n^2 + u_n^2 + \frac{2\epsilon^2}{p+1} u_n^{p+1} \right). \tag{9}$$

# Outline

# Approximations of the Fermi-Pasta-Ulam lattice dynamics [Cont...]

**Theorem 5**

*Let* $W \in C([-\tau_0, \tau_0], H^6(\mathbb{R}))$ *be a solution to the gKDV equation* (4) *for any* $\tau_0 > 0$. *Then there exists positive constants* $\epsilon_0$ *and* $C_0$ *such that, for all* $\epsilon \in (0, \epsilon_0)$, *when initial data* $(u_{in,\epsilon}, q_{in,\epsilon}) \in l^2(\mathbb{Z})$ *are given such that*

$$||u_{in,\epsilon} - W(\epsilon\cdot, 0)||_{l^2} + ||q_{in,\epsilon} - P_\epsilon(\epsilon\cdot, 0)||_{l^2} \leq \epsilon^{\frac{3}{2}}, \tag{10}$$

*the unique solution* $(u_\epsilon, q_\epsilon)$ *to the FPU lattice equation* (8) *with initial data* $(u_{in,\epsilon}, q_{in,\epsilon})$ *belongs to* $C^1([-\tau_0\epsilon^{-3}, \tau_0\epsilon^{-3}], l^2(\mathbb{Z}))$ *and satisfy for every* $t \in [-\tau_0\epsilon^{-3}, \tau_0\epsilon^{-3}]$ :

$$||u_\epsilon(t) - W(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} + ||q_\epsilon(t) - P_\epsilon(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} \leq C_0\epsilon^{\frac{3}{2}}. \tag{11}$$

# Approximations of the Fermi-Pasta-Ulam lattice dynamics [Cont...]

**Proof**

- Decompose the solution

$$u_n(t) = W(\epsilon(n-t), \epsilon^3 t) + \mathcal{U}_n(t), \quad q_n = P_\epsilon(\epsilon(n-t), \epsilon^3 t) + \mathcal{P}_n(t), \quad (12)$$

  where $W(\xi, \tau)$ is a smooth solution to the gKDV equation (4)and $P_\epsilon$ is constructed in such a way that $(W, P_\epsilon)$ solves the first equation in system (8) up to the $\mathcal{O}(\epsilon^4)$ terms.

- Substituting the decomposition (12) into the FPU lattice system (8), we obtain the evolutionary problem for the error terms as

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**Proof**

$$\begin{cases} \dot{\mathcal{U}}_n = \mathcal{P}_{n+1} - \mathcal{P}_n + Res_n^1, \\ \dot{\mathcal{P}}_n = \mathcal{U}_n - \mathcal{U}_{n-1} + p\epsilon^2 \left( W(\epsilon(n-t), \epsilon^3 t))^{p-1} \mathcal{U}_n \right. \\ \quad \left. - W(\epsilon(n-1-t), \epsilon^3 t)^{p-1} \mathcal{U}_{n-1} \right) + \mathcal{R}_n(W, \mathcal{U})(t) + Res_n^2(t), \end{cases}$$

- These residual terms can be bounded as

$$\left|\left|Res^1\right|\right|_{l^2} + \left|\left|Res^2\right|\right|_{l^2} \leq C_W \epsilon^{\frac{9}{2}}, \quad (13)$$

and

$$||\mathcal{R}(W, \mathcal{U})||_{l^2} \leq \epsilon^2 C_{W,\mathcal{U}} \, ||\mathcal{U}||_{l^2}^2 \,, \quad (14)$$

where $C_W$ and $C_{W,\mathcal{U}}$ are constant proportional to $||W||_{H^6} + ||W||_{H^6}^p$ and $||W||_{H^6}^{p-2} + ||\mathcal{U}||_{l^2}^{p-2}$ respectively.

# Approximations of the Fermi-Pasta-Ulam lattice dynamics [Cont...]

**Proof**

- Let us define for a fixed $C > 0$ :

$$\mathcal{T}_C := \sup \left\{ T \in [0, \tau_0 \epsilon^{-3}] : \quad \mathcal{Q}(t) \leq C\,\epsilon, \;\; t \in [-T, T] \right\}. \tag{15}$$

- $\mathcal{Q} = E^{\frac{1}{2}}$, and $E$ is defined as:

$$E(t) := \frac{1}{2} \sum_{n \in \mathbb{Z}} \left[ \mathcal{P}_n^2 + \mathcal{U}_n^2 + \epsilon^2 p W(\epsilon(n-t), \epsilon^3 t)^{p-1} \mathcal{U}_n^2(t) \right]. \tag{16}$$

