Solitary Waves in Granular Chains : Logarithmic Korteweg–De Vries equation

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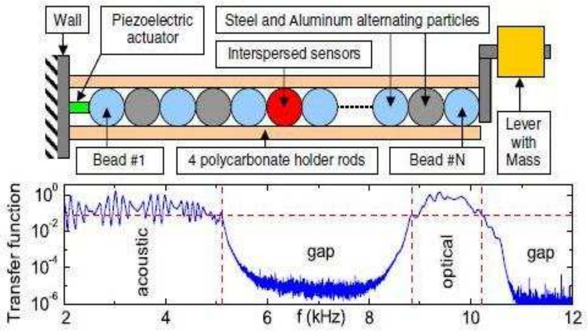
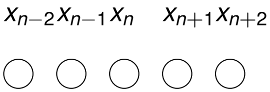
Introduction



- Granular chains contain densely packed, elastically interacting particles with Hertzian contact forces.
- Experimental works focus on transmission of solitary and periodic traveling waves.

The granular chain



Newton's equations of motion define 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.

The interaction potential for spherical beads is

$$V(x) = \frac{1}{1+\alpha} |x|^{1+\alpha} H(-x), \quad \alpha = \frac{3}{2},$$

where H is the step (Heaviside) function.

H. Hertz, *J. Reine Angewandte Mathematik* **92** (1882), 156

Nesterenko's solitary wave

Let $u_n = x_n - x_{n-1}$ and consider traveling wave $u_n(t) = w_n(n-t)$.

$$\frac{d^2 w}{dz^2} = \Delta(w|w|^{\alpha-1}), \quad z \in \mathbb{R},$$

with $(\Delta w)(z) = w(z+1) - 2w(z) + w(z-1)$.

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Expanding $\Delta = \partial_z^2 + \frac{1}{12}\partial_z^4$ and integrating twice yield ODE

$$w = w|w|^{\alpha-1} + \frac{1}{12}\frac{d^2}{dz^2} w|w|^{\alpha-1}, \quad z \in \mathbb{R},$$

which has compacton solutions

$$w_{\rm c}(z) = \begin{cases} A\cos^{\frac{2}{\alpha-1}}(Bz), & |z| \leq \frac{\pi}{2B}, \\ 0, & |z| \geq \frac{\pi}{2B}, \end{cases}$$

where

$$A = \left(\frac{1+\alpha}{2\alpha}\right)^{\frac{1}{1-\alpha}}, \quad B = \frac{\sqrt{3}(\alpha-1)}{\alpha}.$$

No small parameter justifies this approximation.

Boussinesq approximation

The fully nonlinear Boussinesq equation takes the form

$$u_{tt} = (u|u|^{\alpha-1})_{xx} + \frac{1}{12}(u|u|^{\alpha-1})_{xxxx}.$$

V.F. Nesterenko, (1983); K. Ahnert–A. Pikovsky (2009).

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Based on the differential–difference equation, one can prove

- existence of a solitary wave in $H^1(\mathbb{R})$
  [G. Friesecke–J. Wattis (1994), A. Stefanov–P. Kevrekidis, (2012)]
- the double-exponential decay of a solitary wave
  [J. English–R. Pego, (2005)]

Korteweg–de Vries approximation

Consider the FPU lattice

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with $V(x) \sim |x|^{1+\alpha} H(-x)$. No reduction exists for small-amplitude waves unless a precompression is used with $u_n \leq C < 0$, $\forall n \in \mathbb{Z}$.

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If $\alpha = 1 + \varepsilon^2$, then one can write

$$\left(\frac{d^2}{dt^2} - \Delta \right) u_n = \Delta f_\varepsilon(u_n), \quad n \in \mathbb{Z},$$

where

$$f_\varepsilon(u) := u\left(|u|^\varepsilon - 1\right) = \varepsilon\, u \ln|u| + \mathcal{O}(\varepsilon^2).$$

Experimental data: For the chains of hollow spherical particles of different width, α is defined in the range $1.1 \leq \alpha \leq 1.5$.

