Bifurcations, resonances, and stability of multi-site breathers

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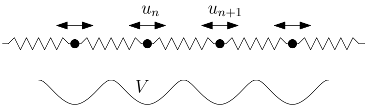
Joint work with A. Sakovich (PhD student)

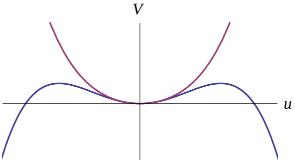
Klein-Gordon lattice

Klein-Gordon (KG) lattice models a chain of coupled anharmonic oscillators with nearest-neighbour interactions

$$\ddot{u}_n + V'(u_n) = \epsilon(u_{n-1} - 2u_n + u_{n+1}),$$

where $\{u_n(t)\}_{n\in\mathbb{Z}} : \mathbb{R} \to \mathbb{R}^{\mathbb{Z}}$, dot represents time derivative, ϵ is the coupling constant, and $V : \mathbb{R} \to \mathbb{R}$ is an on-site potential.





Applications:

- dislocations in crystals (e.g. Frenkel & Kontorova '1938)
- oscillations in biological molecules (e.g. Peyrard & Bishop '1989)

Anharmonic oscillator

We make the following assumptions:

- $V'(u) = u \pm u^3 + \mathcal{O}(u^5)$, where $+/-$ corresponds to hard/soft potential;
- $0 < \epsilon \ll 1$: oscillators are weakly coupled.

In the anti-continuum limit ($\epsilon = 0$), each oscillator is governed by

$$\ddot{\varphi} + V'(\varphi) = 0, \quad \Rightarrow \quad \frac{1}{2}\dot{\varphi}^2 + V(\varphi) = E,$$

where $\varphi \in H^2_{per}(0, T)$.

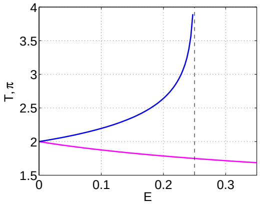


Figure : Period versus energy in hard (magenta) and soft (blue) V.

The period of the oscillator is

$$T(E) = \sqrt{2} \int_{-a(E)}^{a(E)} \frac{dx}{\sqrt{E - V(x)}},$$

where $a(E)$, the amplitude, is the smallest root of $V(a) = E$.

Multi-breathers in the anti-continuum limit

Breathers are spatially localized time-periodic solutions to the Klein-Gordon lattice. Multi-breathers are constructed by parameter continuation in ϵ from $\epsilon = 0$.

For $\epsilon = 0$ we take

$$\mathbf{u}^{(0)}(t) = \sum_{k \in S} \sigma_k \varphi(t) \mathbf{e}_k \quad \in \quad l^2(\mathbb{Z}, H^2_{per}(0,T)),$$

where $S \subset \mathbb{Z}$ is the set of excited sites and $\mathbf{e}_k$ is the unit vector in $l^2(\mathbb{Z})$ at the node k. The oscillators are in phase if $\sigma_k = +1$ and out-of-phase if $\sigma_k = -1$.

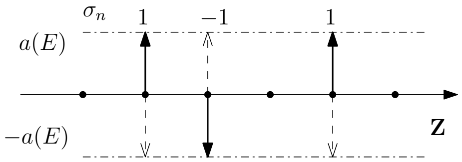


Figure : An example of a multi-site discrete breather at $\epsilon = 0$.

Persistence of multi-breathers

Theorem (MacKay & Aubry '1994)

Fix the period $T \neq 2\pi n$, $n \in \mathbb{N}$ and the T-periodic solution $\varphi \in H^2_{per}(0,T)$ of the anharmonic oscillator equation for $T'(E) \neq 0$. There exist $\epsilon_0 > 0$ and $C > 0$ such that $\forall \epsilon \in (-\epsilon_0, \epsilon_0)$ there exists a solution $\mathbf{u}^{(\epsilon)} \in l^2(\mathbb{Z}, H^2_{per}(0,T))$ of the Klein–Gordon lattice satisfying

$$\left\| \mathbf{u}^{(\epsilon)} - \mathbf{u}^{(0)} \right\|_{l^2(\mathbb{Z}, H^2(0,T))} \leq C\epsilon.$$

