Nonlinear Localized Excitations in Discrete Systems

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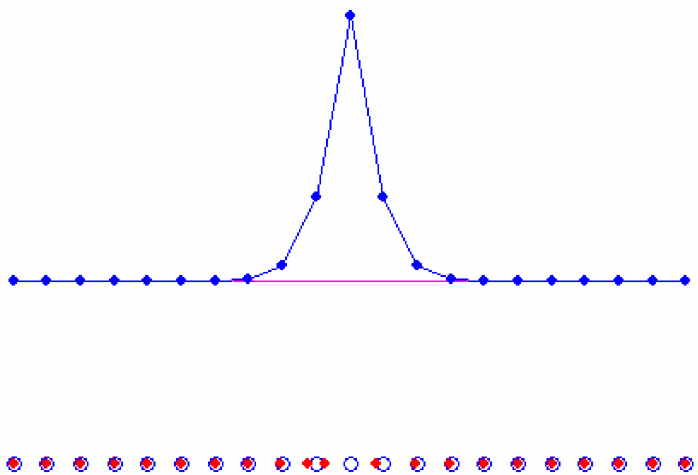
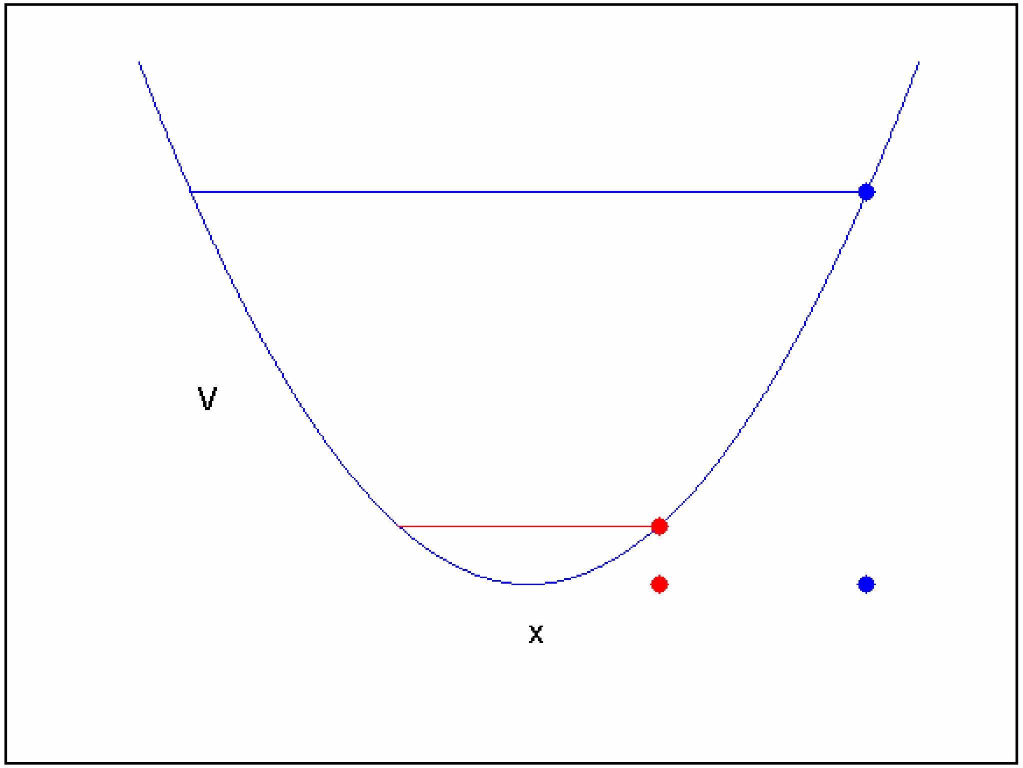
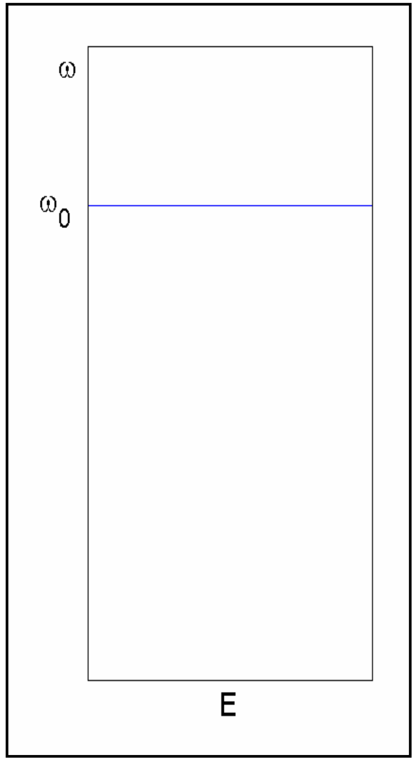
Discrete breathers. Nonlinear localization

- Nonlinear Discrete systems.
- Vibrational state and exact solution
- No Anderson localization



