

INTRINSIC LOCALIZED MODES AND DISCRETE
BREATHERS IN NONLINEAR LATTICES

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Multibreathers Stability Theorems and Applications

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Klein–Gordon systems with linear coupling

Dynamical equations

$$\ddot{u}_n + V'(u_n) + \varepsilon \sum_{m=1}^N C_{nm} u_m = 0 \quad n = 1, \dots, N$$

Coupling examples ($\varepsilon > 0$):

- Elastic attractive coupling: $\sum_{m=1}^N C_{nm} u_m = 2u_n - u_{n+1} - u_{n-1}$
- Next–neighbor, dipole–dipole repulsive coupling: $\sum_{m=1}^N C_{nm} u_m = u_{n+1} + u_{n-1}$
- Dipolar long–range interaction repulsive coupling: $\sum_{m=1}^N C_{nm} u_m = \sum_{m=1}^N \frac{u_m}{r_{nm}^3}$

Notation $|u\rangle = \begin{bmatrix} u_1(t) \\ \vdots \\ u_N(t) \end{bmatrix}$; $V(u) = \sum_{n=1}^N V(u_n)$; $|\dot{u}\rangle = \begin{bmatrix} \frac{du}{dt} \\ \vdots \\ \frac{du_N}{dt} \end{bmatrix}$; $|V'(u)\rangle = \begin{bmatrix} \frac{\partial V}{\partial u_1} \\ \vdots \\ \frac{\partial V}{\partial u_N} \end{bmatrix}$

Linear stability and Newton operator

- Dynamical equation: $|\ddot{u}\rangle + |V'(u)\rangle + \varepsilon C |u\rangle = 0$ $|u\rangle$ time-reversible and periodic with frequency $\omega_b = \frac{2\pi}{T}$

- (Linear) stability equation

$$\mathcal{N}_\varepsilon(u) |\xi\rangle \equiv |\ddot{\xi}\rangle + V''(u) \cdot |\xi\rangle + \varepsilon C |\xi\rangle = E |\xi\rangle$$

Newton operator: \mathcal{N}_ε

- The Floquet Matrix: $\begin{bmatrix} \{\xi_n(T)\} \\ \{\dot{\xi}_n(T)\} \end{bmatrix} = \mathcal{F}_E \begin{bmatrix} \{\xi_n(0)\} \\ \{\dot{\xi}_n(0)\} \end{bmatrix}$

- Floquet multipliers of \mathcal{F}_E and arguments:

$$\lambda_i = \exp(i\theta_i) \quad ; \quad i = 1, \dots, 2N$$

- Band structure

$$(\{\theta_l\}, E) \quad \text{with} \quad \theta_l \in \mathcal{R}$$

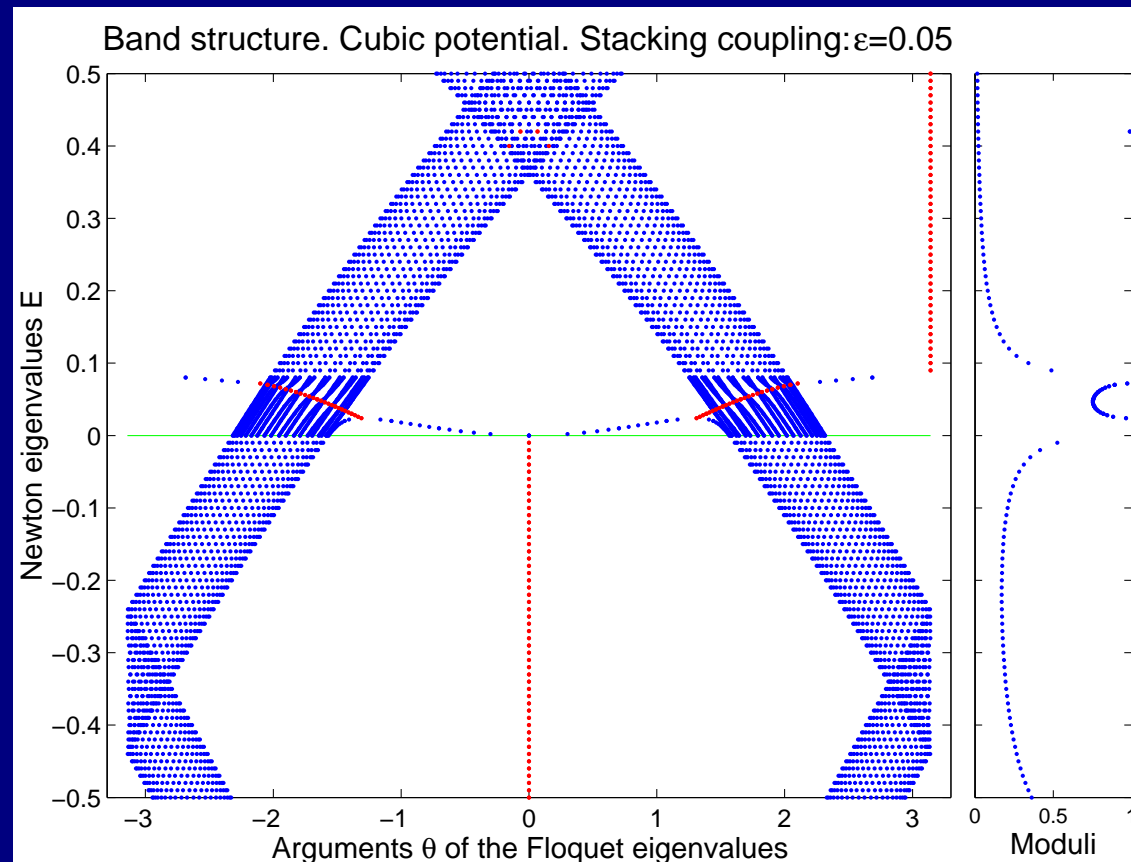
- Stability:

The solution $|u\rangle$ is linearly stable if there are $2N$ band intersections or tangent points with their multiplicity with the axis $E = 0$.

S Aubry. *Physica D*, 103:201–250, 1997.

Example of bands

Cubic potential, attractive elastic coupling, $\varepsilon = 0.05$.
Stable single breather.



Bands figures from:

A Alvarez, JFR Archilla, J Cuevas and FR Romero, *Dark breathers in Klein-Gordon lattices. Band analysis of their stability properties*. New Journal of Physics 4:72.1-72.19 (2002).