Korteweg–de Vries approximation

Let $\alpha = 1 + \varepsilon^2$ and use the asymptotic multi-scale expansion

$$u_n(t) = v(\xi, \tau) + \text{higher order terms},$$

where

$$\xi := 2\sqrt{3}\varepsilon\,(n - t), \quad \tau := \sqrt{3}\varepsilon^3\, t.$$

The FPU chain is reduced to the KdV equation with the logarithmic nonlinearity (log-KdV) [A.Chatterjee (1999); G.James–D.P (2014)]:

$$\frac{\partial v}{\partial \tau} + \frac{\partial}{\partial \xi}(v \log v) + \frac{\partial^3 v}{\partial \xi^3} = 0, \quad (\tau, \xi) \in \mathbb{R}^+ \times \mathbb{R}.$$

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Justification of the KdV equation for smooth FPU chains is known [G. Schneider–C.E. Wayne (1998); D.Bambusi–A.Ponno (2006); G.Friesecke–R.L.Pego (1999-2004)].

Justification of the log–KdV equation can only be proved under precompression [E.Duma–D.P (2014)].

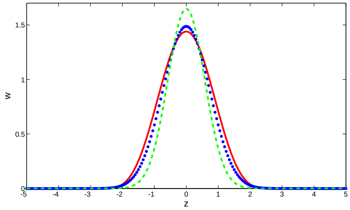
Traveling solitary wave

Log-KdV equation for traveling waves can be integrated once to get

$$\frac{d^2 v}{d\xi^2} + v \ln|v| = 0,$$

which admits the Gaussian solitary wave

$$v(\xi) = e^{1/2 - \xi^2/4}.$$



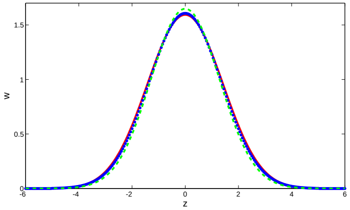


Figure : Solitary waves (blue) in comparison with the compactons (red) and the Gaussian solitons (green) for $\alpha = 1.5$ (left) and $\alpha = 1.1$ (right).

Numerical evidence of convergence of the approximation

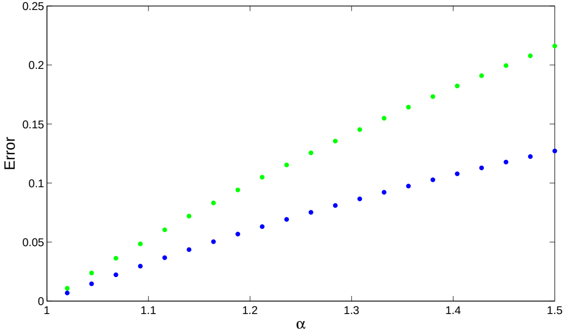


Figure : The L^∞ distance between solitary waves of the FPU chain and either Nesterenko compactons (blue dots) or Gaussian solitons (green dots) vs. α.

Numerical evidence of stability

Lattice of $N = 2000$ particles is excited with the initial impact

$$\dot{x}_n(0) = 0.1\delta_{n,0}, \quad \dot{x}_n(0) = 0 \text{ for all } n \geq 1.$$

A Gaussian solitary wave is formed asymptotically as t evolves.

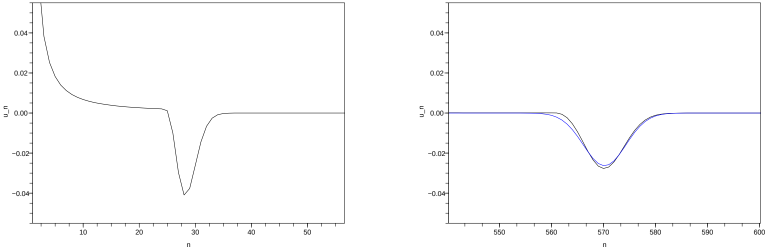


Figure : Formation of a Gaussian wave (blue curve) in the Hertzian FPU lattice with $\alpha = 1.01$: $t \approx 30.5$ (left) and $t \approx 585.6$ (right).