Linear oscillator. F=-kx, $V(x)=1/2kx^2$

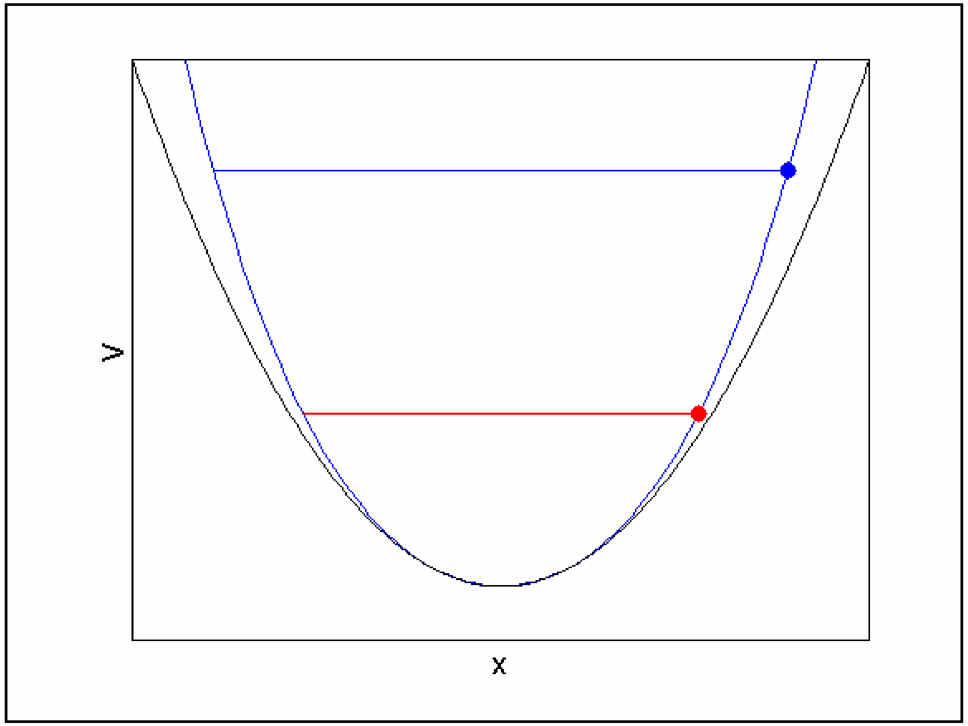


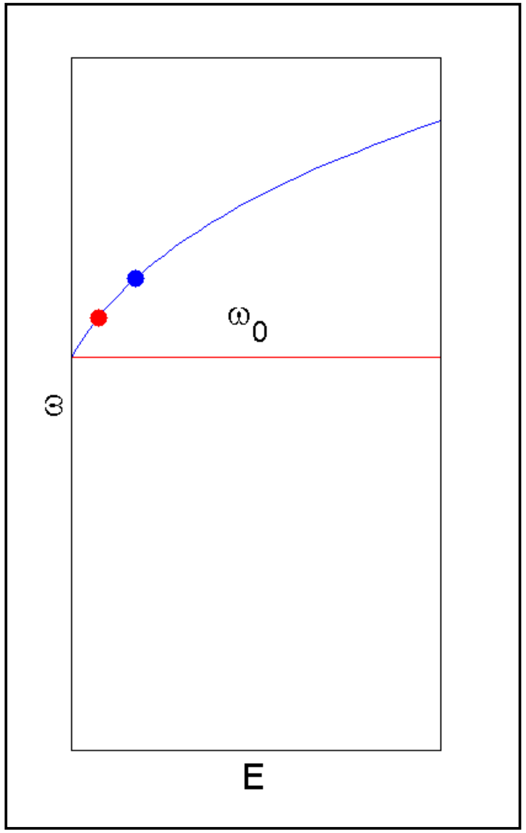


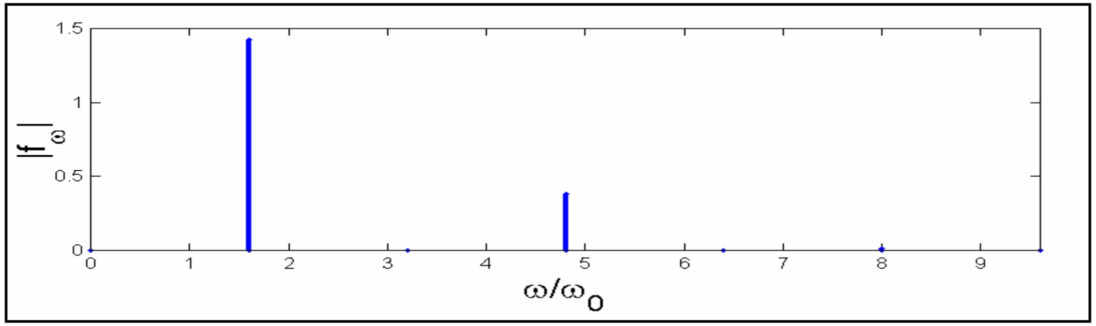
$x = A\cos(\omega_0 t + \varphi_0)$

$\omega_0 \neq \omega_0(E)$

Nonlinear hard oscillator

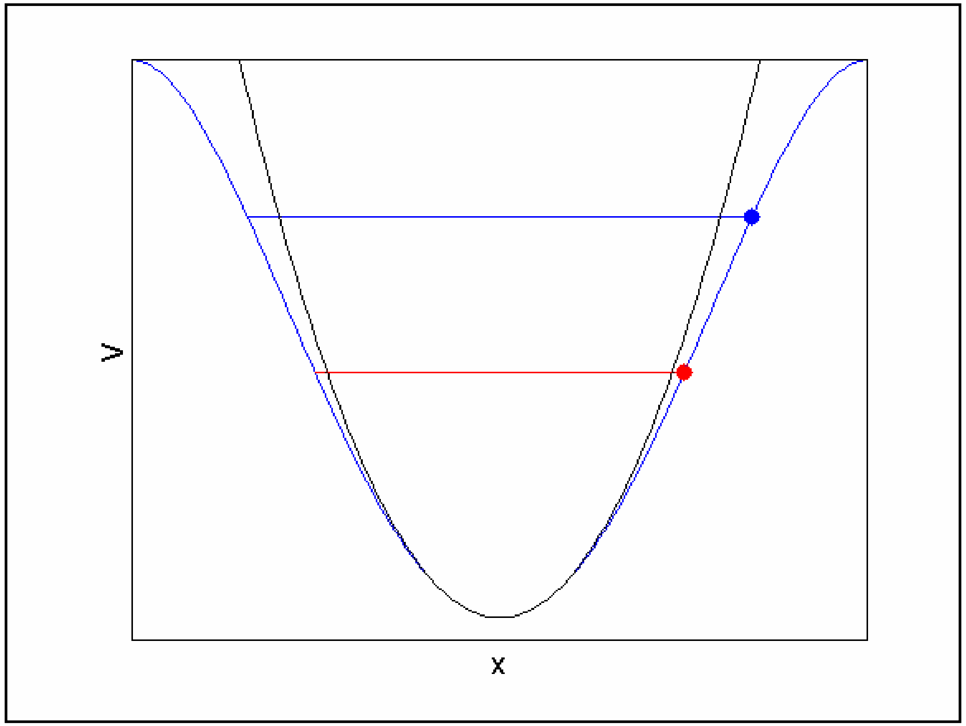


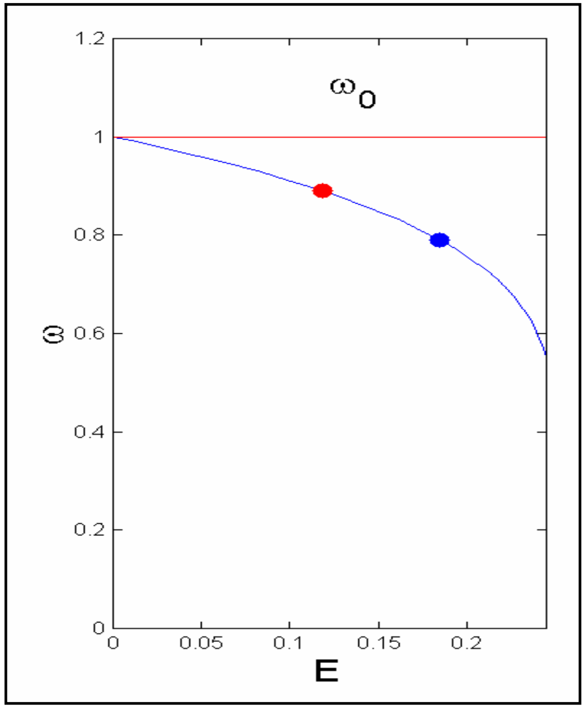




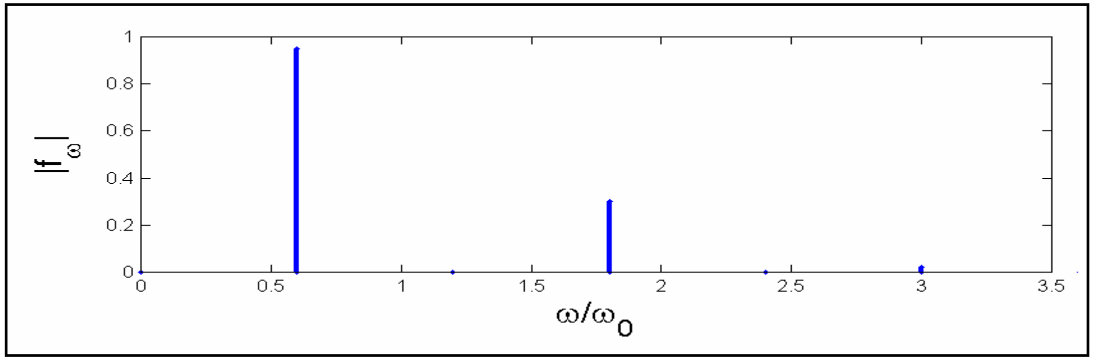
$$V=\tfrac{1}{2}(\omega_0)^2x^2+\tfrac{1}{4}x^4$$