- For $\epsilon_0 < \min \left( 1, ||2pW(\epsilon(\cdot - t))^{p-1}||_{L^\infty}^{-\frac{1}{2}} \right)$, and $\epsilon \in (0, \epsilon_0)$, we have

$$||\mathcal{P}||_{l^2}^2 + ||\mathcal{U}||_{l^2}^2 \leq 4E(t), \;\; t \in (0, \mathcal{T}_C). \tag{17}$$

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# Approximations of the Fermi-Pasta-Ulam lattice dynamics

**Proof**

- Differentiating $E$and then choosing $\mathcal{Q} = E^{\frac{1}{2}}$, we arrive at

$$\left|\frac{d\mathcal{Q}}{dt}\right| \leq \hat{C}_{W,\mathcal{U}}\left(\epsilon^{\frac{9}{2}} + (1+C)\epsilon^3\mathcal{Q}\right),$$

- Using the Gronwall's inequality, we arrive at

$$\mathcal{Q}(t) \leq \left(C_0 + \hat{C}_{W,\mathcal{U}}\tau_0\right)\epsilon^{\frac{3}{2}}e^{(1+C)\hat{C}_{W,\mathcal{U}}\tau_0}, \quad t \in (-\mathcal{T}_C, \mathcal{T}_C). \quad (18)$$

- Finally, choose $\epsilon_0$ sufficiently small such that the bound $\mathcal{Q}(t) \leq C\,\epsilon$ is preserved.

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- Finally, choose $\epsilon_0$ sufficiently small such that the bound $\mathcal{Q}(t) \leq C\,\epsilon$ is preserved.

# Outline

# Main results

From Theorem 2, we know that there exists a constant $c_s$, such that

$$\delta = \sup_{\tau \in [-\tau_0, \tau_0]} ||W(t)||_{H^6} \leq c_s. \tag{19}$$

# Main results

## Theorem 6

*Let $W \in C(\mathbb{R}, H^6(\mathbb{R}))$ be a global solution to the gKDV equation* (4) *with $p = 2, 3$. For fixed $r \in \left(0, \frac{1}{2}\right)$, there exists positive constants $\epsilon_0$ and $C_0$ such that, for all $\epsilon \in (0, \epsilon_0)$, when initial data $(u_{in,\epsilon}, q_{in,\epsilon}) \in l^2(\mathbb{Z})$ are given such that*

$$||u_{in,\epsilon} - W(\epsilon\cdot, 0)||_{l^2} + ||q_{in,\epsilon} - P_\epsilon(\epsilon\cdot, 0)||_{l^2} \leq \epsilon^{\frac{3}{2}}, \tag{20}$$

*the unique solution $(u_\epsilon, q_\epsilon)$ to the FPU lattice equation* (8) *with initial data $(u_{in,\epsilon}, q_{in,\epsilon})$ belongs to $C^1\left(\left[-\frac{r|\log(\epsilon)|}{k_0}\epsilon^{-3}, \frac{r|\log(\epsilon)|}{k_0}\epsilon^{-3}\right], l^2(\mathbb{Z})\right)$, where $k_o$ is $\epsilon$-independent and $(u_\epsilon, q_\epsilon)$ satisfy*

$$||u_\epsilon(t) - W(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} + ||q_\epsilon(t) - P_\epsilon(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} \leq C_0\epsilon^{\frac{3}{2}-r}, \tag{21}$$

*for every $t \in \left[-\frac{r|\log(\epsilon)|}{k_0}\epsilon^{-3}, \frac{r|\log(\epsilon)|}{k_0}\epsilon^{-3}\right]$.*

# Main results

**Proof**

- Following the same lines as in Theorem 5 and using equation (19), we arrive at

$$\mathcal{Q}(t) \leq \left( \mathcal{Q}(0) + \frac{C_\delta}{k_0} \epsilon^{\frac{3}{2}} \right) e^{k_0 \tau_0(\epsilon)}. \tag{22}$$

- To achieve the required extension of time interval, we assume that

$$e^{k_0 \tau_0(\epsilon)} = \frac{\mu}{\epsilon^r}, \tag{23}$$

where $\mu$ is a fixed constant and so is $r \in \left(0, \frac{1}{2}\right)$.

