Approximations of dynamics of nonlinear lattices on the extended time scale

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Introduction

Asymptotic approximations of the lattice dynamics are obtained by using reduction of lattice differential equations to evolution equations.

- Small-amplitude uni-directional long travelling waves of the Fermi–Pasta–Ulam lattice are reduced to the KdV equation.

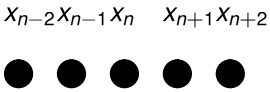
  G. Schneider–C.E. Wayne (2000); D. Bambusi–A. Ponno (2006).

- Small-amplitude envelopes of discrete breathers of the Klein–Gordon lattice are reduced to the discrete NLS equation.

  G. James (2003); D.P.–T.Penati–S.Paleari (2015)

Main question: Can these reductions be useful to obtain existence and stability of coherent states (travelling solitons and discrete breathers) in lattice differential equations?

The FPU chain



Newton's equations define the FPU (Fermi-Pasta-Ulam) lattice:

$$\frac{d^2 x_n}{dt^2} = V'(x_{n+1} - x_n) - V'(x_n - x_{n-1}), \quad n \in \mathbb{Z},$$

where x_n is the displacement of the nth particle from an equilibrium and $V(u)$ is the interaction potential defined in $u_n = x_{n+1} - x_n$.

Let us consider the example of a slightly unharmonic potential:

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

where ε is a small parameter and $p \geq 2$ is an integer.

Formal derivation of the KdV equation

Consider the FPU lattice for relative displacements $u_n := x_{n+1} - x_n$,

$$\frac{d^2 u_n}{dt^2} - (\Delta u)_n = \varepsilon^2 (\Delta u^p)_n, \quad n \in \mathbb{Z},$$

where $(\Delta u)_n = u_{n+1} - 2u_n + u_{n-1}$.

Using the asymptotic multi-scale expansion

$$u_n(t) = W(\varepsilon(n-t), \varepsilon^3 t) + \text{error terms},$$

we derive the generalized KdV equation at the order $\mathcal{O}(\varepsilon^4)$

$$2\partial_\tau W + \frac{1}{12}\partial_\xi^3 W + \partial_\xi W^p = 0.$$

There exists a positive solitary wave for every $p \geq 2$.

Justification of the KdV approximation

Theorem 1 (Schneider-Wayne, 2000; E.Dumas–D.P., 2014)

Let $W \in C([-\tau_0,\tau_0], H^s(\mathbb{R}))$ be a solution to the KdV equation for some integer $s \geq 6$ and some $\tau_0 > 0$. There exist positive constants ε_0 and C_0 s.t. for all $\varepsilon \in (0,\varepsilon_0)$, when initial data $u_{\mathrm{ini},\varepsilon} \in l^2(\mathbb{R})$ are given s.t.

$$\|u_{\mathrm{ini},\varepsilon} - W(\varepsilon\cdot,0)\|_{l^2} \leq \varepsilon^{3/2},$$

the unique solution u_ε to the FPU lattice belongs to $C^1([-\tau_0\varepsilon^{-3},\tau_0\varepsilon^{-3}], l^2(\mathbb{Z}))$ and satisfies

$$\|u_\varepsilon(t) - W(\varepsilon(\cdot - t),\varepsilon^3 t)\|_{l^2} \leq C_0\varepsilon^{3/2}, \quad t \in \left[-\tau_0\varepsilon^{-3},\tau_0\varepsilon^{-3}\right].$$

Remarks:

- The proof relies on the energy method and Gronwall inequality.
- The result suggests correlation between stability of KdV and FPU travelling waves.

Approximate nonlinear stability of FPU solitons

Theorem 2 (E.Dumas–D.P., 2014)

For every $\tau_0 > 0$*, there exist positive constants* ε_0*,* δ_0 *and* C_0 *s.t. for all* $\varepsilon \in (0, \varepsilon_0)$*, when initial data* $u_{\mathrm{ini},\varepsilon} \in l^2(\mathbb{R})$ *satisfy* $\delta := \|u_{\mathrm{ini},\varepsilon} - u_{\mathrm{trav},\varepsilon}(0)\|_{l^2} \leq \delta_0$*, then the unique solution* u_ε *to the FPU lattice belongs to* $C^1([-\tau_0\varepsilon^{-3}, \tau_0\varepsilon^{-3}], l^2(\mathbb{Z}))$ *and satisfies*

$$\|u_\varepsilon(t) - u_{\mathrm{trav},\varepsilon}(t)\|_{l^2} \leq C_0\delta, \quad t \in \left[-\tau_0\varepsilon^{-3}, \tau_0\varepsilon^{-3}\right].$$

Remarks:

- The proof relies on the energy method and Gronwall inequality.
- The travelling waves of the FPU lattice are stable w.r.t. modulations of any spatial scales, up to the time scale of $\mathcal{O}(\varepsilon^{-3})$.

