

# Periodic Travelling Waves in Diatomic Granular Chains

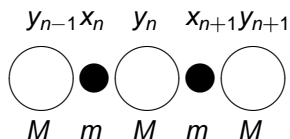
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# Introduction

- Granular crystal chains are chains of densely packed, elastically interacting particles.
- Recent work focuses on periodic travelling waves in granular chains; said to be more relevant to physical experiments.
- Periodic travelling waves in homogeneous granular chains (**monomers**) were approximated numerically [Yu. Starosvetsky and A.F. Vakakis, 2011; G. James, 2012].
- Our work focuses on the periodic travelling waves in chains of beads of alternating masses (**dimers**).

## The Dimer Model



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

$$\begin{cases} m\ddot{x}_n = V'(y_n - x_n) - V'(x_n - y_{n-1}), \\ M\ddot{y}_n = V'(x_{n+1} - y_n) - V'(y_n - x_n), \end{cases} \quad n \in \mathbb{Z},$$

where the interaction potential for spherical beads is

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

and  $H$  is the step (Heaviside) function.

To study small mass ratios  $\varepsilon^2 = \frac{m}{M}$ , we make the substitutions:

$$n \in \mathbb{Z}: \quad x_n(t) = u_{2n-1}(\tau), \quad y_n(t) = \varepsilon w_{2n}(\tau), \quad t = \sqrt{m}\tau$$

The FPU lattice is transformed into the equivalent form:

$$\begin{cases} \ddot{u}_{2n-1} = V'(\varepsilon w_{2n} - u_{2n-1}) - V'(u_{2n-1} - \varepsilon w_{2n-2}), \\ \ddot{w}_{2n} = \varepsilon V'(u_{2n+1} - \varepsilon w_{2n}) - \varepsilon V'(\varepsilon w_{2n} - u_{2n-1}), \end{cases} \quad n \in \mathbb{Z}.$$

Periodicity and travelling wave conditions:

$$u_{2n-1}(\tau) = u_{2n-1}(\tau + 2\pi), \quad w_{2n}(\tau) = w_{2n}(\tau + 2\pi), \quad \tau \in \mathbb{R}, \quad n \in \mathbb{Z}.$$

$$u_{2n+1}(\tau) = u_{2n-1}(\tau + 2q), \quad w_{2n+2}(\tau) = w_{2n}(\tau + 2q), \quad \tau \in \mathbb{R}, \quad n \in \mathbb{Z},$$

where  $q \in [0, \pi]$  is a free parameter.

## The Monomer Model

In the limit of equal mass ratio,  $\varepsilon = 1$  we apply the reduction:

$$n \in \mathbb{Z}: \quad u_{2n-1}(\tau) = U_{2n-1}(\tau), \quad w_{2n}(\tau) = U_{2n}(\tau).$$

This substitution, reduces the dimer system to the monomer system:

$$\ddot{U}_n = V'(U_{n+1} - U_n) - V'(U_n - U_{n-1}), \quad n \in \mathbb{Z}.$$

Periodic travelling waves for the monomer system has been considered before [Starosvetsky & Vakakis, 2011; James, 2012].

Note that travelling waves of the dimer model with  $\varepsilon = 1$  do not have to obey the reductions to the monomer model.

## Differential Advance-Delay Equation

Expressing the travelling waves as:

$$u_{2n-1}(\tau) = u_*(\tau + 2qn), \quad w_{2n}(\tau) = w_*(\tau + 2qn), \quad \tau \in \mathbb{R}, \quad n \in \mathbb{Z}.$$

we obtain the differential advance-delay equations for  $(u_*, w_*)$ :

$$\begin{cases} \ddot{u}_*(\tau) = V'(\varepsilon w_*(\tau) - u_*(\tau)) - V'(u_*(\tau) - \varepsilon w_*(\tau - 2q)), \\ \ddot{w}_*(\tau) = \varepsilon V'(u_*(\tau + 2q) - \varepsilon w_*(\tau)) - \varepsilon V'(\varepsilon w_*(\tau) - u_*(\tau)), \end{cases} \quad \tau \in \mathbb{R}.$$

For particular values  $q = \frac{\pi m}{N}$  with  $1 \leq m \leq N$ , the differential advance-delay equation is equivalently represented by the system of  $2mN$  second-order differential equations closed subject to the periodic boundary conditions.