Nonlinear soft oscillator



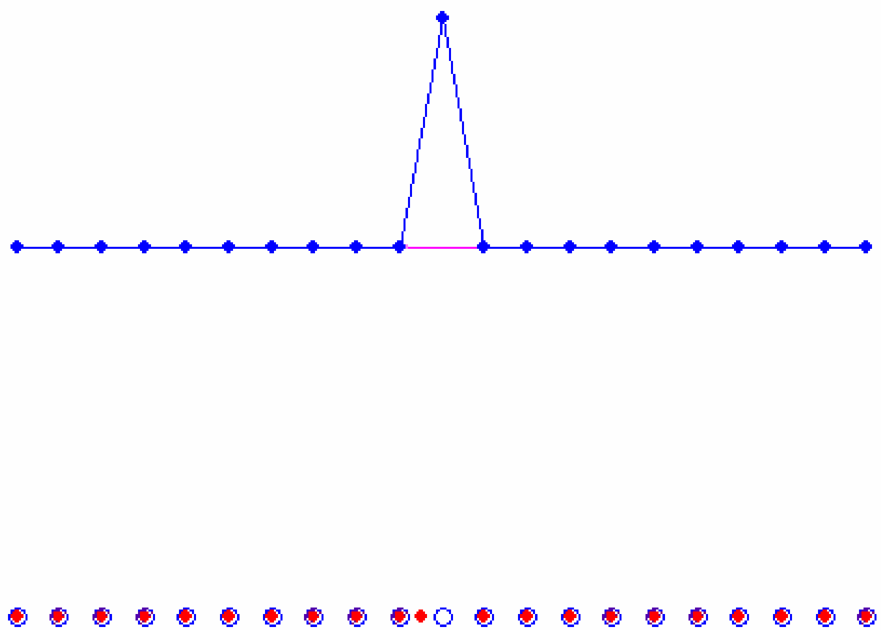


$V = \frac{1}{2} (\omega_0)^2 x^2 - \frac{1}{4} x^4$

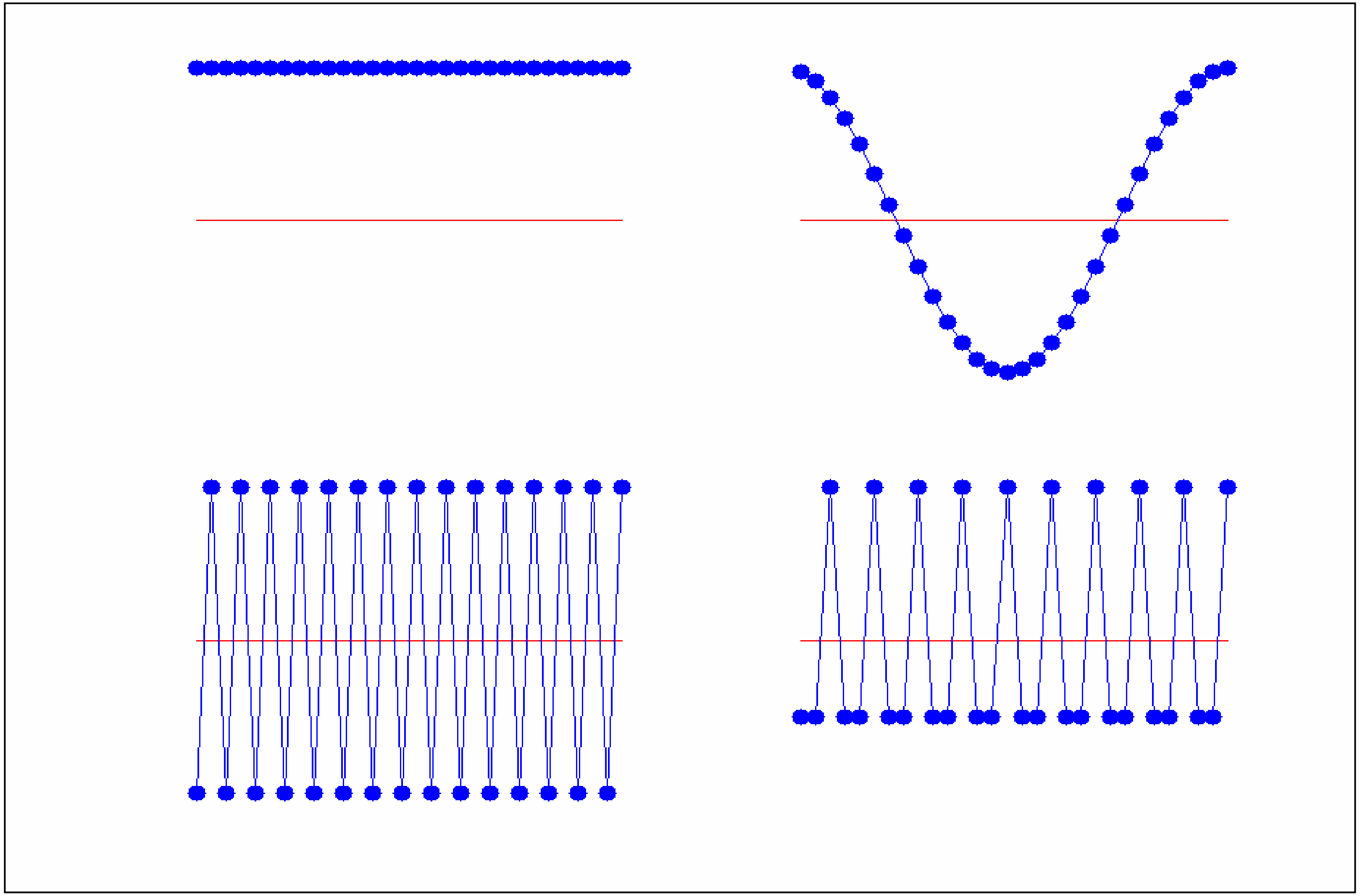


Coupled linear oscillators

$$V=\sum 1/2(\omega_0)X_n^{\,2}+C/2(X_n-X_{n+1})^2$$

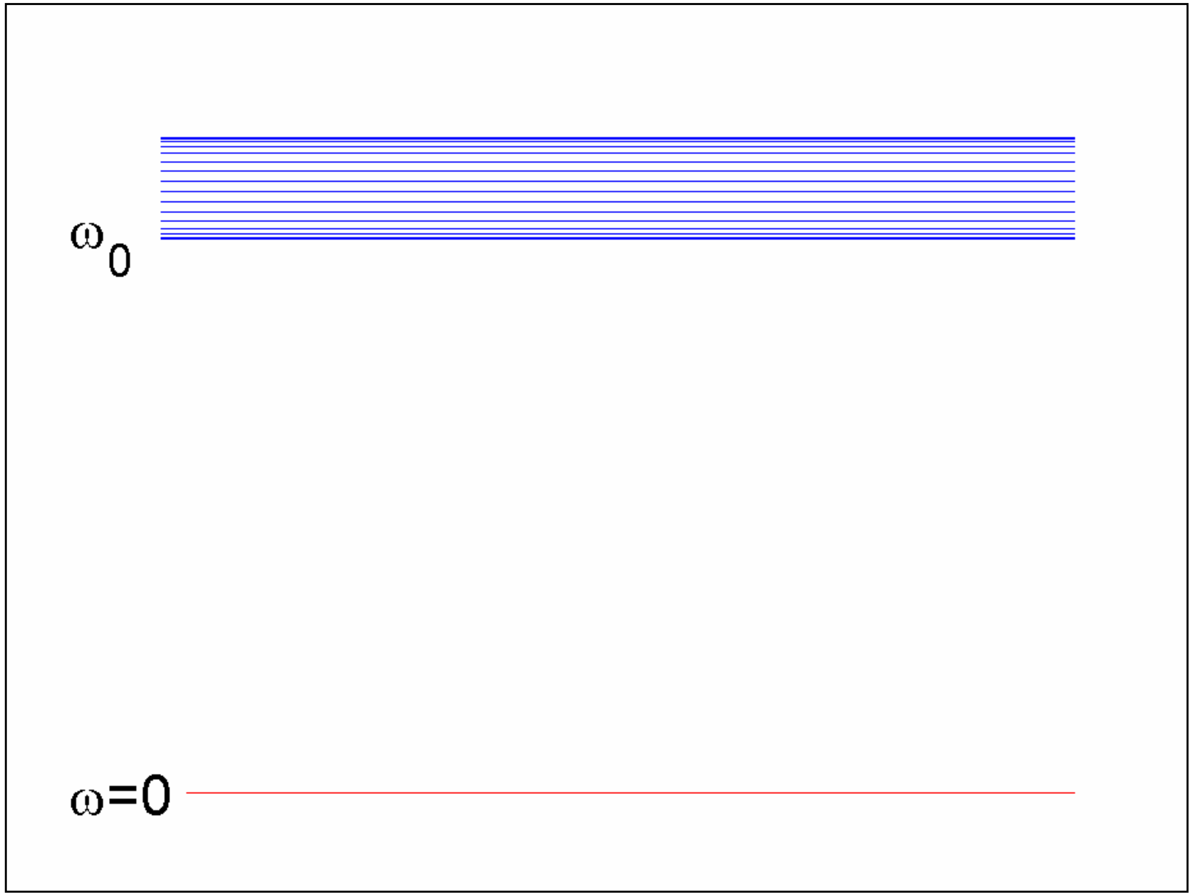


Linear lattices. Normal modes



Phonons

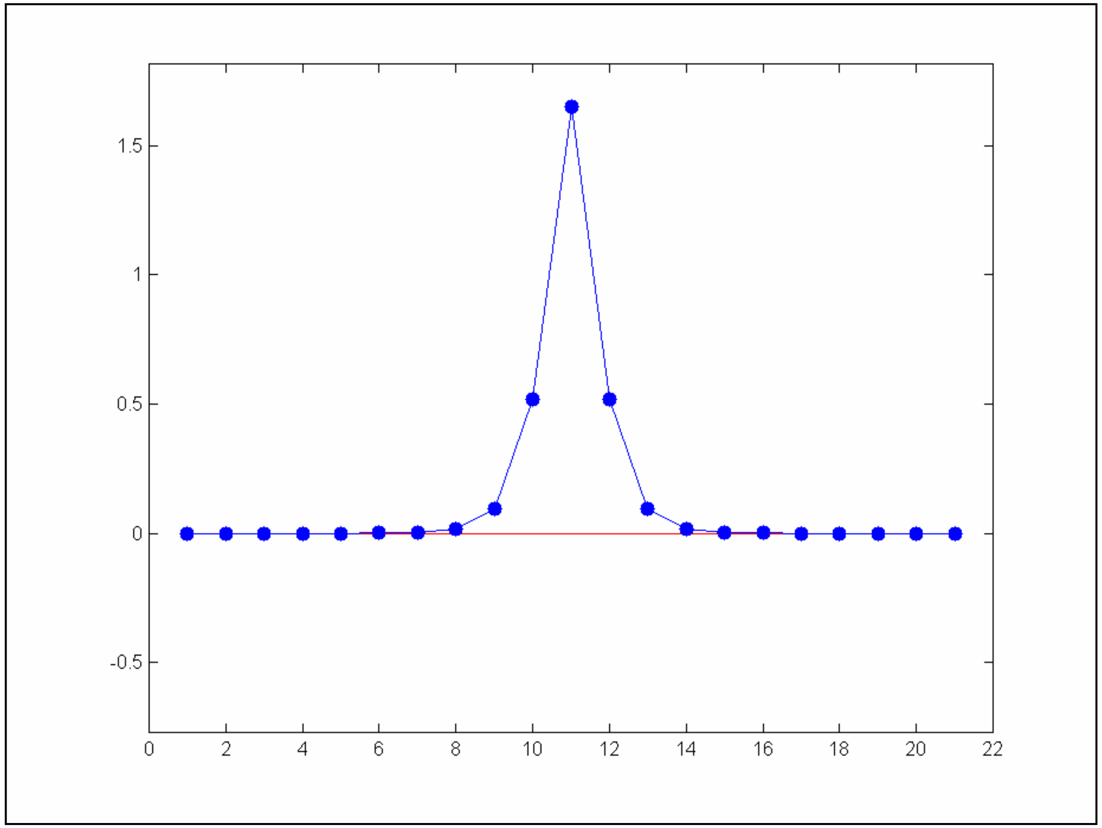
- Frequency band $\omega^2_{ph} = w^2_0 + 4\ C \sin^2 q/2$
- Non localized states



