Discrete breathers in silicate layers

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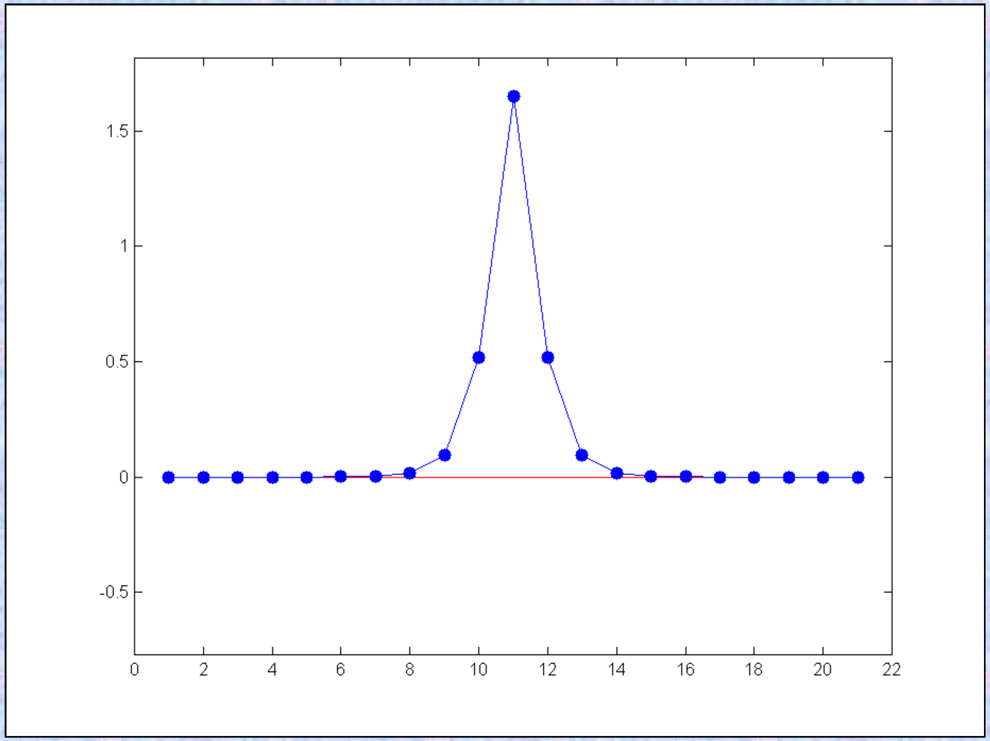
NEMI 2012: 1st International Workshop on
Nonlinear Effects in Materials under Irradiation
12-17 February, 2012. Pretoria, South Africa

Breathers, where they appear?

- In systems of coupled nonlinear oscillators.

What are they?

- Vibrations
- Localized
- Exact



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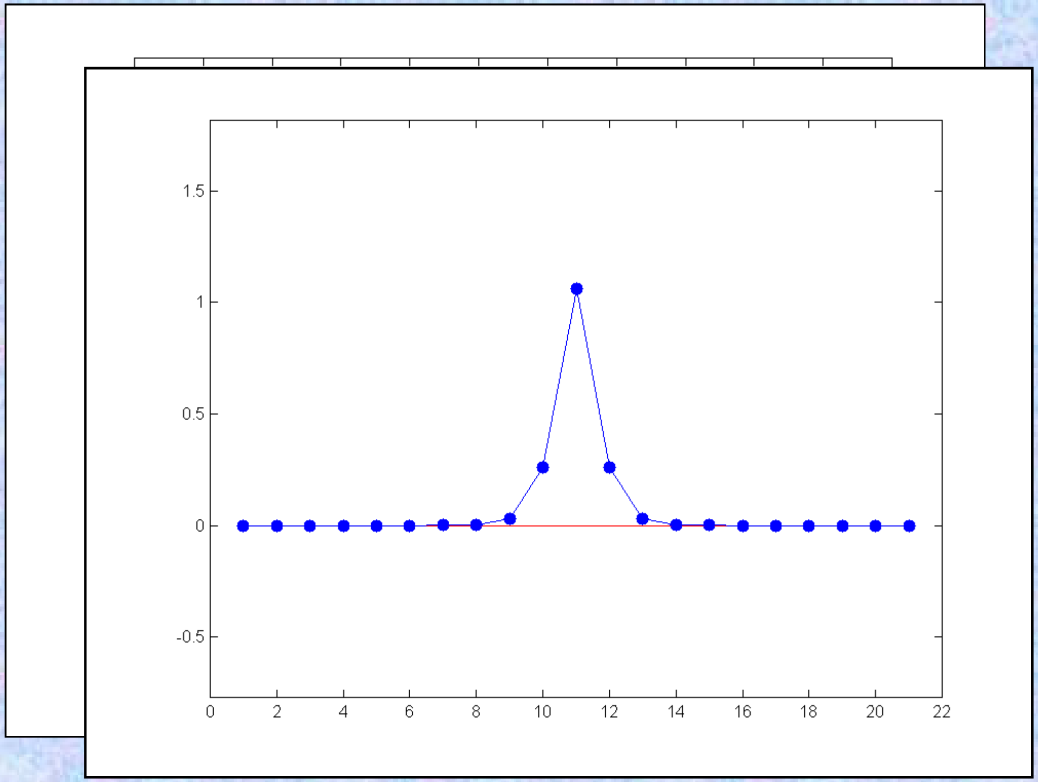

