Stationary and moving breathers in curved alpha–helix proteins

JFR Archilla, Yu B Gaididei, PL Christiansen and J Cuevas

Nonlinear Physics Group (GFNL), University of Sevilla, Spain

http://www.us.es/gfnl

Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine

Informatics and Mathematical Modelling, DTU, Lyngby, Denmark

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Localization in curved chains

- Models
  - Nonlinear Schrödinger equations
  - FPU models
  - Klein–Gordon Models
  - DNA models
- Objectives
  - Role of the bending points in biomolecules
  - Can or cannot localized excitations travel across them?
  - Is energy stored at the bending points?
  - Do bending points play a biological function?

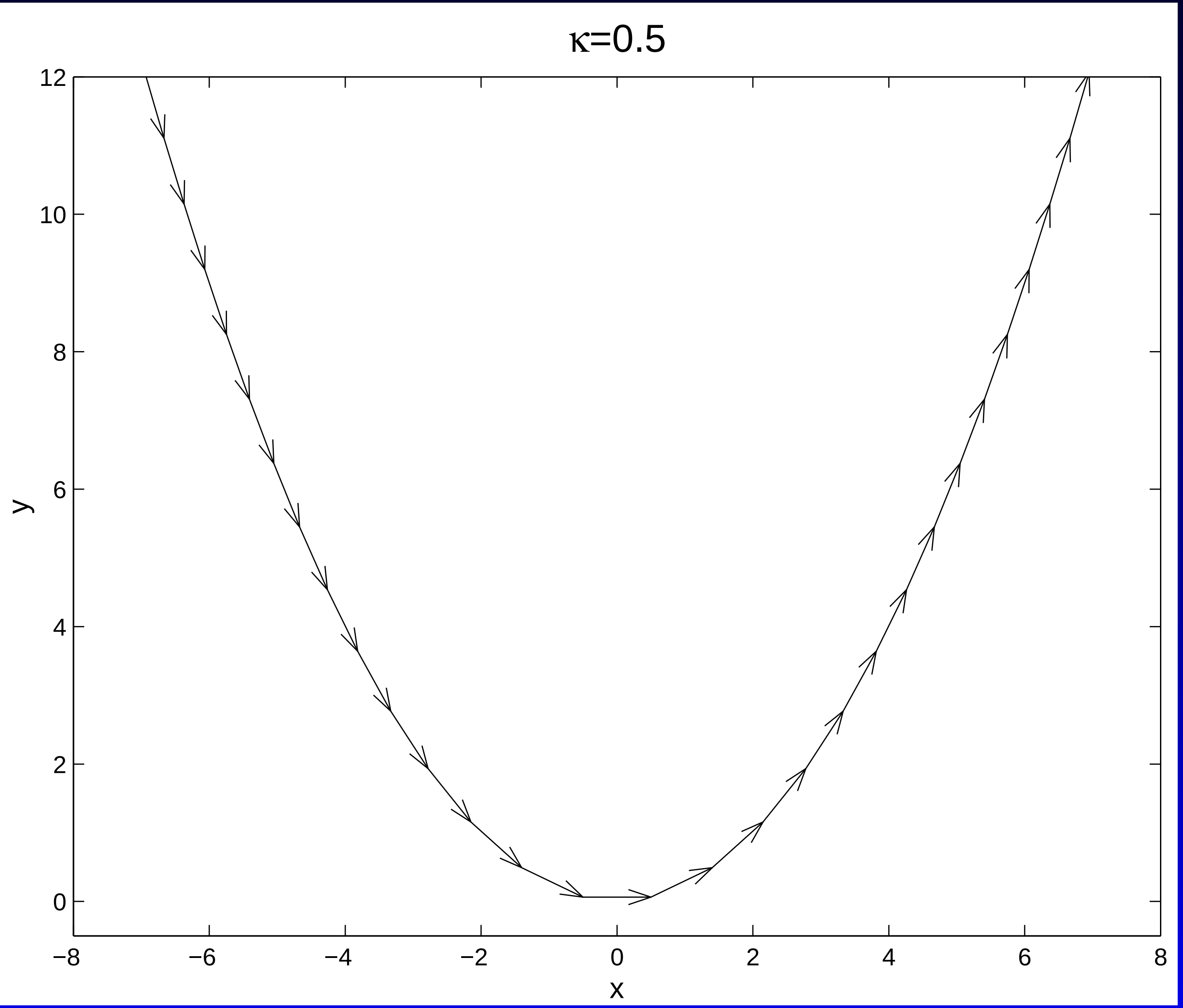
How the geometry is felt?

- Mechanisms:
  - Interaction between nearest and next neighbours
  - Angle–dependent potentials
  - Long–range interaction
- Effects of a curved chain:
  - Localized linear modes due to the inhomogeneity
  - Competition between these modes and nonlinear localized modes
  - Barrier to moving breathers
  - Reflection, transmission or trapping

The alpha–helix protein model

- Peptide groups with dipole moments
- Interaction between the Amide-I excitations
- Theoretical interest
  - Dipole moments parallel to the chain
  - Nearest–neighbour interaction
  - Attempt to generalize the role of the bending points

Sketch of the model



Model description

- Hamiltonian

$$H = \sum_n \frac{1}{2}\dot{u}_n^2 + \frac{1}{2}\omega_0^2 u_n^2 + \Psi(u_n) +$$

$$\frac{1}{2}\varepsilon(u_{n+1} - u_n)^2 + \mu(\mathbf{t}_{n+1} - \mathbf{t}_n)^2 u_n u_{n+1}$$