Bands at the anticontinuous limit ($\varepsilon = 0$)

Stability equation: $\mathcal{N}_0(u) |\xi\rangle \equiv |\ddot{\xi}\rangle + V''(u) \cdot |\xi\rangle = E |\xi\rangle$,

- $N - p$ excited oscillators. Code $\sigma_n = \pm 1$

$$\ddot{\xi}_n + V''(u_n) \xi_n = E \xi_n$$

With $E = 0$:

Phase mode (periodic): \dot{u}_n

Growth mode (unbounded): $\frac{\partial u_n}{\partial \omega_b}$

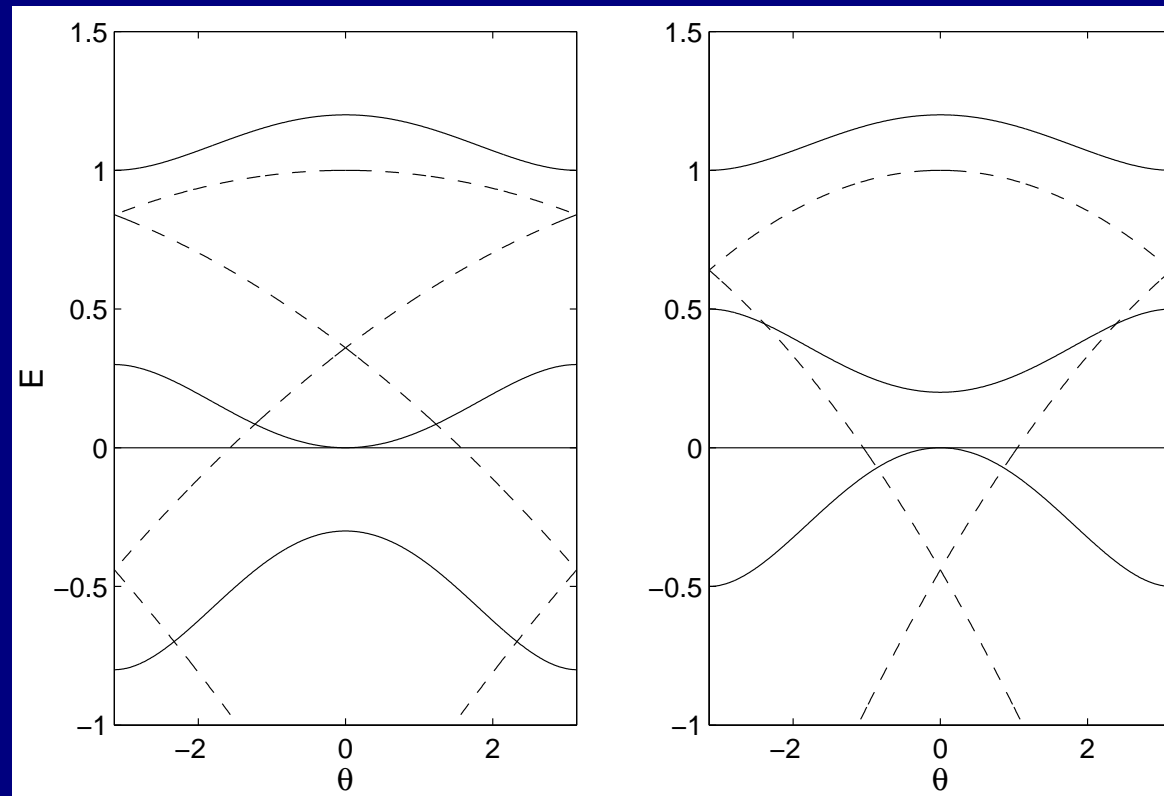
- p rest oscillators. Code $\sigma_n = 0$

$$\ddot{\xi}_n + (\omega_0)^2 \xi_n = E \xi_n \quad ; \quad \omega_0 = \sqrt{V''(0)}$$

Bands

- Excited oscillators ($N - p$): Tangent from above (soft) or below (hard)
- Rest oscillators (p): $E = \omega_0^2 - \omega_b^2(\theta/T)^2$