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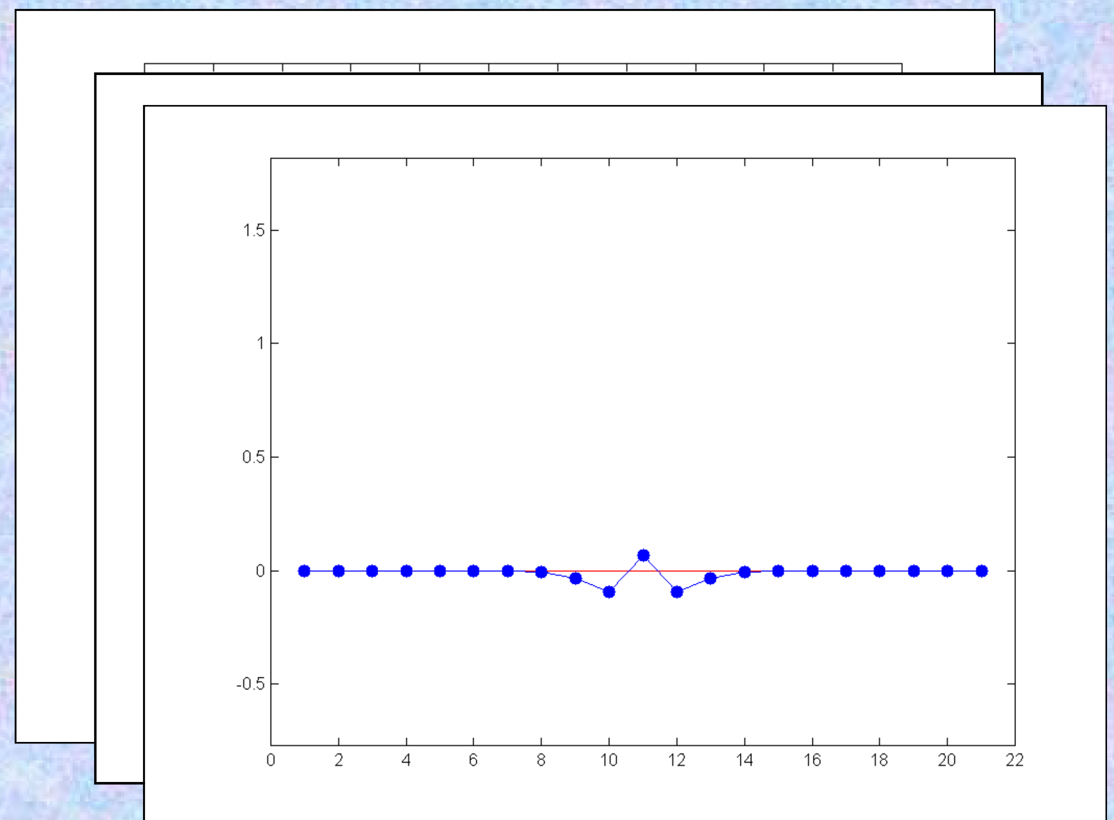

