Gaussian Solitary Waves in Granular Chains

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Introduction

- Granular crystal chains are chains of densely packed, elastically interacting particles.

- Recent works focus on solitary and periodic travelling waves in granular chains; said to be more relevant to physical experiments.

- Periodic travelling waves in granular chains were approximated numerically and analytically
  - G. James, *J. Nonlinear Sci.* **22** (2012), 813
On solitary travelling waves in homogeneous granular chains

Proofs of existence of solitary waves were developed from the variational theory based on the differential–difference equation.


- A. Stefanov and P. Kevrekidis, *J. Nonlinear Sci.* **22** (2012), 327 - proof of the bell-shaped profile of the solitary waves
Experimental setups (CalTECH)

Figure: N. Boechler, G. Theocharis, S. Job, P.G. Kevrekidis, M.A. Porter, and C. Daraio, PRL 104, 244302 (2010)

Figure: Y. Man, N. Boechler, G. Theocharis, P.G. Kevrekidis, and C. Daraio, Phys. Rev. E 85, 037601 (2012)
The granular 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 \( n \)th particle from a reference position versus time \( t \).

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

For the chains of hollow spherical particles of different width, we have other values of \( \alpha \) in the range \( 1.2 \leq \alpha \leq 1.5 \).
Travelling waves and the Boussinesq approximation

Using the relative displacements $u_n = x_n - x_{n-1}$ and applying the travelling wave reduction $u_n(t) = w_n(n - t)$, we obtain

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

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

Expanding $\Delta = \partial_z^2 + \frac{1}{12} \partial_z^4$ and integrating twice, we obtain

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

which has compactons

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

where

$$A = \left( \frac{1 + \alpha}{2\alpha} \right)^{\frac{1}{1-\alpha}}, \quad B = \frac{\sqrt{3}(\alpha-1)}{\alpha}.$$
Ill-posedness of the Boussinesq equation

The fully nonlinear Boussinesq equation takes the form

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


We will show that the Cauchy problem for the Boussinesq equation is ill-posed (according to Hille-Joshida Theorem).

Linearized Boussinesq equation

Linearizing the Boussinesq equation at the compact solution

\[ u(x, t) = w(x - t) + U(x - t) e^{\lambda t}, \]

we arrive at the spectral problem

\[ (\lambda - \partial_z)^2 U = \left( \partial_z^2 + \frac{1}{12} \partial_z^4 \right) (k_\alpha U), \]

where

\[ k_\alpha(z) := \alpha w^{\alpha-1}(z) = \alpha A^{\alpha-1} \cos^2(Bz) 1_{[-\pi/2B, \pi/2B]}(z). \]

The spectral problem can be closed on the compact interval \([-\pi/2B, \pi/2B]\) subject to the boundary conditions

\[ U\left( \pm \frac{\pi}{2B} \right) = 0, \quad U'\left( \pm \frac{\pi}{2B} \right) = 0. \]
Figure: Eigenvalues of the spectral problem (blue dots) for $\alpha = 1.05$ (left) and $\alpha = 1.2$ (right). The red dotted curves show the continuous spectrum obtained in the limit case $\alpha \to 1^+$. 
Korteweg–de Vries equation in the case of precompression

Consider again the FPU lattice

\[
\frac{d^2 u_n}{dt^2} = V'(u_{n+1}) - 2V'(u_n) + V'(u_{n-1}), \quad n \in \mathbb{Z}.
\]

If \( V \in C^3 \) with \( V''(0) = \kappa > 0 \) and \( V'''(0) \neq 0 \), then the asymptotic multi-scale expansion

\[
u_n(t) = \kappa (4V'''(0))^{-1} \varepsilon^2 y(\xi, \tau) + \text{higher order terms},
\]

where \( \xi := \varepsilon (n - c_s t) \), \( \tau := \varepsilon^3 c_s t/24 \), and \( c_s := \sqrt{\kappa} \) is the “sound velocity” of linear waves, shows that \( y \) satisfies the KdV equation

\[
\partial_\tau y + 3y \partial_\xi y + \partial^3_\xi y = 0.
\]

The KdV equation admits the solitary waves \( y = \text{sech}^2((\xi - \tau)/2) \).
Relevant results

- The KdV equation can be justified at a time scale of order $\varepsilon^{-3}$.

