Periodic Travelling Waves in Diatomic Granular Chains

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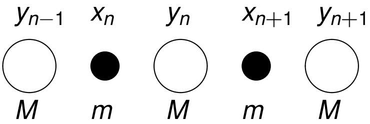
22 May 2012

Introduction

- Granular crystal chains are chains of densely packed, elastically interacting particles.
- Popular area of study in the past decade.
- Recent work focuses on periodic travelling waves in granular chains; said to be more relevant to physical experiments.
- Existence of periodic travelling waves was proved for a homogeneous granular chain (a **monomer**) [James 2011].
- We show existence of periodic travelling waves and stability results for chains of beads of alternating masses (a **dimer**).

The Model



The discrete FPU (Fermi-Pasta-Ulam) lattice:

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

where the interaction potential for spherical beads:

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

where H is the step (Heaviside) function.

We make the substitutions:

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

We transform FPU lattice:

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

where $\varepsilon^2 = \frac{m}{M}$.
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.

Monomer Reduction

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:

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

Existence of periodic travelling waves for the monomer system has previously been proved [James 2011].

Differential Advance-Delay Equation

We express travelling waves as:

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

where (u_*, w_*) solve the differential advance-delay equations:

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

Differential advance-delay systems are well-studied:

- Travelling waves in two-dimensional lattices [Cahn, Mallet-Paret, van Vleck 1998].
- Delay population models [Allen 2006; Murray 2002].

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:

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

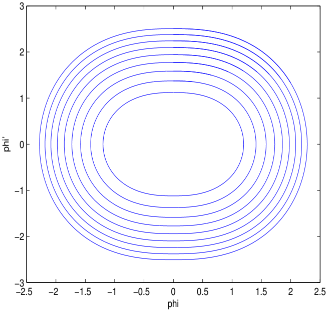


Figure: Phase portrait of the nonlinear oscillator in the $(\varphi, \dot{\varphi})$-plane.

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:

$$q = \frac{\pi}{2} : \quad u_{2n-1}(\tau) = \varphi(\tau + n\pi), \quad w_{2n}(\tau) = 0$$

$$q = \{0, \pi\} : \quad u_{2n-1}(\tau) = \frac{\varphi(\tau)}{(1+\varepsilon^2)^3}, \quad w_{2n}(\tau) = \frac{-\varepsilon\varphi(\tau)}{(1+\varepsilon^2)^3}.$$

Goal: To consider persistence of the limiting solutions in ε.

Spaces

For construction arguments based on the Implicit Function Theorem we shall work in the following spaces for u and w:

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

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

We add these constraints to deal with the two symmetries of the differential advance-delay equations: Translational symmetry in τ and the shift of (u, w) in $(\varepsilon, 1)$.

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 $(u_*, w_*) \in H^2_u \times H^2_w$ of the system of differential advance-delay equations (4) such that

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

Proof

We prove the Theorem by way of the Implicit Function Theorem. We are looking for zeroes of the nonlinear functions:

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

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 since V is C^2.

At $(\varphi, 0, 0)$, $(f_u, f_w) = (0, 0)$.

The Jacobian operator

$$\left[\begin{array}{cc} D_u f_u & D_u f_w \\ D_w f_u & D_w f_w \end{array}\right]_{(u,w,\varepsilon)=(\varphi,0,0)} = \left[\begin{array}{cc} \frac{d^2}{d\tau^2} + \alpha|\varphi|^{\alpha-1} & 0 \\ 0 & \frac{d^2}{d\tau^2} \end{array}\right] = \left[\begin{array}{cc} L & 0 \\ 0 & L_0 \end{array}\right]$$

is invertible in the constrained spaces since L and L_0 have zero-dimensional kernels in H_u^2 and H_w^2 respectively.

Then, the Implicit Function Theorem can be applied.

Linearization

We use the linearization of the dimer lattice 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:

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

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 sufficiently small positive ε. Consider the linear eigenvalue problem subject to $2mN$-periodic boundary conditions. There is a $\varepsilon_0 > 0$ such that, for every $\varepsilon \in (0, \varepsilon_0)$, there exists $q_0(\varepsilon) \in \left(0, \frac{\pi}{2}\right)$ such that for all $q \in (0, q_0(\varepsilon))$ and $q \in (\pi - q_0(\varepsilon), \pi]$, no values of λ with $\mathrm{Re}(\lambda) \neq 0$ exist, whereas for $q \in (q_0(\varepsilon), \pi - q_0(\varepsilon))$, there exist some values of λ with $\mathrm{Re}(\lambda) > 0$.