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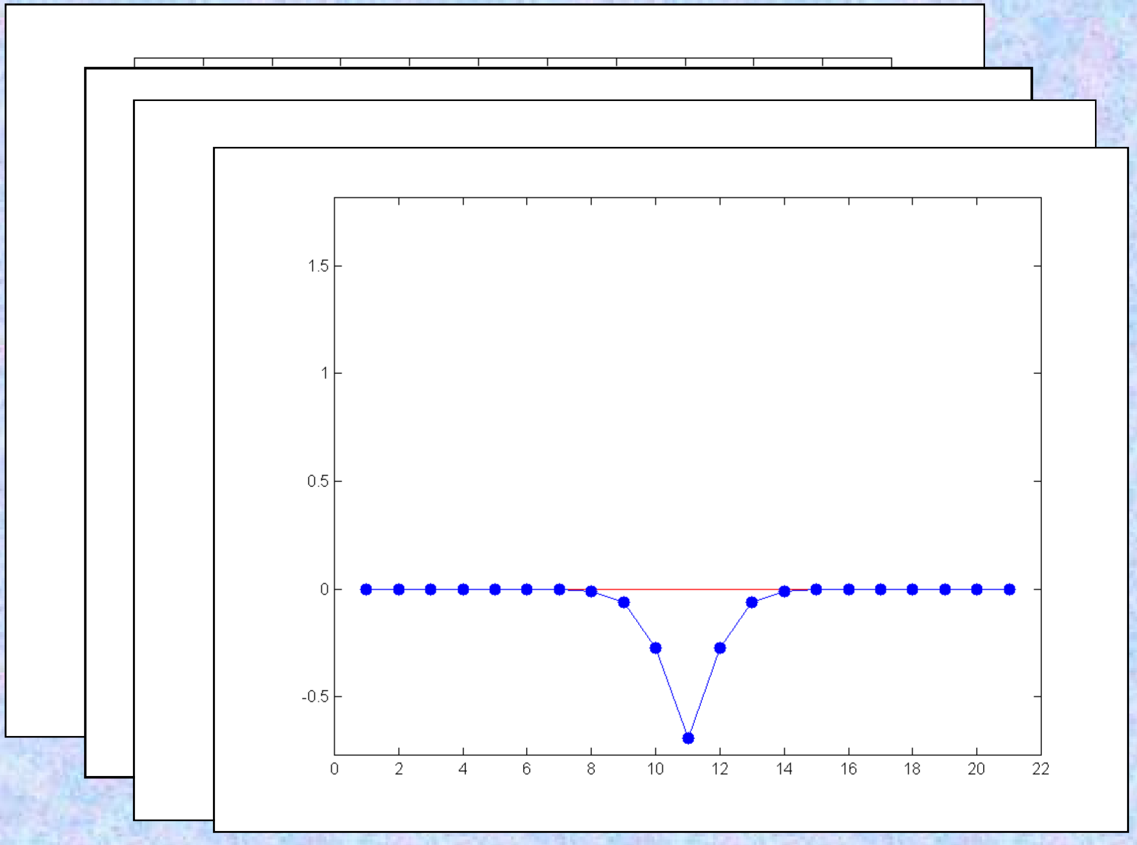

