Justification of the KdV, KP-II, and Toda equations from the Fermi–Pasta–Ulam particle system

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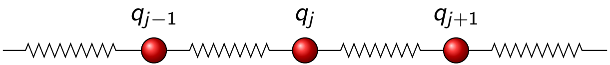
The Fermi-Pasta-Ulam particle system



- System of particles on the line
- Hamiltonian for nearest neighbour interactions is given by $H = \sum_j \frac{1}{2}\dot{q}_j^2 + V(q_{j+1} - q_j)$
- Equations of motion are given by $\ddot{q}_j = V'(q_{j+1} - q_j) - V'(q_j - q_{j-1})$
- Potential $V(q) = \frac{1}{2}q^2 + \frac{1}{3}\alpha q^3 + \frac{1}{4}\beta q^4 + \dots$
- Numerical experiments showed long-time recurrent formations of solitary waves (FPU, 1955)

Main question: Can we describe dynamics by reducing the FPU to an integrable system?

KdV limit for small-amplitude and long-scale waves

- Ansatz in the strain variables:

$$r_j(t) = q_{j+1}(t) - q_j(t) := \varepsilon^2 R\left(\varepsilon\left(j-t\right), \varepsilon^3 t\right) + \mathrm{error}$$

- Approximation satisfies the FPU system up to $O(\varepsilon^6)$ if R satisfies the KdV equation:

$$\partial_\tau R + \alpha R \partial_\xi R + \frac{1}{24}\partial_\xi^3 R = 0$$

KdV is an integrable system with asymptotic stability of solitons and stability of periodic solutions.

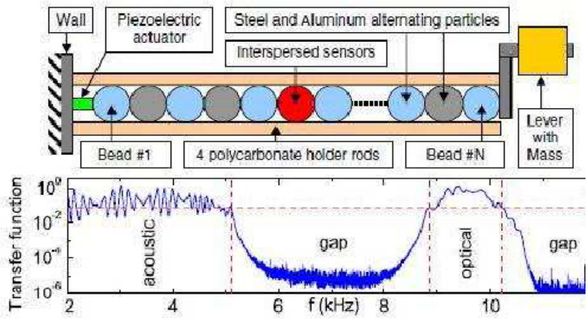
- First derivation: N. Zabusky and M. Kruskal (1965)
- Rigorous justification:
  Schneider–Wayne (1999), Friesecke–Pego (1999-2004), Bambusi–Ponno (2005-2006)
- Follow-up: generalized KdV (Dumas–P., 2014), KdV on extended time intervals (Khan–P, 2017), polyatomic case (Gaison–Moskow–Wright–Zhang, 2014), nonlocal interaction (Herrmann–Mikikits–Leitner, 2016), and more. Recent: Hong–Kwak–Yang, ARMA (2021)

Algorithm for justification of reduced models from FPU models

1. Find the best coordinates to transform the problem.
2. Check that the reduced model formally arises in the appropriate limit of the transformed equations.
3. Define **error terms** to **the leading-order terms** and obtain **residual equations**.
4. Control the error terms from the residual equations in suitable norms by using the energy conservation, approximation estimates, and Gronwall inequality.
5. Check that the reduced models have smooth solutions which are compatible with the estimates.

I will illustrate this algorithm with three recent examples.

Case Study 1: Modeling of granular chains



- Granular chains contain densely packed, elastically interacting particles with Hertzian forces.
- N. Boechler, G. Theocharis, P.G. Kevrekidis, M.A. Porter, C. Daraio (2001-present days).

Logarithmic KdV equation

Granular chains are modeled with Newton's equations of motion:

$$\ddot{q}_j = V'(q_{j+1} - q_j) - V'(q_j - q_{j-1})$$

where V is the contact interaction potential for spherical beads (H. Hertz, 1882):

$$V(q) = \begin{cases} |q|^{1+\alpha}, & q < 0, \\ 0, & q > 0 \end{cases} \qquad \alpha = \frac{3}{2}.$$

For beads with hollows, $\alpha \to 1$. If $\alpha = 1 + \epsilon^2$, then one can write for $r_j = -(q_{j+1} - q_j) \geq 0$:

$$\ddot{r}_j - \Delta r_j = \Delta \left[r_j \left(|r_j|^{\epsilon} - 1 \right) \right] = \epsilon \, \Delta r_j \log r_j + \mathcal{O}(\epsilon^2).$$

If $r_j(t) = R(\xi, \tau) + \text{error}$ with $\xi := 2\sqrt{3}\epsilon \, (j - t)$, $\tau := \sqrt{3}\epsilon^3 \, t$, then we obtain the log-KdV equation

$$\partial_\tau R + \partial_\xi (R \log R) + \partial_\xi^3 R = 0.$$

A.Chatterjee (1999); G.James–D.P (2014).

Justification of log-KdV

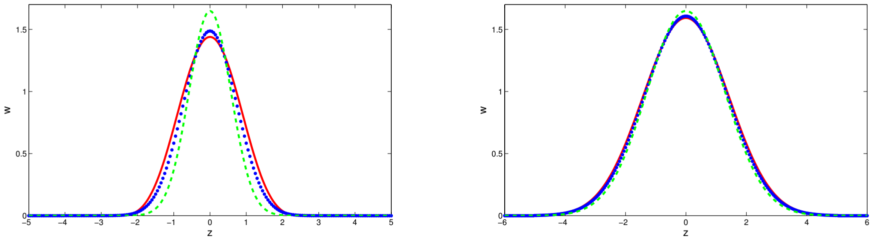


Figure: Solitary waves of the FPU system (blue) in comparison with the Gaussian solitons of the log-KdV equation (green) for $\alpha = 1.5$ (left) and $\alpha = 1.1$ (right).

$$\partial_\tau R + \partial_\xi (R \log R) + \partial_\xi^3 R = 0 \quad \Rightarrow \quad R(\xi,\tau) = c e^{-(\xi - c\tau)^2/4 + 1/2}.$$