- Nonlinear stability of small amplitude FPU solitons can be proved.

- Existence and stability of $N$-soliton solutions can be proved.
  A. Hoffman and C.E. Wayne, *Nonlinearity* 21 (2008), 2911;
Korteweg–de Vries equation without precompression

Consider again the FPU lattice

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

where

\[ f_\alpha(u) := u(|u|^{\alpha-1} - 1) = (\alpha - 1) u \ln |u| + O((\alpha - 1)^2). \]

Let \( \alpha = 1 + \varepsilon^2 \). Using the asymptotic multi-scale expansion

\[ u_n(t) = \nu(\xi, \tau) + \text{higher order terms}, \]

where \( \xi := 2\sqrt{3}\varepsilon (n - t), \tau := \sqrt{3}\varepsilon^3 t, \) we obtain the KdV equation with the logarithmic nonlinearity (log-KdV)

\[ \partial_\tau \nu + \partial_\xi (\nu \log \nu) + \partial_\xi^3 \nu = 0. \]
Stationary solutions

Stationary log-KdV equation can be integrated once to get

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

which admits the Gaussian solitons

\[ v(\xi) = \sqrt{e} e^{-\xi^2/4}. \]

Figure: Solitary waves (blue dotted line) of the differential advance-delay equation in comparison with the compactons (red solid line) and the Gaussian solitons (green dashed line) for \( \alpha = 1.5 \) (left) and \( \alpha = 1.1 \) (right).
Convergence of the approximation

Figure: The $L^\infty$ distance between solitary waves of the differential advance-delay equation and either the compactons (blue dots) or the Gaussian solitons (green dots) versus parameter $\alpha$. 
Travelling solitary waves

A more general Gaussian solution with the speed \( v_s = 1 + c(\alpha - 1) \):

\[
  u_n(t) \approx \pm e^{2c + \frac{1}{2} - 3(\alpha - 1)(n - v_s t - \xi_0)^2},
\]

On the other hand, a more general solitary wave of the differential advance-delay equation may travel with any speed \( v_s \) because of the scaling transformation:

\[
  u_n(t) = |v_s|^2 \frac{2}{\alpha - 1} w(n - v_s t - \xi_0).
\]

Convergence may only occur if the velocity \( v_s \) convergence to unity as \( \alpha \to 1 \).
Numerical evidence of stability

Lattice of $N = 2000$ particles is excited with the initial condition of zero $x_n(0)$ and

$$\dot{x}_0(0) = 0.1, \quad \dot{x}_n(0) = 0 \text{ for all } n \geq 1.$$ 

A Gaussian solitary wave is formed asymptotically as $t$ evolves.

Figure: Formation of a localized wave in the Hertzian FPU lattice with $\alpha = 1.01$: left at $t \approx 30.5$, right at $t \approx 585.6$. The Gaussian approximation is shown by blue curve.
Energy functional

The log-KdV equation

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

can be written in the Hamiltonian form

$$\partial_\tau v = \partial_\xi E'(v),$$

where the energy functional is

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

Gaussian solitary wave $v_0 = \sqrt{e} e^{-\xi^2/4}$ is a critical point of $E(v)$, hence $E'(v_0) = 0$. 
Linear stability

The Hessian operator at the critical point $v_0 = \sqrt{e} e^{-\xi^2/4}$ is

$$L = E''(v_0) = -\frac{\partial^2}{\partial \xi^2} - 1 - \log |v^0| = -\frac{\partial^2}{\partial \xi^2} - \frac{3}{2} + \frac{\xi^2}{4}.$$  

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

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

The spectrum of $L$ consists of simple eigenvalues at integers $n - 1$, where $n \in \mathbb{N}_0$ (the set of natural numbers including zero).