Discussion

What is known about the generalized KdV equation?

$$2\partial_\tau W + \frac{1}{12}\partial_\xi^3 W + \partial_\xi W^p = 0.$$

- KdV solitary waves are orbitally stable for $p = 2, 3, 4$ and unstable for $p \geq 5$.
- Global solutions exists in $H^s(\mathbb{R})$ for $s \geq 1$ for $p = 2, 3, 4$ and, if the norm in $H^{s_0}(\mathbb{R})$ is small, $s_0 = \frac{p-5}{2(p-1)}$, for $p \geq 5$.

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Contradiction?

- Result of Theorem 1 suggests correlation of stability of FPU solitons and KdV solitons for $p \geq 2$.
- Result of Theorem 2 suggests stability of all small FPU travelling waves up to the time scale of $\mathcal{O}(\varepsilon^{-3})$ for any $p \geq 2$.

Proof of (Stability) Theorem 2

The scalar FPU lattice equation can be written in the vector form

$$\left\{ \begin{array}{l} \dot{u}_n = p_{n+1} - p_n, \\ \dot{p}_n = V'(u_n) - V'(u_{n-1}), \end{array} \right. \qquad n \in \mathbb{Z}.$$

The energy functional is conserved at any $(u,p) \in C^1(\mathbb{R}, l^2(\mathbb{Z}))$:

$$H := \sum_{n \in \mathbb{Z}} \frac{1}{2} p_n^2 + \frac{1}{2} u_n^2 + \frac{\varepsilon^2}{p+1} u_n^{p+1}.$$

Let $(u_{\rm trav}, p_{\rm trav}) \in C^1(\mathbb{R}, l^2(\mathbb{Z}))$ denote the travelling wave to the FPU lattice with the speed c. Then, $u_{\rm trav}(t) = u_{\rm stat}(n - ct)$ satisfy

$$\left\{ \begin{array}{l} -c u'_{\rm stat}(z) = p_{\rm stat}(z+1) - p_{\rm stat}(z), \\ -c p'_{\rm stat}(z) = V'(u_{\rm stat}(n-ct)) - V'(u_{\rm stat}(n-1-ct)), \end{array} \right. \qquad z \in \mathbb{R}.$$

Decomposition and the energy method

For any fixed c, we decompose

$$u(t) = u_{\mathrm{trav}}(t) + \mathcal{U}(t), \quad p(t) = p_{\mathrm{trav}}(t) + \mathcal{P}(t),$$

such that $H = H_0 + H_1 + H_2 + H_R$ with

$$\begin{aligned}
H_0 &= \frac{1}{2}\sum_{n\in\mathbb{Z}} p_{\mathrm{stat}}^2(n-ct) + \sum_{n\in\mathbb{Z}} V(u_{\mathrm{stat}}(n-ct)), \\
H_1 &= \sum_{n\in\mathbb{Z}} p_{\mathrm{stat}}(n-ct)\mathcal{P}_n + \sum_{n\in\mathbb{Z}} V'(u_{\mathrm{stat}}(n-ct))\,\mathcal{U}_n, \\
H_2 &= \frac{1}{2}\sum_{n\in\mathbb{Z}} \mathcal{P}_n^2 + \frac{1}{2}\sum_{n\in\mathbb{Z}} V''(u_{\mathrm{stat}}(n-ct))\,\mathcal{U}_n^2,
\end{aligned}$$

and

$$|H_R| \leq C_\rho \sup_{z\in\mathbb{R}} |V'''(u_{\mathrm{stat}}(z))|\, \|\mathcal{U}\|_{l^2}^3 \leq C_\rho \varepsilon^2 \|\mathcal{U}\|_{l^2}^3,$$

as long as $\|\mathcal{U}\|_{l^2} \leq \rho$.