Bands at the anticontinuous limit



Soft

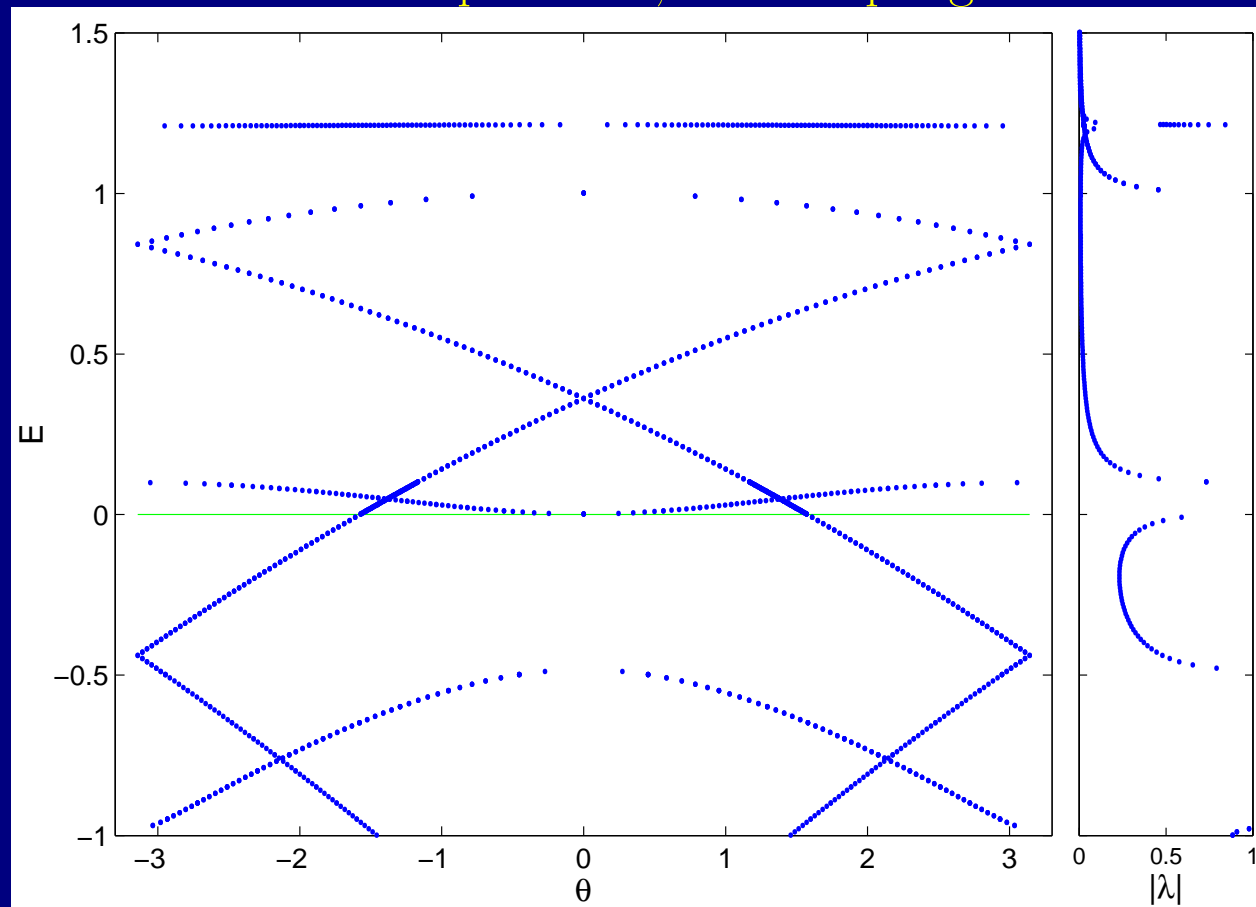
Hard

---- Rest oscillators

— Excited oscillators

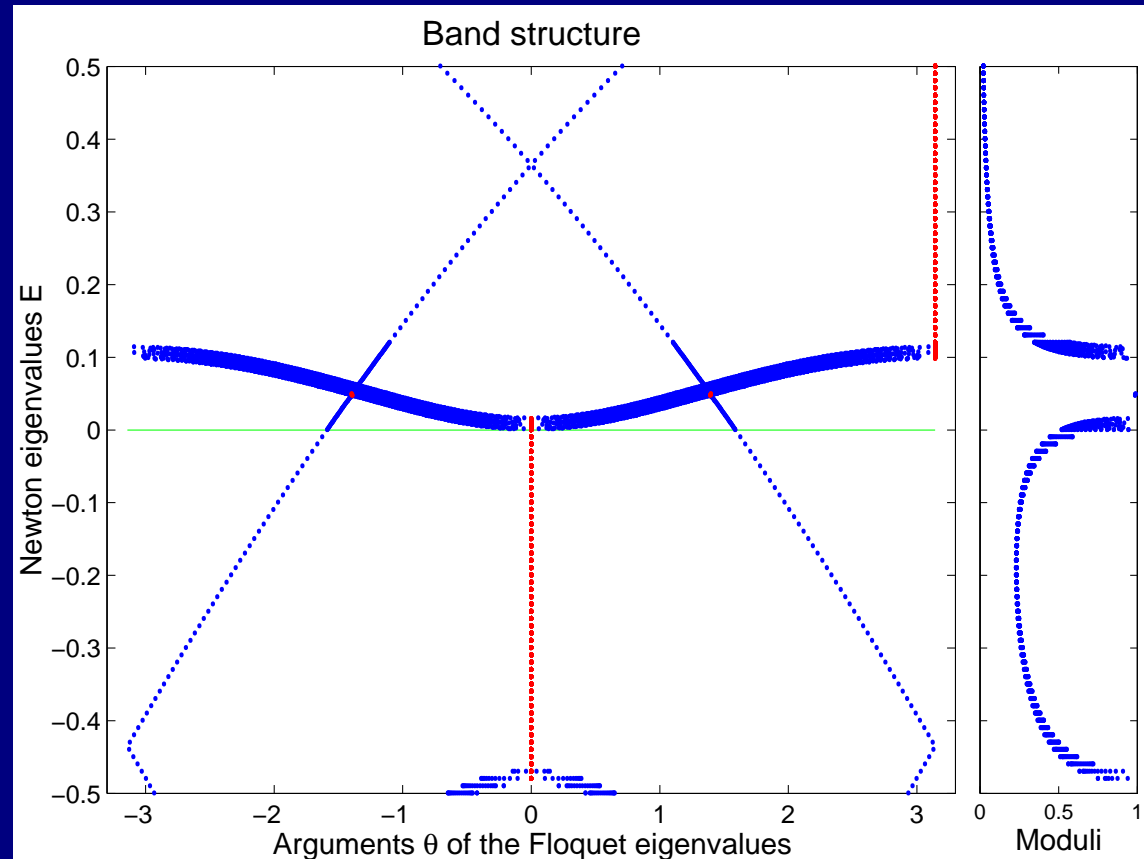
Example of bands at $\varepsilon = 0$

Cubic potential, zero coupling



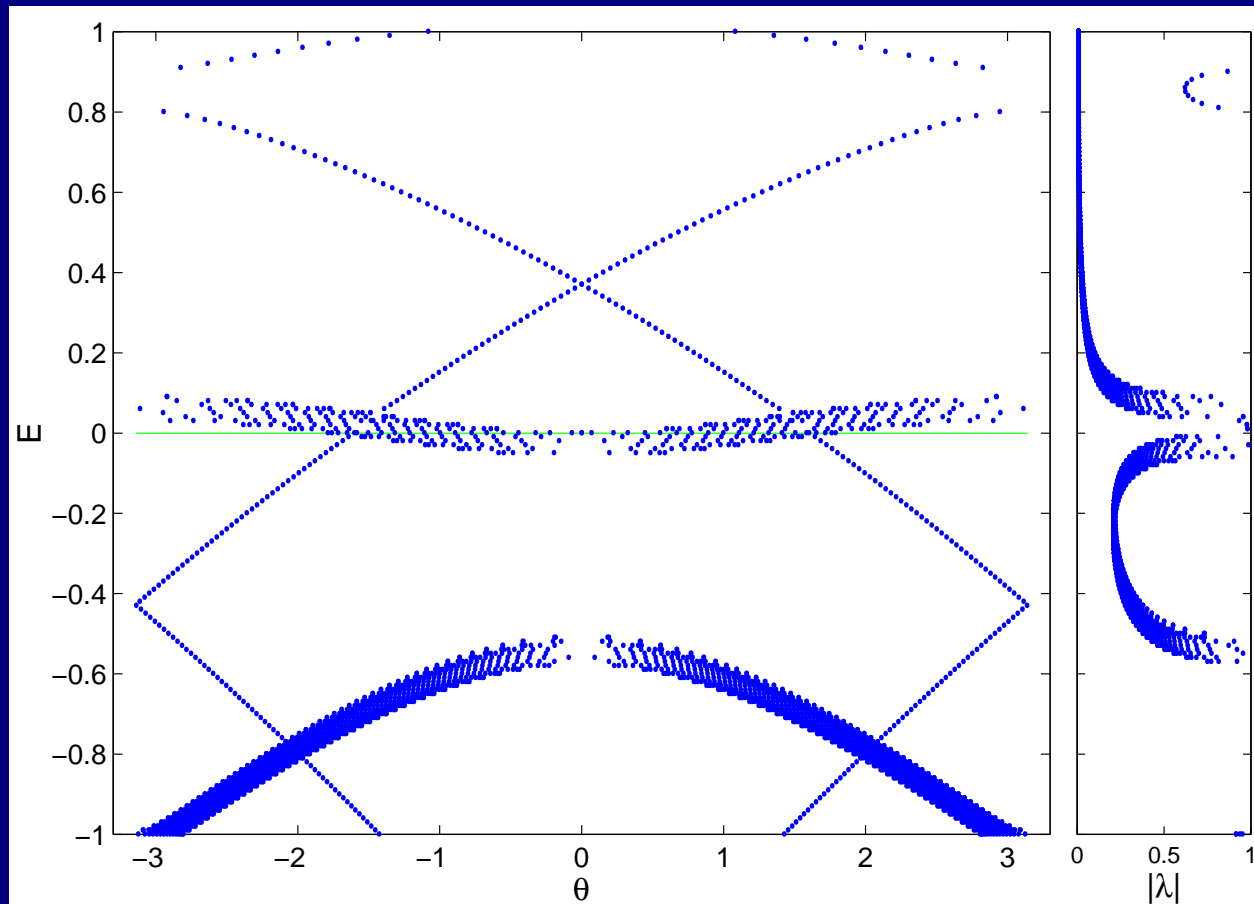
Example of unstable bands

Dark breather. Cubic potential, attractive coupling $\varepsilon = 0.004$



Example of stable bands

Dark breather. Cubic potential, repulsive coupling, $\varepsilon = 0.015$



Degenerate perturbation theory

If \mathcal{N}_0 is a linear operator with a degenerate eigenvalue E_0 , with eigenvectors $\{|v_n\rangle\}$, which are orthonormal with respect to a scalar product, i.e., $\langle v_n|v_m\rangle = \delta_{nm}$, and if $\varepsilon\tilde{\mathcal{N}}$ is a perturbation of \mathcal{N}_0 , with ε small; then, to first order in ε , the eigenvalues of $\mathcal{N}_0 + \varepsilon\tilde{\mathcal{N}}$ are $E_0 + \varepsilon\lambda_i$, with λ_i being the eigenvalues of the perturbation matrix Q with elements $Q_{nm} = \langle v_n|\tilde{\mathcal{N}}|v_m\rangle$.

