# Gaussian Solitary Waves in Granular Chains

Guillaume James[1], Dmitry Pelinovsky[2]

[1] INRIA Grenoble Rhône-Alpes and Laboratoire Jean Kuntzmann, Université de Grenoble and CNRS
[2] Department of Mathematics, McMaster University, Canada

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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
  - K.R. Jayaprakash, Yu. Starosvetsky and A.F. Vakakis, *Phys. Rev. E* **83** (2011), 036606
  - G. James, *J. Nonlinear Sci.* **22** (2012), 813
  - M. Betti and D. Pelinovsky, *J. Nonlinear Sci.* **23** (2013), 619

# 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.

- G. Friesecke and J. Wattis, *Commun. Math. Phys.* **161** (1994), 391 - proof of existence for a general FPU lattice
- R. MacKay, *Phys. Lett. A* **251** (1999), 191 - adaptation of this method to granular chains
- J. English and R. Pego, *Proc. Amer. Math. Soc.* **133** (2005), 1763 - proof of the double-exponential tails of the solitary waves
- A. Stefanov and P. Kevrekidis, *J. Nonlinear Sci.* **22** (2012), 327 - proof of the bell-shaped profile of the solitary waves

# Experimental setups (CalTECH)

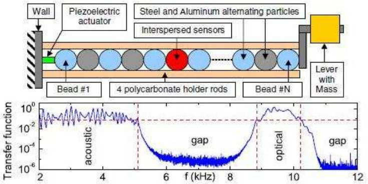


Figure : N. Boechler, G. Theocharis, S. Job, P.G. Kevrekidis, M.A. Porter, and C. Daraio, PRL **104**, 244302 (2010)

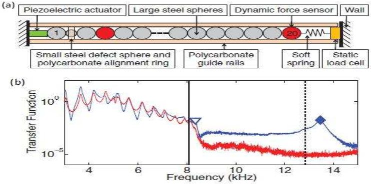


Figure : Y. Man, N. Boechler, G. Theocharis, P.G. Kevrekidis, and C. Daraio, Phys. Rev. E **85**, 037601 (2012)

# 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

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

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

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

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

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

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

V.F. Nesterenko, *J. Appl. Mech. Tech. Phys.* **24** (1983), 733
K. Ahnert and A. Pikovsky, *Phys. Rev. E* **79** (2009), 026209.

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

D.M. Ambrose, G. Simpson, J.D. Wright, and D.G. Yang, *Nonlinearity* **25** (2012), 2655.

# 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

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

The spectral problem can be closed on the compact interval $\left[-\frac{\pi}{2B},\frac{\pi}{2B}\right]$ subject to the boundary conditions

$$U\left(\pm\frac{\pi}{2B}\right) = 0, \quad U'\left(\pm\frac{\pi}{2B}\right) = 0.$$

# Numerical results

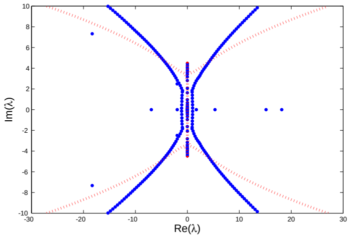


Figure : Eigenvalues of the spectral problem (blue dots) for $\alpha = 1.05$ (left) and $\alpha = 1.2$ (right). The red dotted curves show the continuous spectrum obtained in the limit case $\alpha \to 1^+$.

# 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

$$\partial_\tau y + 3y\partial_\xi y + \partial_\xi^3 y = 0.$$

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

# Relevant results

- The KdV equation can be justified at a time scale of order $\varepsilon^{-3}$.
  G. Schneider and C.E. Wayne, *International Conference on Differential Equations Appl.* **5** (1998) 69
  D. Bambusi, A. Ponno, *Comm. Math. Phys.* **264** (2006), 539

- Nonlinear stability of small amplitude FPU solitons can be proved.
  G. Friesecke and R.L. Pego, *Nonlinearity* **12** (1999), 1601; **15** (2002), 1343; **17** (2004), 207; **17** (2004), 229.

- Existence and stability of $N$-soliton solutions can be proved.
  A. Hoffman and C.E. Wayne, *Nonlinearity* **21** (2008), 2911;
  *J. Dyn. Diff. Equat.* **21** (2009), 343.
  T. Mizumachi, *Commun. Math. Phys.* **288** (2009), 125; *SIMA* **43** (2011), 2170; *Arch. Rat. Mech. Anal.* **207** (2013), 393.

# 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

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

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

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

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)

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

# 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

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

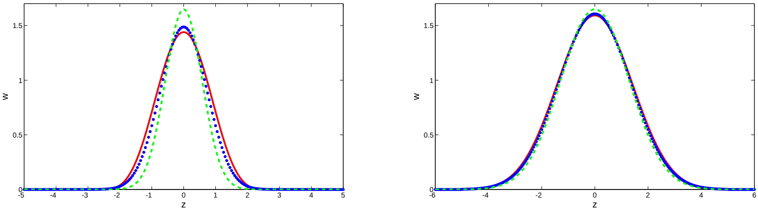


Figure : Solitary waves (blue dotted line) of the differential advance-delay equation in comparison with the compactons (red solid line) and the Gaussian solitons (green dashed line) for $\alpha = 1.5$ (left) and $\alpha = 1.1$ (right).

