LOCNET TASK 6
Randomness and nonlinearity

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Three types of localization

- Anderson localization
  - Disordered systems
  - Linear localized modes
  - Prevents energy transfer
  - Prevents charge transfer
- Localization due to inhomogeneities
  - Localized linear modes at the inhomogeneities
  - Can act as a energy trap
- Nonlinear localization
  - Due to nonlinearity and discreteness
  - Breathers
  - Moving breathers

Two types of disorder

- Spatial disorder
  - Random masses and molecular bonds
  - Media interfaces
  - Isolated impurities
  - Shape, bending points
- Temporal disorder
  - Temperature or noise
  - Random influence of the surrounding media
  - Do static breathers survive?
  - Do moving breathers survive?

DNA and biopolymers

Systems of choice

- Composed of large groups or atoms
- Macroscopic description
- Essentially monodimensional
- Disordered
- Shape and conformation
- Energy transfer: information
- Energy accumulation:
  - DNA denaturation
  - Biological function
- Charge transfer: bioconductivity

Two main types of models

- Klein–Gordon models
  - Internal degrees of freedom
    - Base pair stretching in DNA
    - C=0 vibrations in proteins

$$\ddot{u}_n = -V_n'(u_n) - \varepsilon[(u_{n+1} - u_n) - (u_n - u_{n-1}]$$

- FPU models
  - No internal degrees of freedom
  - Crystals and polymers

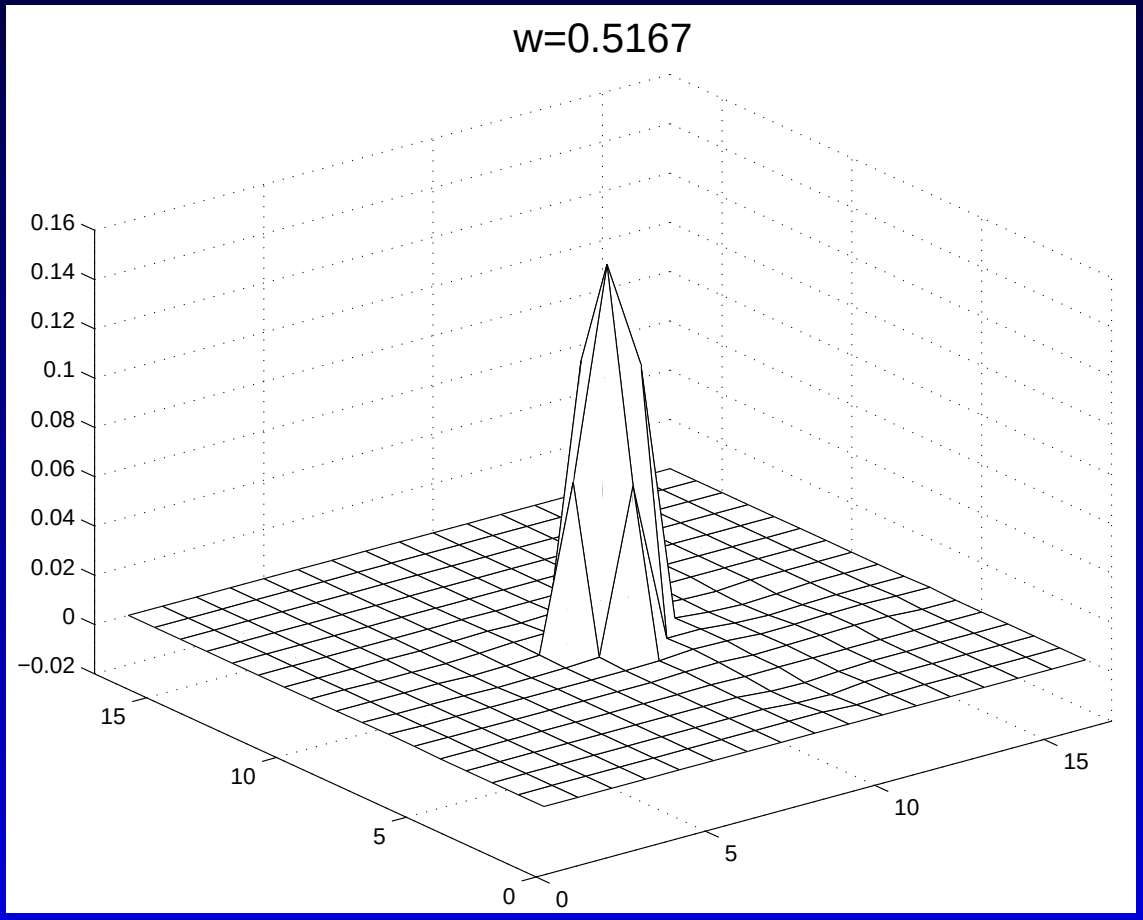
$$\ddot{u}_n = -\varepsilon[W'(u_{n+1} - u_n) - W'(u_n - u_{n-1}]$$