The proof is based on the Implicit Function Theorem and uses invertibility of the linearization operators

$$\begin{aligned} \mathcal{L}_0 &= \partial_t^2 + 1 : H^2_{per}(0,T) \to L^2_{per}(0,T), \qquad T \neq 2\pi n, \\ \mathcal{L}_e &= \partial_t^2 + V''(\varphi(t)) : H^2_{per,even}(0,T) \to L^2_{per,even}(0,T), \qquad T'(E) \neq 0. \end{aligned}$$

Three-site KG lattice

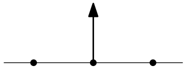
Consider a three-site KG lattice with a *soft* potential and Dirichlet boundary conditions,

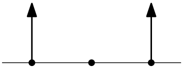
$$\left\{ \begin{array}{c} \ddot{u}_0 + u_0 - u_0^3 = 2\epsilon(u_1 - u_0) \\ \ddot{u}_1 + u_1 - u_1^3 = \epsilon(u_0 - 2u_1) \\ u_{-1} = u_1, \end{array} \right.$$

Two limiting configurations are of interest:

$$\mathbf{u}^{(0)}(t) = \varphi(t)\mathbf{e}_0 \qquad \mathbf{u}^{(0)}(t) = \varphi(t)(\mathbf{e}_{-1} + \mathbf{e}_1)$$

Fundamental breather   Breather with a "hole"

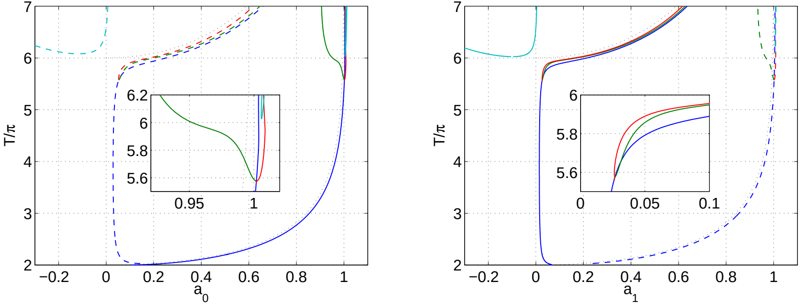




Breather solutions

Periodic solutions are computed with the shooting method for $\epsilon = 0.01$ starting with the initial conditions:

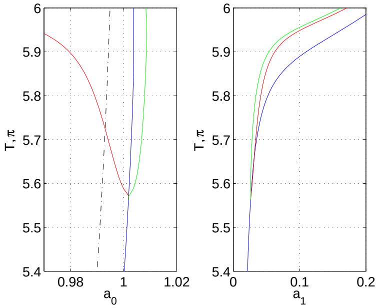
$$u_0(0) = a_0(T), \quad \dot{u}_0(0) = 0, \quad u_1(0) = a_1(T), \quad \dot{u}_1(0) = 0$$

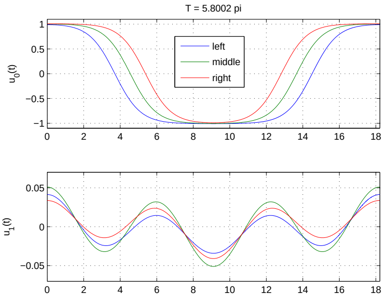


Solid – fundamental breather. Dashed – breather with a "hole".

Fundamental breather

Fundamental breather with $\mathbf{u}^{(0)}(t) = \varphi(t)\mathbf{e}_0$ undertakes a pitchfork (symmetry-breaking) bifurcation near $T = 6\pi$ (1:3 resonance).





Fundamental breather

The middle branch becomes unstable after the pitchfork bifurcation. Left and right branches are born stable, but also become unstable for larger T.