Questions for the log–KdV equation

The log-KdV equation

$$\frac{\partial v}{\partial \tau} + \frac{\partial}{\partial \xi}(v \log v) + \frac{\partial^3 v}{\partial \xi^3} = 0, \quad (\tau, \xi) \in \mathbb{R}^+ \times \mathbb{R}.$$

1. Existence of global solutions for the initial data v_0 in the energy space $H^1(\mathbb{R})$
2. Linear orbital stability of the Gaussian solitary wave in $H^1(\mathbb{R})$.
3. Spectrum of the linearized operator and semi-group estimates.
4. Nonlinear stability of global solutions in the neighborhood of Gaussian solitary waves.

Global existence of solutions

The log-KdV equation has the associated energy functional

$$E(v) = \frac{1}{2}\int_{\mathbb{R}} \left[\left(\frac{\partial v}{\partial \xi}\right)^2 - v^2 \left(\log v - \frac{1}{2}\right)\right] d\xi,$$

defined in the set

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

Theorem 1 (R. Carles–D.P, 2014)

For any $v_0 \in X$, there exists a global solution $v \in L^\infty(\mathbb{R}, X)$ to the log–KdV equation such that

$$\|v(\tau)\|_{L^2} \le \|v_0\|_{L^2}, \quad E(v(\tau)) \le E(v_0), \quad \text{for all } \tau > 0.$$

Proof of global existence [Th. Cazenave (1980)]

1. Construct an approximation of the logarithmic nonlinearity, e.g.

$$f^{\varepsilon}(v) = \begin{cases} v\log(v), & |v| \geq \varepsilon, \\ \left(\log(\varepsilon) - \frac{3}{4}\right) v + \frac{1}{\varepsilon^2} v^3 - \frac{1}{4\varepsilon^4} v^5, & |v| \leq \varepsilon, \end{cases}$$

hence $f^{\varepsilon} \in C^2(\mathbb{R})$ and $f^{\varepsilon}(v) \to v\log(v)$ as $\varepsilon \to 0$ for every $v \in \mathbb{R}$.

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2. Obtain existence of the global approximating solutions $v^{\varepsilon} \in C(\mathbb{R}, H^1(\mathbb{R}))$ to the generalized KdV equations

$$\begin{cases} v^{\varepsilon}_{\tau} + v^{\varepsilon}_{\xi\xi\xi} + f'_{\varepsilon}(v^{\varepsilon}) v^{\varepsilon}_{\xi} = 0, & \tau > 0, \\ v^{\varepsilon}|_{\tau=0} = v_0. \end{cases}$$

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3. Obtain uniform estimates for all $\varepsilon > 0$ and $\tau \in \mathbb{R}$:

$$\|v^{\varepsilon}(\tau)\|_{H^1} + \|(v^{\varepsilon}(\tau))^2 \log(v^{\varepsilon}(\tau))\|_{L^1} \leq C(v_0).$$

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4. Pass to the limit $\varepsilon \to 0$ and obtain a global solution $v \in L^{\infty}(\mathbb{R}, X)$ to the log–KdV equation.

Uniqueness

Lemma: *Assume that a solution* $v \in L^\infty(\mathbb{R}, X)$ *to the log–KdV equation satisfies the additional condition*

$$\partial_\xi \log|v| \in L^\infty([-\tau_0, \tau_0] \times \mathbb{R}).$$

Then, the solution $v(t) \in X$ *is unique for every* $\tau \in (-\tau_0, \tau_0)$*, depends continuously on the initial data* $v_0 \in X$*, and satisfies* $\|v(\tau)\|_{L^2} = \|v_0\|_{L^2}$ *and* $E(v(\tau)) = E(v_0)$ *for all* $\tau \in (-\tau_0, \tau_0)$*.*

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- If $v(\xi) = e^{\frac{2-\xi^2}{4}}$ (the Gaussian solitary wave), then $\partial_\xi \log|v|$ is unbounded as $|\xi| \to \infty$.
- Question of the nonlinear orbital stability of the Gaussian solitary wave is open.