In other words,

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

We use a discrete Fourier transform on perturbation expansions of linearized equations using our substitution and compute the characteristic polynomial:

$$D(\Lambda;\theta) = K\Lambda^4 + 4\Lambda^2(M_1 + KM_2 + L_1 L_2)\sin^2(\theta) + 16 M_1 M_2 \sin^4(\theta) = 0.$$

where

$$K = -\frac{4\pi^2}{T'(E_0)}, \quad M_2 = \frac{2}{\pi T'(E_0)(\dot{\varphi}(0))^2}, \quad L_1 = 2\pi L_2 = \frac{2(2\pi - T'(E_0)(\dot{\varphi}(0))^2)}{T'(E_0)\dot{\varphi}(0)},$$

and

$$M_1 = -\frac{2}{\pi}(\dot{\varphi}(0))^2 + I(q),$$

where

$$I(q) = I(\pi - q) := -\int_{\pi-2q}^{\pi} \ddot{\varphi}(\tau)\ddot{\varphi}(\tau + 2q)d\tau, \quad q \in \left[0, \frac{\pi}{2}\right].$$

To classify the nonzero roots of the characteristic polynomial, we define

$$\Gamma := M_1 + KM_2 + L_1 L_2, \quad \Delta := 4KM_1 M_2.$$

The two pairs of roots are determined in the following table.

Coefficients	Roots
$\Delta < 0$	$\Lambda_1^2 > 0,\ \Lambda_2^2 < 0$
$0 < \Delta \leq \Gamma^2, \Gamma > 0$	$\Lambda_1^2 < 0,\ \Lambda_2^2 < 0$
$0 < \Delta \leq \Gamma^2, \Gamma < 0$	$\Lambda_1^2 > 0,\ \Lambda_2^2 > 0$
$\Delta > \Gamma^2$	$\mathrm{Re}(\Lambda_1^2) > 0,\ \mathrm{Re}(\Lambda_2^2) < 0$

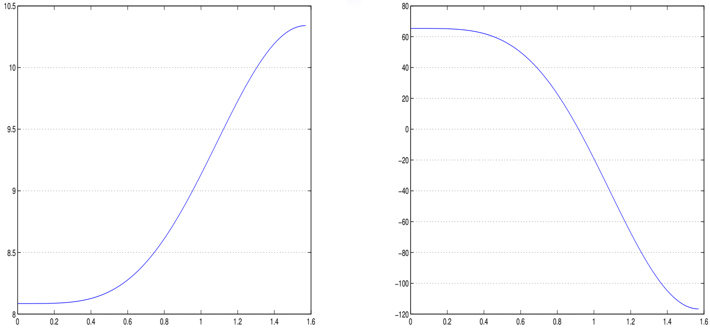


Figure: Coefficients Γ (left) and Δ (right) versus q.

We can show analytically that $\Gamma > 0$ and $\Delta \leq \Gamma^2$. The quantity Δ changes sign at $q_0 \approx 0.915$.

$$0 < q < q_0, \quad \pi - q_0 < q < \pi \quad \Rightarrow \quad \Lambda_1^2, \Lambda_2^2 < 0$$
$$q_0 < q < \pi - q \quad \Rightarrow \quad \Lambda_1^2 > 0, \quad \Lambda_2^2 < 0.$$

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:

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

with

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

We use the shooting method with $2N$ shooting parameters to approximate solutions.

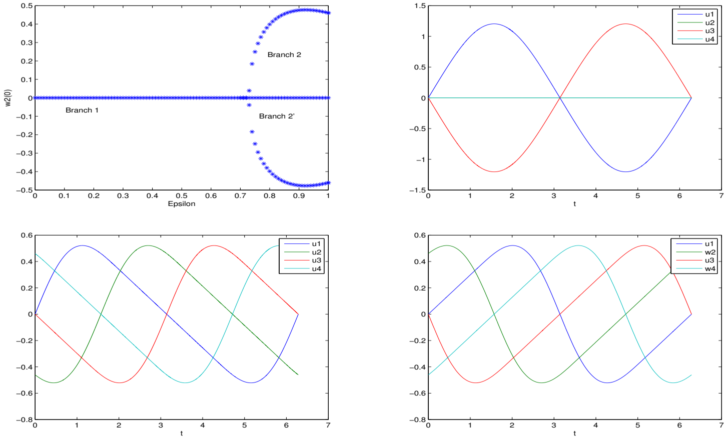


Figure: Travelling wave solutions for $q = \frac{\pi}{2}$: the solution of the dimer chain continued from $\varepsilon = 0$ to $\varepsilon = 1$: branch 1 (top right), branch 2 (bottom left), and branch 2' (bottom right).