Energy estimates

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- H_1 is controlled in terms of H_2:

$$\frac{dH_1}{dt} = \frac{c}{2}\sum_{n\in\mathbb{Z}} u'_{\mathrm{stat}}(n-ct)V'''(u_{\mathrm{stat}}(n-ct))\left(\mathcal{U}_n^2 + \mathcal{O}(\mathcal{U}_n^3)\right).$$

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Hence, we have

$$\left|\frac{dH_1}{dt}\right| \leq C_\rho \varepsilon^3 \|\mathcal{U}\|_{l^2}^2 \leq 2C_\rho \varepsilon^3 H_2,$$

and

$$H_1(t) - H_1(0) \geq -2C_\rho \varepsilon^3 \int_0^{|t|} H_2(t')dt'.$$

End of the proof of Theorem 2

By using the energy expansion, we have

$$H - H_0 - H_1(0) \geq -2C_\rho \varepsilon^3 \int_0^{|t|} H_2(t')dt' + H_2(t)(1 - C_\rho \varepsilon^2 \rho).$$

By Gronwall's inequality, we obtain

$$H_2(t) \leq \frac{H - H_0 - H_1(0)}{1 - C_\rho \varepsilon^2 \rho} e^{2C_\rho \varepsilon^3 |t|} \leq \frac{H_2(0) + H_R(0)}{1 - C_\rho \varepsilon^2 \rho} e^{2C_\rho \varepsilon^3 |t|} \leq \tilde{C}_\rho^2 \delta^2 e^{2C_\rho \tau_0}.$$

Theorem 2 is proved in the ball in $l^2(\mathbb{Z})$ with radius $\rho := C_0 \delta$, where

$$C_0 := \tilde{C}_\rho e^{C_\rho \tau_0}.$$

Remark: The proof of nonlinear stability uses the KdV limit scaling of small ε, but does not rely on the stability of KdV travelling waves.

Proof of (Justification) Theorem 1

Let us now use the decomposition

$$u_n(t) = W(\varepsilon(n-t), \varepsilon^3 t) + \mathcal{U}_n(t), \quad p_n(t) = P(\varepsilon(n-t), \varepsilon^3 t) + \mathcal{P}_n(t),$$

where $W(\xi, \tau)$ is a solution of the generalized KdV equation

$$2\partial_\tau W + \frac{1}{12}\partial_\xi^3 W + \partial_\xi W^p = 0.$$

and $P(\xi, \tau)$ satisfies the approximation problem

$$P(\xi + \varepsilon, \tau) - P(\xi, \tau) = -\varepsilon \partial_\xi W + \varepsilon^3 \partial_\tau W,$$

up to and including the order of $\mathcal{O}(\varepsilon^4)$.

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The perturbation terms satisfy

$$\begin{aligned}
\dot{\mathcal{U}}_n(t) &= \mathcal{P}_{n+1}(t) - \mathcal{P}_n(t) + \varepsilon^5 \mathrm{Res}_n^{(1)}(t), \\
\dot{\mathcal{P}}_n(t) &= \mathcal{P}_n(t) - \mathcal{P}_{n-1}(t) + p\varepsilon^2 W^{p-1}\mathcal{U}_n(t) - p\varepsilon^2 W(\cdot - \varepsilon)^{p-1}\mathcal{U}_{n-1}(t) \\
&\quad + \varepsilon^2 \mathcal{R}_n(W, \mathcal{U})(t) + \varepsilon^5 \mathrm{Res}_n^{(2)}(t),
\end{aligned}$$

where $R(W, \mathcal{U})$ is quadratic in $\mathcal{U}$ in the $l^2(\mathbb{Z})$ norm.

Energy estimates

Approximation Lemma:

There exists $C > 0$ such that for all $X \in H^1(\mathbb{R})$ and $\varepsilon \in (0,1]$,

$$\|x\|_{l^2} \leq C\varepsilon^{-1/2}\|X\|_{H^1},$$

where $x_n := X(\varepsilon n)$, $n \in \mathbb{Z}$.

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The energy quadratic form is

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

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The energy balance equation:

$$\left|\frac{d\mathcal{E}}{dt}\right| \leq C_W \mathcal{E}^{1/2}\left(\varepsilon^{9/2} + \varepsilon^3\mathcal{E}^{1/2} + \varepsilon^2\mathcal{E}\right),$$

where C_W depends on $\|W\|_{H^6}$.

