Periodic Travelling Waves in Diatomic Granular Chains

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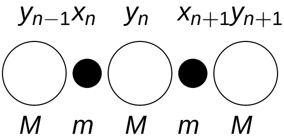
Introduction

- 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:

$$\left\{\begin{array}{l} m\ddot{x}_n = V'(y_n - x_n) - V'(x_n - y_{n-1}), \\ M\ddot{y}_n = V'(x_{n+1} - y_n) - V'(y_n - x_n), \end{array}\right. \qquad n \in \mathbb{Z},$$

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:

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

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_*):

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

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.

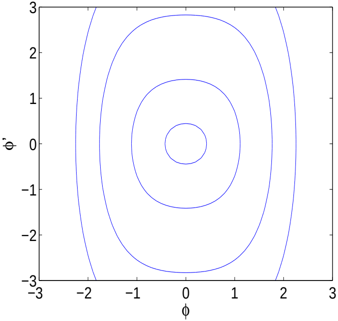
Anti-continuum Limit

Let φ 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 2π-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 ε 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:

$$H_u^2 = \left\{u \in H^2_{\rm per}(0,2\pi): \quad u(-\tau) = -u(\tau),\ \tau \in \mathbb{R}\right\},$$

and

$$H_w^2 = \left\{w \in H^2_{\rm per}(0,2\pi): \quad w(\tau) = -w(-\tau-2q)\right\},$$

Theorem 1

Fix $q \in [0, \pi]$. There is a unique C^1 continuation of 2π-periodic travelling wave in ε. 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*

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

Proof

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

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

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 $H^2_u \times H^2_w \times \mathbb{R}$ to $L^2_u \times L^2_w$ since $V \in C^2$.
- At $(\varphi, 0, 0)$, $(f_u, f_w) = (0, 0)$.
- The Jacobian operator

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

is invertible in the constrained spaces since the linear operators have zero-dimensional kernels in H^2_u and H^2_w 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:

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

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 2π-periodic functions of τ.

Admissible λ are called the **characteristic exponents**. They define Floquet multipliers μ:

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

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 λ 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 ε, 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:

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

- 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 $U_{2n-1} = c_{2n-1}\dot{\varphi}(\tau+2qn) + \mathcal{O}(\varepsilon)$ and $W_{2n} = a_{2n} + \mathcal{O}(\varepsilon)$:

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

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

where $q_0 \approx 0.915$

Ideas of the proof

- Because of $2mN$-periodic boundary conditions, the admissible values of θ 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 $\lambda = \varepsilon\Lambda + \mathrm{o}(\varepsilon)$ 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:

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

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

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.

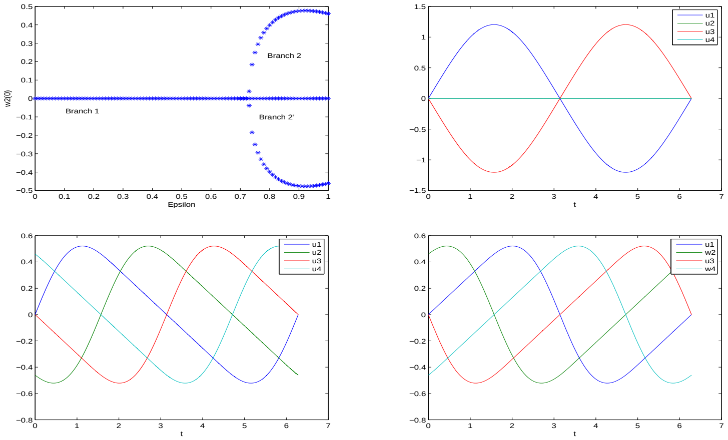


Figure: Travelling wave solutions for $q = \frac{\pi}{2}$: branch 1 (top right), branch 2 (bottom left), and branch 2' (bottom right) at $\varepsilon = 1$.