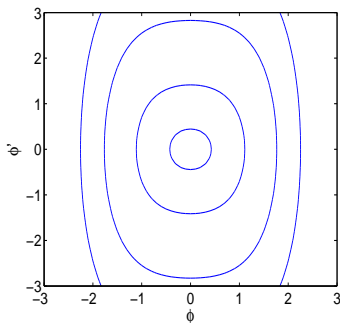
## Anti-continuum Limit

Let  $\varphi$  be a solution of the nonlinear oscillator equation,

$$\ddot{\varphi} = V'(-\varphi) - V'(\varphi) \quad \rightarrow \quad \ddot{\varphi} + |\varphi|^{\alpha-1}\varphi = 0.$$

For a unique  $2\pi$ -periodic solution we set:

$$\varphi(0) = 0, \quad \dot{\varphi}(0) > 0$$



## Special Solutions

For  $\varepsilon = 0$ , we can construct a limiting solution to the differential advance-delay equations:

$$\varepsilon = 0 : \quad u_*(\tau) = \varphi(\tau), \quad w_*(\tau) = 0, \quad \tau \in \mathbb{R},$$

Two solutions are known exactly for all  $\varepsilon \geq 0$ :

$$q = \frac{\pi}{2} : \quad u_*(\tau) = \varphi(\tau), \quad w_*(\tau) = 0$$

and

$$q = \pi : \quad u_*(\tau) = \frac{\varphi(\tau)}{(1 + \varepsilon^2)^3}, \quad w_*(\tau) = \frac{-\varepsilon\varphi(\tau)}{(1 + \varepsilon^2)^3}.$$

**Goal:** To consider persistence of the limiting solutions in  $\varepsilon$  for any fixed  $q \in [0, \pi]$ .



## Symmetries and Spaces

If  $\{u_{2n-1}(\tau), w_{2n}(\tau)\}_{n \in \mathbb{Z}}$  is a solution, then

- $\{u_{2n-1}(\tau + c), w_{2n}(\tau + c)\}_{n \in \mathbb{Z}}$  is a solution because of the translational invariance
- $\{u_{2n-1}(\tau) + c\varepsilon, w_{2n}(\tau) + c\}_{n \in \mathbb{Z}}$  is a solution because of the symmetry w.r.t. the change of coordinates.

For persistence analysis based on the Implicit Function Theorem, we shall work in the following spaces for  $u$  and  $w$ :

$$H_u^2 = \{u \in H_{\text{per}}^2(0, 2\pi) : u(-\tau) = -u(\tau), \tau \in \mathbb{R}\},$$

and

$$H_w^2 = \{w \in H_{\text{per}}^2(0, 2\pi) : w(\tau) = -w(-\tau - 2q)\},$$

## Theorem 1

*Fix  $q \in [0, \pi]$ . There is a unique  $C^1$  continuation of  $2\pi$ -periodic travelling wave in  $\varepsilon$ . In other words, there is an  $\varepsilon_0 > 0$  such that for all  $\varepsilon \in (0, \varepsilon_0)$  there exist a positive constant  $C$  and a unique solution  $(u_*, w_*) \in H_u^2 \times H_w^2$  of the system of differential advance-delay equations (4) such that*

$$\|u_* - \varphi\|_{H_{\text{per}}^2} \leq C\varepsilon^2, \quad \|w_*\|_{H_{\text{per}}^2} \leq C\varepsilon.$$