- On site potential:
  $V(u_n) = \frac{1}{2}\omega_0^2 u_n^2 + \Psi(u_n)$ with $\omega_0 = 1$
- Dynamical equations:

$$\ddot{u}_n + \omega_0^2 u_n + \Psi'(u_n) + \varepsilon(2\, u_n - u_{n+1} - u_{n-1}) +$$

$$\mu((\mathbf{t}_{n+1} - \mathbf{t}_n)^2 u_{n+1} + (\mathbf{t}_{n-1} - \mathbf{t}_n)^2 u_{n-1}) = 0$$

Linear modes

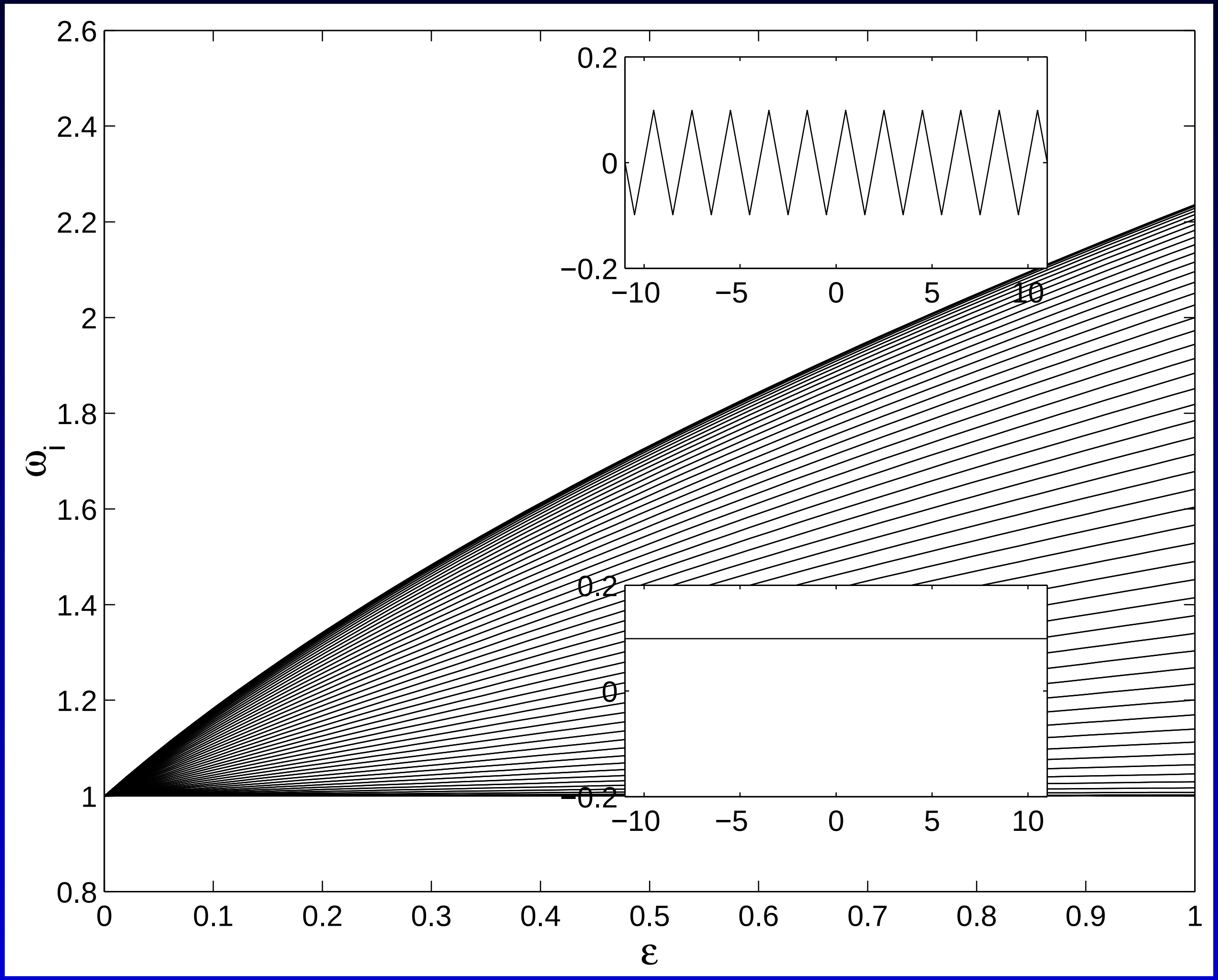
Dependence on the parameters:

- Stacking coupling parameters ε
- Curvature κ
- Dipole coupling parameter μ

Result:

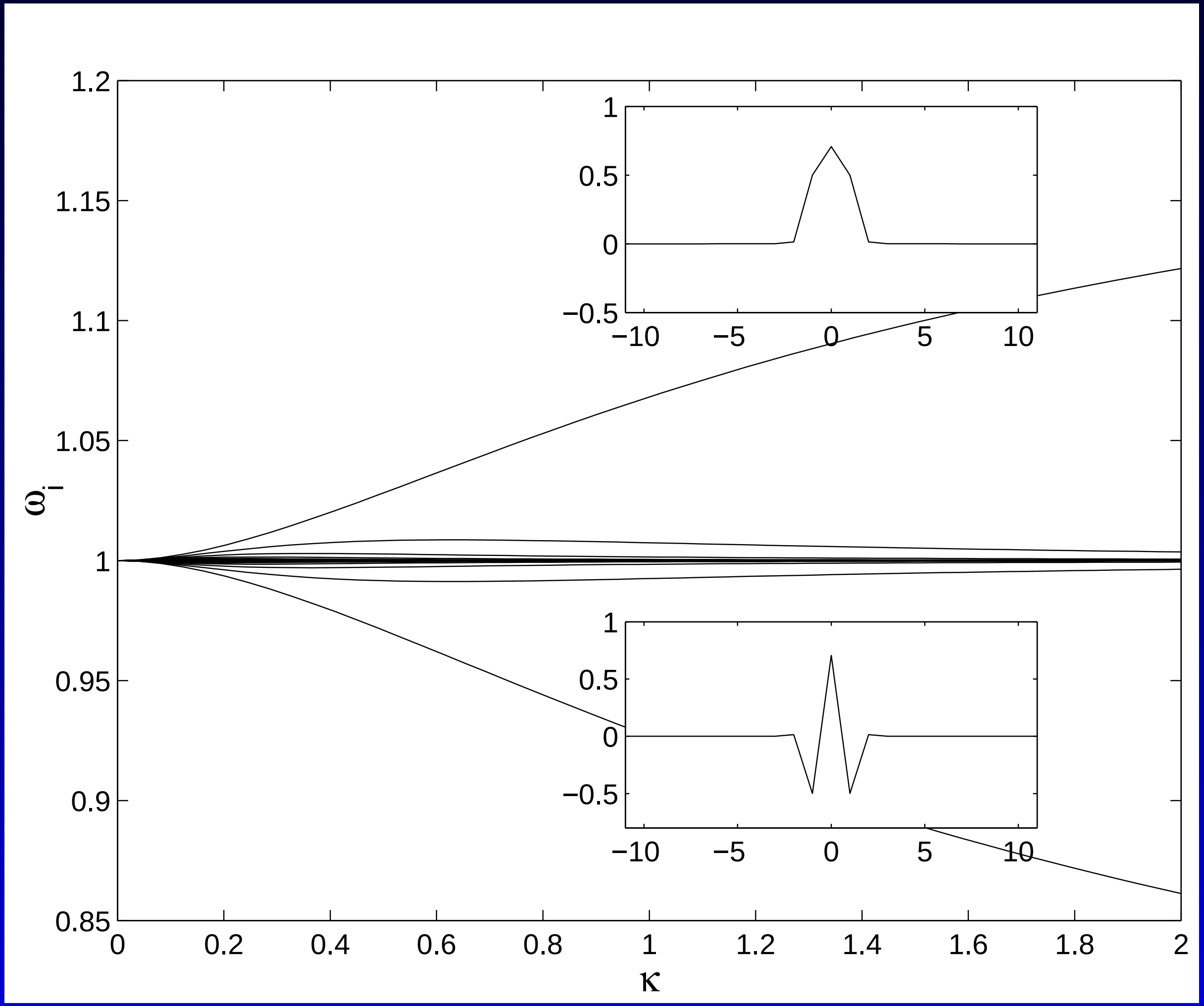
Different top and bottom localized linear modes when $\kappa \neq 0$ and $\mu \neq 0$