End of the proof of Theorem 1

Let $\mathcal{Q} := \mathcal{E}^{1/2}$ and the time span be defined by

$$\mathcal{T}_C(\varepsilon) := \sup\left\{ T_0 \in (-\tau_0\varepsilon^{-3}, \tau_0\varepsilon^{-3}] : \quad \mathcal{Q}(t) \le C\varepsilon, \; t \in [-T_0, T_0] \right\}.$$

Then, the energy balance estimate is

$$\left| \frac{d\mathcal{Q}}{dt} \right| \le C_W \left(\varepsilon^{9/2} + \varepsilon^3 (1 + C) \mathcal{Q} \right)$$

By Gronwall's inequality, we obtain

$$\mathcal{Q}(t) \le \left(\mathcal{Q}(0) + C_W \varepsilon^{9/2} |t| \right) e^{C_W (1+C) \varepsilon^3 t}, \quad t \in (-\mathcal{T}_C, \mathcal{T}_C).$$

Since $\mathcal{Q}(0) \le \varepsilon^{3/2}$ and $\varepsilon^{3/2} \ll \varepsilon$, then $\mathcal{T}_C$ is extended to the full time span $\tau_0 \varepsilon^{-3}$ with the constant

$$C_0 := (1 + C_W \tau_0)\, e^{C_W (1+C) \tau_0}.$$

Discussion

Recall that from the generalized KdV equation

$$2\partial_\tau W + \frac{1}{12}\partial_\xi^3 W + \partial_\xi W^p = 0,$$

KdV solitary waves are orbitally stable for $p = 2, 3, 4$ and unstable for $p \geq 5$.

Is there a contradiction?

- Result of Theorem 1 suggests correlation of stability of FPU solitons and KdV solitons for $p \geq 2$.
- Result of Theorem 2 suggests stability of all small FPU travelling waves up to the time scale of $\mathcal{O}(\varepsilon^{-3})$ for any $p \geq 2$.

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There is no contradiction:
C_0 depends exponentially on τ_0 in both theorems.

KdV approximation on the extended time span

For the modified KdV equations ($p = 2, 3$), integrability implies

$$\exists C_s > 0 : \quad \|W(\cdot, \tau)\|_{H^s} \leq C_s \quad \forall \tau,$$

for every integer s.

Theorem 3 (A.Khan–D.P., 2015)

Let $W \in C(\mathbb{R}, H^6(\mathbb{R}))$ be a global solution to the KdV equation with $p = 2, 3$. For fixed $r \in (0, \frac{1}{2})$, there exist positive constants ε_0 and C_0 s.t. for all $\varepsilon \in (0, \varepsilon_0)$, when initial data $u_{\mathrm{ini},\varepsilon} \in l^2(\mathbb{R})$ are given s.t.

$$\|u_{\mathrm{ini},\varepsilon} - W(\varepsilon \cdot, 0)\|_{l^2} \leq \varepsilon^{3/2},$$

the unique solution u_ε to the FPU lattice belongs to $C^1([-\tau_0 \varepsilon^{-3}, \tau_0 \varepsilon^{-3}], l^2(\mathbb{Z}))$ with $\tau_0 = \mathcal{O}(|\log(\varepsilon)|)$ and satisfies

$$\|u_\varepsilon(t) - W(\varepsilon(\cdot - t), \varepsilon^3 t)\|_{l^2} \leq C_0 \varepsilon^{3/2 - r}, \quad t \in \left[-\tau_0 \varepsilon^{-3}, \tau_0 \varepsilon^{-3}\right].$$

Proof of Theorem 3

It is the same framework as in the (Justification) Theorem 1. The initial time span is defined by

$$\mathcal{T}_C(\varepsilon) := \sup\left\{ T_0 \in (-\tau_0(\varepsilon)\varepsilon^{-3}, \tau_0(\varepsilon)\varepsilon^{-3}] : \quad \mathcal{Q}(t) \leq C\varepsilon,\ t \in [-T_0, T_0] \right\}.$$

where τ_0 depends on ε.

Then, the energy balance estimate is

$$\left|\frac{d\mathcal{Q}}{dt}\right| \leq C_s\varepsilon^{9/2} + \varepsilon^3 k_s \mathcal{Q},$$

where k_s depends on C_s and C.