Nonlinear coupled oscillators

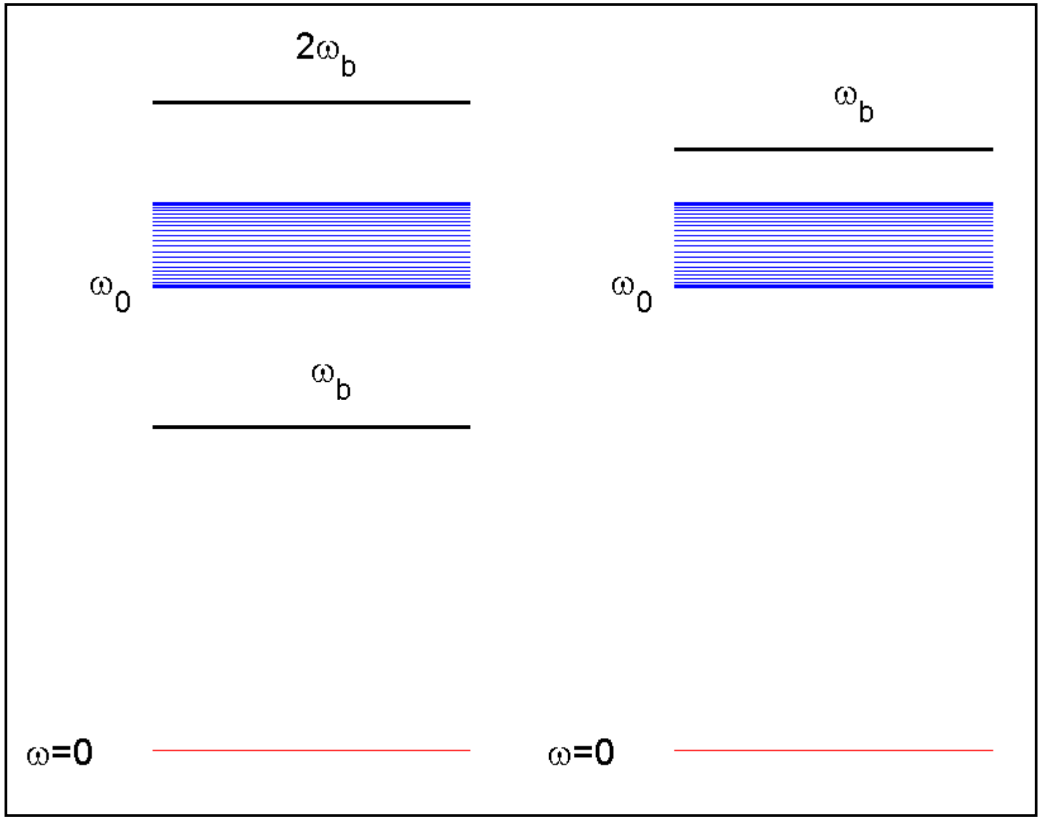
$$V=\sum V(X_n)+C\,W(X_n,X_{n+1})$$

- Exact, periodic and localized solution



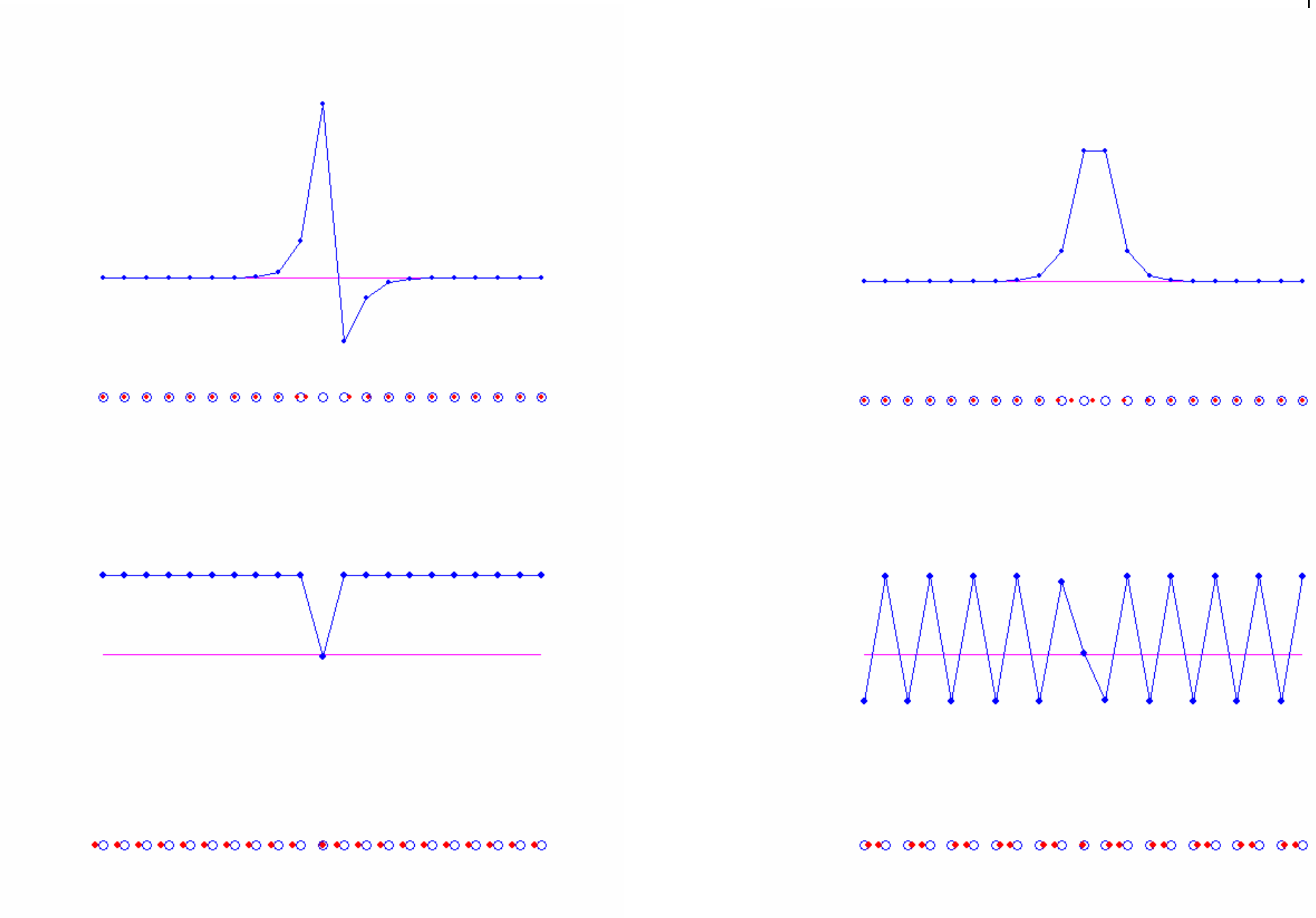
Existence of breathers (1994)

Soft Hard



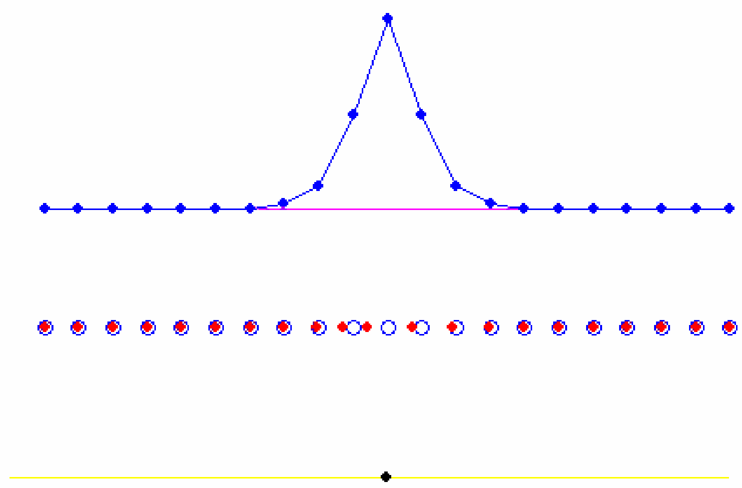
$n\,\omega_b \notin [\omega_0, \omega_{f,máx}], \quad \omega_b'(E) \neq 0$

“Breathers and Multibreathres”



Discrete moving breathers

- Discrete breathers can move and transport coherently energy through the lattice



Nonlinear lattices

- Klein Gordon lattices (mechanical systems as coupled pendulum, Josephson junction arrays)
- FPU lattices (crystals)
- DNLS (Discrete Nonlinear Schrödinger)
  - Nonlinear wave arrays
  - Photonic crystals
  - Bose-Einstein condensates
- Biomolecules (DNA, proteins…). Klein Gordon, FPU, DNLS…

Theoretical and numerical works

- Classical systems
  - Mathematical and numerical extensive work. Existence and properties well known.(For a review, see, i.e. T. Dauxois et al. (Eds) Energy Localisation and Transfer, *Advanced Series in Nonlinear Dynamics 22*, World Scientific, 2004).
- Discrete Quantum breathers
  - Open problems. (V. Fleurov. *Discrete quantum breathers: What do we know about them?.* Chaos 13, 676, 2003).

Experimental results

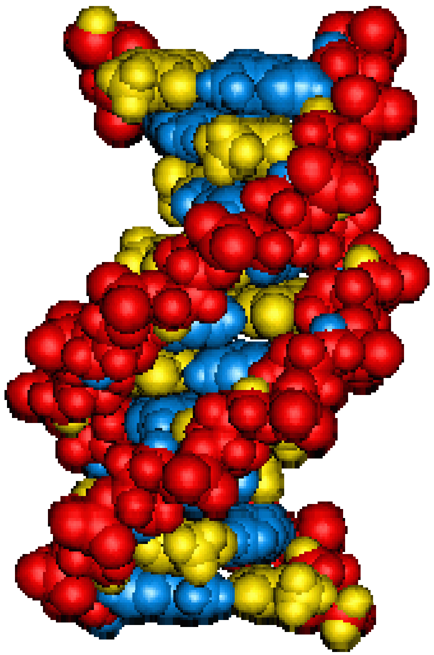
- Real materials (crystals, magnetic systems, i.e. M.E. Manley et al. *Formation of a new dynamical mode in alpha-uranium observed by inelastic X-ray and neutron scattering*, Phys. Rev. Lett. 96, 125501, 2006.)
- Artificial systems as Josephson Junctions arrays, micromechanical cantilever and coupled optical waveguides (see, i.e. D.K. Campbell et al. *Localizing energy through Nonlinearity and Discreteness*, Physics Today, p. 43-49, January 2004.)
- Biomolecules?. Results not clear

Research lines

- Biomolecules. Discrete breathers in DNA?
- Defect migration in solids.
- Breathers and reconstructive transformations in the Mica muscovite
- Quantum breathers

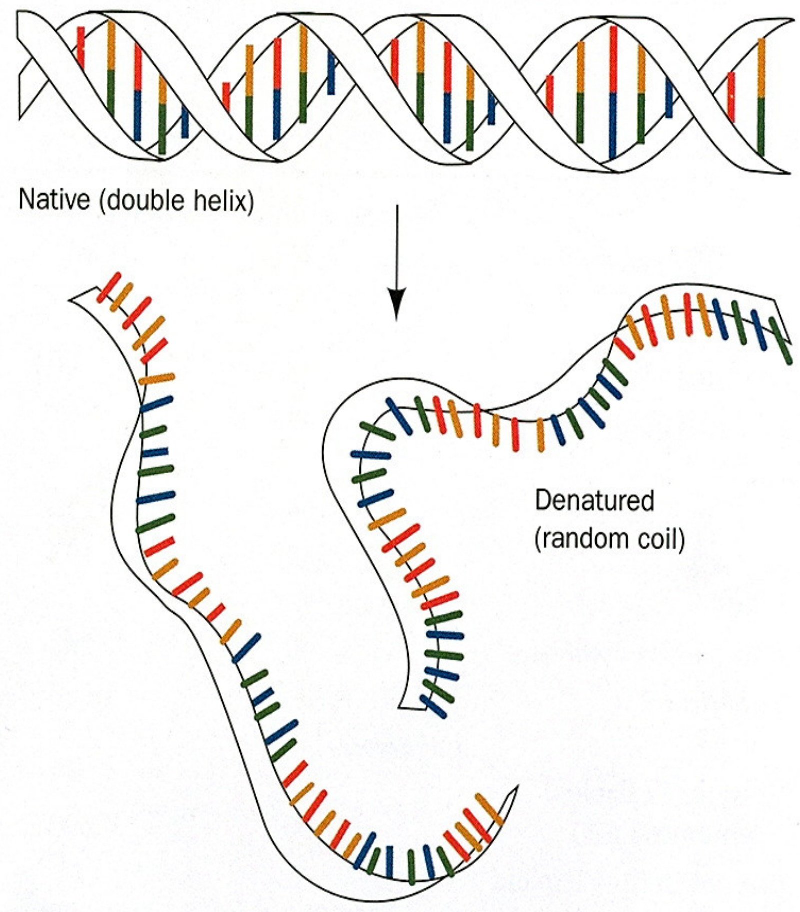
Breathers in DNA?

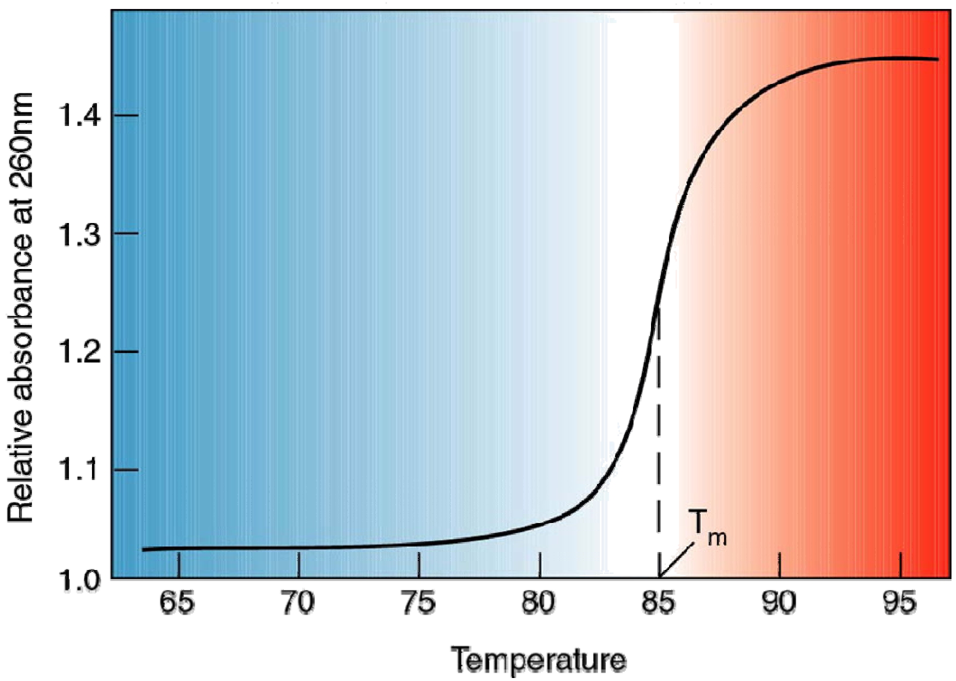
- Breathers are thought to play a role in processes such as the formations of local fluctuations openings in DNA molecules (M. Peyrard. *Nonlinear Dynamics and statistichal Physics of DNA*, Nonlinearity 17, 1-40, 2004).