Spatial randomness

- Heraklion, Saclay
  - Continuation of breathers inside the phonon band
  - Intraband discrete multibreathers
  - Energy propagation is restored by the nonlinearity
  - Physica, 2000, Phys Rev Lett, 2000
- Sevilla
  - Continuous path from nonlinearity to disorder
  - Pitchfork: localization if preserved
  - Saddle–node: breather annihilation
  - J. Phys. A, 2001

Anderson localization

- 2D disordered linear system

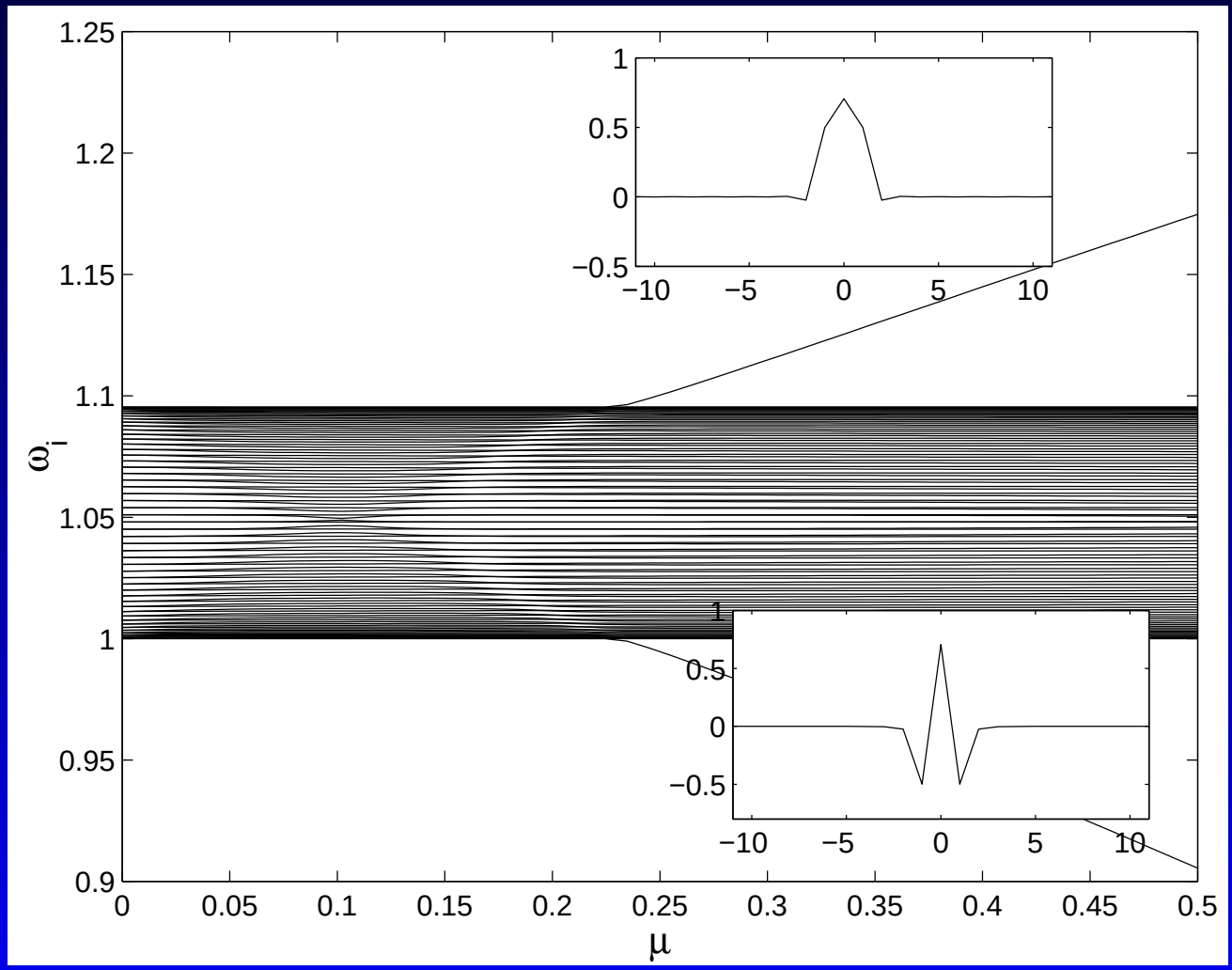


Inhomogeneities I

- Lyngby and Sevilla
  - Effect of shape and LRI in models for DNA and alpha–helix proteins
  - DNLS and Klein-Gordon models
  - Bending points can act as a trap for excitations
  - Nonlinear impurity modes
  - Conditions for trapping at a impurity
  - Effect of DNA helicity
  - Characteristic frequencies at the bending points
  - Phys. Rev. E, 2000, 2001, 2002; J. Phys. Cond. Matter, 2000; Jou. Phys. A, 2001, 2002(2); Phys. Rev. E, 2001(2), 2002; Phys. Lett. A. 2002;