- Finally, we arrive at

$$\mathcal{Q}(t) \leq C \epsilon^{\frac{3}{2} - r}, \tag{24}$$

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# Main results

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# Outline

# Previous result

Let us assume that there exist $C_s$ and $k_s$ such that

$$\delta(\tau_0) = \sup_{\tau \in [-\tau_0, \tau_0]} ||W(\cdot, \tau)||_{H^6} \leq C_s e^{k_s \tau_0}. \tag{25}$$

# Main results

## Theorem 7

*Let* $W \in C(\mathbb{R}, H^6(\mathbb{R}))$ *be a global solution to the gKDV equation* (4) *for* $p = 5$. *For fixed* $r \in \left(0, \frac{1}{2}\right)$ *there exist positive constants* $\epsilon_0$ *and* $C_0$ *such that, for all* $\epsilon \in (0, \epsilon_0)$, *when initial data* $(u_{in,\epsilon}, q_{in,\epsilon}) \in l^2(\mathbb{Z})$ *are given such that*

$$||u_{in,\epsilon} - W(\epsilon\cdot, 0)||_{l^2} + ||q_{in,\epsilon} - P_\epsilon(\epsilon\cdot, 0)||_{l^2} \le \epsilon^{\frac{3}{2}}, \tag{26}$$

*the unique solution* $(u_\epsilon, q_\epsilon)$ *to the FPU lattice equation* (8) *with initial data* $(u_{in,\epsilon}, q_{in,\epsilon})$ *belongs to* $C^1\left(\left[-\frac{1}{2k_s(p-1)}\log(|\log(\epsilon)|)\epsilon^{-3}, \frac{1}{2k_s(p-1)}\log(|\log(\epsilon)|)\epsilon^{-3}\right], l^2(\mathbb{Z})\right)$, *where* $k_s$ *is* $\epsilon$*-independent , and satisfy*

$$||u_\epsilon(t) - W(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} + ||q_\epsilon(t) - P_\epsilon(\epsilon(\cdot - t), \epsilon^3 t)||_{l^2} \le C_0\epsilon^{\frac{3}{2} - r}, \tag{27}$$

*for every* $t \in \left[-\frac{1}{2k_s(p-1)}\log(|\log(\epsilon)|)\epsilon^{-3}, \frac{1}{2k_s(p-1)}\log(|\log(\epsilon)|\epsilon^{-3}\right]$.

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- Following the same lines as in the Proof of Theorem 5 and using (25), we arrive at

$$\mathcal{Q}(t) \leq \left( \mathcal{Q}(0) + \tilde{\tilde{\mathcal{C}}} \epsilon^{\frac{3}{2}} \right) e^{\frac{\mathcal{C}_s}{2(p-1)k_s}(e^{2(p-1)k_s \tau_0} - 1)}. \quad (28)$$

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we established the following results.

- In Theorem 2, we showed that the upper bound on the $H^s(\mathbb{R})$ norm of the solution of the gKDV equation (4) with $p = 2, 3$ does not depend on time for any $s \in \mathbb{N}$.
- In Theorem 4, we showed that the upper bound on the $H^s(\mathbb{R})$ norm of the solution of the gKDV equation (4) with $p = 5$ grows like

$$||W||_{H^s(\mathbb{R})} \leq c_s e^{k_s \int_0^\tau ||W_\xi||_{L^\infty} d\tau}.$$

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- In Theorem 5, we approximated dynamics of the FPU lattice (8) with solutions of the gKDV equation (4) on standard time scale.
- In Theorem 6 and 7, we approximated dynamics of the FPU lattice (8) with solutions of the gKDV equation (4) for $p = 2, 3, 5$ on extended time scale.

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# Approximations of the Fermi-Pasta-Ulam lattice dynamics

Based on our results we claim the following

- Solitary waves of the FPU lattice (8) with $p = 2, 3$ can be approximated by the stable solitary waves of the gKDV equation (4) with $p = 2, 3$ on an extended time interval up to $\mathcal{O}(|\log(\epsilon)|\epsilon^{-3})$.
- Dynamics of small-norm solution to the FPU lattice (8) with $p = 5$ can be approximated by globally small-norm solution to the gKDV equation (4) with $p = 5$ on an extended time interval up to $\mathcal{O}(\log|\log(\epsilon)|\epsilon^{-3})$.

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# Approximations of the Fermi-Pasta-Ulam lattice dynamics

Finally, we present open problems which are left for further studies

- We are not able to extend the time scale of the gKDV equation (4) with $p = 4$ by a logarithmic factor. The difficulty is that we ere unable to find suitable energy estimate on the growth of $||W||_{H^6}$.
- Another problem is that the result of Theorem 7 for $p = 5$ excludes the solitary waves because the initial data has small $L^2(\mathbb{R})$ norm.
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