Stacking coupling parameter ε



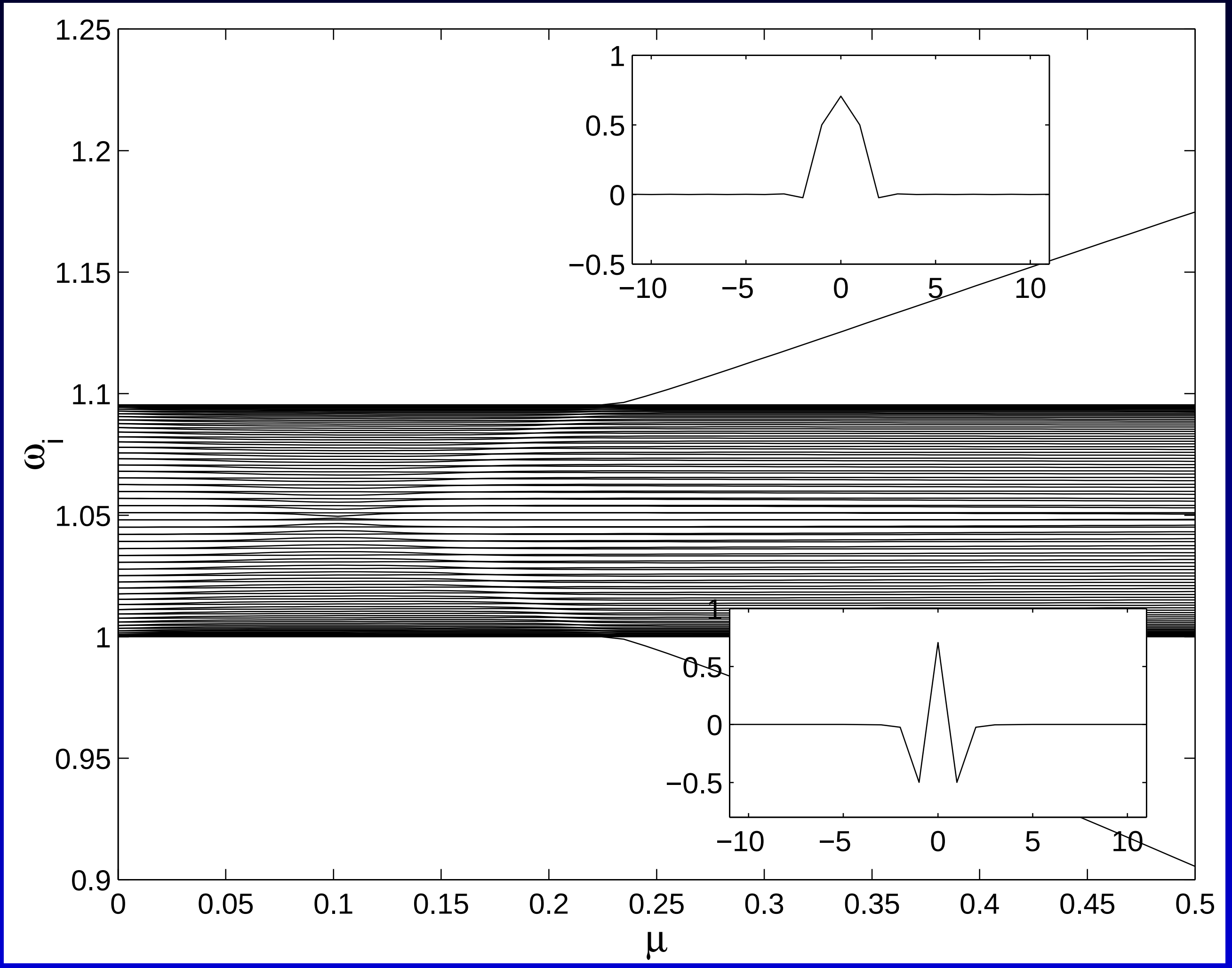
Straight chain

Curvature κ



$\varepsilon = 0$ and $\mu = 0.2$

Dipole coupling parameter μ



$\varepsilon = 0.05$ and $\kappa = 1$

Breathers

- Different on–site potentials
  - Breathers with ϕ^4 hard potential

$$V(u_n) = \frac{1}{2}\omega_0^2 u_n^2 + 1/4\, u_n^4$$

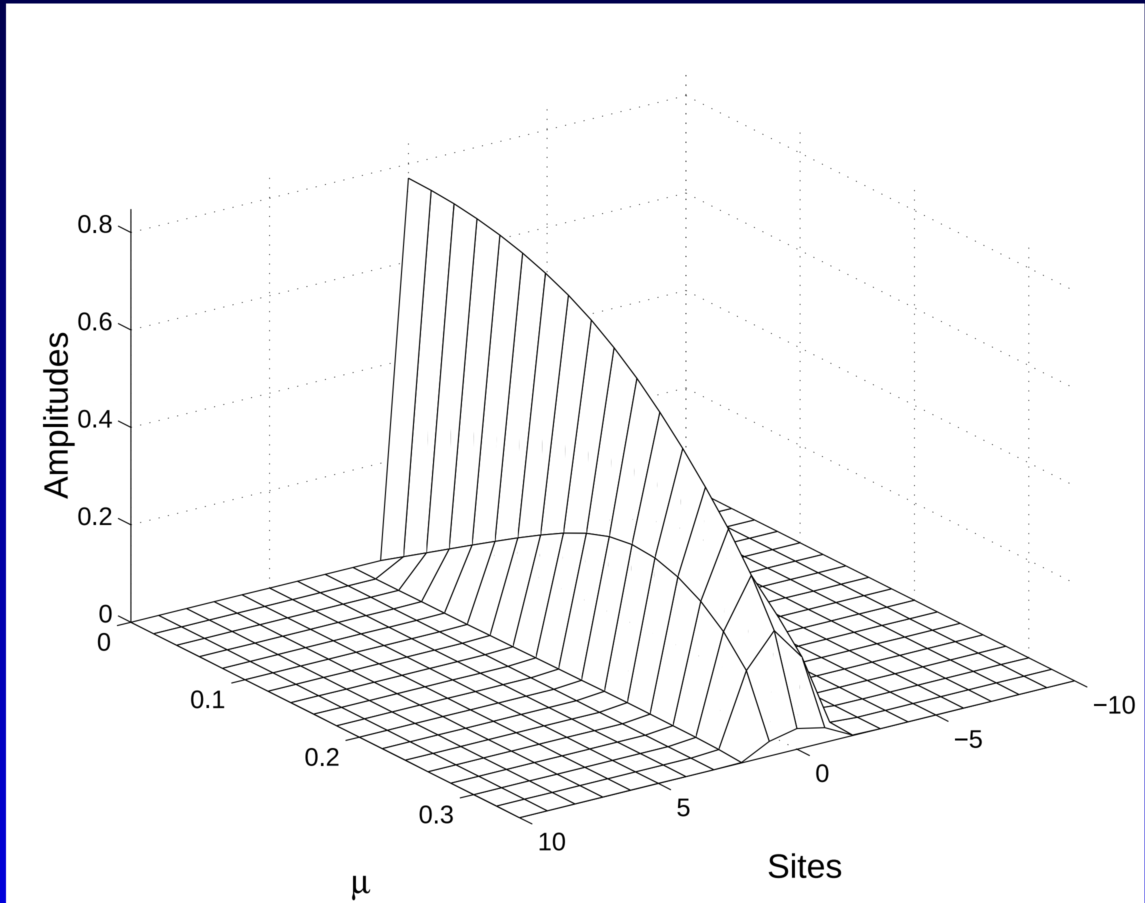
  - Breathers with soft potential

$$V(u_n) = D(\exp(-b\, u_n) - 1)^2$$

- Continuation with respect to the different parameters
  - At constant frequency ω_{b}
  - At constant energy E