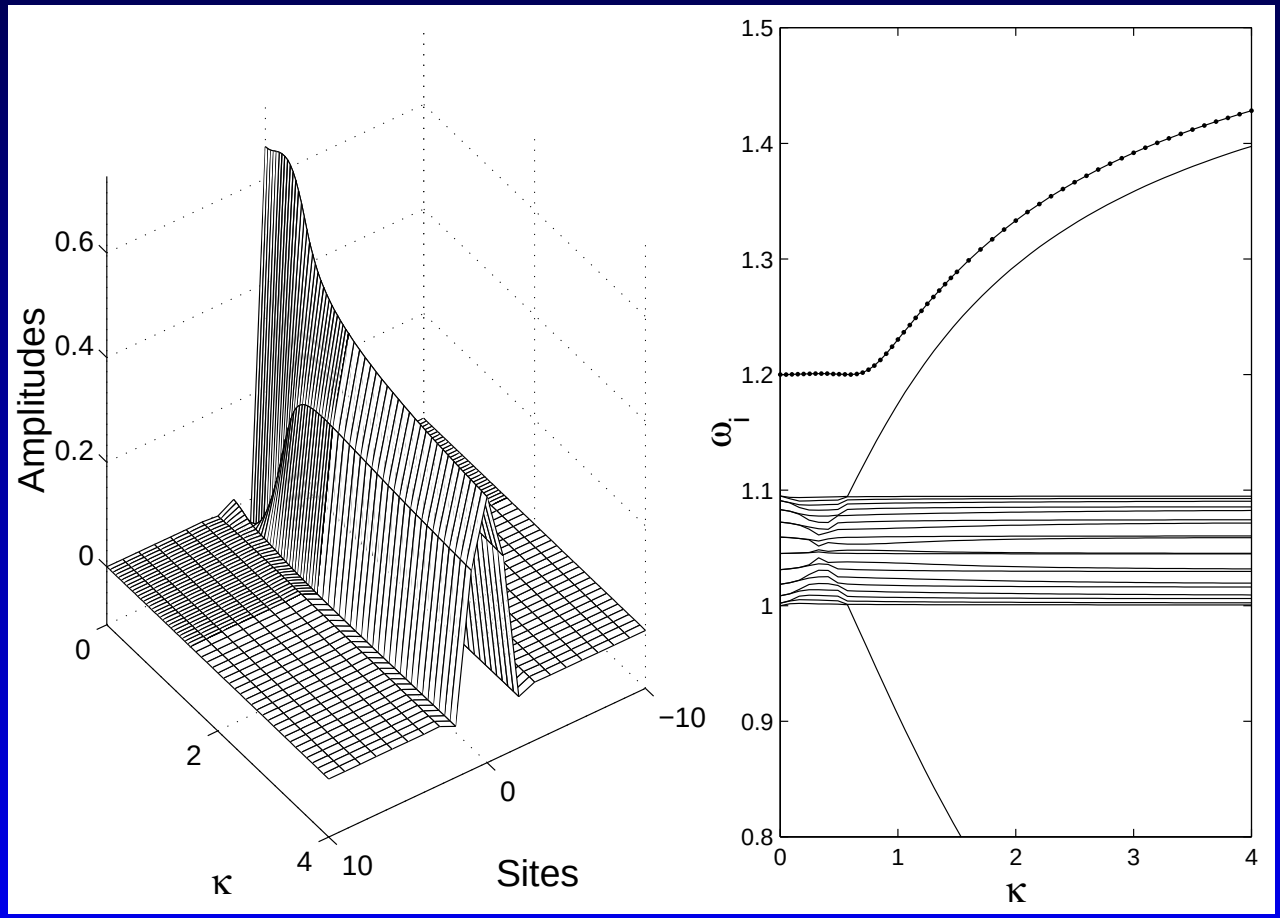
Bending points I

- Linear curved alpha–helix proteins



Bending points II

- Interaction inhomogeneity–nonlinearity
- Nonlinear curved alpha–helix proteins



Inhomogeneities II

- Barcelona, Heraklion
  - Breather mobility in FPU models for biopolymers
  - Energy transport across bending points
  - Conditions for transport on chains with different masses
  - Curved segments as gates
  - Conditions for trapping, re¤exion, transmision or spliting in terms of the Peierls–Nabarro potential.
  - Jou. Phys. A, 2001; Europhys. Lett. 2002; Phys. Rev. E, 2002 (2)