Linearization at the Gaussian solitary wave

Gaussian wave $v_0 = e^{\frac{2-\xi^2}{4}}$ is a critical point of the energy function in X

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

Although $E(v)$ is not C^2 at $v = 0$, its second variation is well defined at v_0 by the quadratic form $\langle Lw, w \rangle_{L^2}$ for the perturbation $w = v - v_0$, where

$$L = -\frac{\partial^2}{\partial \xi^2} - 1 - \log(v_0) = -\frac{\partial^2}{\partial \xi^2} - \frac{3}{2} + \frac{\xi^2}{4}$$

is the Schrödinger operator for a quantum harmonic oscillator.

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The time evolution of the perturbation $w(\tau, \xi) = v(\tau, \xi) - v_0(\xi)$ is given by the linearized log–KdV equation

$$\frac{\partial w}{\partial \tau} = \frac{\partial}{\partial \xi} L w.$$

Spectral stability

If $w(\tau,\xi) = W(\xi)e^{\lambda\tau}$, we arrive to the linear eigenvalue problem

$$\partial_\xi L W = \lambda W.$$

The operator L is self-adjoint in $L^2(\mathbb{R})$ with domain

$$\mathrm{Dom}(L) = \{ u \in H^2(\mathbb{R}), \xi^2 u \in L^2(\mathbb{R}) \}.$$

The spectrum of L consists of simple eigenvalues at integers:

$$\sigma(L) = \{n - 1, \quad n \in \mathbb{N}_0\}.$$

The eigenfunctions of L are given by Hermite functions and decay like the Gaussian wave $v_0(\xi) = e^{\frac{2-\xi^2}{4}}$.

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Theorem 2 (R. Carles–D.P, 2014)

The spectrum of $\partial_x L$ in $L^2(\mathbb{R})$ is purely discrete and consists of a double zero eigenvalue and a sequence of simple eigenvalues $\{\pm i\omega_n\}_{n\in\mathbb{N}}$ s.t. $\omega_n \to \infty$ as $n \to \infty$. The eigenfunctions for nonzero eigenvalues are smooth in ξ but decay algebraically as $|\xi| \to \infty$.

Construction of eigenfunctions

Consider eigenfunctions of the linear eigenvalue problem $AW = \lambda W$,

$$A := \partial_\xi L = -\frac{\partial^3}{\partial \xi^3} + \frac{1}{4}(\xi^2 - 6)\frac{\partial}{\partial \xi} + \frac{1}{2}\xi.$$

If $\lambda \neq 0$, W belongs to $X_A := \mathrm{Dom}(A) \cap \dot{H}^{-1}(\mathbb{R})$,

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By using the Fourier transform, the linear eigenvalue problem can be written in the form $\hat{A}\hat{W} = \lambda \hat{W}$, where

$$\hat{A} = \frac{i}{4} k \left(-\partial_k^2 + 4k^2 - 6 \right).$$

If $W \in X_A$, then $\hat{W} \in \hat{X}_A$ with

$$\hat{X}_A = \left\{ \hat{u} \in H^1(\mathbb{R}) : \; k\partial_k^2 \hat{u} \in L^2(\mathbb{R}),\; k^3 \hat{u} \in L^2(\mathbb{R}),\; k^{-1}\hat{u} \in L^2(\mathbb{R}) \right\}.$$

It makes sense to write $\lambda = \frac{i}{4}E$.