Scalar product $\langle \xi_1|\xi_2\rangle = \sum_{n=1}^N \int_{-T/2}^{T/2} \xi_1^*(t)\xi_2(t) dt$

Basis $N - p$ elements (excited oscillators):

$$|n\rangle = \frac{1}{\mu} \begin{bmatrix} \vdots \\ 0 \\ \dot{u}^0 \\ 0 \\ \vdots \end{bmatrix} ; \quad \mu = \sqrt{\int_{-T/2}^{T/2} (\dot{u}^0)^2 dt}$$

Operators

$$\begin{aligned} \mathcal{N}_\varepsilon(u)|\xi\rangle &= \overbrace{|\ddot{\xi}\rangle + V''(u) \cdot |\xi\rangle}^{\mathcal{N}_0|\xi\rangle} + \varepsilon \overbrace{(V'''(u) \cdot u_\varepsilon \cdot |\xi\rangle + C|\xi\rangle)}^{\tilde{\mathcal{N}}|\xi\rangle} = \\ &= \underbrace{\left(\begin{matrix} E_0 \\ 0 \end{matrix} + \varepsilon\lambda_i \right)}_0 |\xi\rangle \end{aligned}$$

Demonstration (1)

Deriving with respect to ε , at $\varepsilon = 0$, the dynamical equations we obtain:

$$|\ddot{u}_\varepsilon\rangle + V''(u) \cdot |u_\varepsilon\rangle + C |u\rangle = 0 \quad \text{or} \quad N_0 |u_\varepsilon\rangle = -C |u\rangle. \quad (1)$$

$\tilde{C}_{nm} = \langle n | C | m \rangle$ is C without the columns and rows corresponding to the oscillators at rest.

$$\begin{aligned} \langle n | V'''(u) \cdot u_\varepsilon | m \rangle = \\ \frac{1}{\mu^2} \int_{-T/2}^{T/2} [\dots, 0, \dot{u}_n^0, 0, \dots] [\dots, 0, V'''(u^0) u_{m,\varepsilon} \dot{u}_m^0, 0, \dots]^\dagger dt = \\ \frac{\delta_{nm}}{\mu^2} \int_{-T/2}^{T/2} \dot{u}^0 V'''(u^0) u_{n,\varepsilon} \dot{u}^0 dt, \end{aligned} \quad (2)$$

with $u_{n,\varepsilon} = \left(\frac{\partial u_n}{\partial \varepsilon}\right)_{\varepsilon=0}$. Thus, $\langle n | V'''(u) \cdot u_\varepsilon \cdot | n \rangle = 0$ if $n \neq m$

To calculate the last integral in (2) we will integrate by parts and use that the integral in a period of the derivative of a periodic function is zero. Besides, the functions $u_{n,\varepsilon}$ are periodic as the coefficients of their Fourier series are given by the derivatives with respect to ε of the Fourier coefficients of u_n . In the deduction below, all the integral limits are $-T/2$ and $T/2$, and the terms between brackets from integration by parts will be zero.

Demonstration (2)

The last integral in Eq. (2) becomes:

$$\begin{aligned}
 & [\dot{u}^0 u_{n,\varepsilon} V''(u^0)]_{-T/2}^{T/2} - \int V''(u^0) \dot{u}^0 \dot{u}_{n,\varepsilon} dt - \int V''(u^0) \ddot{u}^0 u_{n,\varepsilon} dt = \\
 & - [V'(u^0) \dot{u}_{n,\varepsilon}]_{-T/2}^{T/2} + \int V'(u^0) \ddot{u}_{\varepsilon,n} dt - \int V''(u^0) \ddot{u}^0 u_{n,\varepsilon} dt = \\
 & - \int \ddot{u}^0 (\ddot{u}_{n,\varepsilon} + V''(u^0) u_{n,\varepsilon}) dt \quad (3)
 \end{aligned}$$

The term between parentheses, is the n component of the lhs of Eq. (1), i.e., it becomes $-\sum_m C_{nm} u_m^0$, where $u_m^0 = u^0$, if the oscillator m is excited, and zero otherwise, i.e., it is $-\sum_m \tilde{C}_{nm} u^0 = -(\sum_m \tilde{C}_{nm}) u^0$. Equation (3) becomes:

$$\begin{aligned}
 & \left(\sum_m \tilde{C}_{nm} \right) \int \ddot{u}^0 u^0 dt = \\
 & \left(\sum_m \tilde{C}_{nm} \right) \left([\dot{u}^0 u^0]_{-T/2}^{T/2} - \int (\dot{u}^0)^2 dt \right) = - \left(\sum_m \tilde{C}_{nm} \right) \mu^2. \quad (4)
 \end{aligned}$$

That is, equation (2), leads to:

$$\langle n | V'''(u) \cdot u_\varepsilon \cdot | n \rangle = - \sum_m \tilde{C}_{nm} \quad \text{at } \varepsilon = 0. \quad (5)$$

Demonstration (3)

Therefore the diagonal elements of the perturbation matrix Q are

$$Q_{nn} = - \sum_m \tilde{C}_{nm} + \tilde{C}_{nn} = - \sum_{\forall m \neq n} \tilde{C}_{nm} = \sum_{\forall m \neq n} Q_{nm}. \quad (6)$$

To summarize, the perturbation matrix Q is given by:

$$Q_{nm} = \tilde{C}_{nm}, \quad n \neq m \quad , \quad Q_{nn} = - \sum_{\forall m \neq n} Q_{nm}, \quad (7)$$

\tilde{C} being the coupling matrix without the p rows and columns corresponding to oscillators at rest.

Perturbation matrix. Oscillators in phase

Modified coupling matrix \tilde{C} Identical to C but without the rows and columns for the rest oscillators

Perturbation matrix Q $Q_{nm} = \tilde{C}_{nm}$, $n \neq m$
 $Q_{nn} = -\sum_{\forall m \neq n} Q_{nm}$

Example : 3-site breather. Code [1, 1, 1,]. Elastic attractive interaction

$$C = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}; \tilde{C} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}; Q = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$$

Eigenvalues: $\lambda_1 = 0$, $\lambda_2 = 1$, $\lambda_3 = 3$

$\lambda_1 = 0$: phase mode

λ_2, λ_3 positive

Conclusion If $\varepsilon > 0$ Unstable for V soft
 Stable for V hard

Perturbation matrix. Oscillators not in phase. V symmetric

Code matrix $\sigma = \begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_N \end{bmatrix}$

Perturbation matrix Q

$$Q_{nm} = \begin{cases} \tilde{C}_{nm} & \text{if } \sigma_n = \sigma_m \\ -\tilde{C}_{nm} & \text{if } \sigma_n \neq \sigma_m \end{cases} \quad n \neq m$$

$$Q_{nn} = - \sum_{\forall m \neq n} Q_{nm}$$

Symmetric multibreathers stability theorem

Example : 3-site breather. Code $[-1, 1, -1]$. Elastic attractive coupling.

$$C = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}; \tilde{C} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}; Q = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix}$$

Eigenvalues: $\lambda_1 = 0$ (phase mode), $\lambda_2 = -1$, $\lambda_3 = -3$ (both negative)

Conclusion: If $\varepsilon > 0$: Stable for V soft, Unstable for V hard.