# Proof

To apply the Implicit Function Theorem, we rewrite the existence problem as the root-finding problem for the nonlinear operators:

$$\begin{cases} f_u(u, w, \varepsilon) := \frac{d^2 u}{d\tau^2} - F_u(u, w, \varepsilon), \\ f_w(u, w, \varepsilon) := \frac{d^2 w}{d\tau^2} - F_w(u, w, \varepsilon). \end{cases}$$

where

$$\begin{cases} F_u(u(\tau), w(\tau), \varepsilon) := V'(\varepsilon w(\tau) - u(\tau)) - V'(u(\tau) - \varepsilon w(\tau - 2q)), \\ F_w(u(\tau), w(\tau), \varepsilon) := \varepsilon V'(u(\tau + 2q) - \varepsilon w(\tau)) - \varepsilon V'(\varepsilon w(\tau) - u(\tau)), \end{cases}$$

- $f_u$  and  $f_w$  are  $C^1$  maps from  $H_u^2 \times H_w^2 \times \mathbb{R}$  to  $L_u^2 \times L_w^2$  since  $V \in C^2$ .
- At  $(\varphi, 0, 0)$ ,  $(f_u, f_w) = (0, 0)$ .
- The Jacobian operator

$$\left[ \begin{array}{cc} D_u f_u & D_u f_w \\ D_w f_u & D_w f_w \end{array} \right]_{(u,w,\varepsilon)=(\varphi,0,0)} = \left[ \begin{array}{cc} \frac{d^2}{d\tau^2} + \alpha|\varphi|^{\alpha-1} & 0 \\ 0 & \frac{d^2}{d\tau^2} \end{array} \right]$$

is invertible in the constrained spaces since the linear operators have zero-dimensional kernels in  $H_u^2$  and  $H_w^2$  respectively.

The result follows by the Implicit Function Theorem.

## Linearization

We linearize the dimer lattice equations around the travelling waves in order to analyze their stability:

$$\begin{cases} \ddot{u}_{2n-1} = V''(\varepsilon w_*(\tau + 2qn) - u_*(\tau + 2qn))(\varepsilon w_{2n} - u_{2n-1}) \\ \quad - V''(u_*(\tau + 2qn) - \varepsilon w_*(\tau + 2qn - 2q))(u_{2n-1} - \varepsilon w_{2n-2}), \\ \ddot{w}_{2n} = \varepsilon V''(u_*(\tau + 2qn + 2q) - \varepsilon w_*(\tau + 2qn))(u_{2n+1} - \varepsilon w_{2n}) \\ \quad - \varepsilon V''(\varepsilon w_*(\tau + 2qn) - u_*(\tau + 2qn))(\varepsilon w_{2n} - u_{2n-1}), \end{cases}$$

We use Floquet Theory for the chain of second-order ODEs:

$$\mathbf{u}(\tau + 2\pi) = \mathcal{M} \mathbf{u}(\tau), \quad \tau \in \mathbb{R},$$

where  $\mathbf{u} := [\cdots, w_{2n-2}, u_{2n-1}, w_{2n}, u_{2n+1}, \cdots]$  and  $\mathcal{M}$  is the monodromy operator.

Eigenvalues of the monodromy operator,  $\mathcal{M}$  are found via the substitution:

$$u_{2n-1}(\tau) = U_{2n-1}(\tau)e^{\lambda\tau}, \quad w_{2n}(\tau) = W_{2n}(\tau)e^{\lambda\tau}, \quad \tau \in \mathbb{R},$$

where  $(U_{2n-1}, W_{2n})$  are  $2\pi$ -periodic functions of  $\tau$ .

Admissible  $\hat{\lambda}$  are called the **characteristic exponents**. They define Floquet multipliers  $\mu$ :

$$\mu = e^{2\pi\lambda}$$

For  $\varepsilon = 0$ , the only characteristic exponent is  $\lambda = 0$ . It splits for  $\varepsilon \neq 0$  and the **goal** is to study the splitting of the zero eigenvalue.

**Challenges:**  $V''$  is only continuous.

The spectrum of  $\hat{\lambda}$  is continuous.