Temporal disorder

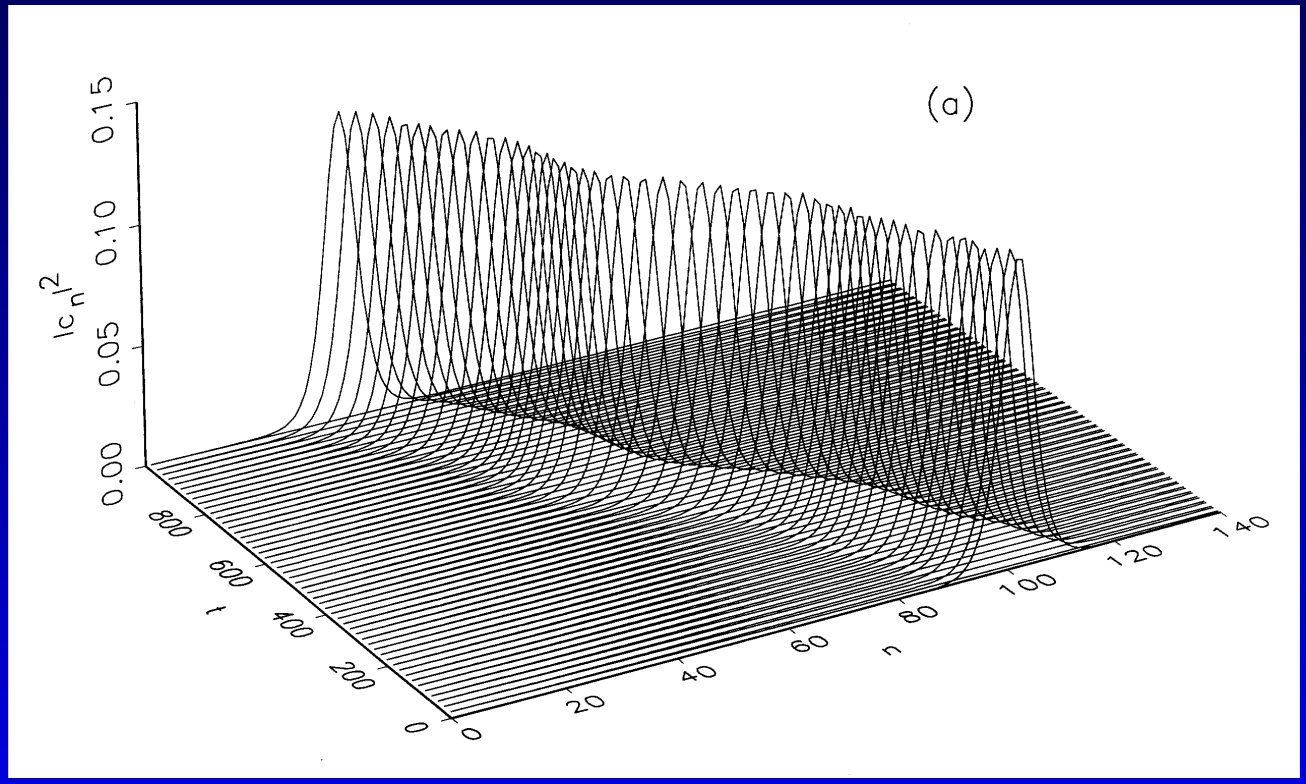
- Barcelona, Heraklion
  - FPU models for curved biopolymers
  - Dissipation
  - Temperature
  - Survival of breather mobility
  - Jou. Phys. A, 2001; Europhys. Lett. 2002; Phys. Rev. E, 2002.
- Saclay, Heraklion
  - Thermalization of phonons leading to discrete breathers
  - Eur. Phys. Jou. 2002.

Disordered systems

- Berlin, Sevilla
  - DNA 3D model for charge transport
  - Spatial disorder due to random distribution of base pairs
  - Structural (shape) disorder due to interaction with the media
  - Charge transport mediated by polarobreathers survives
  - Coherent with experimental data
  - Physica D, 2002.

Charge transport

- Electron wave function
- Disordered DNA



Some projets

- Lyon
  Actual sequences in DNA
- Warwick, Barcelona, Zaragoza
  Noise induced conductivity on charge density wave materials
- Lyngby, Sevilla
  Moving breathers and DNA interfaces
- Edinburgh, Sevilla
  Interaction of moving breathers with vacancies and other defects