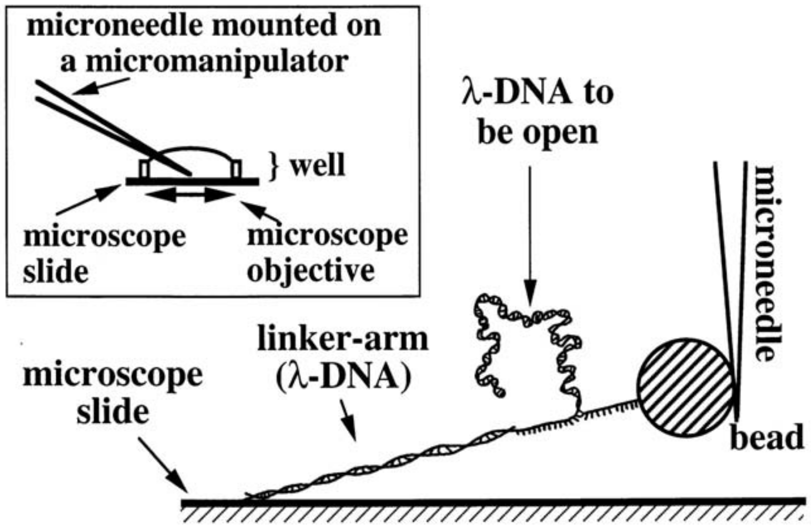
- Double helix structure
- Genetic code as a basis sequence
- ≈ 20 Å diameter
- Human genome ≈ 3.3 x 10^9 bp
- ≈ 25,000 gens
- 1 cromosome = 1 DNA molecule
- 2 m DNA per cell (salamander ≈ 1 km)

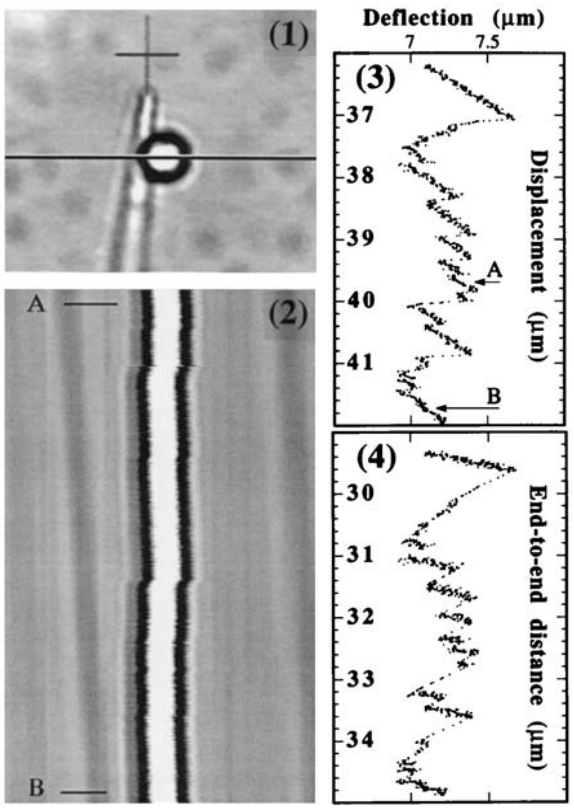
Thermal DNA denaturation



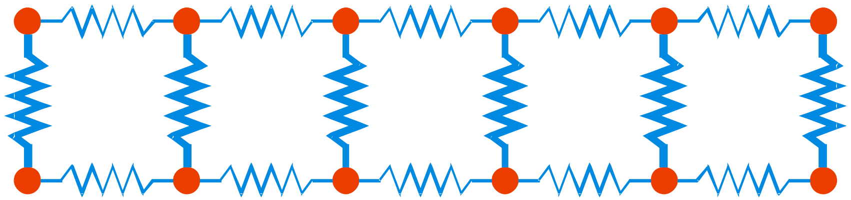


DNA Mechanical denaturation





Peyrad-Bishop model



•Qualitative and cuantitative agreement with experiments!

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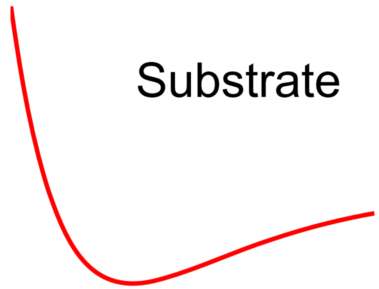
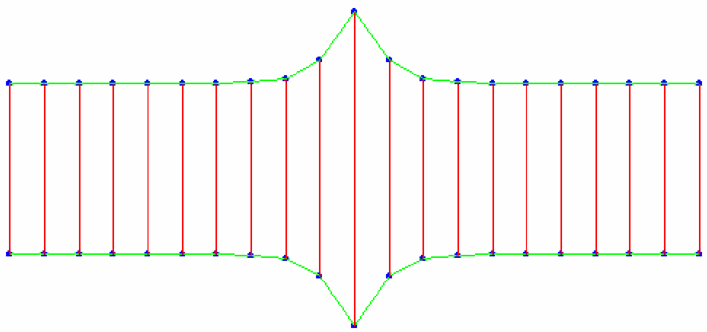


$$H = \sum_n \frac{p_n^2}{2m} + W(y_n, y_{n-1}) + V(y_n), \;\; p_n = m\frac{dy_n}{dt}$$

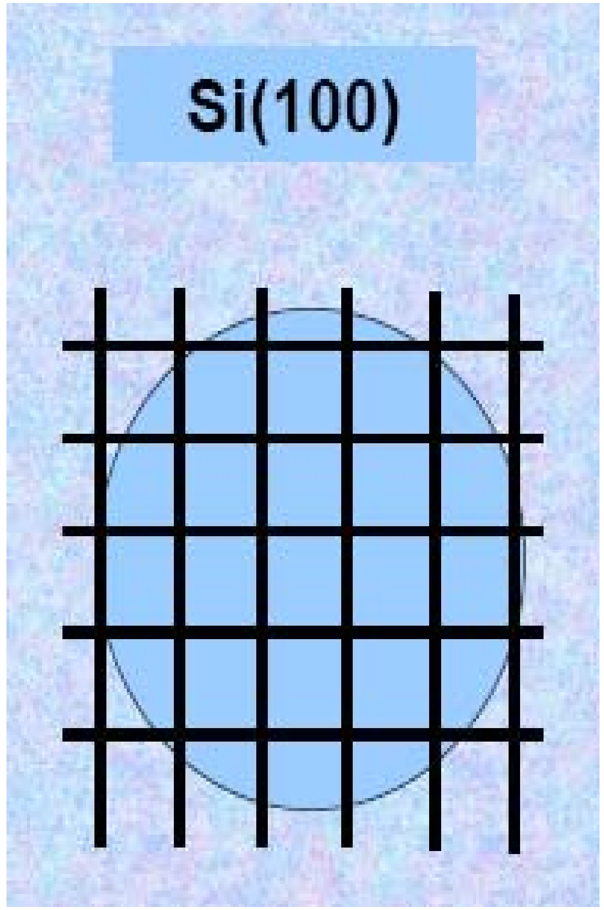
Breathers in PB model

- Existence and mobility
- More complicated structures
- Long range interaction
- Charge transport (polarons)

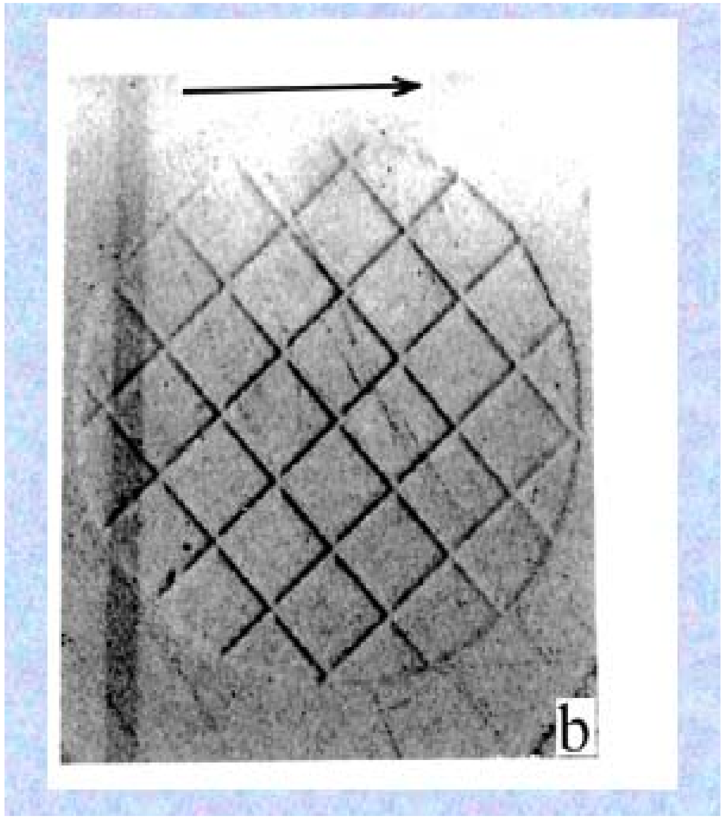


Migracion of defects in solids

- Experiment: Migracion of defects in Silicon due to iteraction with heavy ions (P. Sen et al. Current Science *85, 1723,* 2003).
- Ion (Ag) 100-200 Mev perpendicular
- Ni lattice 5 mm-300 mm