Breather annihilation

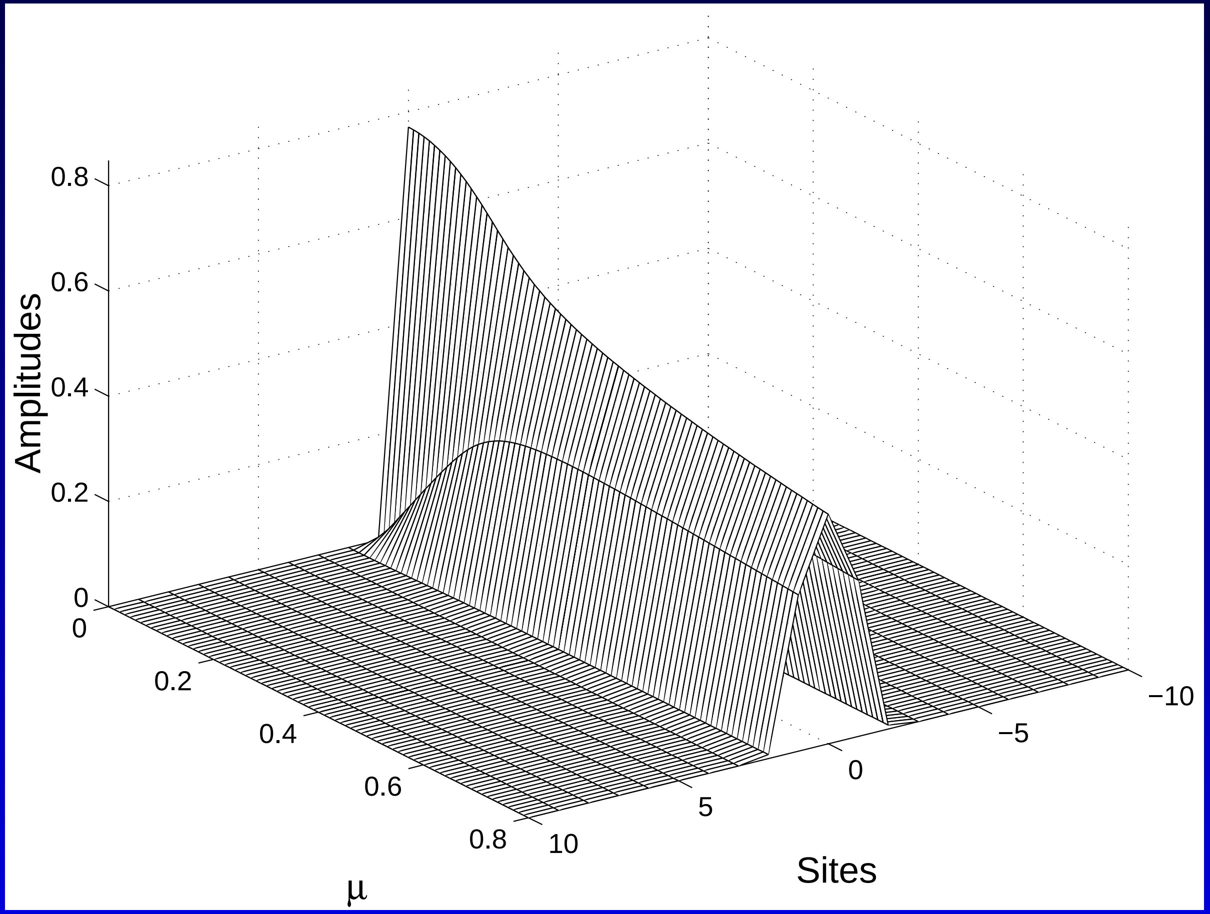
Hard potential. Dependence on the dipole coupling parameter μ. Constant frequency.