By Gronwall's inequality, we obtain

$$\mathcal{Q}(t) \leq \left(\mathcal{Q}(0) + C_s k_s^{-1}\varepsilon^{3/2}\right) e^{k_s\varepsilon^3 t}, \quad t \in (-\mathcal{T}_C, \mathcal{T}_C).$$

If $\tau_0(\varepsilon)$ is chosen s.t. $e^{k_s\tau_0(\varepsilon)} = \mu\varepsilon^{-r}$ for an ε-independent μ, then

$$\mathcal{Q}(t) \leq \left(1 + C_s k_s^{-1}\right)\mu\varepsilon^{\frac{3}{2}-r}, \quad t \in (-\mathcal{T}_C, \mathcal{T}_C).$$

Discussion

The initial time span $\mathcal{T}_C$ is extended to the full time span $\tau_0(\varepsilon)\varepsilon^{-3}$ with the ε-independent constant

$$C_0 := \mu(1 + C_s k_s^{-1}).$$

The KdV time $\tau_0(\varepsilon) = r k_s^{-1} |\log(\varepsilon)| + \mathcal{O}(1)$ is large as $\varepsilon \to 0$. Thus, the approximation result

$$\|u_\varepsilon(t) - W(\varepsilon(\cdot - t), \varepsilon^3 t)\|_{l^2} \leq C_0 \varepsilon^{3/2-r}, \quad t \in \left[-\tau_0 \varepsilon^{-3}, \tau_0 \varepsilon^{-3}\right]$$

holds uniformly on the logarithmically large time scale.

The approximation result justifies also nonlinear stability of small-amplitude FPU solitons with respect to perturbations of the same spatial scale on the time scale of $\mathcal{O}(\varepsilon^{-3})$.

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The approximation result justifies also nonlinear stability of small-amplitude FPU solitons with respect to perturbations of the same spatial scale on the time scale of $\mathcal{O}(\varepsilon^{-3})$.

Remark: Similar extension of the KdV approximation can be obtained even if $\|W(\cdot,\tau)\|_{H^s}$ grows at most exponentially in τ, which may be relevant for the generalized KdV equation with $p \geq 4$.

The Klein–Gordon chain

Coupled nonlinear oscillators satisfy the discrete KG equation

$$\frac{d^2 x_n}{dt^2} + x_n + x_n^3 = \varepsilon(x_{n+1} - 2x_n + x_{n-1}), \quad n \in \mathbb{Z},$$

where $V(u)$ is the onsite potential and ε is the coupling constant.

Using the asymptotic multi-scale expansion

$$u_n(t) = \varepsilon^{1/2} X_n(t) + \text{error terms}, \quad X_n(t) := a_n(\varepsilon t)e^{it} + \bar{a}_n(\varepsilon t)e^{-it},$$

we derive the discrete NLS equation at the order $\mathcal{O}(\varepsilon^{3/2})$

$$2i\dot{a}_n + 3|a_n|^2 a_n = a_{n+1} - 2a_n + a_{n-1}, \quad n \in \mathbb{Z}.$$

Solitary waves of dNLS correspond to discrete breathers of KG.

Justification of the dNLS approximation

Theorem 4 (D.P.-Penati–Paleari, 2015)

For every $\tau_0 > 0$, there are positive constants C_0 and ε_0 such that for every $\varepsilon \in (0, \varepsilon_0)$, for which the initial data satisfies

$$\|\mathbf{u}(0) - \varepsilon^{1/2}\mathbf{X}(0)\|_{l^2} \leq \varepsilon^{3/2},$$

the solution of the dKG equation satisfies for every $t \in [-\tau_0\varepsilon^{-1}, \tau_0\varepsilon^{-1}]$,

$$\|\mathbf{u}(t) - \varepsilon^{1/2}\mathbf{X}(t)\|_{l^2} \leq C_0\varepsilon^{3/2}.$$

Remarks:

- The constant C_0 again grows exponentially in τ_0.
- The proof relies on the energy method and Gronwall inequality.

Extended time scale

To relate existence and stability of discrete breathers in

$$\frac{d^2 x_n}{dt^2} + x_n + x_n^3 = \varepsilon(x_{n+1} - 2x_n + x_{n-1}), \quad n \in \mathbb{Z},$$

with existence and stability of discrete solitons in

$$2i\dot{a}_n + 3|a_n|^2 a_n = a_{n+1} - 2a_n + a_{n-1}, \quad n \in \mathbb{Z}.$$

we can justify the dNLS approximation on the logarithmically extended time scale $\mathcal{O}(|\log(\varepsilon)|\varepsilon^{-1})$. This is always possible since solutions of the dNLS equation enjoy global estimates in $\ell^2(\mathbb{Z})$ norm.

Remark: dNLS approximation is different from the tools developed in the anti-continuum limit $\varepsilon \to 0$ for nearly compact KG breathers.