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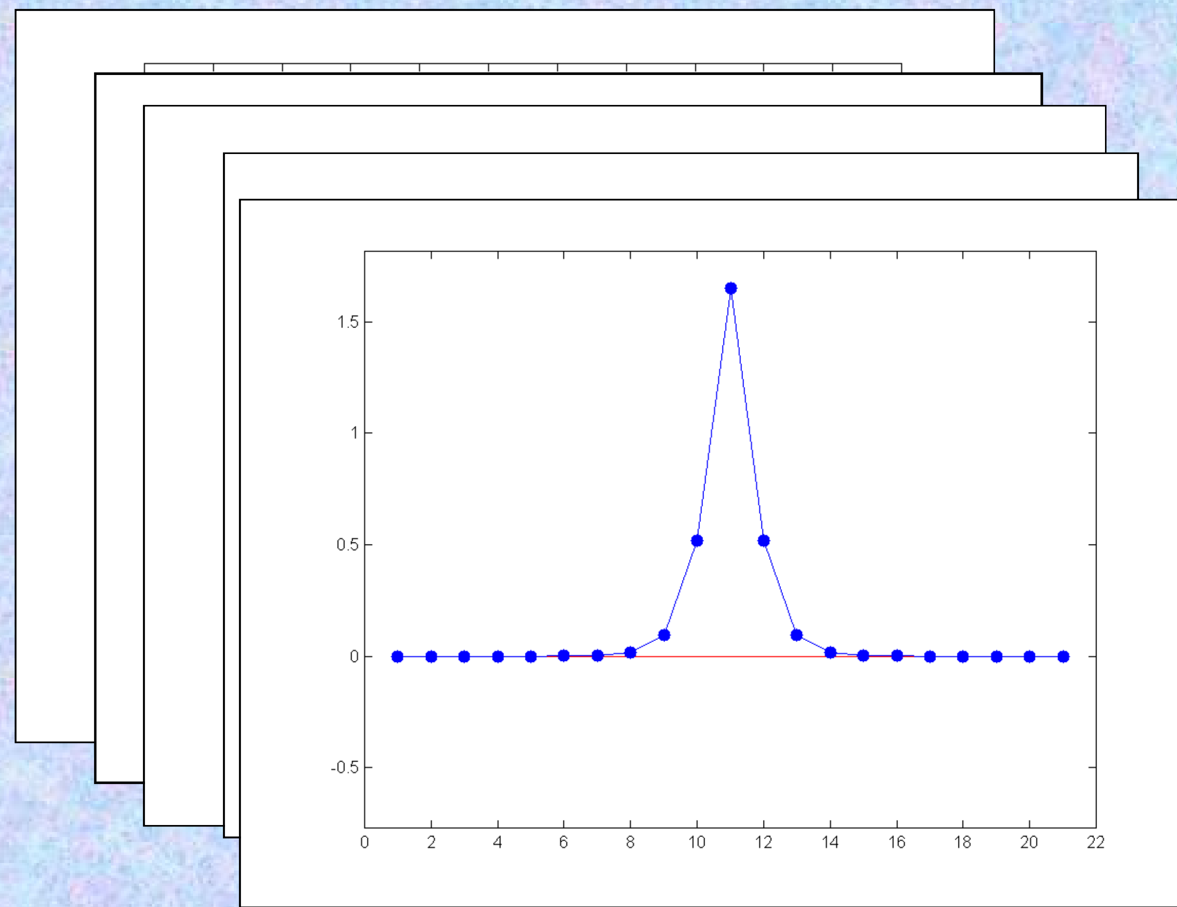


Theoreticians in breathers

An experimentalist knows the question but not the anwer.

A theoretician knows the answer but doesn’t know the question.

If breathers are the answer, what is the question? GP Tsironis, Chaos 13, 657 (2003)