## Theorem 2

Fix  $q = \frac{\pi m}{N}$  for some positive integers  $m$  and  $N$  such that  $m \leq N$ . Let  $(u_*, w_*) \in H_u^2 \times H_w^2$  be defined by Theorem 1. For a sufficiently small  $\varepsilon$ , there exists  $q_0 \in (0, \pi/2)$  such that the travelling periodic waves in the linear eigenvalue problem closed at the  $2mN$ -periodic boundary conditions are:

$$\begin{aligned} 0 < q < q_0, \quad \pi - q_0 < q < \pi &\Rightarrow \text{stable} \\ q_0 < q < \pi - q &\Rightarrow \text{unstable} \end{aligned}$$

- Special solution with  $q = \pi$  is stable.
- Special solution with  $q = \pi/2$  is unstable.

## Ideas of the proof

- Renormalization by using the derivative expansion

$$\begin{aligned}\ddot{u}_*(\tau) &= V''(\varepsilon w_*(\tau) - u_*(\tau))(\varepsilon \dot{w}_*(\tau) - \dot{u}_*(\tau)) \\ &\quad - V''(u_*(\tau) - \varepsilon w_*(\tau - 2q))(\dot{u}_*(\tau) - \varepsilon \dot{w}_*(\tau - 2q)),\end{aligned}$$

to avoid the problem of discontinuity of  $V'''$ .

- Formal expansion for the eigenvalue  $\lambda = \varepsilon\Lambda + o(\varepsilon)$  and the eigenvectors  $U_{2n-1} = c_{2n-1}\dot{\phi}(\tau + 2qn) + o(\varepsilon)$  and  $W_{2n} = a_{2n} + o(\varepsilon)$ :

$$\begin{cases} K\Lambda^2 c_{2n-1} = M_1(c_{2n+1} + c_{2n-3} - 2c_{2n-1}) + L_1\Lambda(a_{2n} - a_{2n-2}), \\ \Lambda^2 a_{2n} = M_2(a_{2n+2} + a_{2n-2} - 2a_{2n}) + L_2\Lambda(c_{2n+1} - c_{2n-1}), \end{cases}$$

where  $K > 0$ ,  $M_1(q)$ ,  $M_2$ ,  $L_1$ ,  $L_2 < 0$  are numerical coefficients.



## Ideas of the proof

- Using a discrete Fourier transform, e.g.  $c_{2n-1} = Ce^{i\theta(2n-1)}$ , we transform difference equations to the characteristic polynomial:

$$D(\Lambda; \theta) = K\Lambda^4 + 4\Lambda^2(M_1 + KM_2 + L_1L_2)\sin^2(\theta) + 16M_1M_2\sin^4(\theta) = 0.$$

- To classify the nonzero roots of  $D(\Lambda; \theta)$ , we define

$$\Gamma := M_1 + KM_2 + L_1L_2, \quad \Delta := 4KM_1M_2.$$

- The two pairs of roots are determined in the following table:

Coefficients	Roots	$q$ Values
$\Delta < 0$	$\Lambda_1^2 < 0 < \Lambda_2^2$	$q_0 < q < \pi - q$
$0 < \Delta \leq \Gamma^2, \Gamma > 0$	$\Lambda_1^2 \leq \Lambda_2^2 < 0$	$0 < q < q_0$
$0 < \Delta \leq \Gamma^2, \Gamma < 0$	$\Lambda_1^2 \geq \Lambda_2^2 > 0$	
$\Delta > \Gamma^2$	$\text{Re}(\Lambda_1^2) > 0, \text{Re}(\Lambda_2^2) < 0$	

where  $q_0 \approx 0.915$

## Ideas of the proof

- Because of  $2mN$ -periodic boundary conditions, the admissible values of  $\theta$  are discrete and finite:

$$\theta = \frac{\pi k}{mN} \equiv \theta_k(m, N), \quad k = 0, 1, \dots, mN - 1.$$

We count  $4mN$  eigenvalues  $\lambda = \varepsilon\Lambda + o(\varepsilon)$  but some are double because  $\sin(\theta) = \sin(\pi - \theta)$ .