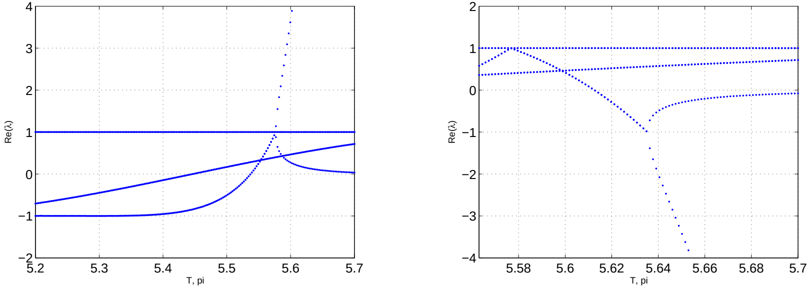


Figure : Real part of the Floquet multipliers versus period T.

Asymptotic theory of pitchfork bifurcation

Recall the discrete Klein–Gordon equation

$$\ddot{u}_n + V'(u_n) = \epsilon(u_{n-1} - 2u_n + u_{n+1}).$$

When $T \neq 2\pi n$ is fixed, breather solutions are represented by the expansion

$$\left\{ \begin{array}{lclcl} u_0(t) & = & \varphi(t) - 2\epsilon\psi_1(t) & + & \mathcal{O}_{H^2_{\rm per}(0,T)}(\epsilon^2), \\ u_{\pm 1}(t) & = & + \epsilon\varphi_1(t) & + & \mathcal{O}_{H^2_{\rm per}(0,T)}(\epsilon^2), \\ u_{\pm n}(t) & = & & + & \mathcal{O}_{H^2_{\rm per}(0,T)}(\epsilon^2), \quad n \geq 2, \end{array} \right.$$

where φ can be expanded in the Fourier series,

$$\varphi(t) = \sum_{n \in \mathbb{N}_{\rm odd}} c_n(T) \cos\left(\frac{2\pi nt}{T}\right).$$

and the first-order correction is found from $\ddot{\varphi}_1 + \varphi_1 = \varphi$:

$$\varphi_1(t) = \sum_{n \in \mathbb{N}_{\rm odd}} \frac{T^2 c_n(T)}{T^2 - 4\pi^2 n^2} \cos\left(\frac{2\pi nt}{T}\right).$$

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Near $T = 6\pi$, the norm $\|u_{\pm 1}\|_{H^2_{\rm per}(0,T)}$ is much larger than $\mathcal{O}(\epsilon)$ if $c_3(6\pi) \neq 0$.

Lyapunov–Schmidt reduction (for $V'(u) = u - u^3$)

Using the scaling transformation,

$$T = \frac{6\pi}{1+\delta\epsilon^{2/3}}, \quad \tau = (1+\delta\epsilon^{2/3})t, \quad u_n(t) = (1+\delta\epsilon^{2/3})U_n(\tau),$$

where δ is ϵ-independent, U is 6π-periodic, and

$$\ddot{U}_n + U_n - U_n^3 = \beta U_n + \gamma(U_{n+1} + U_{n-1}), \quad n \in \mathbb{Z},$$

where

$$\beta = 1 - \frac{1+2\epsilon}{(1+\delta\epsilon^{2/3})^2} = \mathcal{O}(\epsilon^{2/3}), \quad \gamma = \frac{\epsilon}{(1+\delta\epsilon^{2/3})^2} = \mathcal{O}(\epsilon).$$

Hence we have at the central site:

$$\ddot{U}_0 + U_0 - U_0^3 = \beta U_0 + 2\gamma U_1$$

whereas at the first site:

$$\ddot{U}_1 + U_1 - U_1^3 = \beta U_1 + \gamma U_2 + \gamma U_0.$$

Decomposition

Let us represent an even 6π-periodic function U_0 by the Fourier series,

$$U_0(\tau) = \sum_{n \in \mathbb{N}_{\rm odd}} b_n \cos\left(\frac{n\tau}{3}\right).$$

If $U_0(\tau) \to \varphi(\tau)$ as $\epsilon \to 0$, then $b_n \to c_n(6\pi)$ as $\epsilon \to 0$.