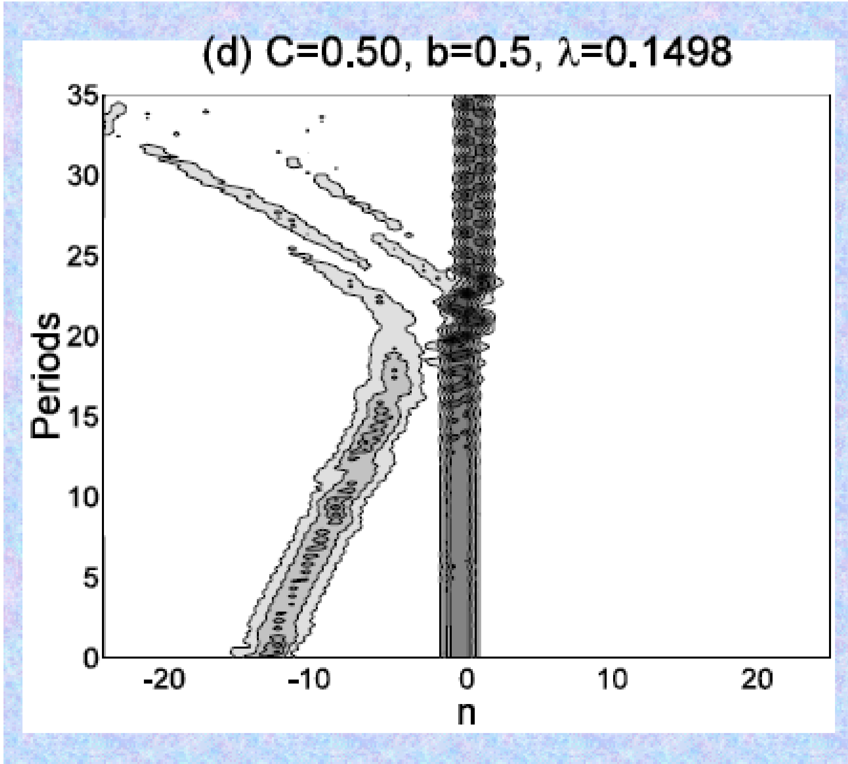
Results



- Defects move through interfaz
- Irradated area free of defects
- Breathers can be the origen of defect migration?

Numerical simulations

- Numerical simulations show that moving breathers can move a vacancy (even backwards or forward).



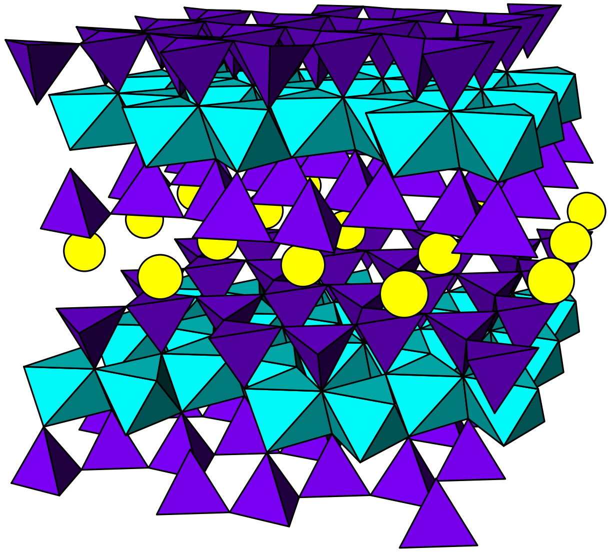
Reconstructive transformation of Mica muscovite

moscovite

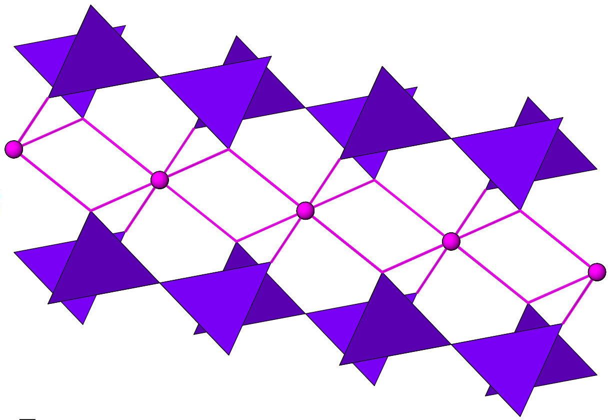
$K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4$

Disilicate of Lutetium

$Lu_2Si_2O_7$



Lu^{3+}



300° C, 3 days

K^+

Lu^{3+}

36% of moscovite transforms

¿What is special in the reconstructive transformation of mica and other layered silicates?

• Reconstructive transformations had been observed in silicates only about 1000 C

• **Some of the authors (MDA, MN, JMT) have recently achieved low temperature reconstructive transformations (LTRT) at temperatures 500 C lower than the lowest temperature reported before**

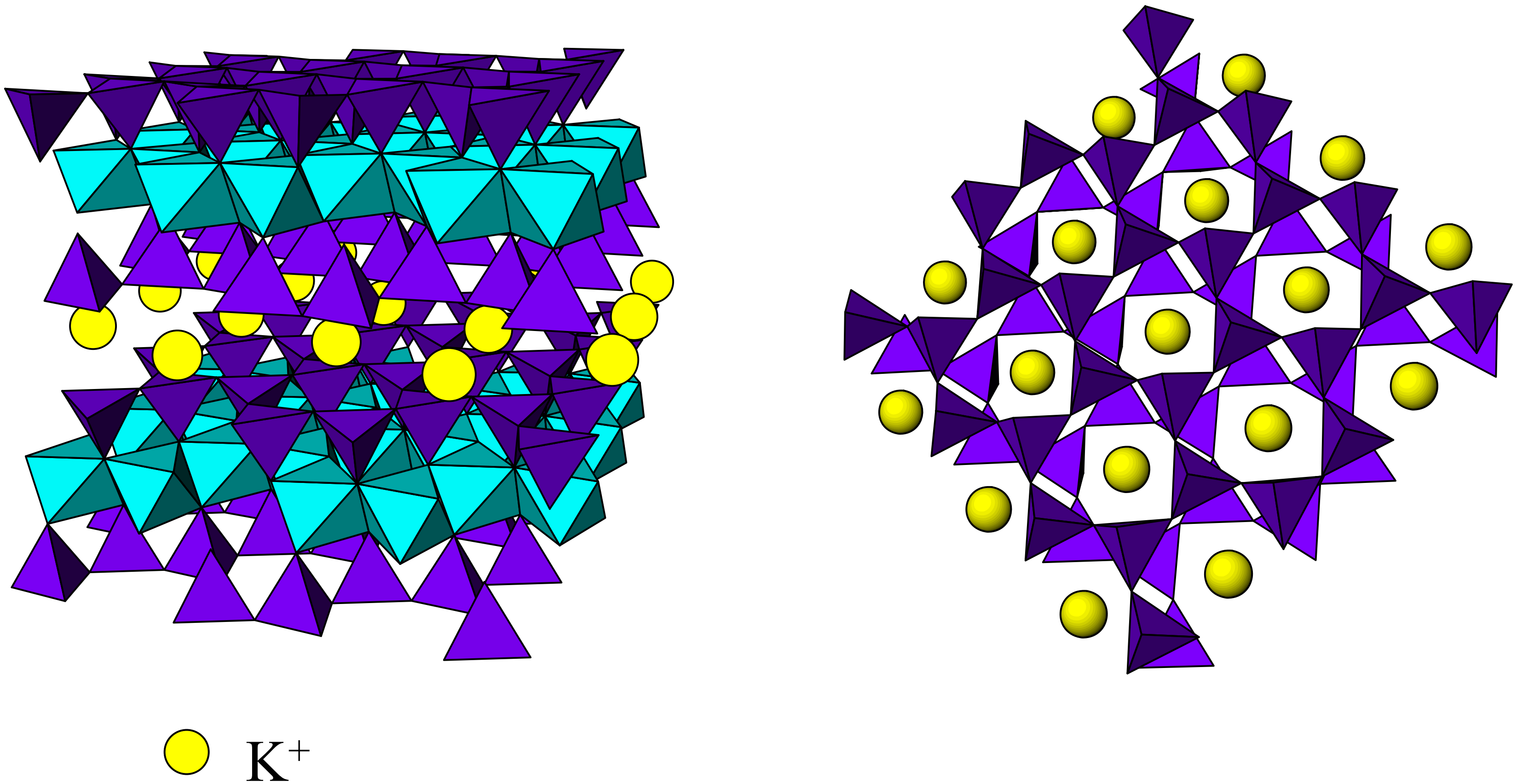
• **LTRT:** Low temperature reconstructive transformations.

• **UP TO NOW THERE WAS NO EXPLICATION**

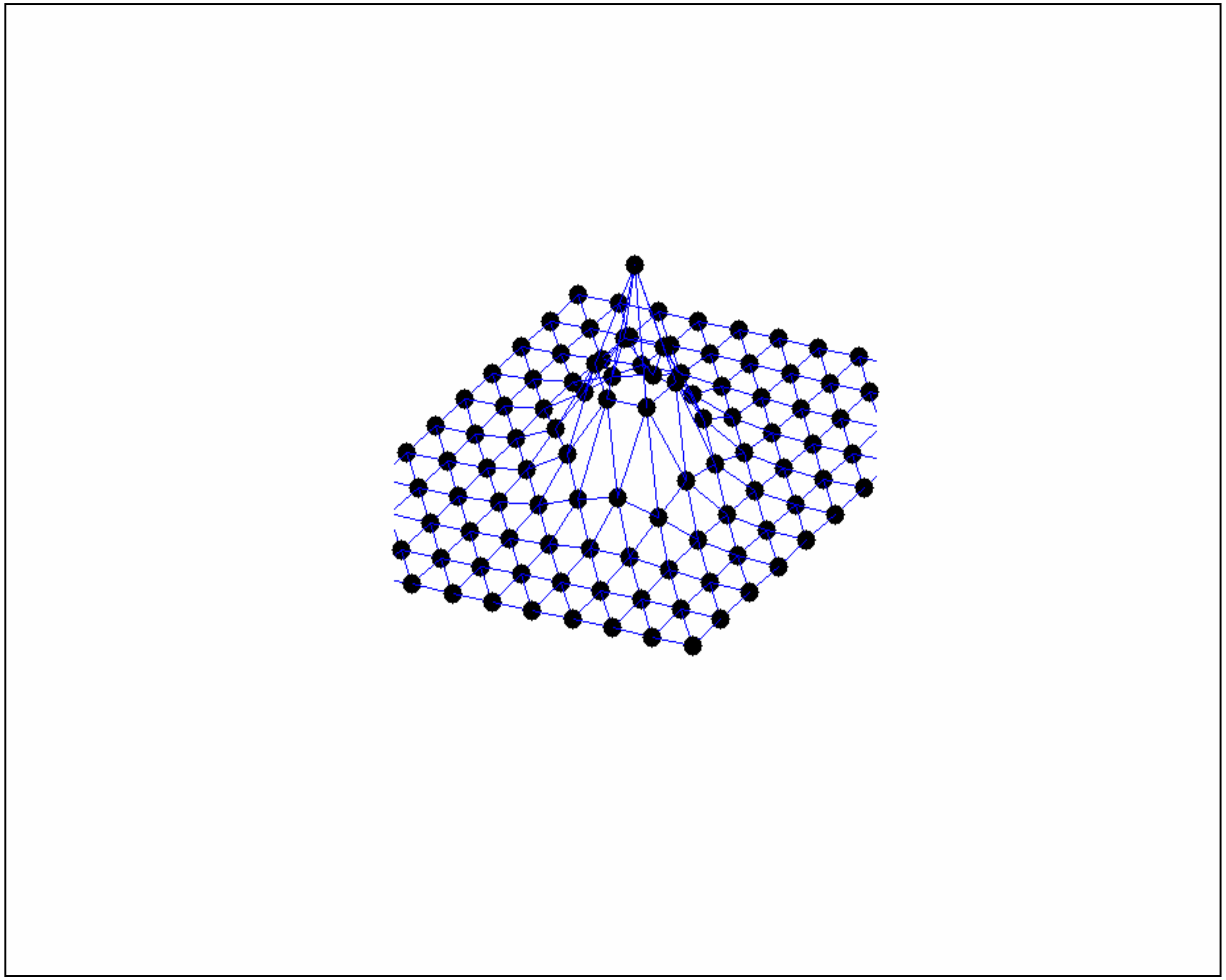
¿Could breathers be the explanation?