- The semi-simple eigenvalues  $\lambda \in i\mathbb{R}$  have the same (nonzero) Krein signature:

$$\begin{aligned} \sigma &= i \sum_{n \in \mathbb{Z}} [u_{2n-1} \dot{\bar{u}}_{2n-1} - \bar{u}_{2n-1} \dot{u}_{2n-1} + w_{2n} \dot{\bar{w}}_{2n} - \bar{w}_{2n} \dot{w}_{2n}] \\ &= \varepsilon \sigma^{(1)} + o(\varepsilon^2). \end{aligned}$$

Semi-simple eigenvalues  $\lambda \in i\mathbb{R}$  are structurally stable w.r.t.  $\varepsilon$ .

## Numerical Results

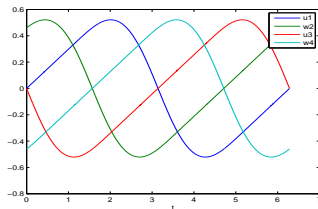
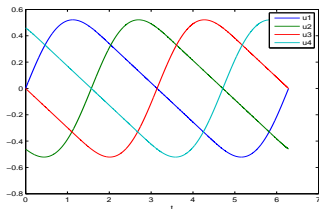
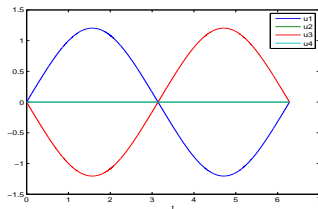
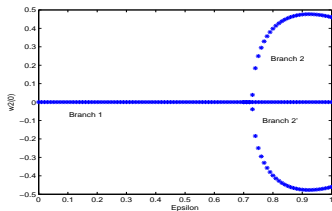
We close the infinite chain of beads into a chain of  $2N$  (i.e.  $q = \frac{\pi}{N}$ ) beads with periodic boundary conditions:

$$\begin{cases} \ddot{u}_{2n-1}(t) = (\varepsilon w_{2n}(t) - u_{2n-1}(t))_+^\alpha - (u_{2n-1}(t) - \varepsilon w_{2n-2}(t))_+^\alpha, \\ \ddot{w}_{2n}(t) = \varepsilon(u_{2n-1}(t) - \varepsilon w_{2n}(t))_+^\alpha - \varepsilon(\varepsilon w_{2n}(t) - u_{2n+1}(t))_+^\alpha, \end{cases}$$

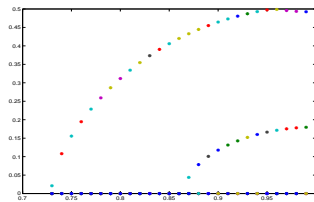
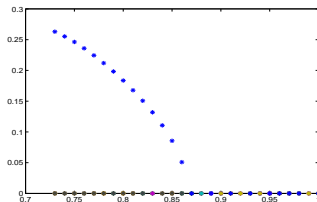
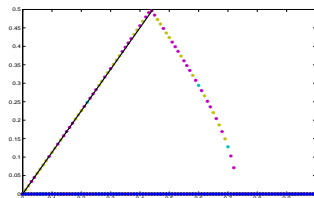
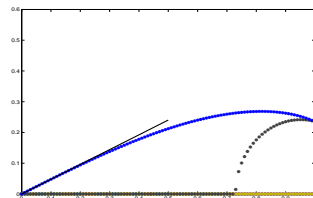
where  $1 \leq n \leq N$  and the periodic boundary conditions are used:

$$u_{-1} = u_{2N-1}, \quad u_{2N+1} = u_1, \quad w_0 = w_{2N}, \quad w_{2N+2} = w_2.$$

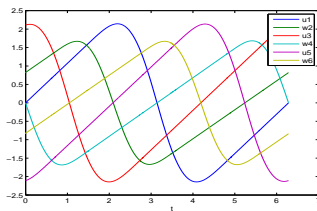
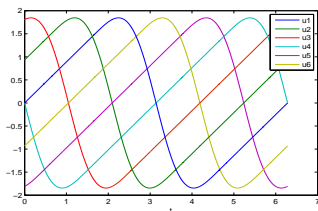
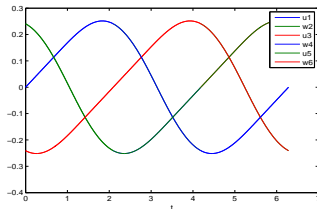
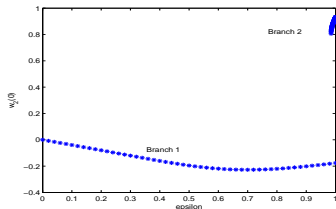
- We use the shooting method with  $N$  shooting parameters to approximate the travelling wave solutions.
- Then, we compute Floquet multipliers from the monodromy matrix of the linearized system.