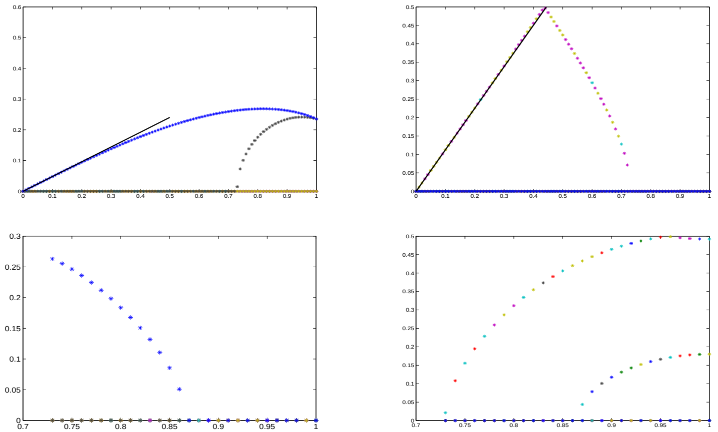


Figure: Real (left) and imaginary (right) parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{2}$ for branch 1 (top) and branch 2 (bottom).

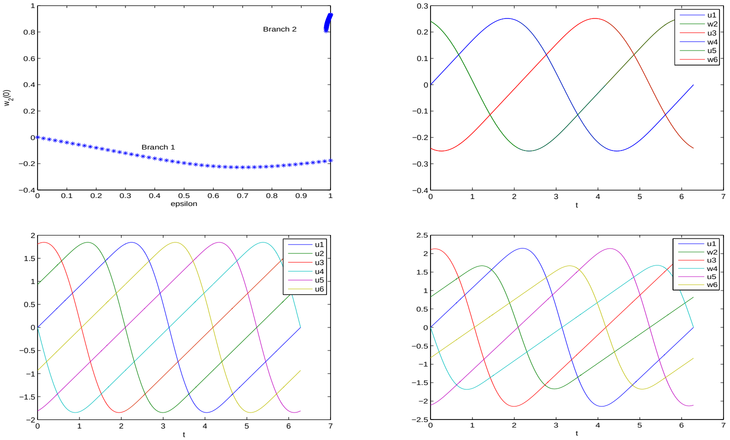


Figure: Travelling wave solutions for $q = \frac{\pi}{3}$: the solution of branch 1 is continued from $\varepsilon = 0$ to $\varepsilon = 1$ (top right) and the solution of branch 2 is continued from $\varepsilon = 1$ (bottom left) to $\varepsilon = 0.985$ (bottom right).

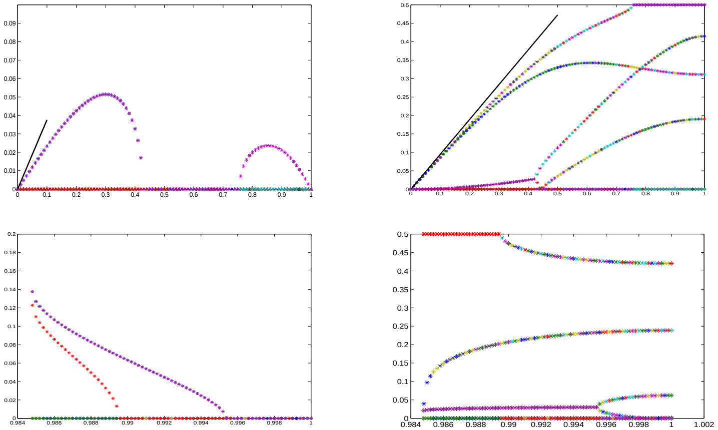


Figure: Real (left) and imaginary (right) parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{3}$ for branch 1 (top) and branch 2 (bottom).

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

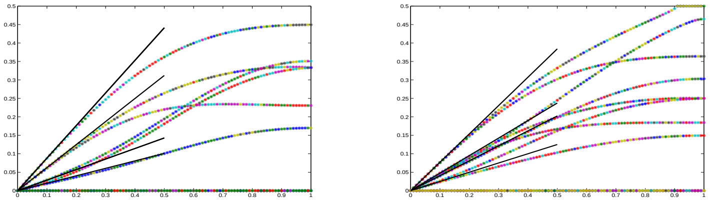


Figure: Imaginary parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{4}$ (left) and $q = \frac{\pi}{5}$ (right). The real part of all the exponents is zero.

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 $\varepsilon \gtrapprox \varepsilon_*$.

- We would like to understand the hidden symmetry which explains why coalescent eigenvalues remain stable for branch 1 for all $\varepsilon \in [0,1]$.