Non-symmetric on-site potentials

Symmetry coefficient γ :
$$\gamma = - \frac{\int_{-T/2}^{T/2} \dot{u}^0(t) \dot{u}^0(t + T/2) dt}{\int_{-T/2}^{T/2} \dot{u}^0(t) \dot{u}^0(t) dt}$$

Properties of γ

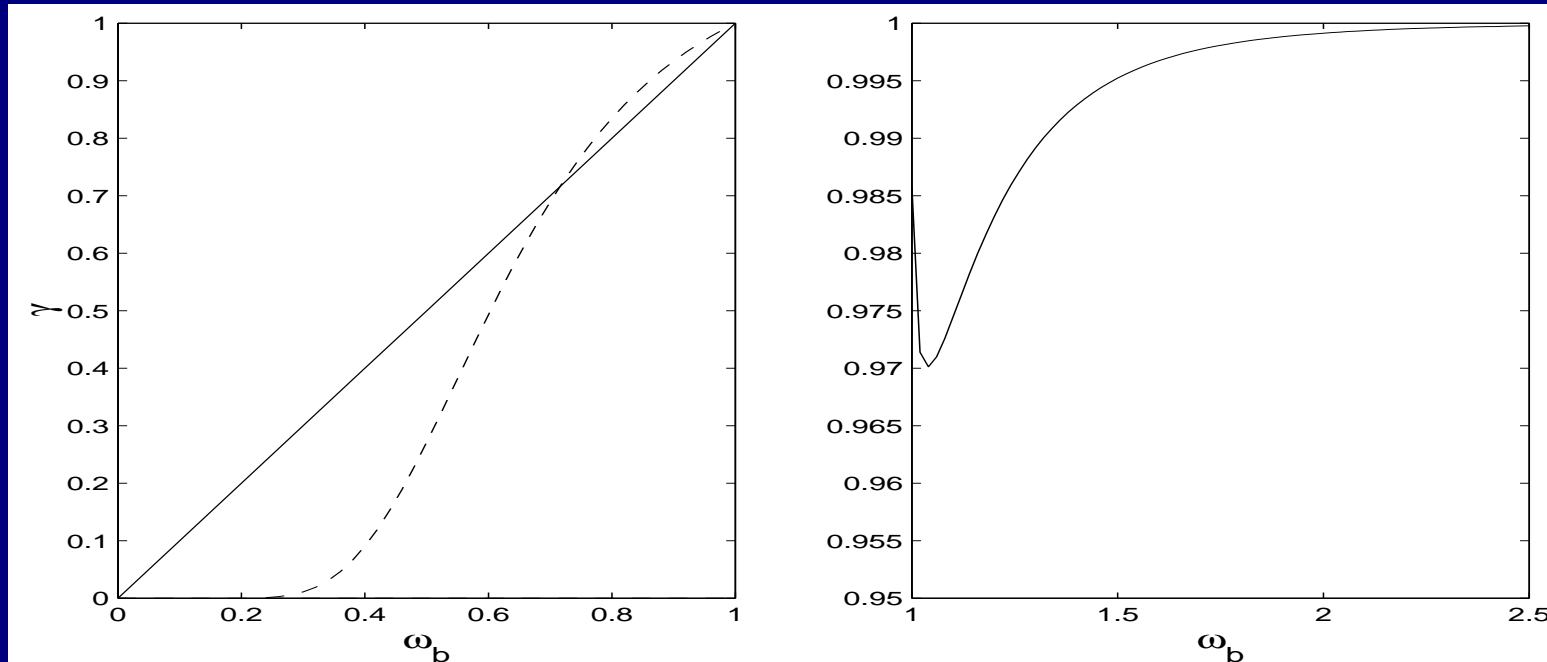
- 1) $\gamma = \gamma(\omega_b)$
- 2) $0 < \gamma < 1$
- 3) If V is symmetric $\gamma = 1$
- 4) $\omega_b \longrightarrow \omega_0 \Rightarrow \gamma \longrightarrow 1$
- 5) Numerically: Fourier coefficients
- 6) Analytically: Morse potential: $\gamma = \omega_b$

Perturbation matrix Q

$$Q_{nm} = \begin{cases} \tilde{C}_{nm} & \text{if } \sigma_n = \sigma_m \\ -\gamma \tilde{C}_{nm} & \text{if } \sigma_n \neq \sigma_m \end{cases} \quad n \neq m$$
$$Q_{nn} = - \sum_{\forall m \neq n} Q_{nm}$$

Non-symmetric multibreather stability theorem

The symmetry coefficient γ versus ω_b



Soft

----- $V(u_n) = \frac{1}{2}u_n^2 - \frac{1}{3}u_n^3$
 ————— $V(u_n) = \frac{1}{2}(\exp(-u_n) - 1)^2$

Hard

$V(u_n) = \frac{1}{2}u_n^2 + \frac{1}{3}u_n^3 + \frac{1}{4}u_n^4$

Rest frequency $\omega_0 = 1$

Application. 2-site breathers

$$C = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ -1 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

$$\text{Code } \pm[1, 1]: \quad \tilde{C} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}; \quad Q = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}; \quad (\lambda_1, \lambda_2) = (0, +2)$$

$$\text{Code } \pm[-1, 1]: \quad \tilde{C} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}; \quad Q = \begin{bmatrix} -\gamma & \gamma \\ \gamma & -\gamma \end{bmatrix}; \quad (\lambda_1, \lambda_2) = (0, -2\gamma)$$

$\pm[1, 1]$	Attractive	Repulsive	$\pm[1, -1]$	Attractive	Repulsive
Soft	Unstable	Stable	Soft	Stable	Unstable
Hard	Stable	Unstable	Hard	Unstable	Stable

Theorem by Aubry for the symmetric case in:

JL Marín. *PhD thesis*, June 1997.