Applying the decomposition

$$U_n(\tau) = A_n \cos(\tau) + V_n(\tau), \quad \langle V_n, \cos(\cdot) \rangle_{L^2_{\rm per}(0,6\pi)} = 0,$$

we obtain for $n = 1$:

$$\beta A_1 + \gamma A_2 + \gamma b_3 = -\frac{1}{3\pi} \int_0^{6\pi} \cos(\tau)(A_1 \cos(\tau) + V_1(\tau))^3 d\tau$$

and

$$\begin{aligned} \ddot{V}_1 + V_1 \quad = \quad & \beta V_1 + \gamma V_2 + \gamma \sum_{k \in \mathbb{N}_{\rm odd} \backslash \{3\}} b_k \cos\left(\frac{k\tau}{3}\right) \\ & + (A_1 \cos(\tau) + V_1)^3 - \cos(\tau) \frac{\langle \cos(\cdot), (A_1 \cos(\cdot) + V_1)^3 \rangle_{L^2_{\rm per}(0,6\pi)}}{\langle \cos(\cdot), \cos(\cdot) \rangle_{L^2_{\rm per}(0,6\pi)}}. \end{aligned}$$

Reduction

By the Implicit Function Theorem, for small ϵ and small $\|\mathbf{A}\|$, there is $C > 0$:

$$\|\mathbf{V}\|_{l^2(\mathbb{N},H^2_{\rm per}(0,6\pi))} \leq C(\epsilon + \|\mathbf{A}\|^3_{l^\infty(\mathbb{N})}).$$

Then, V_n can be substituted in the system of algebraic equations, e.g. for $n = 1$,

$$\beta A_1 + \gamma A_2 + \gamma b_3 = -\frac{1}{3\pi}\int_0^{6\pi} \cos(\tau)(A_1\cos(\tau) + V_1(\tau))^3 d\tau$$

Recall that $\beta = 2\delta\epsilon^{2/3} - 2\epsilon + \mathcal{O}(\epsilon^{4/3})$ and $\gamma = \epsilon + \mathcal{O}(\epsilon^{5/3})$ as $\epsilon \to 0$. Using the scaling transformation $A_n = \epsilon^{1/3} a_n$, we obtain

$$\begin{aligned} 2\delta a_1 + \frac{3}{4}a_1^3 + b_3 &= \epsilon^{1/3}(2a_1 - a_2) + \mathcal{O}(\epsilon^{2/3}), \\ 2\delta a_n + \frac{3}{4}a_n^3 &= \epsilon^{1/3}(2a_n - a_{n+1} - a_{n-1}) + \mathcal{O}(\epsilon^{2/3}), \quad n \geq 2. \end{aligned}$$

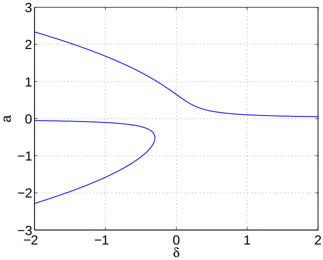
If $\delta \neq 0$, then for small ϵ and finite a_1, there is $C > 0$: $\|\mathbf{a}\|_{l^2(\mathbb{N}\backslash\{1\})} \leq C\epsilon^{1/3}$.

Normal form for 1:3 resonance

Assume that $U_0(\tau) \to \varphi(\tau)$ as $\epsilon \to 0$, then $b_n \to c_n(6\pi)$ as $\epsilon \to 0$. For fixed $\delta \neq 0$, let $a(\delta)$ be a root of the cubic equation

$$2\delta a(\delta) + \frac{3}{4} a^3(\delta) + c_3(6\pi) = 0,$$

and assume that $8\delta + 9a^2(\delta) \neq 0$.