Justification of log-KdV

1. Find the best coordinates to transform the problem.
2. Check that the reduced model formally arises in the appropriate limit of the transformed equations.
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Justification of log-KdV

Theorem (R. Carles–D.P, 2014)

For any $R_0 \in X$ in the set

$$X := \left\{ R \in H^1(\mathbb{R}) : \quad R\sqrt{|\log|R||} \in L^2(\mathbb{R}) \right\}.$$

there exists a global solution $R \in L^\infty(\mathbb{R}, X)$ to the log–KdV equation such that

$$\|R(\tau,\cdot)\|_{L^2} \leq \|R_0\|_{L^2}, \quad E(R(\tau,\cdot)) \leq E(R_0), \quad \text{for all} \quad \tau > 0,$$

where

$$E(R) = \frac{1}{2}\int_{\mathbb{R}} \left[(R_\xi)^2 - R^2 \log|R| \right] d\xi.$$

A way around the problem is to consider pre-compression with strictly positive solutions: $R(\tau,\xi) \geq R_0 > 0$ for every (τ,ξ).

Justification of log-KdV

Theorem (E. Dumas–D.P, 2014)

Let $R \in C^0([0,\tau_0], H^s_{\rm loc}(\mathbb{R}))$ be a solution of the log–KdV equation for some $s \geq 6$ and $\tau_0 > 0$ such that $R(t,\cdot) \geq R_0 > 0$ for $\tau \in [0,\tau_0]$. Then there exist $\epsilon_0 > 0$ and $C_0 > 0$ such that for every $\epsilon \in (0,\epsilon_0)$, the unique solution $r \in C^1([0,\tau_0/\epsilon^3], \ell^2(\mathbb{Z}))$ with appropriately choosen initial data satisfies

$$\|r(t) - R(2\sqrt{3}\epsilon(\cdot - t), \sqrt{3}\epsilon^3 t)\|_{\ell^2} \leq C_0 \epsilon^{3/2}, \quad t \in [0,\tau_0/\epsilon^3].$$

The approximation result between solutions on the grid and solutions on the line is given by

$$\|u\|_{\ell^2(\mathbb{Z})} \leq C_s \varepsilon^{-1/2} \|U\|_{H^s(\mathbb{R})},$$

where $u_j = U(\varepsilon j)$ with $U \in H^s(\mathbb{R})$ for integer $s \geq 1$.

Proof of the approximation result

Lemma

$$\|u\|_{\ell^2(\mathbb{Z})} \leq C_s \varepsilon^{-1/2} \|U\|_{H^s(\mathbb{R})},$$

where $u_j = U(\varepsilon j)$ *with* $U \in H^s(\mathbb{R})$ *for integer* $s \geq 1$.

The proof is based on the Fourier transform

$$\hat{u}(\theta) := \sum_{j \in \mathbb{Z}} u_j e^{-ij\theta}, \quad u_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{u}(\theta) e^{ij\theta},$$

and

$$\begin{aligned} u_j &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{U}(k)\, e^{ik\epsilon j} \mathrm{d}k = \frac{1}{2\pi\epsilon} \int_{-\infty}^{\infty} \hat{U}\left(\frac{p}{\epsilon}\right) e^{ipj} \mathrm{d}p \\ &= \frac{1}{2\pi\epsilon} \sum_{m \in \mathbb{Z}} \int_{(2m-1)\pi}^{(2m+1)\pi} \hat{U}\left(\frac{p}{\epsilon}\right) e^{ipj} \mathrm{d}p = \frac{1}{2\pi\epsilon} \sum_{m \in \mathbb{Z}} \int_{-\pi}^{\pi} \hat{U}\left(\frac{\theta + 2\pi m}{\epsilon}\right) e^{ij\theta} \mathrm{d}\theta \end{aligned}$$

so that $\hat{u}(\theta) = \epsilon^{-1} \sum_{m \in \mathbb{Z}} \hat{U}\left(\frac{\theta + 2\pi m}{\epsilon}\right)$.

By Parseval's equality,

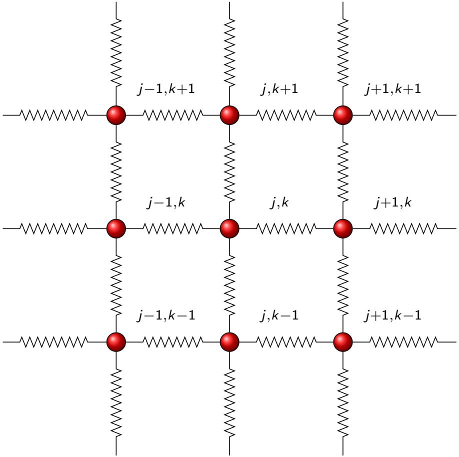
$$\begin{aligned}\|u\|_{l^2}^2 &= \frac{1}{2\pi\epsilon^2}\int_{-\pi}^{\pi}\Big|\sum_{m\in\mathbb{Z}}\hat{U}\left(\frac{\theta+2\pi m}{\epsilon}\right)\Big|^2 \mathrm{d}\theta \\ &\leq \frac{1}{2\pi\epsilon^2}\sum_{m_1,m_2\in\mathbb{Z}}\int_{-\pi}^{\pi}\left|\hat{U}\left(\frac{\theta+2\pi m_1}{\epsilon}\right)\right|\left|\hat{U}\left(\frac{\theta+2\pi m_2}{\epsilon}\right)\right|\mathrm{d}\theta \\ &\leq \frac{1}{2\pi\epsilon^2}\left(\sum_{m_1\in\mathbb{Z}}\frac{1}{1+\pi^2 m_1^2/\epsilon^2}\right)\left(\sum_{m_2\in\mathbb{Z}}\left(1+\frac{\pi^2 m_2^2}{\epsilon^2}\right)\int_{-\pi}^{\pi}\left|\hat{U}\left(\frac{\theta+2\pi m_2}{\epsilon}\right)\right|^2\mathrm{d}\theta\right).\end{aligned}$$