Application. 3-site breathers

		Attractive coupling	Repulsive coupling
Code $\pm [1, 1, 1]$:	Soft	Unstable	Stable
	Hard	Stable	Unstable

		Attractive coupling	Repulsive coupling
Code $\pm [-1, 1, -1]$:	Soft	Stable	Unstable
	Hard	Unstable	Stable

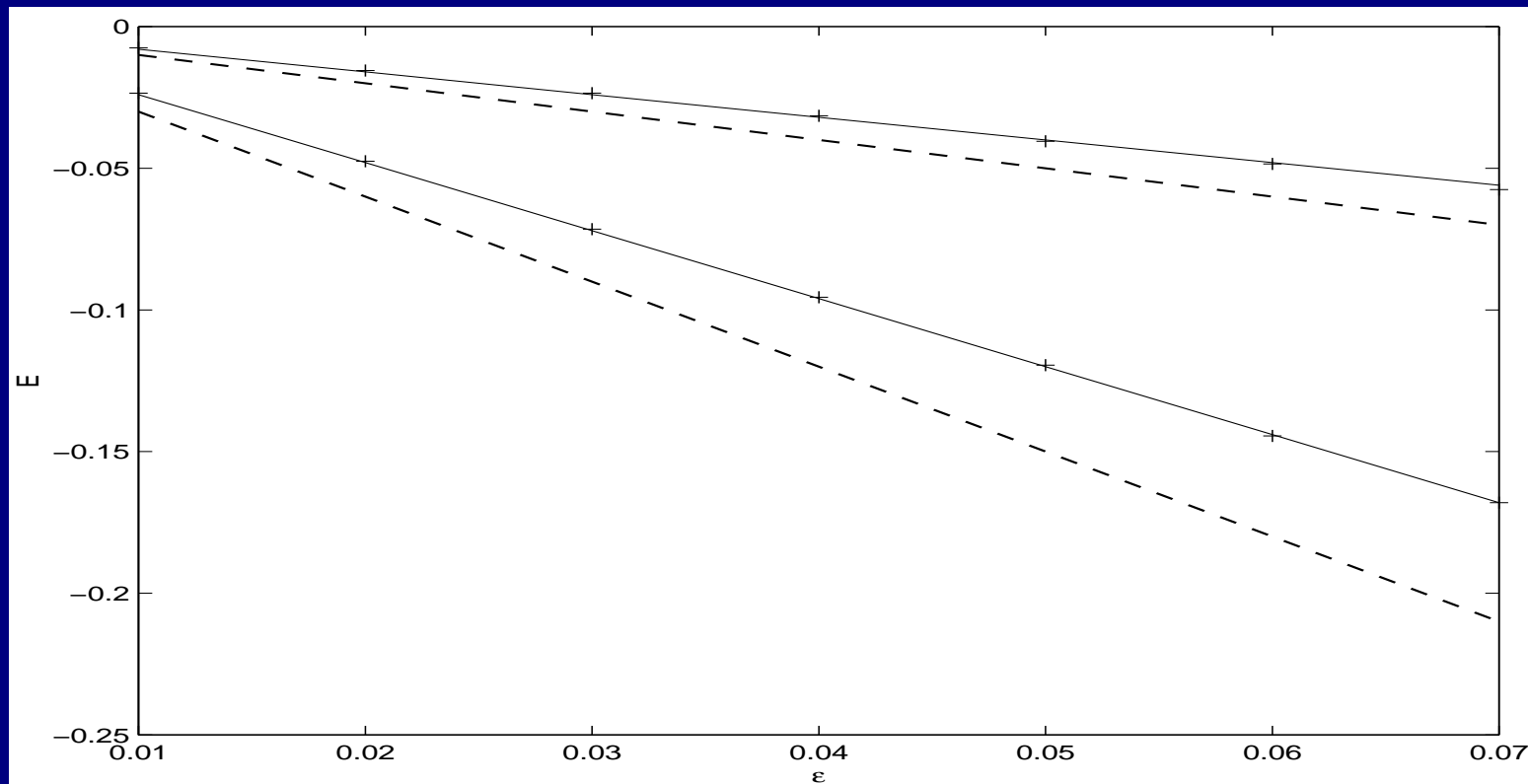
Code $\pm [1, 1, -1]$:	Always unstable
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MST versus *exact* numerical

Morse potential. Elastic attractive coupling. Code $[-1, 1, -1]$.

Frequency $\omega_b = \gamma = 0.8$.

Eigenvalues E of the Newton operator versus the coupling ε



+ Numerical. ---- Symmetric MST. —— Non-symmetric MST

Multibreathers

Group of contiguous oscillators excited at $\varepsilon = 0$

In-phase (wave vector $q = 0$)	:		Attractive coupling	Repulsive coupling
		Soft	Unstable	Stable
		Hard	Stable	Unstable

Out-of-phase (wave vector $q = \pi$)	:		Attractive coupling	Repulsive coupling
		Soft	Stable	Unstable
		Hard	Unstable	Stable

Mixed :

Always unstable

Phonobreathers

All oscillators excited at zero coupling

- With **free–ends** or **fixed–ends** boundary conditions: as multibreathers

Coherent with:

I. Daumont, T. Dauxois, and M. Peyrard.

Nonlinearity, 10:617–630, 1997. (Modulational instability).

AM Morgante, M Johansson, G Kopidakis, and S Aubry.

Phys. D, 162:53, 2002. (DNLS)

S Aubry. *Physica D*, 103:201–250, 1997. (Theorem 9, action properties)

- With **periodic** boundary conditions: **Parity instabilities**

Dark breathers

- **Free-ends** of **fixed-ends**: almost as multibreathers:

There is a degenerate 0-eigenvalue of $Q \Rightarrow$

If the eigenvalues of Q correspond to instability: instability

If the eigenvalues of Q correspond to stability: undefined

- Periodic boundary conditions: **Parity instabilities**

- **Parity instabilities. Example.**

Dark breather. Attractive coupling. Soft on-site potential.

Code $\sigma = [\dots, 1, -1, 0, 1, -1, \dots]$

N **odd** ($N = 5$):

$\sigma = [1, -1, 0, 1, -1]$: **stable**

N **even** ($N = 6$): $\sigma = [1, -1, 0, 1, -1, 1]$

equivalent to $\sigma = [-1, 0, 1, -1, 1, 1]$: **unstable**.

But with code $\sigma = [\dots, -1, 1, 0, 1, -1, \dots]$ the conditions are reversed.

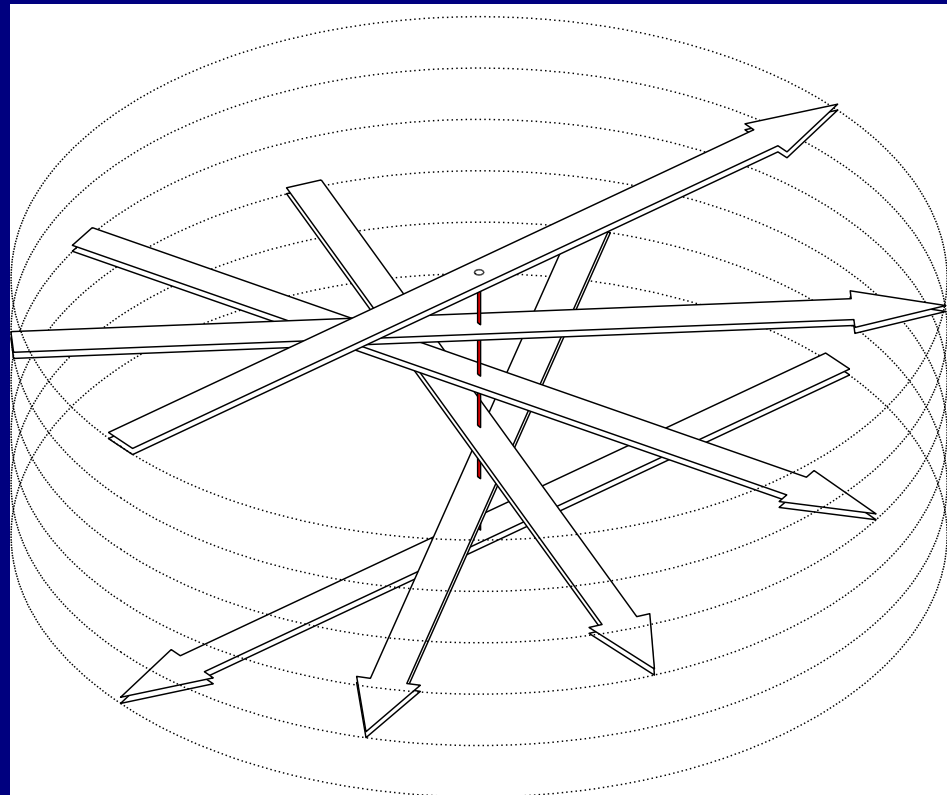
A model with LRI (1)