We have thus obtained the periodic solution in the form of the expansion

$$\begin{cases} U_{\pm 1}(\tau) = \epsilon^{1/3} a(\delta) \cos(\tau) + \mathcal{O}_{H^2_{\rm per}(0,6\pi)}(\epsilon^{2/3}), \\ U_{\pm n}(\tau) = \mathcal{O}_{H^2_{\rm per}(0,6\pi)}(\epsilon^{2/3}), \quad n \geq 2. \end{cases}$$

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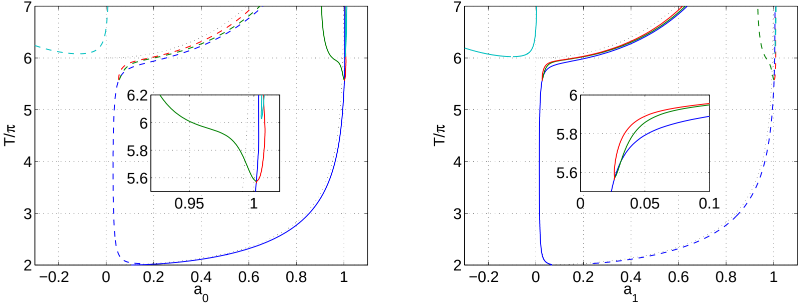

Solid – fundamental breather. Dashed – breather with a "hole".

6π-periodic solutions of the discrete Klein–Gordon equation

For any root $a(\delta)$, U_0 is found from the Duffing oscillator with a periodic force:

$$\ddot{U}_0 + U_0 - U_0^3 = \beta U_0 + \nu \cos(\tau)$$

where $\nu = 2\gamma\epsilon^{1/3} a(\delta) = \mathcal{O}(\epsilon^{4/3})$ and $\beta = \mathcal{O}(\epsilon^{2/3})$.

Theorem (D.P. & A. Sakovich '12)

For small ϵ and any finite $\delta \neq 0$, there exists a unique 6π-periodic solution of the discrete Klein–Gordon equation satisfying

$$\|U_0 - \varphi\|_{H^2_{\rm per}} \leq C\epsilon^{4/3}, \quad \|U\|_{l^2(\mathbb{N}, H^2_{\rm per})} \leq C\epsilon^{1/3}.$$

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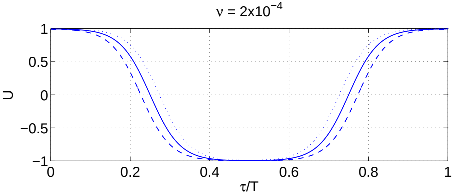
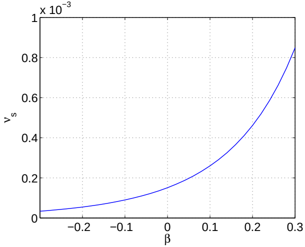
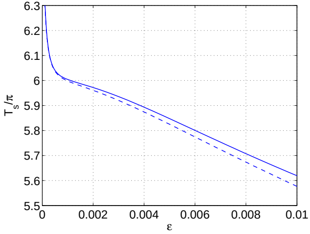
Nevertheless, for $\beta = 0$ and $\nu = 0.0002$, we obtain three 6π-periodic solutions, which are generated by the pitchfork bifurcation:



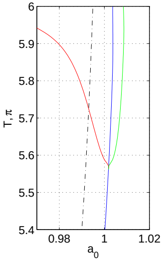
Comparison of pitchfork bifurcations

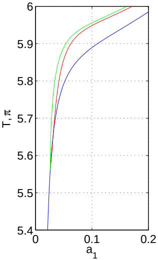
Pitchfork bifurcation within the Duffing equation:

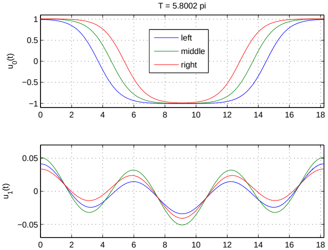




Pitchfork bifurcation in the original Klein–Gordon lattice:







Stability of discrete breathers

Discrete Klein–Gordon equation:

$$\ddot{u}_n + V'(u_n) = \epsilon(u_{n-1} - 2u_n + u_{n+1}),$$

Stability of multi-site breathers:

- Morgante, Johansson, Kopidakis, Aubry '2002 - numerical results
- Archilla, Cuevas, Sánchez-Rey, Alvarez '2003 - Aubry's spectral band theory
- Koukouloyannis, Kevrekidis '2009 - MacKay's action-angle averaging
- Yoshimura '2012 - KG unharmonic lattice
- Rapti' 2013 - next-neighbors interactions