$\kappa = 2$, $\varepsilon = 0$ and $\omega_{\mathrm{b}} = 1.2$

Frequency choosing

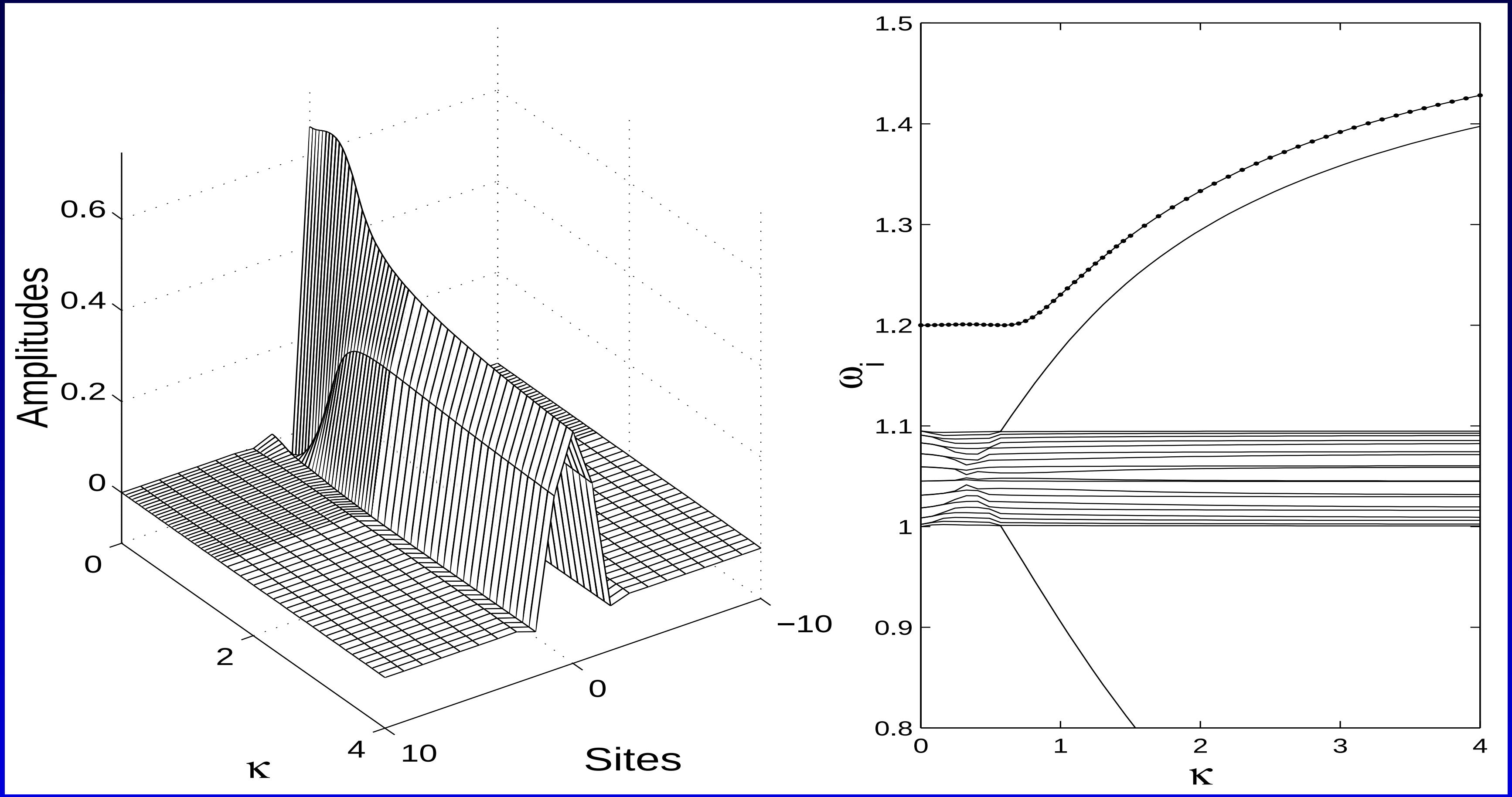
Hard potential. Dependence on the dipole coupling parameter μ. Constant energy.



$\kappa = 2$, $\varepsilon = 0$ and $E = 0.38$

Adiabatic bending

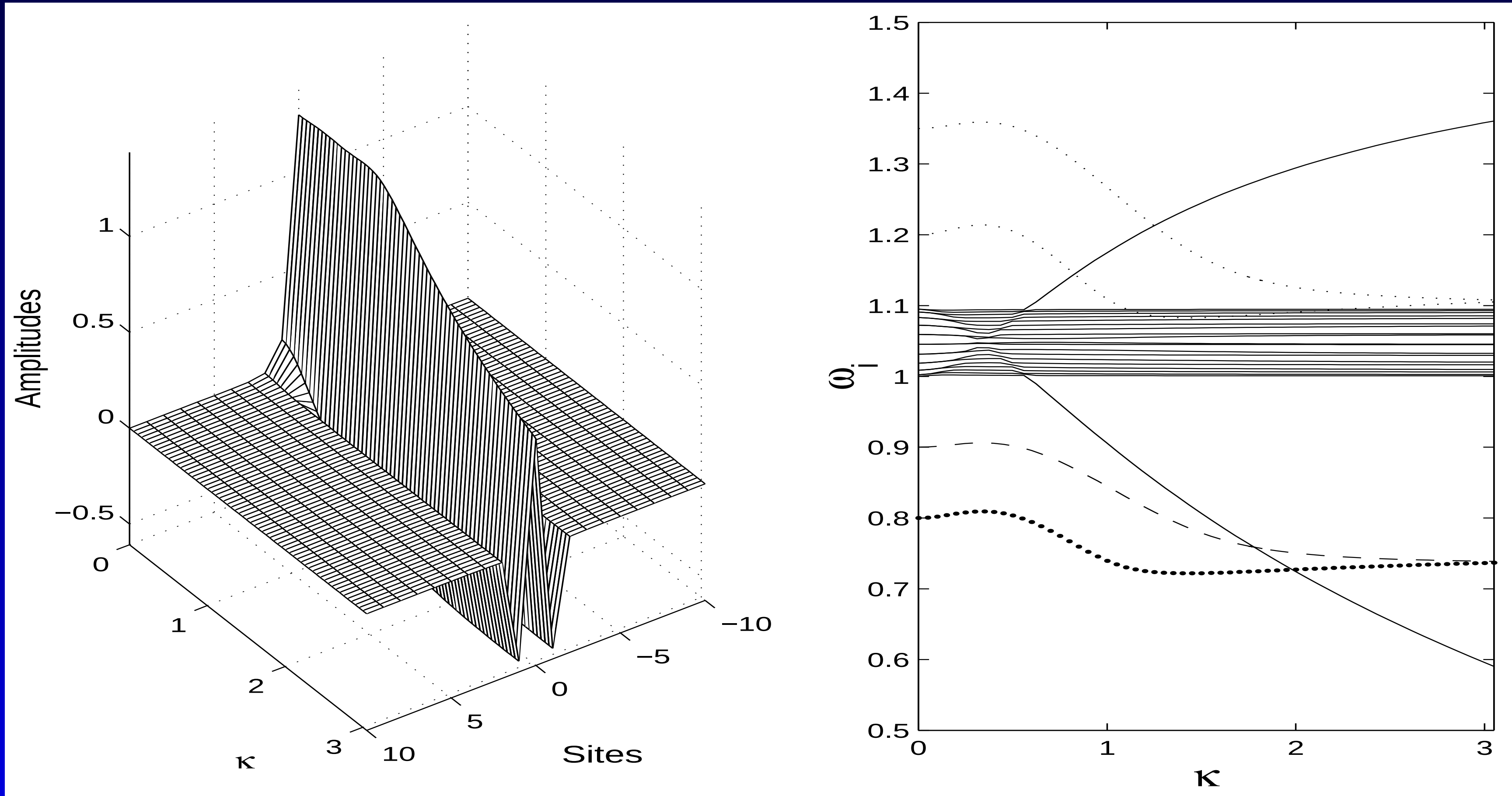
Hard potential. Dependence on the curvature κ. Constant energy.