For $\epsilon \in (0,1]$, the first term in the product takes values between 1 and $\sum_{m\in\mathbb{Z}}(1+\pi^2 m^2)^{-1} < \infty$. The second term can be compared with the H^1 norm of U:

$$\begin{aligned}\|U\|_{H^1}^2 &= \frac{1}{2\pi}\int_{-\infty}^{\infty}(1+k^2)\left|\hat{U}(k)\right|^2\mathrm{d}k \\ &= \frac{1}{2\pi\epsilon}\sum_{m\in\mathbb{Z}}\int_{-\pi}^{\pi}\left(1+\frac{(\theta+2\pi m)^2}{\epsilon^2}\right)\left|\hat{U}\left(\frac{\theta+2\pi m}{\epsilon}\right))\right|^2\mathrm{d}\theta.\end{aligned}$$

For any $m \in \mathbb{Z}$, $\theta \in [-\pi,\pi]$, we have $(\theta+2\pi m)^2 \geq \pi^2 m^2$, so that the factor $(1+(\theta+2\pi m)^2/\epsilon^2)$ is bounded from below by $(1+\pi^2 m^2/\epsilon^2)$.

Case Study 2: Modeling of transverse modulations



KP-II limit for small-amplitude, long-scale, transversely modulated waves

There exist two versions of the two-dimensional generalization of the KdV equation:

$$\text{(KP-I)} \quad \partial_\xi(\partial_\tau R + \alpha R \partial_\xi R + \frac{1}{24}\partial_\xi^3 R) - \partial_\eta^2 R = 0$$

and

$$\text{(KP-II)} \quad \partial_\xi(\partial_\tau R + \alpha R \partial_\xi R + \frac{1}{24}\partial_\xi^3 R) + \partial_\eta^2 R = 0$$

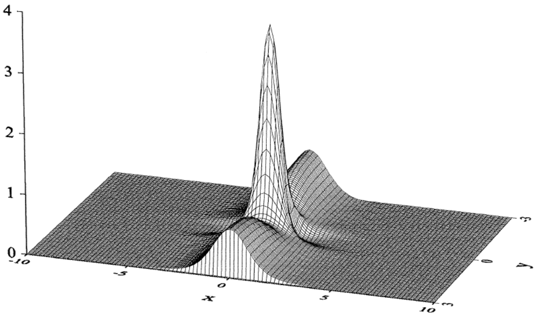
For water waves, (KP-I) arises for problems with surface tension and (KP-II) arises for gravity waves.

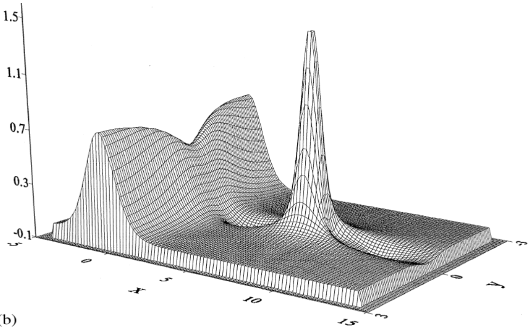
For Bose–Einstein condensates (defocusing Gross–Pitaevskii equation), only (KP-I) arises in the asymptotic reduction on the nonzero background.

For the FPU lattice on the square lattice, only (KP-II) arises in the asymptotic reduction.

KP-I limit

Line solitary and periodic waves are unstable for KP-I and the perturbations evolve into two-dimensional solitons called lumps.

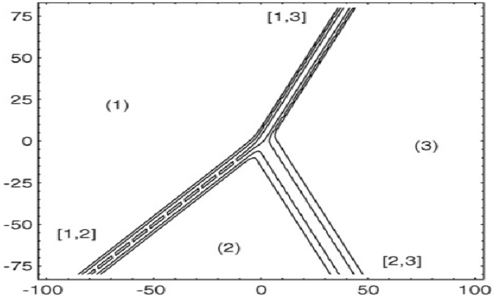


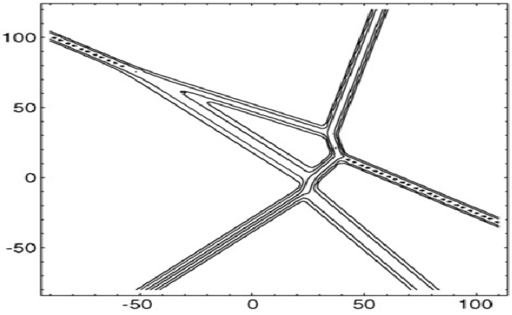


(b)

KP-II limit

Line solitary and periodic waves are transversally stable for KP-II (Mizumachi, 2015; Haragus, Li, P, 2017), and form stable web patterns in the plane.





Scalar 2D FPU model

$$H = \sum_{(m,n)} \frac{1}{2}\dot{q}_{m,n}^2 + \frac{1}{2}(q_{m+1,n} - q_{m,n})^2 + \frac{1}{3}\alpha(q_{m+1,n} - q_{m,n})^3 + \frac{1}{2}\varepsilon^2(q_{m,n+1} - q_{m,n})^2$$

- Duncan–Eilbeck–Zakharov (1991) formally derived KP-II equation

$$\partial_\xi(\partial_\tau R + \alpha R \partial_\xi R + \frac{1}{24}\partial_\xi^3 R) + \partial_\eta^2 R = 0$$

- Rigorous justification of the KP-II limit has been an open problem for 30 years!
- It was only justified recently: Gallone–Pasquali (Nonlinearity, 2021) on $\mathbb{T}^2$; Hristov–P (ZAMP, 2022) on $\mathbb{R}^2$; P–Schneider (SIAM J. Appl. Math., 2023) on $\mathbb{T}^2$ for oblique propagation.