In our work

- no restriction to small-amplitude approximation
- multi-site breathers with "holes"

Floquet Multipliers

Linearize about the breather solution to the dKG by replacing $\mathbf{u}$ with $\mathbf{u} + \mathbf{w}$, where $\mathbf{w} : \mathbb{R} \to \mathbb{R}^{\mathbb{Z}}$ is a small perturbation, and collect the terms linear in $\mathbf{w}$:

$$\ddot{w}_n + V''(u_n) w_n = \epsilon(w_{n-1} - 2w_n + w_{n+1}), \qquad n \in \mathbb{Z}.$$

In the anti-continuum limit, it is easy to find the Floquet multipliers:

- on "holes", $n \in \mathbb{Z} \backslash S$,

$$\ddot{w}_n + w_n = 0, \qquad \begin{pmatrix} w_n(T) \\ \dot{w}_n(T) \end{pmatrix} = \begin{pmatrix} \cos T & \sin T \\ -\sin T & \cos T \end{pmatrix} \begin{pmatrix} w_n(0) \\ \dot{w}_n(0) \end{pmatrix},$$

  Floquet multipliers are $\mu_{1,2} = e^{\pm iT}$

- on excited sites, $n \in S$,

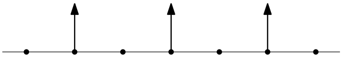
$$\ddot{w}_n + V''(\varphi) w_n = 0, \qquad \begin{pmatrix} w_n(T) \\ \dot{w}_n(T) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ T'(E)\left(V'(a)\right)^2 & 1 \end{pmatrix} \begin{pmatrix} w_n(0) \\ \dot{w}_n(0) \end{pmatrix},$$

  Floquet multipliers are $\mu_{1,2} = 1$ of geometric multiplicity 1 and algebraic multiplicity 2.

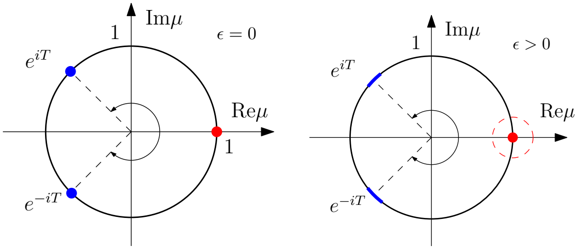
Splitting of the unit Floquet multiplier

Introduce a limiting configuration $\mathbf{u}^{(0)}(t)$ that has M excited sites with $N-1$ "holes" in between them:

$$\mathbf{u}^{(0)}(t) = \sum_{j=1}^{M} \sigma_j \varphi(t) \mathbf{e}_{jN}$$



For $\epsilon > 0$, Floquet multipliers split as follows:



Floquet exponents

A Floquet multiplier μ can be written as $\boxed{\mu = e^{\lambda T}}$.

Theorem (D.P., A. Sakovich, 2012)

For small $\epsilon > 0$ the linearized stability problem has $2M$ small Floquet exponents $\lambda = \epsilon^{N/2}\Lambda + \mathcal{O}\left(\epsilon^{(N+1)/2}\right)$, where Λ is determined from the eigenvalue problem

$$-\frac{T(E)^2}{2T'(E)K_N}\Lambda^2 \mathbf{c} = \mathcal{S}\mathbf{c}, \quad \mathbf{c} \in \mathbb{C}^M.$$

Here $\mathcal{S} \in \mathbb{R}^{M\times M}$ is a tridiagonal matrix with elements

$$\mathcal{S}_{i,j} = -\sigma_j\left(\sigma_{j-1} + \sigma_{j+1}\right)\delta_{i,j} + \delta_{i,j-1} + \delta_{i,j+1}, \qquad 1 \leq i,j \leq M,$$

and K_N is defined by

$$K_N = \int_0^T \dot{\varphi}(t)\dot{\varphi}_{N-1}(t)dt, \quad \left(\partial_t^2 + 1\right)\varphi_k = \varphi_{k-1}, \quad \varphi_0 = \varphi.$$