First suggested in: Mackay and Aubry [Nonlinearity, **7**, 1623 (1994)]

Mica muscovite. A two dimensional model



A 2D breather in the cation layer



Hypothesis: inclucence of discrete breathers on the reaction speed

Objectives:

- Calculate 2D breathers in the cation layer of mica moscovite
- ¿Have they large enough energy to bring about the increse in reaction speed?
- ¿Is their number large enough?

Estimations

For E_a~100-200 kJ/mol, T=573 K:

$$\frac{\text{Number of breathers}}{\text{Number of phonons}} = 10^4\text{-}10^5 \qquad (\text{with } E \geq E_a)$$

Reaction time without breathers: 80 a 800 years,

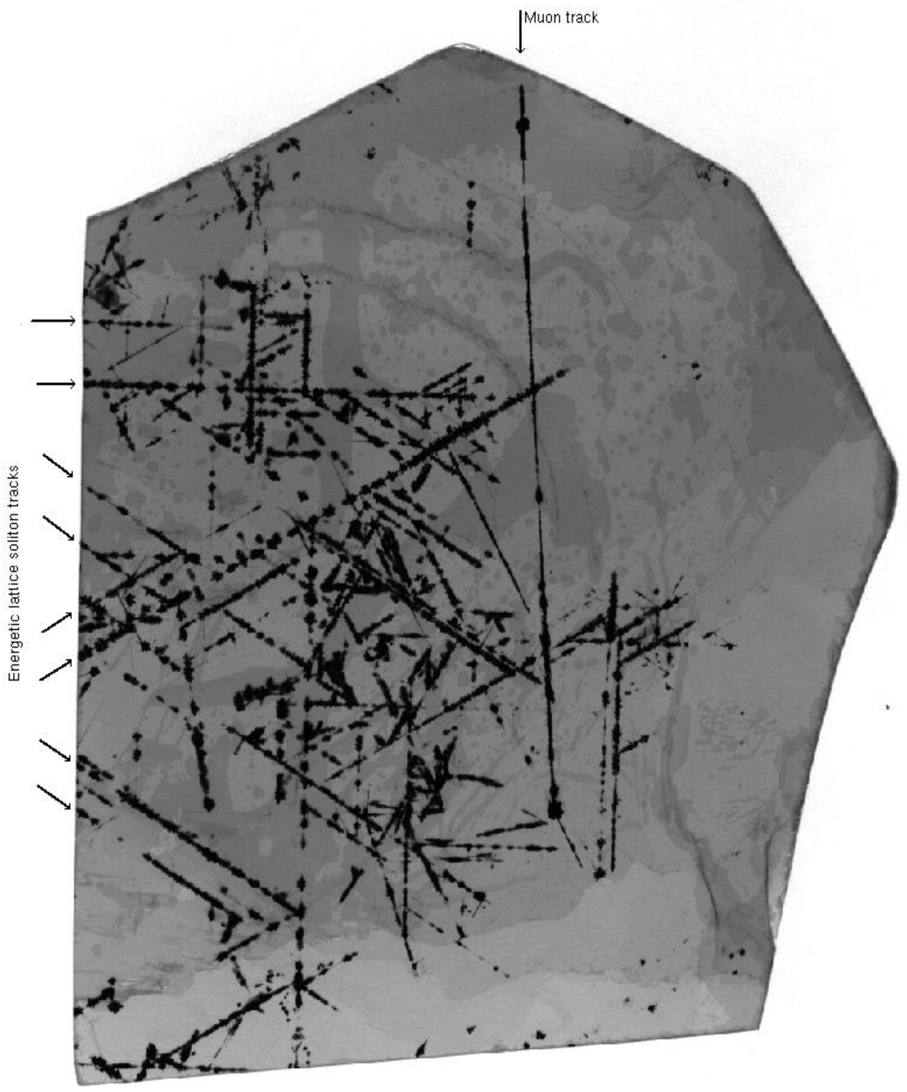
Moreover, breather can localize more the energy delivered, which will increse further the reaction speed

THERE ARE MUCH LESS BREATHERS THAN LINEAR MODES, BUT MUCH MORE WITH ENERGY ABOVE THE ACTIVATION ENERGY

Other possible evidences for breather existence in mica muscovite

- Black tracks in natural mica
- Numerical studies of moving breathers
- Sputtering

Quodons in mica moscovite



Black tracks: Fe_3O_4

Cause:

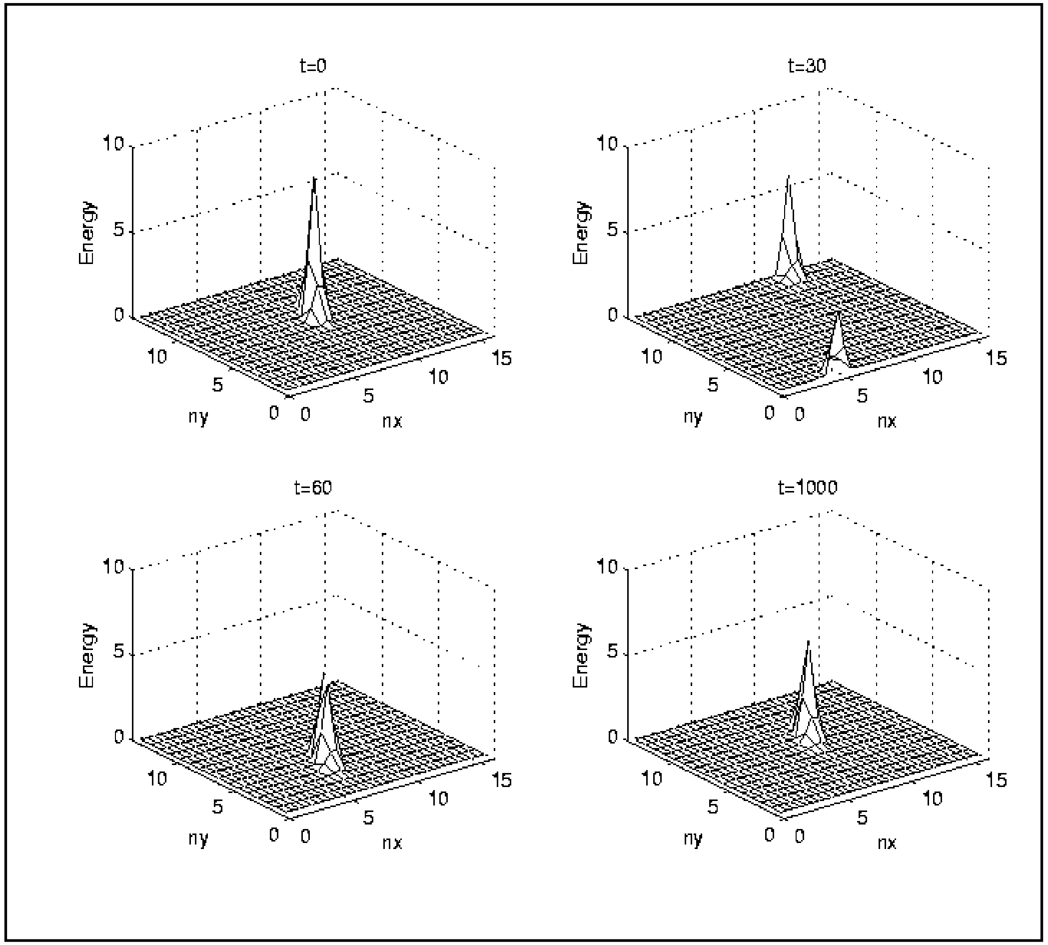
- 0.1% Particles:
  - muons: produced by interaction with neutrines
  - Positrons: produced by muons' electromagnetic interaction and K decay

- 99.9% **Unknown**

¿Lattice localized vibrations: quodons?

Black traks are alogn lattice directions within the K^+ layer

Numerical simulations in a 2D hexagonal lattice



No apparent dispersion in 1000~10000 lattice units

Localized moving breathers in a 2D hexagonal lattice. JL Marín, JC Eilbeck, FM Russell, Phys. Lett A 248 (1998) 225

Sputtering

Trayectories along lattice directions within the K^+ layer

Evidence for moving breathers in a layered crystal insulator at 300K
FM Russell and JC Eilbeck, Europhysics Letters 78, 10004, 2007.

Quantum breathers

- Discrete breathers in classical lattices
  - Spatial localization by nonlinearity. General conditions for its existence and stability.
  - Some analytical results. Standard numerical methods.
  - Static and moving breathers.
  - Experimental evidences.
- Quantum systems: Quantum equivalence of discrete breathers is an open question.

Hubbard models (fermions or bosons). QDNLS systems.