Twist model for DNA:

B Sánchez-Rey, JFR Archilla, F Palmero, and FR Romero.

Phys. Rev. E, 66:017601–017604, 2002.

Selected by Virtual Journal of Biological Physics Research 4(1), 2002.



A model with LRI (2)

Dynamical equations

$$\ddot{u}_n + V'(u_n) + \varepsilon \sum_{m=n-N/2}^{n+N/2} \frac{\cos[\theta_{tw}(n-m)]}{|n-m|^3} u_m = 0$$

$V(u_n)$: Morse potential

Coupling matrix $C_{nm} = \frac{\cos[\theta_{tw}(n-m)]}{|n-m|^3}$

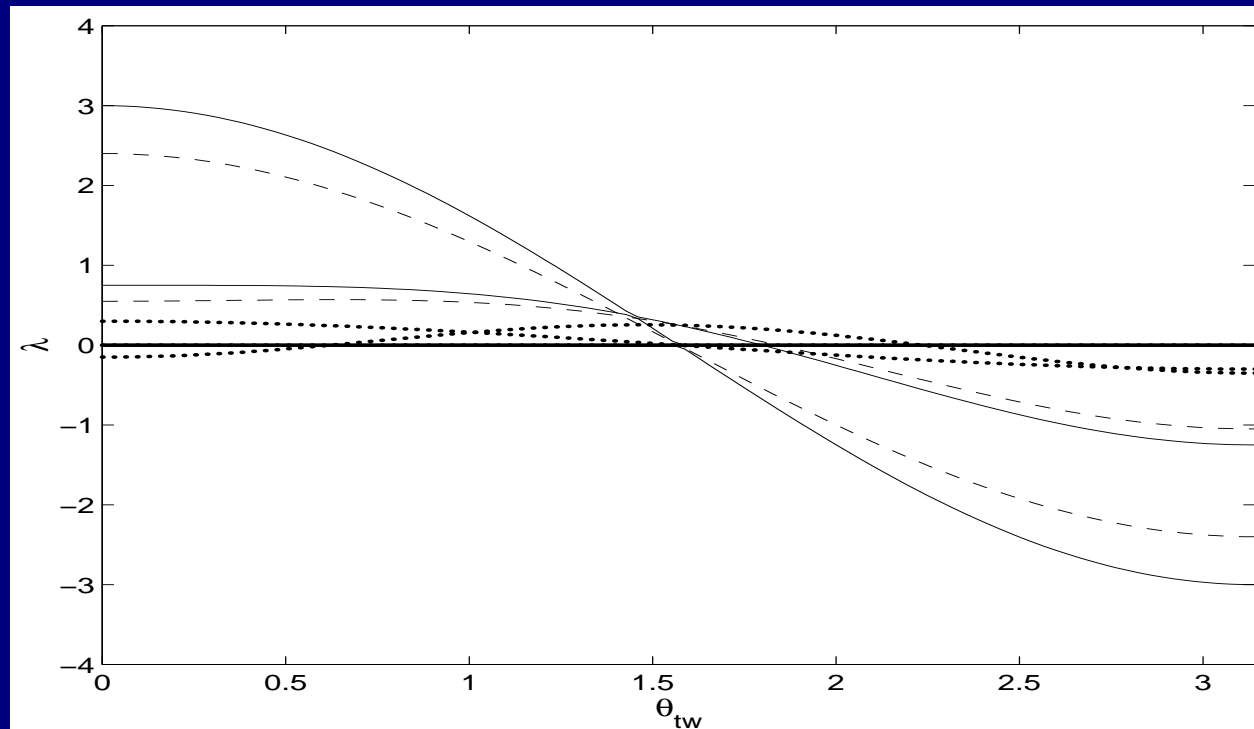
Some results

Code	$\theta_{tw} = 0$	$\theta_{tw} = \pi$
11	Stable	Unstable
1 -1	Unstable	Stable
101	Stable	Stable
111	Stable	Unstable
1-1 1	Unstable	Stable
11-1	Unstable	Stable

A model with LRI (3)

Dependence on the symmetry coefficient $\gamma = \omega_b$. Code $[-1, 1, -1]$.

Eigenvalues λ_i of Q versus the twist angle θ_{tw}



————: $\gamma = \omega_b = 1$ - - - - : $\gamma = \omega_b = 0.8$ · · · · : $\gamma = \omega_b = 0.1$

Instability induced by the nonlinearity for $\gamma = 0.1$ and $\theta_{tw} = 2$ rad.