Construction of eigenfunctions

The linear eigenvalue problem is

$$\frac{d^2\hat{u}}{dk^2} + \left(\frac{E}{k} + 6 - 4k^2\right)\hat{u}(k) = 0, \quad k \in \mathbb{R}.$$

- As $k \to 0$, two linearly independent solutions exist

$$\hat{u}_1(k) = k + \mathcal{O}(k^2), \quad \hat{u}_2(k) = 1 + \mathcal{O}(k\log(k)).$$

  The second solution does not belong to $\hat{X}_A$.

- As $|k| \to \infty$, there exists only one decaying solution satisfying

$$\hat{u}(k) = ke^{-k^2}\left(1 + \mathcal{O}(|k|^{-1})\right).$$

  The shooting problem from $k = 0$ to $k = \pm\infty$ is over-determined.

Construction of eigenfunctions

- The way around is to define eigenfunctions piecewise:

$$\hat{u}(k) = \begin{cases} \hat{u}_+(k), & k > 0, \\ 0, & k < 0, \end{cases} \quad \text{or} \quad \hat{u}(k) = \begin{cases} 0, & k > 0, \\ \hat{u}_-(k), & k < 0, \end{cases}$$

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- For $\hat{u}_+$, we set $\hat{u}_+(k) = k^{1/2}\hat{v}_+(k)$ and obtain

$$k^{1/2}\left(-\frac{d^2}{dk^2} + 4k^2 - 6\right)k^{1/2}\hat{v}_+(k) = E\hat{v}_+(k), \quad k \in (0, \infty),$$

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- For $E = 0$, we have $\hat{v}_+ = k^{1/2}e^{-k^2} > 0$ for $k > 0$. By Sturm's Theorem, the set of eigenvalues $\{E_n\}_{n\in\mathbb{N}_0}$ satisfies $0 = E_0 < E_1 < E_2 < \dots$ and $E_n \to \infty$ as $n \to \infty$.

Numerical illustration

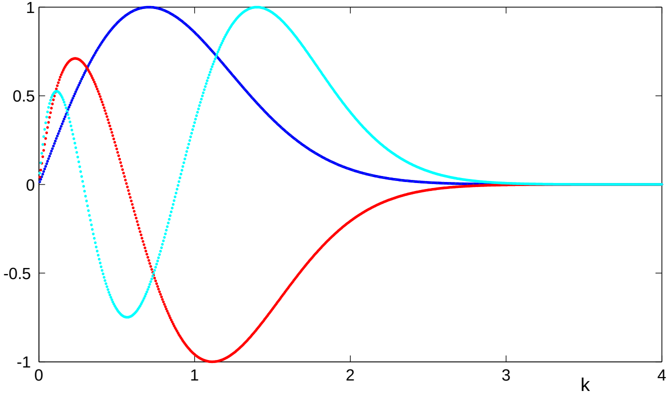

Figure : Eigenfunctions $\hat{u}$ of the spectral problem versus k for the first three eigenvalues $E_0 = 0$, $E_1 \approx 5.411$, and $E_2 \approx 12.308$.

Linear orbital stability

Consider time evolution of the perturbation $w(\tau,\xi) = v(\tau,\xi) - v_0(\xi)$:

$$\begin{cases} \partial_\tau w = \partial_\xi L w, \\ w(0) = w_0. \end{cases}$$

Theorem 3 (G.James–D.P., 2014)

The Gaussian solitary wave is linearly orbitally stable in space $H^1(\mathbb{R})$.

The solitary wave is said to be linearly orbitally stable if for every $w_0 \in \mathrm{Dom}(\partial_x L)$ with $\langle v_0, w_0 \rangle_{L^2} = 0$ there exists constant C such that

$$\|w(\tau)\|_{H^1 \cap L^2_1} \leq C \|w_0\|_{H^1 \cap L^2_1}, \quad \tau > 0,$$

where $\|w_0\|_{L^2_1} = \||\xi| w_0(\xi)\|_{L^2(\mathbb{R})}$.