Recall the justification algorithm

1. Find the best coordinates to transform the problem.
2. Check that the reduced model formally arises in the appropriate limit of the transformed equations.
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4. Control the error terms from the residual equations in suitable norms by using the energy conservation, approximation estimates, and Gronwall inequality.
5. Check that the reduced models have smooth solutions which are compatible with the estimates.

Strain variables

The scalar model can be expressed in the strain variables as:

$$\left\{ \begin{array}{l} \dot{u}_{m,n} = w_{m+1,n} - w_{m,n}, \\ \dot{v}_{m,n} = w_{m,n+1} - w_{m,n}, \\ \dot{w}_{m,n} = V'(u_{m,n}) - V'(u_{m-1,n}) + V'(v_{m,n}) - V'(v_{m,n-1}), \end{array} \right.$$

where $V'(u) = u - u^2$ will be used for simplifications.

We can eliminate $w_{m,n}$ and get

$$\left\{ \begin{array}{l} \ddot{u}_{m,n} = V'(u_{m+1,n}) - 2V'(u_{m,n}) + V'(u_{m-1,n}) \\ \qquad\qquad + V'(v_{m+1,n}) - V'(v_{m+1,n-1}) - V'(v_{m,n}) + V'(v_{m,n-1}), \\ \ddot{v}_{m,n} = V'(v_{m,n+1}) - 2V'(v_{m,n}) + V'(v_{m,n-1}) \\ \qquad\qquad + V'(u_{m,n+1}) - V'(u_{m-1,n+1}) - V'(u_{m,n}) + V'(u_{m-1,n}), \end{array} \right.$$

There exists still a compatibility condition between $u_{m,n}$ and $v_{m,n}$.

Fourier transform

With Fourier transform the system converts into the form:

$$\begin{cases} \partial_t^2 \widehat{u} = -(\omega_k^2 + \omega_l^2)\widehat{u} + \omega_k^2(\widehat{u} * \widehat{u}) - (e^{-ik} - 1)(1 - e^{il})(\widehat{v} * \widehat{v}), \\ \partial_t^2 \widehat{v} = -(\omega_k^2 + \omega_l^2)\widehat{v} + \omega_l^2(\widehat{v} * \widehat{v}) - (e^{-il} - 1)(1 - e^{ik})(\widehat{u} * \widehat{u}). \end{cases}$$

where $\omega_k^2 := 2 - 2\cos(k)$.

The compatibility condition between $u_{m,n}$ and $v_{m,n}$ can be expressed easier in the Fourier form as

$$(e^{-ik} - 1)\widehat{v}(k, l, t) = (e^{-il} - 1)\widehat{u}(k, l, t).$$

Formal limit for arbitrary propagation direction

The leading order approximation for an arbitrary angle ϕ can be expressed by

$$u_{m,n}(t) = \varepsilon^2 A(X, Y, T), \qquad v_{m,n}(t) = \varepsilon^2 B(X, Y, T),$$

where

$$X = \varepsilon((\cos\phi)m + (\sin\phi)n - t), \quad Y = \varepsilon^2(-(\sin\phi)m + (\cos\phi)n), \quad T = \varepsilon^3 t.$$

This yields the KP-II equation

$$-2\partial_X \partial_T A = \frac{1}{12}[(\cos\phi)^4 + (\sin\phi)^4]\partial_X^4 A + \partial_Y^2 A \\ - (\cos\phi)^2 \partial_X^2 (A^2) - (\sin\phi)(\cos\phi))\partial_X^2 (B^2)$$

and the compatibility condition

$$(\cos\phi)\partial_X B = (\sin\phi)\partial_X A$$

up to the leading order. For horizontal propagation, $\phi = 0$ and $B(X, Y, T) = 0$.

Justification result for $\phi = 0$

Theorem (Hristov–P, 2022)

Let $A \in C^0([0,\tau_0], H^s(\mathbb{R}^2))$ be a solution to the KP-II equation with fixed integer $s \geq 9$, whose initial data satisfies $A_0 \in H^s(\mathbb{R}^2)$, $\partial_X^{-2}\partial_Y^2 A_0 \in H^s(\mathbb{R}^2)$, and

$$\partial_X^{-1}\partial_Y^2\left(\partial_X^{-2}\partial_Y^2 A_0 + A_0^2\right) \in H^{s-6}(\mathbb{R}^2).$$

Then there exist $\varepsilon_0 > 0$ and $C_0 > 0$ such that for every $\varepsilon \in (0,\varepsilon_0)$, the unique solution of the 2D FPU system satisfies for $t \in [0, \tau_0\varepsilon^{-3}]$

$$\|u_{m,n}(t) - \varepsilon^2 A(\varepsilon(m-t), \varepsilon^2 n, \varepsilon^3 t)\|_{\ell^2} + \|v_{m,n}(t)\|_{\ell^2} + \|w_{m,n}(t) + \varepsilon^2 A(\varepsilon(m-t), \varepsilon^2 n, \varepsilon^3 t)\|_{\ell^2} \leq C_0 \varepsilon^{5/2}.$$

The approximation result between solutions on the grid and solutions on $\mathbb{R}^2$ is given by

$$\|u\|_{\ell^2(\mathbb{Z}^2)} \leq C_s \varepsilon^{-3/2} \|U\|_{H^s(\mathbb{R}^2)},$$

where $u_j = U(\varepsilon m, \varepsilon^2 n)$ with $U \in H^s(\mathbb{R}^2)$ for integer $s \geq 2$.