Multibreathers in the Peyrard–Bishop DNA model

Dynamical equations Planar model

$$\ddot{u}_n + V'(u_n) + \epsilon(2u_n - u_{n-1} - u_{n+1}) = 0$$

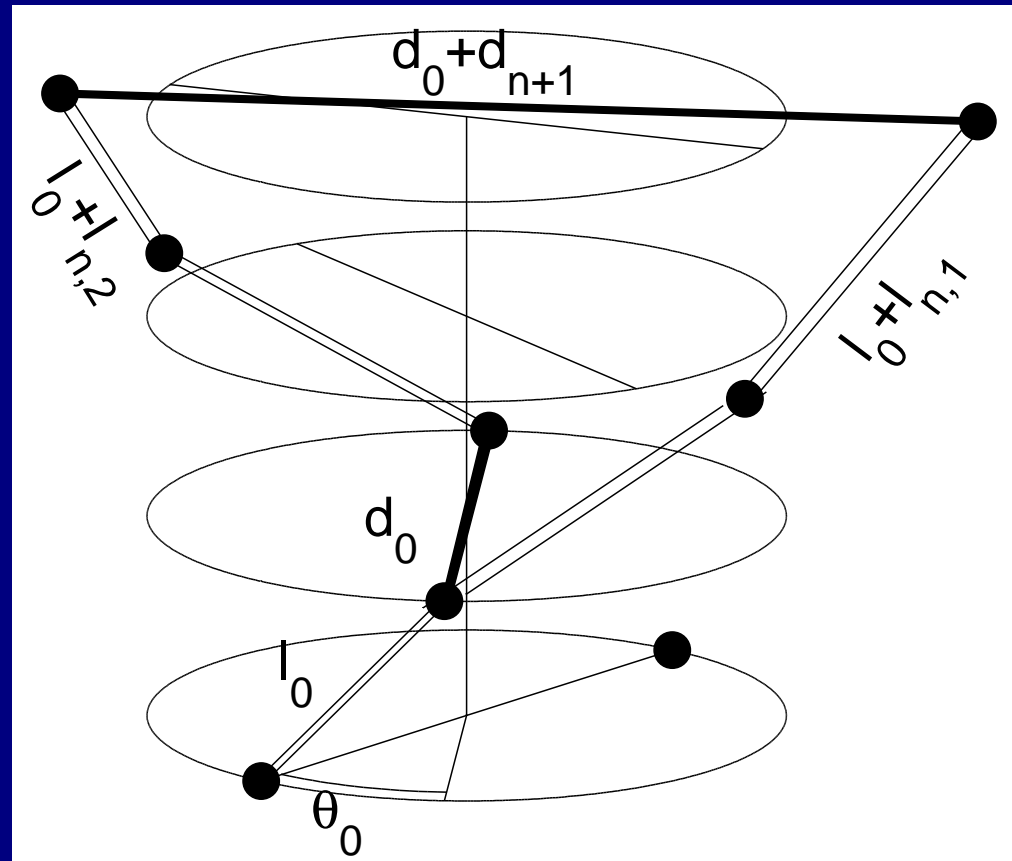
V : Morse potential (soft) and attractive coupling

In-phase multibreathers are unstable

Helical model for DNA

- D Hennig and JFR Archilla, *Multi-site H-bridge breathers in a DNA-shaped double strand*. Preprint, nlin.PS/0301047.
- Simplified variant of:
M. Barbi, S. Cocco and M. Peyrard, *Phys. Lett. A* **253**, 358 (1999). And continuations.

A helical DNA-like model



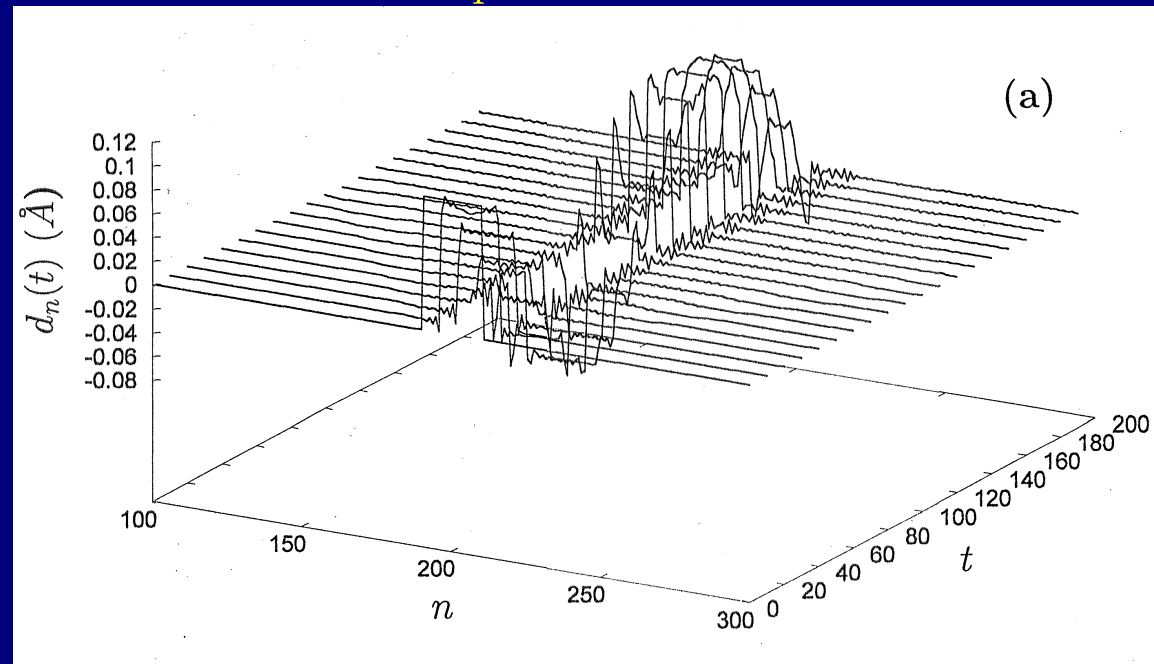
Multibreathers in the helical DNA-like model

Effective repulsive coupling

Linear equations

$$\ddot{r}_n = -\omega_0^2 r_n - \varepsilon \sin^2\left(\frac{\theta_0}{2}\right) (2r_n + r_{n+1} + r_{n-1}) - \varepsilon \sin\left(\frac{\theta_0}{2}\right) \cos\left(\frac{\theta_0}{2}\right) d_0 (\alpha_{n+1} - \alpha_{n-1}),$$

Stable in-phase multibreathers



The helical shape supports in-phase, stable multibreathers

Generalization

Hamiltonian $H = \sum_n \left(\frac{1}{2} m_n \dot{u}_n^2 + V_n(u_n) \right) + \varepsilon W(u)$

Dynamical equations $m_n \ddot{u}_n + V_n'(u_n) + \varepsilon \frac{\partial W(u)}{\partial u_n} = 0$ $V_n(u_n)$ heterogeneous
multiple wells, etc

Given periodic solution at $\varepsilon = 0$: $u^0 = \begin{bmatrix} u_1^0 \\ \vdots \\ u_N^0 \end{bmatrix}$ u_n^0 determined by
 n , well, phase
(non time-reversible)

Basis elements: $|n\rangle = \frac{1}{\mu_n} \begin{bmatrix} \vdots \\ 0 \\ \dot{u}_n^0 \\ 0 \\ \vdots \end{bmatrix}$; $\mu_n = \sqrt{\int_{-T/2}^{T/2} (\dot{u}_n^0)^2 dt}$

Perturbation matrix

$$Q_{nm} = \frac{1}{\mu_n \mu_m} \int_{-T/2}^{T/2} \dot{u}_n^0 \frac{\partial^2 W(u^0)}{\partial u_n \partial u_m} \dot{u}_m^0 dt, \quad n \neq m; \quad Q_{nn} = - \sum_{\forall m \neq n} \frac{\mu_m}{\mu_n} Q_{nm}$$

Generalized multibreathers stability theorem

Conclusions

- 1** A theory for calculating the stability of **any** multibreather in **any** Klein–Gordon system at (relatively) low coupling
- 2** For (relatively) simple systems is very simple
- 3** For complex systems is (relatively) complex
- 4** Application to a number of systems

2–site breathers

3–site breathers

Multibreathers

Phonobreathers

Dark breathers

Parity instabilities

Systems with LRI

Nonlinear instabilities

- 5** Potential consequences for helical DNA models

JFR Archilla, J Cuevas, B Sánchez–Rey and A Alvarez.

Demonstration of the stability or instability of multibreathers at low coupling.

Physica D **180**(3-4):235-255 (2003).

Nonlinear Physics Group (GFNL). University of Sevilla

<http://www.us.es/gfnl>