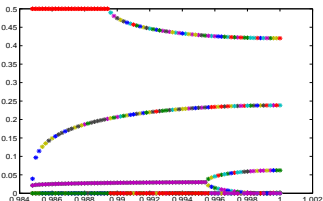
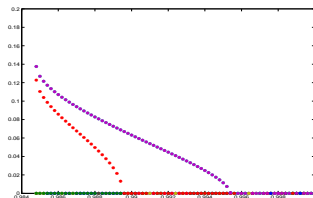
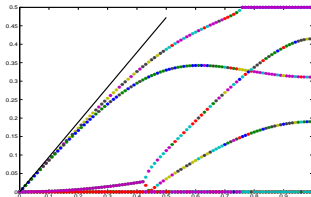
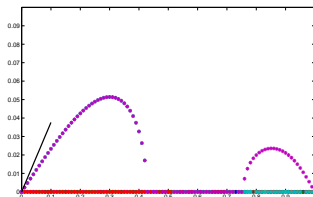
**Figure:** Travelling wave solutions for  $q = \frac{\pi}{2}$ : branch 1 (top right), branch 2 (bottom left), and branch 2' (bottom right) at  $\epsilon = 1$ .



**Figure:** Real (left) and imaginary (right) parts of the characteristic exponents  $\lambda$  versus  $\varepsilon$  for  $q = \frac{\pi}{2}$  for branch 1 (top) and branch 2 (bottom).

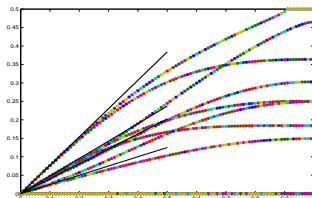
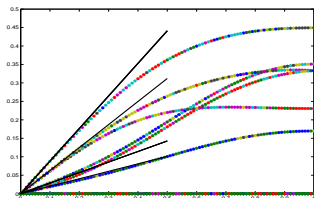


**Figure:** Travelling wave solutions for  $q = \frac{\pi}{3}$ : the solution of branch 1 is continued from  $\epsilon = 0$  to  $\epsilon = 1$  (top right) and the solution of branch 2 is continued from  $\epsilon = 1$  (bottom left) to  $\epsilon = 0.985$  (bottom right).



**Figure:** Real (left) and imaginary (right) parts of the characteristic exponents  $\lambda$  versus  $\varepsilon$  for  $q = \frac{\pi}{3}$  for branch 1 (top) and branch 2 (bottom).

Recall that branch 1 is stable for  $0 < q < q_0 \approx 0.915$ .



**Figure:** Imaginary parts of the characteristic exponents  $\lambda$  versus  $\varepsilon$  for  $q = \frac{\pi}{4}$  (left) and  $q = \frac{\pi}{5}$  (right). The real part of all the exponents is zero.



# Conclusions

- We have shown that the limiting periodic waves are uniquely continued from the anti-continuum limit for small mass ratio parameters.
- We are able to show that periodic waves with wavelengths larger than a certain critical value are spectrally stable for small mass ratios.
- We have used numerical techniques to show that for larger wavelengths the stability of these periodic travelling waves persists all the way to the limit of equal mass ratio.

## Open Problems

- The nature of the bifurcations where Branch 2 terminates at  $\varepsilon_* \in (0, 1)$  needs to be clarified for  $N \geq 3$ . We have been unsuccessful in our attempts to find another solution branch nearby for  $\varepsilon \gtrsim \varepsilon_*$ .
- We would like to understand the hidden symmetry which explains why coalescent eigenvalues remain stable for branch 1 for all  $\varepsilon \in [0, 1]$ .