$\mu = 0.5$, $\varepsilon = 0.05$ and $E = 0.31$

Soft potential

Adiabatic bending. Dependence on the curvature κ. Constant energy.



$\mu = 0.5$, $\varepsilon = 0.05$, $E = 0.35$ ($\cdot\cdot$) and $E = 0.20$ (– –)

Results

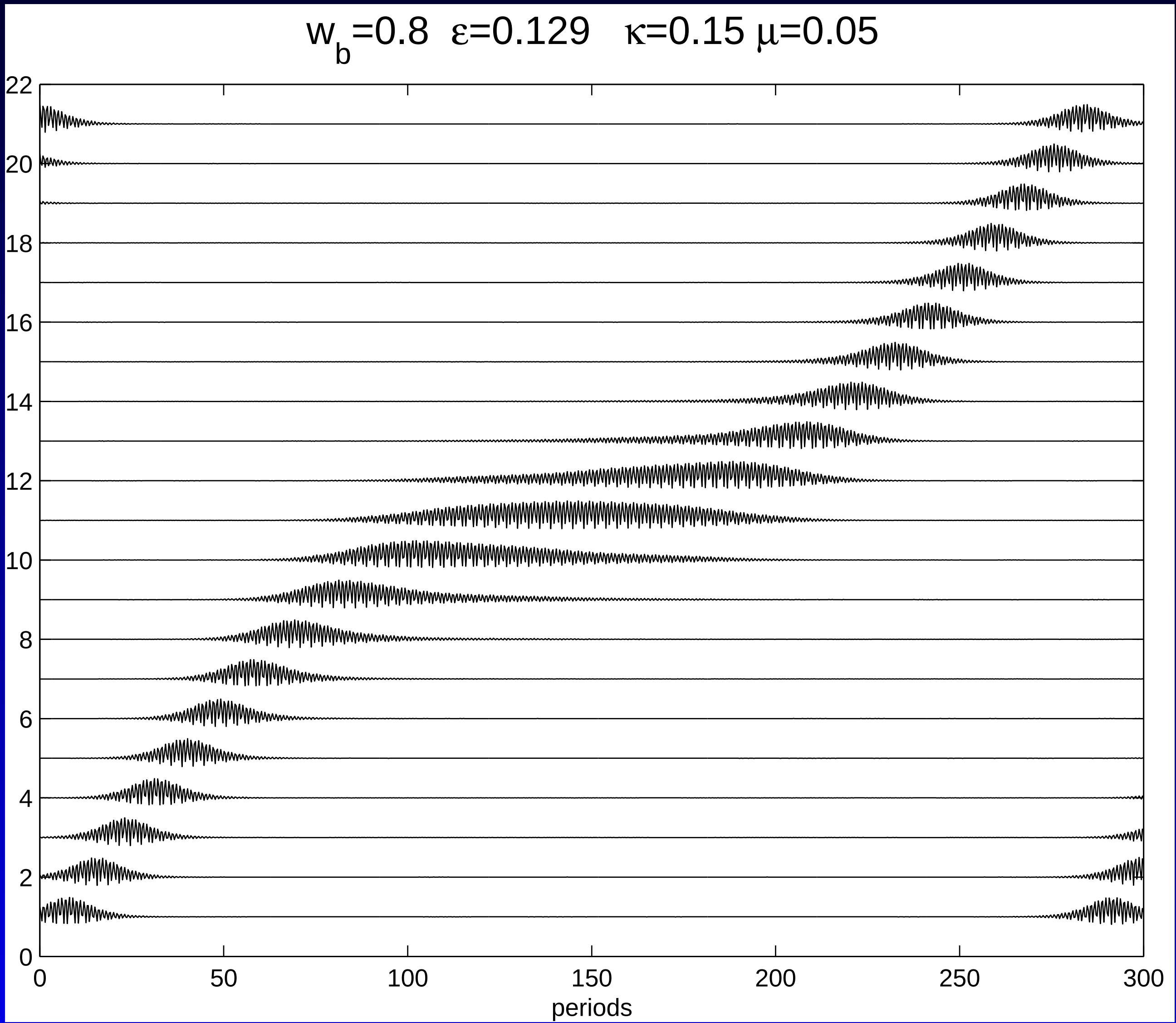
- Breather frequency is curvature dependent
- Hard breathers: stable
- Soft breathers:
    - Instabilities through subharmonic bifurcations
    - Localization is preserved