Expansions to satisfy the compatibility conditions

The scalar model can be expressed in the strain variables as:

$$\begin{cases} \dot{u}_{m,n} = w_{m+1,n} - w_{m,n}, \\ \dot{v}_{m,n} = w_{m,n+1} - w_{m,n}, \\ \dot{w}_{m,n} = V'(u_{m,n}) - V'(u_{m-1,n}) + V'(v_{m,n}) - V'(v_{m,n-1}), \end{cases}$$

- We introduce the following decomposition:

$$\begin{aligned} u_{m,n} &= \varepsilon^2 A(\xi,\eta,\tau) + \varepsilon^2 U_{m,n} \\ v_{m,n} &= \varepsilon^2 B_\varepsilon(\xi,\eta,\tau) + \varepsilon^2 V_{m,n} \\ w_{m,n} &= \varepsilon^2 W_\varepsilon(\xi,\eta,\tau) + \varepsilon^2 W_{m,n} \end{aligned}$$

  where $\xi = \varepsilon(m-t), \eta = \varepsilon^2 n, \tau = \varepsilon^3 t$

- Here B_ε and W_ε are introduced to satisfy the linear equations of motion:

$$\dot{u}_{m,n} = w_{m+1,n} - w_{m,n}, \quad \dot{v}_{m,n} = w_{m,n+1} - w_{m,n}.$$

Expansions to satisfy the compatibility conditions

- These equations are satisfied up to $\mathcal{O}(\varepsilon^5)$ order:

$$\begin{aligned} W_\varepsilon\left(\xi+\varepsilon,\eta\right) - W_\varepsilon\left(\xi,\eta\right) &= -\varepsilon\partial_\xi A(\xi,\eta) + \varepsilon^3\partial_\tau A(\xi,\eta), \\ W_\varepsilon\left(\xi,\eta+\varepsilon^2\right) - W_\varepsilon\left(\xi,\eta\right) &= -\varepsilon\partial_\xi B_\varepsilon(\xi,\eta) + \varepsilon^3\partial_\tau B_\varepsilon(\xi,\eta). \end{aligned}$$

- We seek an approximate solution by expanding $W_\varepsilon, B_\varepsilon$ in orders of ε
- $W_\varepsilon = -A + \varepsilon\left(\frac{1}{2}\partial_\xi A\right) + \varepsilon^2\left(\partial_\xi^{-1}\partial_\tau A - \frac{1}{12}\partial_\xi^2 A\right) - \varepsilon^3\left(\frac{1}{2}\partial_\tau A\right)$
- $B_\varepsilon = \varepsilon\partial_\xi^{-1}\partial_\eta A - \varepsilon^2\left(\frac{1}{2}\partial_\eta A\right) + \varepsilon^3\left(\frac{1}{2}\partial_\xi^{-1}\partial_\eta^2 A + \frac{1}{12}\partial_\xi\partial_\eta A\right)$
- By construction of terms W_ε and B_ε, the residual terms of the two equations vanish to $\mathcal{O}(\varepsilon^5)$.

Control of residual terms

- The last remaining equation is

$$\begin{aligned}\dot{W}_{j,k} &= U_{j,k} - U_{j-1,k} + V_{j,k} - V_{j,k-1} \\ &\quad + \varepsilon^2 \left[2AU_{j,k} - 2A(\xi - \varepsilon, \eta) U_{j-1,k} + (U_{j,k})^2 - (U_{j-1,k})^2 \right] + Res^W_{j,k}\end{aligned}$$

- The residual term is given by:

$$\begin{aligned}Res^W_{j,k} := &\varepsilon \partial_\xi W_\varepsilon - \varepsilon^3 \partial_\tau W_\varepsilon + A(\xi, \eta) - A(\xi - \varepsilon, \eta) \\ &+ B_\varepsilon(\xi, \eta) - B_\varepsilon(\xi, \eta - \varepsilon^2) + \varepsilon^2 \left[A(\xi, \eta)^2 - A(\xi - \varepsilon, \eta)^2 \right],\end{aligned}$$

- Expanding Res^W gives the following formal expansion:

$$\begin{aligned}Res^W_{j,k} = \quad &\varepsilon^3 \left[2\partial_\tau A + \frac{1}{12} \partial_\xi^3 A + \partial_\xi^{-1} \partial_\eta^2 A + \partial_\xi (A^2) \right] \\ &-\varepsilon^4 \left[\partial_\xi \partial_\tau A + \frac{1}{24} \partial_\xi^4 A + \frac{1}{2} \partial_\eta^2 A + \frac{1}{2} \partial_\xi^2 (A^2) \right] + \mathcal{O}(\varepsilon^5).\end{aligned}$$

Control of residual terms

Lemma

Let $A \in C^0(\mathbb{R}, H^s)$ be a solution to the KP-II equation with $s \geq 9$. There is a positive constant C that depend on A such that for all $\varepsilon \in (0,1]$, we have

$$\left\| Res^U_{j,k} \right\|_{\ell^2} + \left\| Res^V_{j,k} \right\|_{\ell^2} + \left\| Res^W_{j,k} \right\|_{\ell^2} \leq C \varepsilon^{\frac{7}{2}}.$$

- The formal expansions of the residual terms are handled using Taylor's theorem, e.g.

$$A(\xi+\varepsilon,\eta) - A(\xi,\eta) = \varepsilon \partial_\xi A + \frac{1}{2}\varepsilon^2 \partial_\xi^2 A + \frac{1}{3!}\varepsilon^3 \partial_\xi^3 A + \frac{1}{4!}\varepsilon^4 \partial_\xi^4 A + \frac{1}{4!}\varepsilon^5 \int_0^1 (1-r)^4 \partial_\xi^5 A(\varepsilon(j+r), \varepsilon^2 k, \varepsilon^3 t) dr$$

- The integral residual terms is estimated in ℓ^2-norm for every r on $[0,1]$
- Since the rigorous bound loses $\mathcal{O}(\varepsilon^{-3/2})$, the formal bound of $\mathcal{O}(\varepsilon^5)$ yields $\mathcal{O}(\varepsilon^{7/2})$ in the ℓ^2-norm.