- Index *j* and *p* a D-dimensional index, ranges over the D-dimensional lattice).
- Conserves the number of quanta

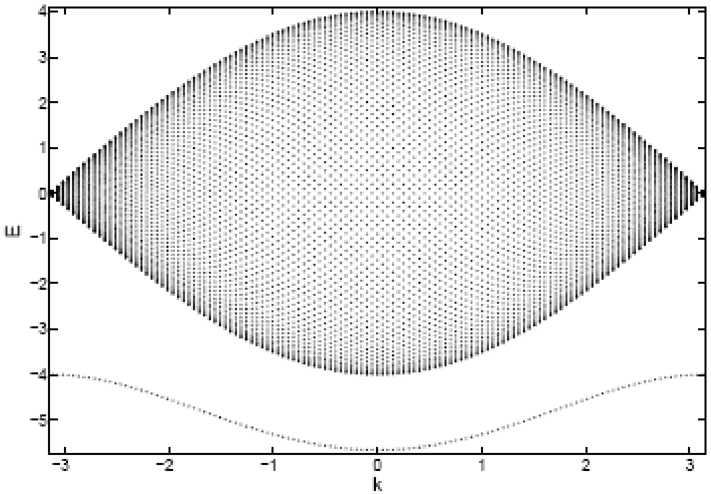
$$\hat{H} = -\sum_{j=1}^{f^D} \frac{\gamma_j}{2} b_j^\dagger b_j^\dagger b_j b_j - \sum_{j=1}^{f^D} \sum_p \epsilon_{jp} b_j^\dagger b_{j+p}.$$

Number of states method

- Main problem: Determination of matrix representation of the Hamiltonian operator and its total/partial spectrum. Block-diagonalize the Hamiltonian for a fixed number of quanta *N*.
- Number of states basis. Symbolic manipulation programs (Maple) allows to obtain the metrix of the system for a fixed number of quanta.

Spectrum

Example: Eigenvalues of the energy $E(k)$ as function of the momentum k for a QDNLS one–dimensional bosons system. $f = 125$ and $n = 2$.

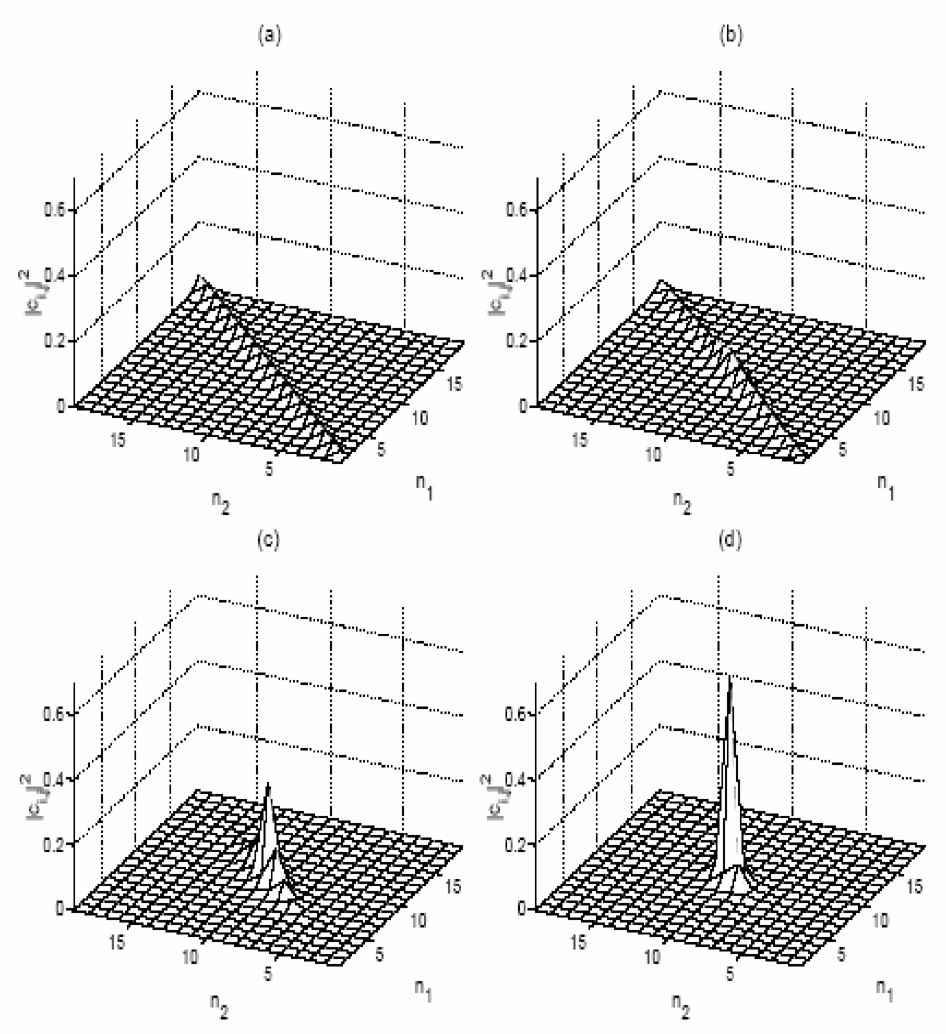


On a lattice of length f, the unnormalized coefficients of the first f terms are equal to unity and the rest are $O(\gamma^{-1})$. At $k = 0$ for simplicity, the ground state is

$$|\Psi\rangle = [20\ldots0] + [020\ldots0] + \cdots + [0\ldots02] + O(\gamma^{-1})$$

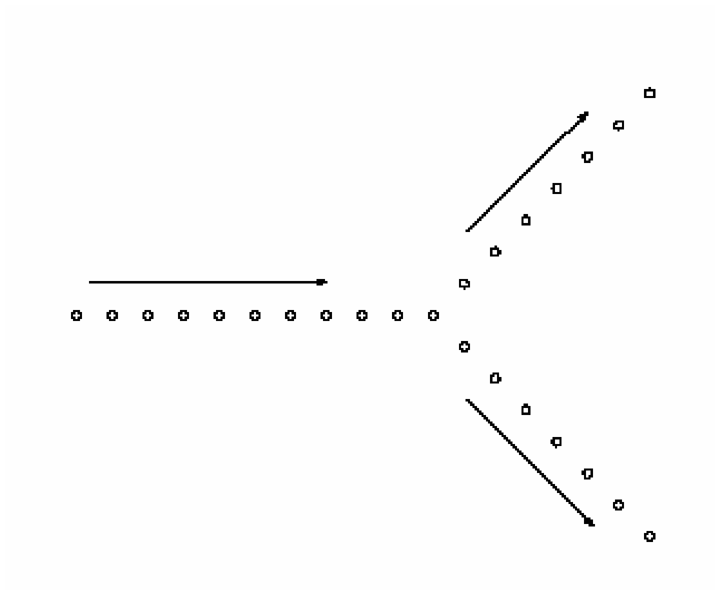
Non-translational invariant systems (I)

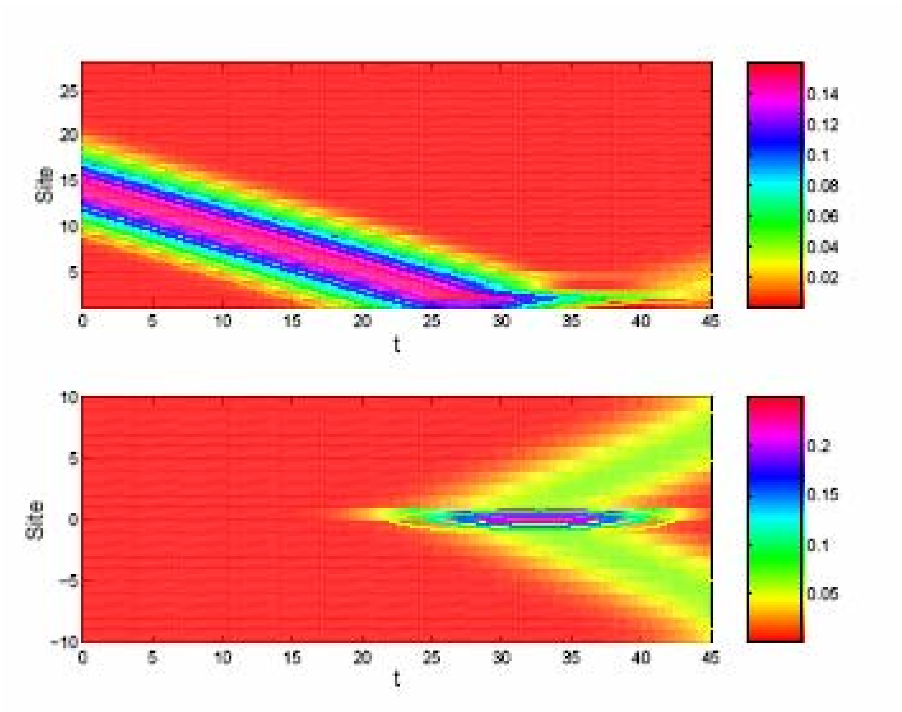
- Inhomogeneities in anharmonic parameter and/or hopping coefficients
- Computational effort increases. Momentum of the system not defined (expected value of k)
- Spatial localization



Solitons wave packets

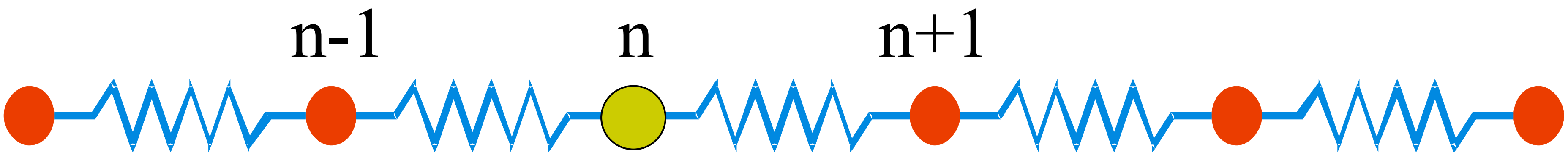
- Boson lattices





Research in SDSU

- One Dimensional DNLS system with a single impurity. (Coupled nonlinear wave guides).



$$i\dot{\psi}_n + \gamma|\psi_n|^2\psi_n + C(\psi_{n+1} + \psi_{n-1} - 2\psi_n) + \alpha_n\psi_n = 0$$

Research Program

- Linear modes. OK
- Stationary states. Bifurcations. OK
- Nucleation Problem. In progress
- Iteration of moving localized states with the defect. Pending
  - Reflection
  - Transmission
  - Trapping
- Two Dimensional system. Future
- Quantum model. In progress

Thank you!