Remarks on the analytical computations

Floquet multipliers $\mu = e^{\lambda T}$ are found from solutions $\mathbf{W} \in l^2(\mathbb{Z}, H^2_{\rm per}(0,T))$ of the linear homogeneous equations

$$\ddot{W}_n + V''(u_n) W_n + 2\lambda \dot{W}_n + \lambda^2 W_n = \epsilon (W_{n+1} - 2W_n + W_{n-1}), \quad n \in \mathbb{Z}.$$

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When $N = 1$ (all excited oscillators are adjacent), the perturbation theory is an easy exercise with $\lambda = \epsilon^{1/2}\Lambda$ and

$$\mathbf{W} = \sum_{j=1}^{M} c_j \sigma_j \dot{\varphi} \mathbf{e}_j - 2\epsilon^{1/2}\Lambda \sum_{j=1}^{M} c_j \sigma_j (L_e^{-1} \ddot{\varphi}) \mathbf{e}_j + \epsilon \tilde{\mathbf{W}}.$$

At the excited sites $n = j$ for $j \in \{1, 2, ..., M\}$, we obtain linear inhomogeneous equations

$$\begin{aligned} \ddot{\tilde{W}}_j + V''(\varphi)\tilde{W}_j &= (c_{j+1} + c_{j-1})\dot{\varphi} - \sigma_j(\sigma_{j+1} + \sigma_{j-1}) c_j V'''(\varphi)\psi_1 \dot{\varphi} \\ &\quad + \Lambda^2 c_j (4 \dot{L}_e^{-1} \ddot{\varphi} - \dot{\varphi}) + \mathcal{O}(\epsilon^{1/2}), \end{aligned}$$

which yield

$$-\frac{T(E)^2}{2T'(E)K_1}\Lambda^2 \mathbf{c} = \mathcal{S}\mathbf{c}, \quad \mathbf{c} \in \mathbb{C}^M.$$

Remarks on the (general) analytical computations

Recall again the problem of finding $\mathbf{W} \in l^2(\mathbb{Z}, H^2_{\rm per}(0,T))$ and λ from solutions of the linear homogeneous equations

$$\ddot{W}_n + V''(u_n) W_n + 2\lambda \dot{W}_n + \lambda^2 W_n = \epsilon (W_{n+1} - 2W_n + W_{n-1}), \quad n \in \mathbb{Z}.$$

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Fundamental breather is a solution $\mathbf{u}^{(\epsilon)} \in l^2(\mathbb{Z}, H^2_e(0,T))$ of the discrete Klein–Gordon equation for small $\epsilon > 0$ for a given $\mathbf{u}^{(0)}(t) = \varphi(t) \mathbf{e}_0$.

$$\mathbf{u}^{(\epsilon)} = \phi^{(\epsilon,N)} + \mathcal{O}_{l^2(\mathbb{Z}, H^2_{\rm per}(0,T))}(\epsilon^{N+1}).$$

Then, we write

$$\mathbf{W} = \sum_{j=1}^{M} c_j \tau_{jN} \partial_t \phi^{(\epsilon,N)} + \epsilon^{N/2} \Lambda \sum_{j=1}^{M} c_j \tau_{jN} \boldsymbol{\mu}^{(\epsilon,N)} + \epsilon^N \tilde{\mathbf{W}},$$

and perform perturbation computations at the order $\mathcal{O}(\epsilon^N)$.