Symplectic decomposition

We know that $\partial_\xi L$ has a double zero eigenvalue because

$$L v_0' = 0, \quad \partial_\xi L\, v_0 = -v_0'.$$

The constraint $\langle v_0, w_0 \rangle_{L^2} = 0$ removes the algebraic growth of perturbations in τ.

Using the decomposition

$$w(\tau,\xi) = a(\tau)\, v_0'(\xi) + b(\tau)\, v_0(\xi) + y(\xi,\tau)$$

with $\langle v_0, y \rangle_{L^2} = 0$ and $\langle \partial_\xi^{-1} v_0, y \rangle_{L^2} = 0$, we obtain

$$\frac{da}{d\tau} + b = 0, \quad \frac{db}{d\tau} = 0, \quad \frac{\partial y}{\partial \tau} = \partial_\xi L\, y.$$

If $\langle v_0, w_0 \rangle_{L^2} = 0$, then $b(\tau) = b(0) = 0$ and $a(\tau) = a(0)$.

Proof of linear orbital stability

Conservation of energy $E_c(y) := \langle Ly, y\rangle_{L^2}$ holds for smooth solutions:

$$\frac{d}{d\tau}\frac{1}{2}\langle Ly, y\rangle_{L^2} = \langle Ly, \partial_\tau y\rangle_{L^2} = \langle Ly, \partial_\xi Ly\rangle_{L^2} = 0.$$

The energy is coercive as follows.

Lemma 4

There exists a constant $C \in (0,1)$ such that for every $y \in H^1(\mathbb{R}) \cap L^2_1(\mathbb{R})$ satisfying the constraints

$$\langle v_0, y\rangle_{L^2} = \langle \partial_x^{-1} v_0, y\rangle_{L^2} = 0,$$

it is true that

$$C\|y\|^2_{H^1\cap L^2_1} \leq \langle Ly, y\rangle_{L^2} \leq \|y\|^2_{H^1\cap L^2_1}.$$

From here, we obtain the Lyapunov stability of the zero equilibrium $y = 0$ and hence linear orbital stability of the Gaussian solitary wave.

Nonlinear orbital or asymptotic stability ?

- Because the spectrum of $\partial_x L$ is purely discrete, no asymptotic stability result can hold for Gaussian solitary waves.
- This agrees with the result of Th. Cazenave (1983):
  the L^p norms for the solution v to the log–NLS equation do not vanish as $t \to \infty$ (or in a finite time) for any $p \geq 2$ including $p = \infty$.

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- Analysis of perturbations to v_0 meets the following obstacle. If $w(\tau,\xi) := v(\tau,\xi) - v_0(\xi)$, then w satisfies

$$w_\tau = \partial_\xi L w - \partial_\xi N(w),$$

where

$$N(w) := w \log\left(1 + \frac{w}{v_0}\right) + v_0 \left[\log\left(1 + \frac{w}{v_0}\right) - \frac{w}{v_0}\right].$$

"Small" $w(\tau,\xi)/v_0(\xi)$ may grow like $e^{\xi^2/4}$.

Another idea explored recently

Consider the decomposition of solutions to the linearized equation

$$\begin{cases} \partial_\tau w = \partial_\xi L w, \\ w(0) = w_0. \end{cases}$$

in terms of Hermite functions

$$w(\tau) = \sum_{n \in \mathbb{N}_0} c_n(\tau) u_n, \quad L u_n = (n-1) u_n.$$

The evolution problem is given by a chain of equations:

$$2 \frac{dc_n}{d\tau} = n\sqrt{n+1}\, c_{n+1} - (n-2)\sqrt{n}\, c_{n-1}, \quad n \in \mathbb{N}_0.$$

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- The constraint $\langle v_0, w_0 \rangle_{L^2} = 0$ yields $c_0(\tau) = 0$ for every $\tau \in \mathbb{R}$.
- The mode c_1 is eliminated by $c_1'(\tau) = c_2(\tau)/\sqrt{2}$.
- If $w \in H^1(\mathbb{R}) \cap L^2_1(\mathbb{R})$, then $\{c_n\}_{n \in \mathbb{N}}$ is defined in $\ell^2_1(\mathbb{N})$.