Energy Estimates

- Recall the total energy of the FPU system in strain variables

$$H = \frac{1}{2} \sum_{(j,k)\in\mathbb{Z}^2} w_{j,k}^2 + (u_{j,k})^2 + (v_{j,k})^2 + \frac{1}{3} \sum_{(j,k)\in\mathbb{Z}^2} (u_{j,k})^3.$$

- This suggests the following energy quantity to control the growth of the approximation error:

$$E(t) = \frac{1}{2} \sum_{j,k\in\mathbb{Z}^2} W_{j,k}^2 + (U_{j,k})^2 + (V_{j,k})^2 + \frac{1}{3}\varepsilon^2 \sum_{j,k\in\mathbb{Z}^2} \left[3A\,(U_{j,k})^2 + (U_{j,k})^3 \right].$$

- The ε-dependent terms in the energy $E(t)$ are chosen such that the growth rate $E'(t)$ does not contain terms up to the formal order $\mathcal{O}(\varepsilon^2)$
- Assume that $E(t) \leq E_0$ for some ε-independent constant $E_0 > 0$ for every $t \in [-\tau_0\varepsilon^{-3}, \tau_0\varepsilon^{-3}]$. There exist some constants $\varepsilon_0 > 0$ and $K_0 > 0$ that depend on A such that

$$K_0 E(t) \leq \|W\|_{\ell^2}^2 + \|U\|_{\ell^2}^2 + \|V\|_{\ell^2}^2 \leq 2K_0 E(t),$$

for each $\varepsilon \in (0, \varepsilon_0)$ and $t \in [-\tau_0\varepsilon^{-3}, \tau_0\varepsilon^{-3}]$.

Bounds on the approximation error in the time evolution

By differentiating $E(t)$, we obtain

$$E'(t) = \sum_{j,k \in \mathbb{Z}^2} W_{j,k} Res^W_{j,k} + U_{j,k} Res^U_{j,k} + V_{j,k} Res^V_{j,k} + \varepsilon^2 \left(-\varepsilon \partial_\xi A + \varepsilon^3 \partial_\tau A\right) (U_{j,k})^2 .$$

- Cauchy-Schwartz and the previous estimates give the differential inequality:

$$|E'(t)| \leq C \left(\varepsilon^{7/2} E(t)^{1/2} + \varepsilon^3 E(t)\right),$$

  for some $C_0 > 0$ as long as $E(t) \leq E_0$ for some $E_0 > 0$.
- By making the substitution $E(t) := \frac{1}{2} Q(t)^2$, we obtain:

$$|Q'(t)| \leq C \left(\varepsilon^{7/2} + \varepsilon^3 Q\right)$$

- Gronwall's lemma yields for $Q(0) \leq C_0 \varepsilon^{1/2}$,

$$Q(t) \leq \varepsilon^{1/2} (1 + C_0) \exp\left(C \tau_0\right)$$

  for each $\varepsilon \in (0, \varepsilon_0)$ and $t \in [-\tau_0 \varepsilon^{-3}, \tau_0 \varepsilon^{-3}]$.

This completes the proof of the justification result for $\phi = 0$

Theorem (Hristov–P, 2022)

Let $A \in C^0([0,\tau_0], H^s(\mathbb{R}^2))$ be a solution to the KP-II equation with fixed integer $s \geq 9$, whose initial data satisfies $A_0 \in H^s(\mathbb{R}^2)$, $\partial_X^{-2}\partial_Y^2 A_0 \in H^s(\mathbb{R}^2)$, and

$$\partial_X^{-1}\partial_Y^2 \left(\partial_X^{-2}\partial_Y^2 A_0 + A_0^2\right) \in H^{s-6}(\mathbb{R}^2).$$

Then there exist $\varepsilon_0 > 0$ and $C_0 > 0$ such that for every $\varepsilon \in (0, \varepsilon_0)$, the unique solution of the 2D FPU system satisfies for $t \in [0, \tau_0 \varepsilon^{-3}]$

$$\|u_{m,n}(t) - \varepsilon^2 A(\varepsilon(m-t), \varepsilon^2 n, \varepsilon^3 t)\|_{\ell^2} + \|v_{m,n}(t)\|_{\ell^2} + \|w_{m,n}(t) + \varepsilon^2 A(\varepsilon(m-t), \varepsilon^2 n, \varepsilon^3 t)\|_{\ell^2} \leq C_0 \varepsilon^{5/2}.$$

Justification result for $\phi \neq 0$

We need to control solutions of the original KP-II equation with additional requirement:

$$\partial_X^{-1}\partial_Y(A^2) \in H^{s-6}$$

However, this is impossible on $\mathbb{R}^2$ (L. Molinet, J.-C. Saut, and N. Tzvetkov, 2002).

On other hand, working on torus $\mathbb{T}^2$ (Bourgain, 1993), if the mean value of A in X is independent of Y, then $\partial_X^{-3}\partial_Y^3 A$ is controllable in $H^s(\mathbb{T}^2)$ and so is $\partial_X^{-1}\partial_Y(A^2)$.

As a result, we have justified the KP-II equation for an arbitrary direction of propagation on $\mathbb{T}^2$, but not on $\mathbb{R}^2$ (P-Schneider, 2023). The justification result also extends to the line solitary waves (no transverse modulations) for an arbitrary direction of propagation (the KdV equation).

Case Study 3: The monoatomic FPU as a limit of a diatomic FPU

The Hamiltonian is

$$H = \sum_{j \in 2\mathbb{Z}} \frac{1}{2} \dot{Q}_j^2 + \frac{1}{2} \varepsilon^2 \dot{q}_{j+1}^2 + V(q_{j+1} - Q_j) + V(Q_j - q_{j-1}),$$

where ε is the mass ratio between light and heavy particles and $V'(u) = u + u^2$ will be used.

Formal limit of small-mass ratio

Equations of motion:

$$\ddot{Q}_j = V'(q_{j+1} - Q_j) - V'(Q_j - q_{j-1}),$$
$$\varepsilon^2 \ddot{q}_{j+1} = V'(Q_{j+2} - q_{j+1}) - V'(q_{j+1} - Q_j),$$

where $j \in 2\mathbb{Z}$.