Stability theorem

Theorem (D.P., A. Sakovich, 2012)

For small $\epsilon > 0$ *the linearized stability problem has* $2M$ *small Floquet exponents* $\lambda = \epsilon^{N/2}\Lambda + \mathcal{O}\left(\epsilon^{(N+1)/2}\right)$, *where* Λ *is determined from the eigenvalue problem*

$$-\frac{T(E)^2}{2T'(E)K_N}\Lambda^2 \mathbf{c} = \mathcal{S}\mathbf{c}, \quad \mathbf{c} \in \mathbb{C}^M.$$

where

$$\mathcal{S}_{i,j} = -\sigma_j \left(\sigma_{j-1} + \sigma_{j+1}\right)\delta_{i,j} + \delta_{i,j-1} + \delta_{i,j+1}, \qquad 1 \leq i,j \leq M,$$

and K_N *is a numerical coefficient.*

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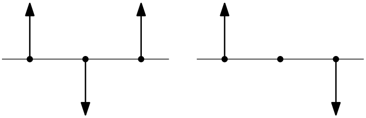
Theorem (B. Sandstede, 1998)

Let n_0 be the numbers of negative elements in the sequence $\{\sigma_j\sigma_{j+1}\}_{j=1}^{M-1}$. Matrix $\mathcal{S}$ has exactly n_0 positive and $M - 1 - n_0$ negative eigenvalues counting their multiplicities, in addition to the simple zero eigenvalue.

Stable configurations of multibreathers



$T'(E)K_N(T) > 0$: anti-phase breathers, $n_0 = M - 1$

$T'(E)K_N(T) < 0$: in-phase breathers, $n_0 = 0$

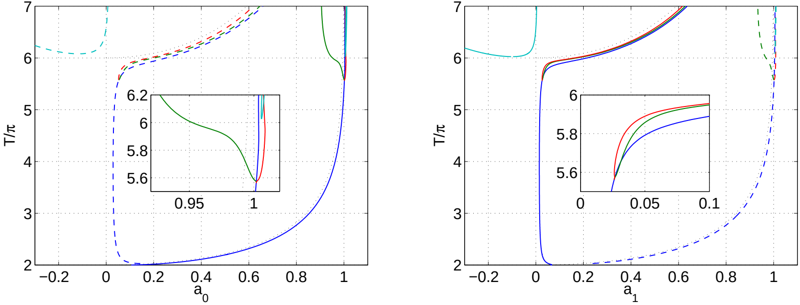
	N odd	N even
$V'(u) = u + u^3$, $T'(E) < 0$	in-phase	anti-phase
$V'(u) = u - u^3$, $T'(E) > 0$	anti-phase	anti: $2\pi < T < T_N^*$ in: $T_N^* < T < 6\pi$

where $K_N(T)$ changes sign at T_N^*, e.g., $T_2^* = 5.476\pi$.

Breather solutions

Periodic solutions are computed with the shooting method for $\epsilon = 0.01$ starting with the initial conditions:

$$u_0(0) = a_0(T), \quad \dot{u}_0(0) = 0, \quad u_1(0) = a_1(T), \quad \dot{u}_1(0) = 0$$



Solid – fundamental breather. Dashed – breather with a “hole”.

Breather with a "hole"

The breather $\mathbf{u}^{(0)}(t) = \varphi(t)(\mathbf{e}_{-1} + \mathbf{e}_1)$ is unstable for $T \in (2\pi, T_2^*)$. It then remains stable until the symmetry-breaking bifurcation occurs.

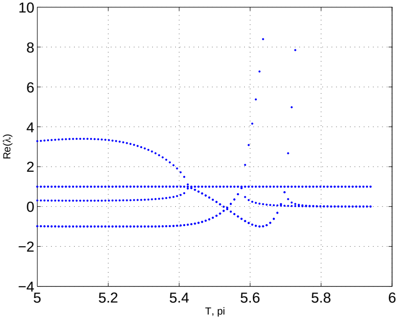


Figure : Real part of the Floquet multipliers versus T.

Conclusions

- We have constructed rigorous asymptotic theory for 1 : 3 resonance of periodic orbits by reduction to the forced Duffing oscillator.

- We have fully characterized the criterion for spectral stability/instability of multi-site breathers of the discrete KG equation near the anti-continuum limit with the reduced linear eigenvalue problem.

- We have discovered new phenomena for soft potentials:
  - Disconnection between solution branches across the resonant periods
  - Symmetry-breaking bifurcation of periodic orbits near the resonant periods
  - Change of stability for breathers with holes

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Merci beaucoup pour votre attention!