Jacobi difference equation

If $\{c_n\}_{n\in\mathbb{N}}$ is defined in $\ell_1^2(\mathbb{N})$, then we can set

$$c_{n+1} = \frac{i^n a_n}{\sqrt{n}}, \quad n \in \mathbb{N},$$

where $\{a_n\}_{n\in\mathbb{N}}$ is defined in $\ell^2(\mathbb{N})$.

The sequence $\{a_n\}_{n\in\mathbb{N}}$ satisfies the evolution problem

$$\frac{da}{dt} = \frac{i}{2} Ja,$$

where J is the Jacobi operator defined by

$$(Ja)_n := \sqrt{n(n+1)(n+2)}a_{n+1} + \sqrt{(n-1)n(n+1)}a_{n-1}, \quad n \in \mathbb{N}.$$

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Applying the theory of difference equations (G. Teschl, 2000):

- The Jacobi operator J has a limit circle at infinity.
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- The spectrum of J consists of a countable set of simple real isolated eigenvalues.

- For every $a(0) \in \ell^2(\mathbb{N})$, there exists a unique solution $a(t) \in \ell^2(\mathbb{N})$ to the evolution problem satisfying $\|a(t)\|_{\ell^2} = \|a(0)\|_{\ell^2}$ for every $t \in \mathbb{R}$.

Eigenvalues and eigenvectors

Solutions of $Jf = zf$ for $z \in \mathbb{R}^+$:

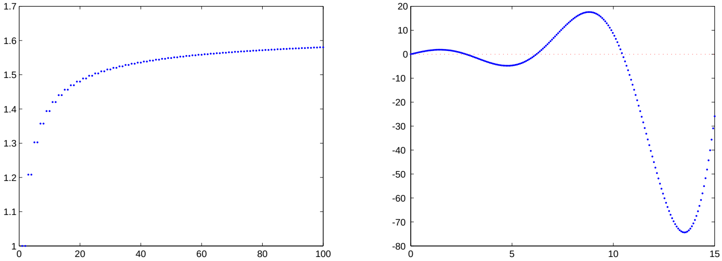

Figure : (a) Convergence of the sequence $\{W_n\}_{n\in\mathbb{N}}$ as $n \to \infty$ for $z = 1$. (b) Oscillatory behavior of W_∞ versus z.

Back to the same problem

If $A_m = f_{2m-1}$ and $B_m = f_{2m}$, then

$$A_m = \mathcal{O}(m^{-3/4}), \quad B_m = \mathcal{O}(m^{-5/4}) \quad \text{as} \quad m \to \infty.$$

The decay rate is too slow for the decomposition

$$y := u - c_1 u_1 = \sum_{n \in \mathbb{N}} \frac{i^n}{\sqrt{n}} f_n u_{n+1} = y_{\rm odd} + i y_{\rm even},$$

so that $y_{\rm odd} \in H^2(\mathbb{R}) \cap L^2_2(\mathbb{R})$, $y_{\rm even} \in H^1(\mathbb{R}) \cap L^2_1(\mathbb{R})$, but $y_{\rm even} \notin H^2(\mathbb{R}) \cap L^2_2(\mathbb{R})$.

If $w(\tau,\xi) := v(\tau,\xi) - v_0(\xi)$, then w satisfies

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"Small" $w(\tau,\xi)/v_0(\xi)$ may grow like an inverse Gaussian function of ξ.

Conclusion

The log-KdV equation

$$\frac{\partial v}{\partial \tau} + \frac{\partial}{\partial \xi}(v \log v) + \frac{\partial^3 v}{\partial \xi^3} = 0, \quad (\tau, \xi) \in \mathbb{R}^+ \times \mathbb{R}.$$

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4. Nonlinear stability of global solutions in the neighborhood of Gaussian solitary waves. Not yet.

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