The small-mass limit $\varepsilon = 0$ is satisfied if

$$q_{j+1} = \frac{Q_{j+2} + Q_j}{2},$$

for which the scalar FPU system arises:

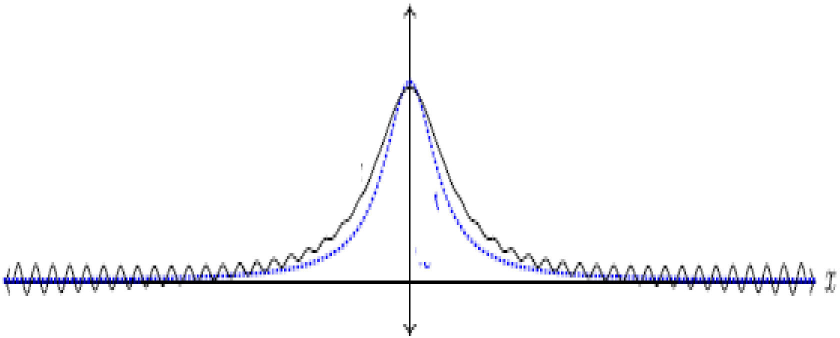
$$\ddot{Q}_j = V'\left(\frac{Q_{j+2} - Q_j}{2}\right) - V'\left(\frac{Q_j - Q_{j-2}}{2}\right).$$

K. Jayaprakash, Y. Starosvetsky, A. Vakakis, PRE 83 (2011) 11

Solitary waves with and without exponentially small tails

Generally, the traveling solitary waves have oscillatory tails which are exponentially small in ε.

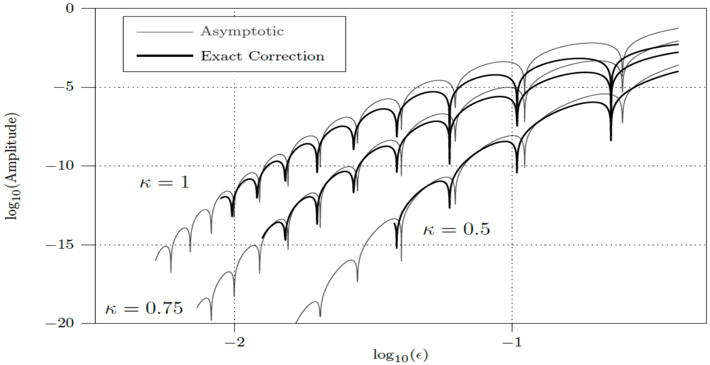
A. Hoffman, J. D. Wright (2017); T. Faver, J. D. Wright (2018); C. Lustri, M. Porter (2018)



Solitary waves with and without exponentially small tails

However, for a sequence of special values of $\{\varepsilon_n\}_{n\in\mathbb{N}}$ such that $\varepsilon_n \to 0$ as $n \to \infty$, the traveling solitary waves are fully localized without oscillatory tails.

K. Jayaprakash, Y. Starosvetsky, A. Vakakis (2011); C. Lustri, M. Porter (2018)



Justification result

Theorem (P–Schneider, 2020)

Assume that $Q^* \in C^1([0,T_0],\ell^2)$ *is a suitable solution to the monoatomic FPU system*

$$\ddot{Q}_j = V'\left(\frac{Q_{j+2}-Q_j}{2}\right) - V'\left(\frac{Q_j - Q_{j-2}}{2}\right).$$

There exist $\varepsilon_0 > 0$ *and* $C_0 > 0$ *such that for all* $\varepsilon \in (0,\varepsilon_0)$ *if* $[Q(0),q(0)] \in \ell^2 \times \ell^2$ *satisfy*

$$\sup_{j\in 2\mathbb{Z}} |Q_j(0) - Q_j^*(0)| + \left| q_{j+1}(0) - \frac{1}{2}(Q_j^*(0) + Q_{j+2}^*(0))\right| \leq \varepsilon,$$

then the unique solution to the diatomic FPU system satisfies for every $t \in [0,T_0]$*:*

$$\sup_{j\in 2\mathbb{Z}} |Q_j(t) - Q_j^*(t)| + \left| q_{j+1}(t) - \frac{1}{2}(Q_j^*(t) + Q_{j+2}^*(t))\right| \leq C_0\varepsilon.$$

Justification result

The approximation result is nontrivial since the right-hand side of the vector field is $\mathcal{O}(\varepsilon^{-2})$:

$$\ddot{Q}_j = V'(q_{j+1} - Q_j) - V'(Q_j - q_{j-1}),$$
$$\ddot{q}_{j+1} = \varepsilon^{-2} \left[V'(Q_{j+2} - q_{j+1}) - V'(q_{j+1} - Q_j) \right].$$

If

$$q_{j+1} = \frac{1}{2}(Q_j + Q_{j+2}) + \mathcal{O}(\varepsilon),$$

then Gronwall's inequlity gives only estimates on the time scale of $\mathcal{O}(\varepsilon)$. The theorem ensures proximity on the natural time scale of $\mathcal{O}(1)$ for which dynamics of the FPU system is nontrivial.

Justification result

1. Find the best coordinates to transform the problem.
2. Check that the reduced model formally arises in the appropriate limit of the transformed equations.
3. Define **error terms** to **the leading-order terms** and obtain **residual equations**.
4. Control the error terms from the residual equations in suitable norms by using the energy conservation, approximation estimates, and Gronwall inequality.
5. Check that the reduced models have smooth solutions which are compatible with the estimates.

Proof of the justification result

1 Find the best coordinates to transform the problem.

We are using the coordnates:

$$U_j := \frac{1}{2}(Q_{j+2} - Q_j) \quad \text{and} \quad w_{j+1} := q_{j+1} - \frac{1}{2}(Q_{j+2} + Q_j).$$

It turns out that the same choice of coordinates was made in A. Hoffman, J. D. Wright (2017).