The linear stability is determined by the time evolution of the perturbation of the solitary wave $v_0$:

$$\partial_{\tau} v = \partial_{\xi} L v.$$  

Spectral stability

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

\[
\frac{\partial}{\partial \xi} L V = \lambda V.
\]

Spectral stability of this KdV type was recently studied in

- D.P., in *Spectral analysis, stability, and bifurcation in modern nonlinear physical systems* (Wiley IST, 2014)

The difference is that \( L \) has purely discrete spectrum and the potential of \( L \) is confining.
Proof of linear stability

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

$$Lv_0' = 0, \quad \partial_\xi L v_0 = -v_0',$$

and no $u \in D(\partial_\xi L)$ exists in $\partial_\xi Lu = v_0$ because $\|\phi_0\|_2^2 \neq 0$.

Using the decomposition

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

with $\langle v_0, y \rangle = 0$ and $\langle \int_0^\xi v_0 dx, y \rangle = 0$, we obtain

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

Alternatively, we can represent \( y = c(\tau)\nu'_0 + w \) with \( \langle \nu_0, w \rangle = 0 \) and \( \langle \nu'_0, w \rangle = 0 \).

Now \( L \) is strictly positive definite on \( \nu_0 \perp \cap \nu'_0 \perp \), hence
\[
\| y \|_L = (Ly, y)^{1/2} = (Lw, w)^{1/2}
\]
defines a norm (equivalent to a weighted \( H^1 \)-norm). From the energy balance,
\[
\frac{d}{d\tau} \frac{1}{2} \| y \|_L^2 = (Ly, \partial_\tau y) = (Ly, \partial_\xi Ly) = 0,
\]
we obtain the Lyapunov stability of the zero equilibrium \( y = 0 \) in the constrained space \( \langle \nu_0, y \rangle = 0 \) and \( \langle \int_0^\xi \nu_0 dx, y \rangle = 0 \). The constrained space corresponds to the modulation of the two parameters of the Gaussian solitary wave.
Further development - justification of convergence

We can rewrite the differential advance-delay equation

$$\frac{d^2 w}{dz^2} = \Delta w^{1+\varepsilon^2}, \quad z \in \mathbb{R},$$

in the equivalent integral Fourier form

$$\hat{w}(k) = \frac{4}{k^2} \sin^2 \left( \frac{k}{2} \right) \hat{w}^{1+\varepsilon^2}(k), \quad k \in \mathbb{R},$$

where $\alpha = 1 + \varepsilon^2$. 
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\]

where \( \alpha = 1 + \varepsilon^2 \).

Divide \( \mathbb{R} \) into two sets: the interval \( I := [-\varepsilon^p, \varepsilon^p] \), where \( p > 0 \) is to be defined, and \( \mathbb{R} \setminus I \). Hence, we decompose

\[
\hat{w}(k) = \hat{V}(k)\chi_I(k) + \hat{W}(k)\chi_{\mathbb{R} \setminus I}(k),
\]

where \( \chi_S \) is the characteristic function of the set \( S \subset \mathbb{R} \).

D.P., G. Schneider, Appl. Anal. 86 (2007), 1017
D. Dohnal, H. Uecker, Physical D 238 (2009), 860
For the Gaussian solitary wave, we have

\[ v(z) = \sqrt{e} e^{-3\varepsilon^2 z^2} \Rightarrow \hat{v}(k) = \sqrt{\frac{\pi e}{3\varepsilon^2}} e^{-\frac{k^2}{12\varepsilon^2}}. \]

Hence, we shall work in the space of even continuous functions with

\[ |w(z)| \leq \alpha e^{-\gamma \varepsilon^2 z^2}, \quad |\hat{w}^{1+\varepsilon^2}(k)| \leq \beta \varepsilon^{-1} e^{-\delta \varepsilon^{-2} k^2}, \]

where \(\alpha, \beta, \gamma,\) and \(\delta\) are positive \(\varepsilon\)-independent constants.
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where \( \alpha, \beta, \gamma, \) and \( \delta \) are positive \( \varepsilon \)-independent constants.