Moving breathers

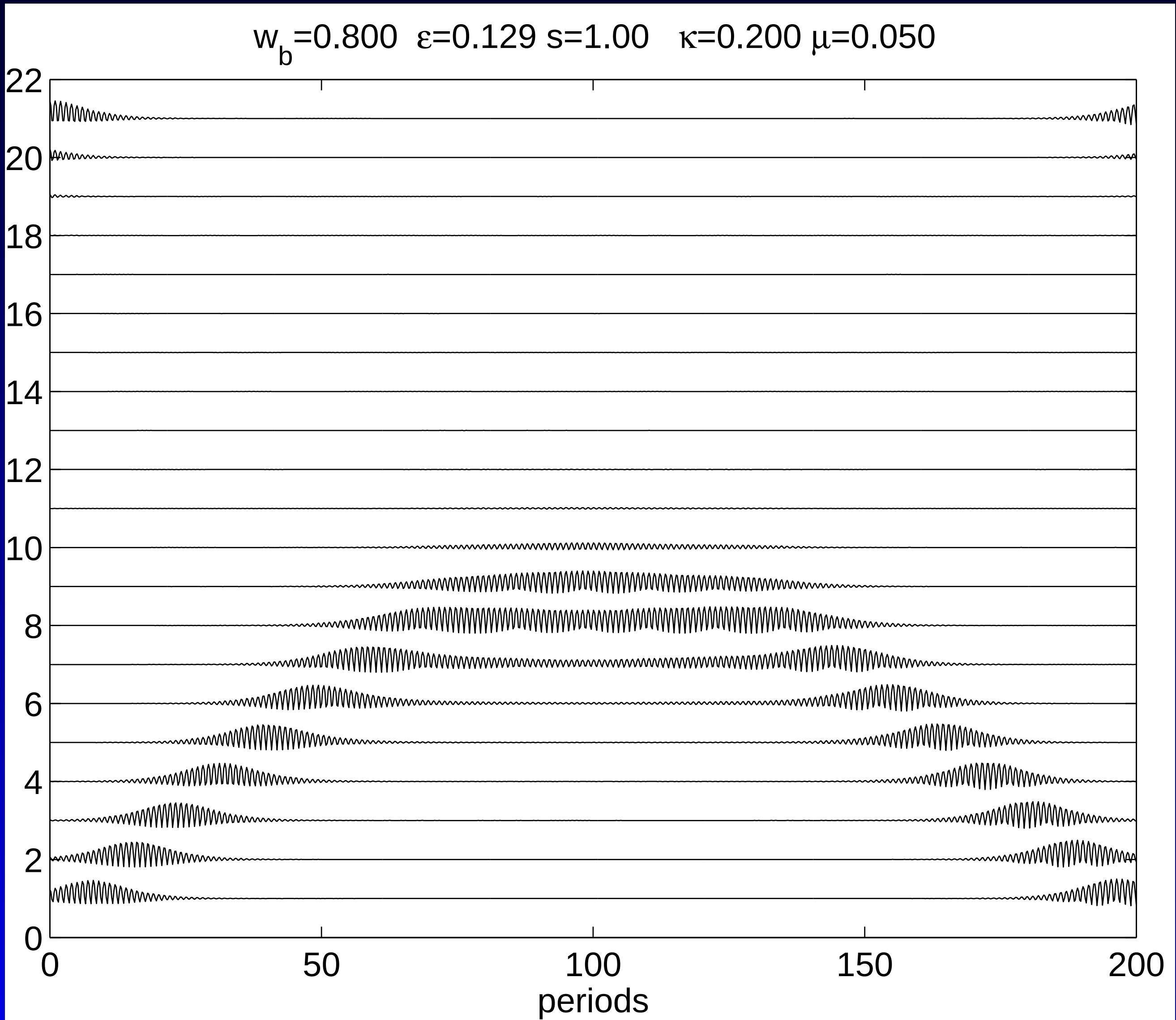
- Soft potential
- Pinning mode method
- Transmitted for $\kappa < \kappa_c$
- Reflected for $\kappa > \kappa_c$
- No trapping

  J Cuevas, F Palmero, JFR Archilla and FR Romero. Moving discrete breathers in a Klein–Gordon chain with an impurity. Submitted to Physical Review E, 2002

Transmitted breather



Reflected breather



Conclusions

- Breathers of fixed frequency become annihilated when the curvature is increased
- Breathers with constant energy choose their frequencies when the curvature is increased
- This frequencies tend to values which depend only on the curvature
- Moving breathers cross over the bending point or become reflected for higher curvatures
- No trapping of moving breathers takes place

Information

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Authors: JFR Archilla, Yu B Gaididei, PL Christiansen and J Cuevas

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