The diatomic FPU system is now written as

$$\ddot{U}_j + V'(U_j) + w_{j+1}^2 = \frac{1}{2}V'(U_{j+2} + w_{j+3}) + \frac{1}{2}V'(U_{j-2} - w_{j-1}),$$

$$\varepsilon^2 \ddot{w}_{j+1} + (2 + \varepsilon^2) w_{j+1}(1 + 2U_j) = -\frac{\varepsilon^2}{2}V'(U_{j+2} + w_{j+3}) + \frac{\varepsilon^2}{2}V'(U_{j-2} - w_{j-1}),$$

where $V'(u) = u + u^2$ is used for simplicity.

Proof of the justification result

2 Check that the reduced model formally arises in the appropriate limit of the transformed equations.

We have rewritten the diatomic FPU system in the form:

$$\ddot{U}_j + V'(U_j) + w_{j+1}^2 = \frac{1}{2}V'(U_{j+2} + w_{j+3}) + \frac{1}{2}V'(U_{j-2} - w_{j-1}),$$
$$\varepsilon^2 \ddot{w}_{j+1} + (2+\varepsilon^2) w_{j+1}(1 + 2U_j) = -\frac{\varepsilon^2}{2}V'(U_{j+2} + w_{j+3}) + \frac{\varepsilon^2}{2}V'(U_{j-2} - w_{j-1}).$$

If $\varepsilon = 0$ and $w_{j+1} = 0$, then the strain variable U_j satisfies the monoatomic FPU lattice

$$\ddot{U}_j = \frac{1}{2}V'(U_{j+2}) + \frac{1}{2}V'(U_{j-2}) - V'(U_j).$$

Proof of the justification result

3 Define **error terms** to **the leading-order terms** and obtain **residual equations**.

We have rewritten the diatomic FPU system in the form:

$$\ddot{U}_j + V'(U_j) + w_{j+1}^2 = \frac{1}{2}V'(U_{j+2} + w_{j+3}) + \frac{1}{2}V'(U_{j-2} - w_{j-1}),$$

$$\varepsilon^2 \ddot{w}_{j+1} + (2 + \varepsilon^2) w_{j+1}(1 + 2U_j) = -\frac{\varepsilon^2}{2}V'(U_{j+2} + w_{j+3}) + \frac{\varepsilon^2}{2}V'(U_{j-2} - w_{j-1}).$$

Let Ψ satisfy

$$\ddot{\Psi}_j = \frac{1}{2}V'(\Psi_{j+2}) + \frac{1}{2}V'(\Psi_{j-2}) - V'(\Psi_j).$$

The error terms are $U - \Psi$ and w. The residual terms are

$$\mathrm{Res}_{U,j} = 0, \quad \mathrm{Res}_{w,j} = -\frac{\varepsilon^2}{2}V'(\Psi_{j+2}) + \frac{\varepsilon^2}{2}V'(\Psi_{j-2}).$$

Proof of the justification result

4 Control the residual terms in suitable norm.

The residual terms are controlled by

$$\sup_{t \in [0, T_0]} \|\mathrm{Res}_w\|_{\ell^2} \leq C\varepsilon^2,$$

as long as $\Psi \in C([0, T_0], \ell^2)$.

Proof of the justification result

4 Control the error term in suitable norm from the energy conservation.

The error terms in the decomposition

$$U_j = \Psi_j + \varepsilon R_j \quad \text{and} \quad w_{j+1} = \varepsilon v_{j+1}.$$

are controlled from the energy function

$$E(t) = \frac{1}{2} \sum_{j \in 2\mathbb{Z}} \dot{R}_j^2 + R_j^2 + \varepsilon^2 \dot{v}_{j+1}^2 + 2v_{j+1}^2 + 2\Psi_j (R_j^2 + 2v_{j+1}^2) + 4\varepsilon R_j v_{j+1}^2,$$

as long as

$$\sup_{t \in [0,T_0]} \sup_{j \in 2\mathbb{Z}} |\Psi_j(t)| < \frac{1}{4}.$$

Proof of the justification result

4 Control the energy function from the balance equation and Gronwall's inequality.

$$\frac{d}{dt}E(t) \leq C_1 E(t)^{1/2} + C_2 E(t) + C_3 \varepsilon E(t)^{3/2}, \quad t \in [0, T_0].$$

$$E(t)^{1/2} \leq \left[E(0)^{1/2} + (2C_2)^{-1} C_1 \right] e^{2C_2 t}, \quad t \in [0, T_0].$$

as long as $\varepsilon E(t)^{1/2} \leq C_2 / C_3$.

Proof of the justification result

5 Check that the reduced models have smooth solutions which are compatible with the estimates.

We have assumed that $\Psi \in C^1([0, T_0], \ell^2)$ is a solution of

$$\ddot{\Psi}_j = \frac{1}{2} V'(\Psi_{j+2}) + \frac{1}{2} V'(\Psi_{j-2}) - V'(\Psi_j)$$

such that

$$\sup_{t \in [0, T_0]} \sup_{j \in 2\mathbb{Z}} |\Psi_j(t)| < \frac{1}{4}.$$

Since the monoatomic system is Hamiltonian with the conserved energy

$$H_{\rm FPU} = \sum_{j \in 2\mathbb{Z}} \frac{1}{2} \dot{\Psi}_j^2 + \Psi_j^2 + \frac{2}{3} \Psi_j^3,$$

the constraint is satisfied at least for sufficiently small initial data.

Summary

- With three motivational examples, I have illustrated the justification analysis of obtaining nice integrable systems as reduction of non-integrable FPU systems.
- One of the main concerns of the justification algorithm is to verify that the reduced system admits nice smooth solutions which would justify the reduction.
- The other points to take home is that the approximation result should hold on times sufficiently long to observe nontrivial dynamics of the reduced system.
- The justification analysis relies on the choice of the energy function which always originates from the energy conservation of the original FPU system. The energy function often suggests the choice of the best coordinates for the justification result.