Then, the integral equation on \( \mathbb{R} \setminus I \) yields

\[ |\hat{W}(k)| \leq \frac{4\beta}{k^2 \varepsilon} e^{-\delta \varepsilon^{-2} k^2}, \quad |k| \geq \varepsilon^p, \]

and

\[ W(z) = \frac{1}{2\pi} \int_{|k| \geq \varepsilon^p} W(k)e^{-ikz} dk \quad \Rightarrow \quad |W(z)| \leq \frac{4\beta}{\pi \varepsilon^{1+p}} e^{-\delta \varepsilon^{2p-2}}, \]

which is small if \( p < 1 \).
The integral equation on $I$ yields

$$\hat{V}(k) = \left( 1 - \frac{k^2}{12} + O(\varepsilon^{4p}) \right) \left( \hat{V}(k) + \varepsilon^2 (V + W) \log(V + W)(k) + \ldots \right).$$

The truncated version of this equation

$$0 = -\frac{k^2}{12} \hat{V}(k) + \varepsilon^2 V \log(V)(k), \quad |k| \leq \varepsilon^p$$

admits the Gaussian solution.

The linearized operator

$$\hat{L}v(k) := \left( \frac{3\varepsilon^2}{2} - \frac{k^2}{12} \right) \hat{v}(k) + 3\varepsilon^2 \frac{d^2 \hat{v}}{dk^2}$$

has a sequence of simple eigenvalues near $\varepsilon^2(1 - n)$, where $n \in \mathbb{N}_0$. Truncation introduces exponentially small perturbations.
The zero eigenvalue of $L$ corresponds to the translational invariance of the system with the eigenfunction $v'(z)$.

In the space of even functions, the zero eigenvalue of $L$ is removed and the correction term to the Gaussian solution satisfies

$$\sup_{z \in \mathbb{R}} |v(z)| \leq C\varepsilon^{4p-2},$$

which is small if $p > \frac{1}{2}$.

Hence, the approximation is justified for $p \in \left(\frac{1}{2}, 1\right)$. 
Further development - the KdV equation with compactons

Beyond order of \((\alpha - 1)^2 = \varepsilon^4\), we can rewrite the nonlinearity of the differential advance-delay equation

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

in the equivalent form:

\[
f_{\alpha}(u) := u(|u|^{\alpha-1} - 1) = (\alpha - 1) u \ln |u| + O((\alpha - 1)^2) = \alpha \left( u - u |u|^{\frac{1}{\alpha}-1} \right) + O((\alpha - 1)^2).
\]

Consequently, we can derive the generalized KdV equation

\[
\partial_\tau \nu + \partial_\xi^3 \nu + \frac{\alpha}{\alpha - 1} \partial_\xi (\nu - \nu |\nu|^{\frac{1}{\alpha}-1}) = 0
\]

at the same order as the log-KdV equation.
The generalized KdV equation with compactons

The generalized stationary KdV equation

\[ \partial^2_{\xi} v + \frac{\alpha}{\alpha - 1} \left( v - v |v|^{\frac{1}{\alpha} - 1} \right) = 0, \]

admit compacton solutions

\[ v_{\alpha}(\xi) = \begin{cases} \tilde{A} \cos^{\frac{2\alpha}{\alpha - 1}} (\tilde{B} \xi), & |\xi| \leq \frac{\pi}{2\tilde{B}}, \\ 0, & |\xi| \geq \frac{\pi}{2\tilde{B}}, \end{cases} \]

where

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

These compactons converge to the Gaussian solitons as \( \alpha \to 1 \).
Open questions

- Stability and convergence of compactons in the generalized KdV equation.
- Local and global well-posedness of the log-KdV and the generalized KdV equations.
- Justification of the time-dependent solutions of the FPU lattice described asymptotically by the log–KdV and generalized KdV equations.
- Proofs of nonlinear (orbital or asymptotic) stability of solitary waves in the FPU lattice with Hertzian nonlinearity.