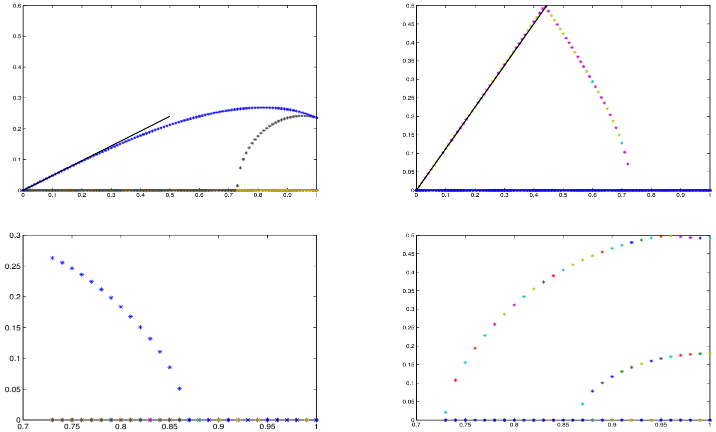


Figure: Real (left) and imaginary (right) parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{2}$ for branch 1 (top) and branch 2 (bottom).

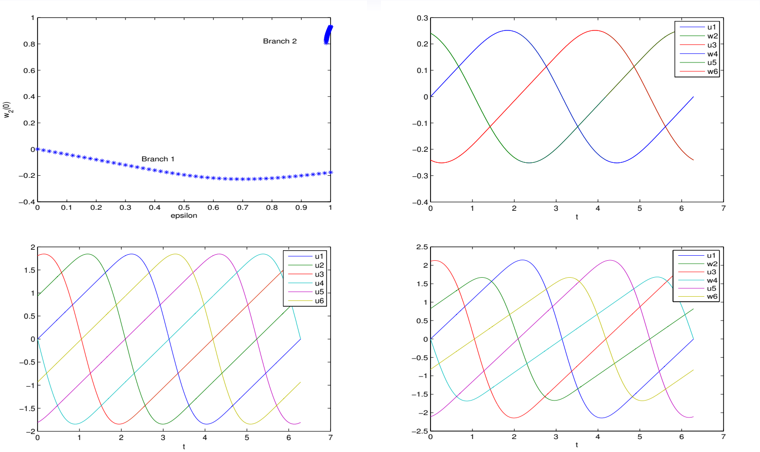


Figure: Travelling wave solutions for $q = \frac{\pi}{3}$: the solution of branch 1 is continued from $\varepsilon = 0$ to $\varepsilon = 1$ (top right) and the solution of branch 2 is continued from $\varepsilon = 1$ (bottom left) to $\varepsilon = 0.985$ (bottom right).

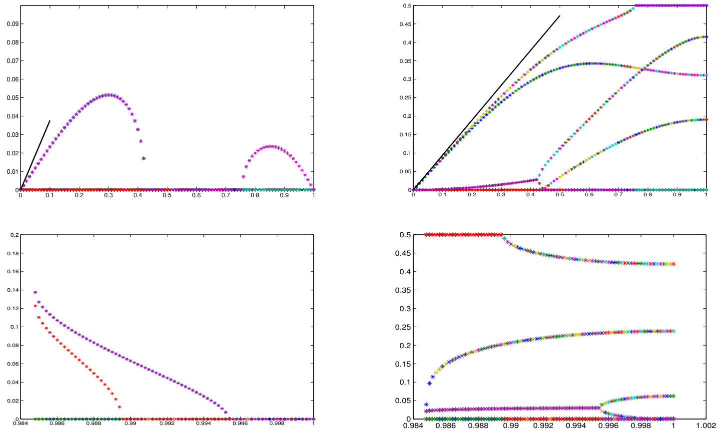


Figure: Real (left) and imaginary (right) parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{3}$ for branch 1 (top) and branch 2 (bottom).

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

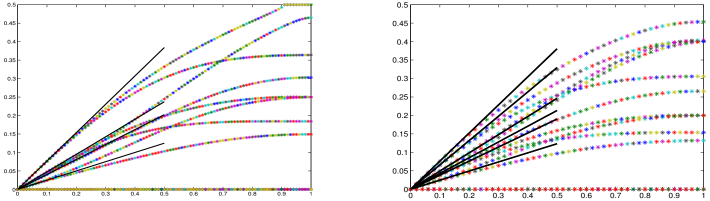


Figure: Imaginary parts of the characteristic exponents λ versus ε for $q = \frac{\pi}{5}$ (left) and $q = \frac{\pi}{6}$ (right). The real part of all the exponents is zero.

Conclusions

- We have shown that the limiting periodic waves are all 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 $q = \frac{\pi}{3}$.
- 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 $q \leq \frac{\pi}{5}$.

Thank you!