# Convergence of the approximation

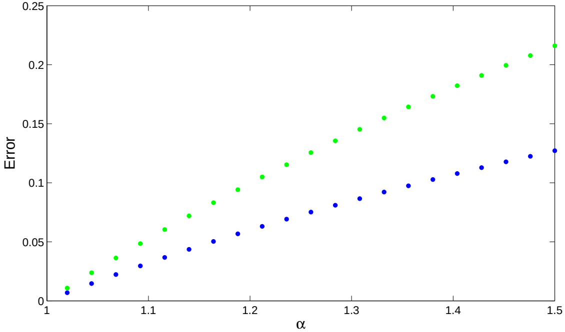


Figure : The $L^\infty$ distance between solitary waves of the differential advance-delay equation and either the compactons (blue dots) or the Gaussian solitons (green dots) versus parameter $\alpha$.

# Travelling solitary waves

A more general Gaussian solution with the speed $v_{\rm s} = 1 + c(\alpha - 1)$:

$$u_n(t) \approx \pm e^{2c + \frac{1}{2} - 3(\alpha-1)(n - v_{\rm s} t - \xi_0)^2},$$

On the other hand, a more general solitary wave of the differential advance-delay equation may travel with any speed $v_{\rm s}$ because of the scaling transformation:

$$u_n(t) = |v_{\rm s}|^{\frac{2}{\alpha-1}} w(n - v_{\rm s} t - \xi_0).$$

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.

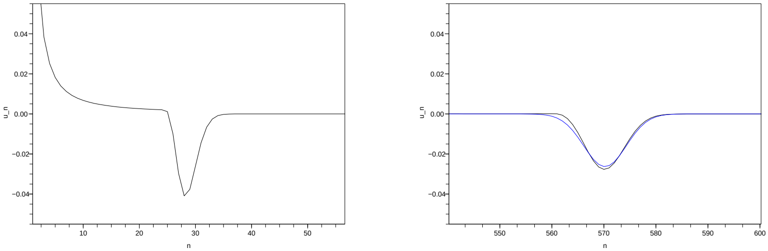


Figure : Formation of a localized wave in the Hertzian FPU lattice with $\alpha = 1.01$: left at $t \approx 30.5$, right at $t \approx 585.6$. The Gaussian approximation is shown by blue curve.

# 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

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

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

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

Spectral stability of this KdV type was recently studied in

- T. Kapitula, A. Stefanov, arXiv: 1210.6005 (2012)
- 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 $\partial_\xi L u = v_0$ 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 $y = c(\tau) v_0' + w$ with $\langle v_0, w \rangle = 0$ and $\langle v_0', w \rangle = 0$.

Now $L$ is strictly positive definite on ${v_0}^{\perp} \cap {v_0'}^{\perp}$, 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 $\langle v_0, y \rangle = 0$ and $\langle \int_0^\xi v_0 dx, y \rangle = 0$. 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

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

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 $\mathbb{R} \backslash I$. Hence, we decompose

$$\hat{w}(k) = \hat{V}(k)\chi_I(k) + \hat{W}(k)\chi_{\mathbb{R}\backslash I}(k),$$

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

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

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

$$|w(z)| \le \alpha e^{-\gamma \varepsilon^2 z^2}, \quad |\widehat{w^{1+\varepsilon^2}}(k)| \le \beta \varepsilon^{-1} e^{-\delta \varepsilon^{-2} k^2},$$

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 $\mathbb{R}\backslash I$ 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

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

The truncated version of this equation

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

admits the Gaussian solution.

The linearized operator

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

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

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

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:

$$\begin{aligned} f_\alpha(u) &:= u\left(|u|^{\alpha-1}-1\right) \\ &= (\alpha-1)\,u\ln|u|+\mathcal{O}((\alpha-1)^2) \\ &= \alpha\left(u-u|u|^{\frac{1}{\alpha}-1}\right)+\mathcal{O}((\alpha-1)^2). \end{aligned}$$

Consequently, we can derive the generalized KdV equation

$$\partial_\tau v+\partial_\xi^3 v+\frac{\alpha}{\alpha-1}\partial_\xi\left(v-v|v|^{\frac{1}{\alpha}-1}\right)=0$$

at the same order as the log-KdV equation.

# The generalized KdV equation with compactons

The generalized stationary KdV equation

$$\partial_\xi^2 v + \frac{\alpha}{\alpha - 1}\left(v - v|v|^{\frac{1}{\alpha}-1}\right) = 0,$$

admit compacton solutions

$$v_\alpha(\xi) = \begin{cases} \tilde{A}\cos^{\frac{2\alpha}{\alpha-1}}(\tilde{B}\xi), & |\xi| \le \frac{\pi}{2\tilde{B}}, \\ 0, & |\xi| \ge \frac{\pi}{2\tilde{B}}, \end{cases}$$

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.
- Development of numerical methods for the log–KdV and generalized KdV equations.