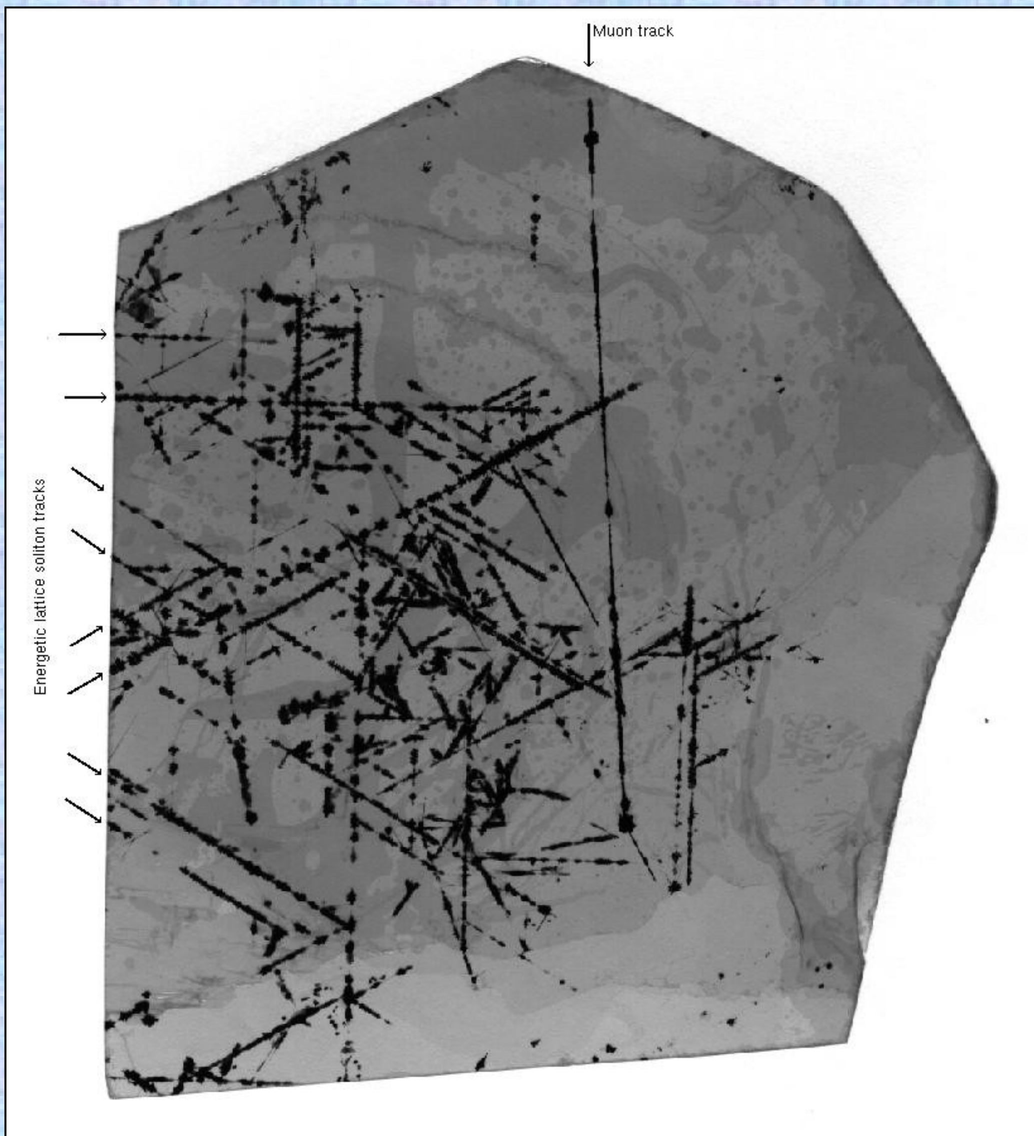
Two questions on mica

- Dark tracks: Russell, Eilbeck

- Low Temperature Reconstructive Transformations (LTRT).

Sevilla Materials Science Group:Alba, Becerro, Naranjo, Trillo (MSG)

Dark traks in mica moscovite: Quodons (Russell)



Black tracks: Fe_3O_4

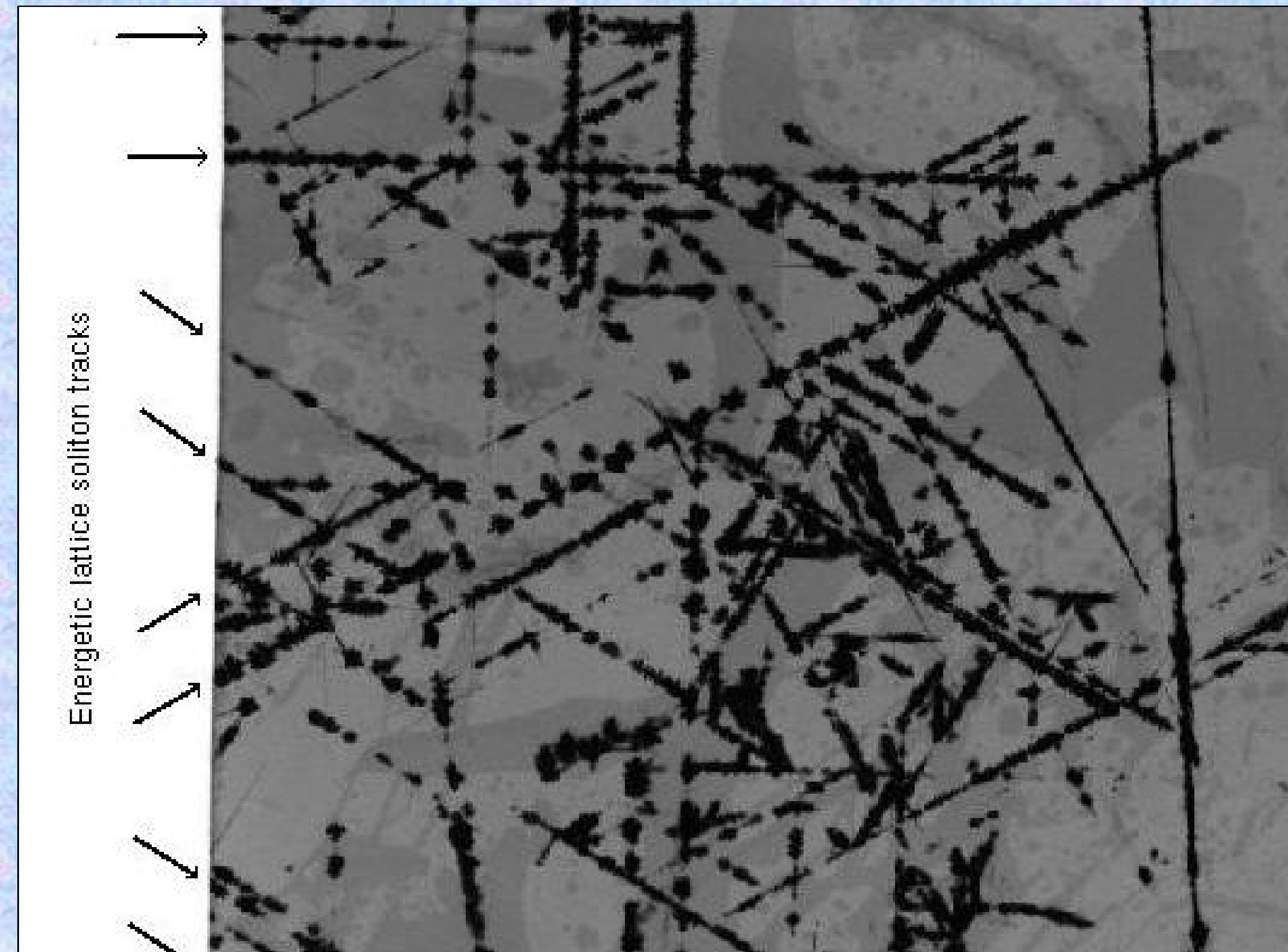
Cause:

- 0.1% Particles:
  - muons: produced by interaction with neutrinos
  - 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



Reconstructive transformation of muscovite

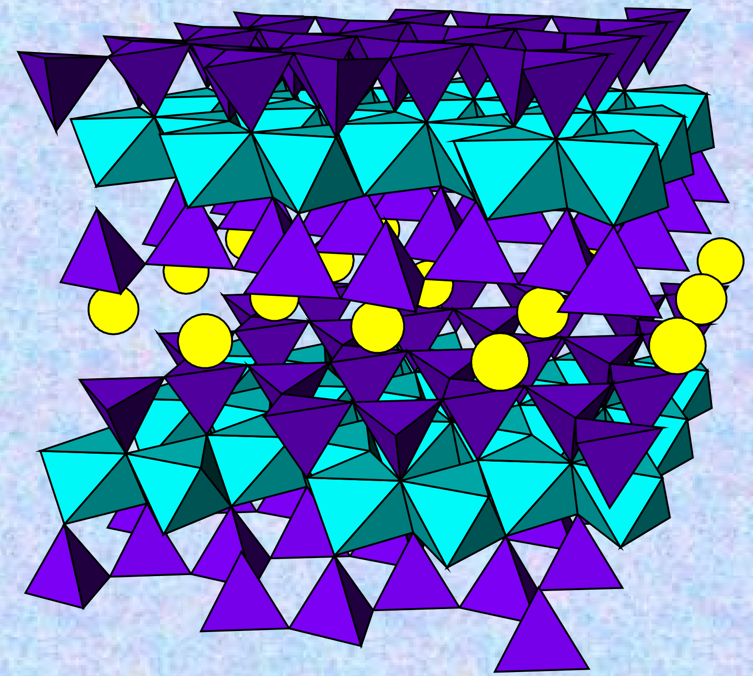
Muscovite

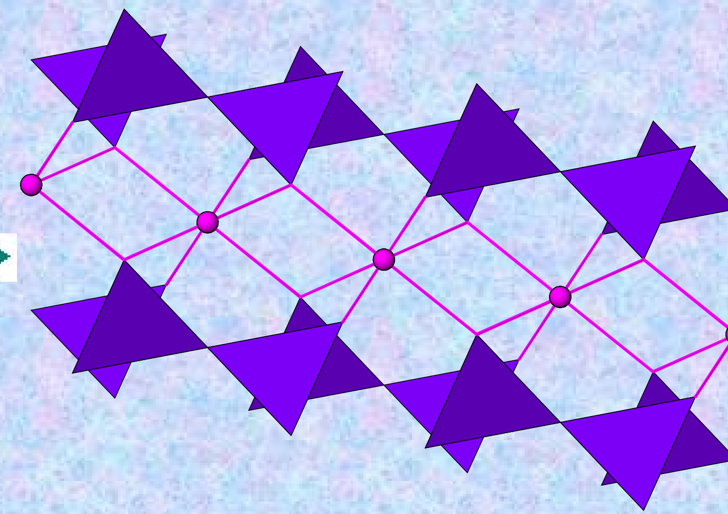
$K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4$

Disilicate of Lutetium

$Lu_2Si_2O_7$

Lu^{3+}



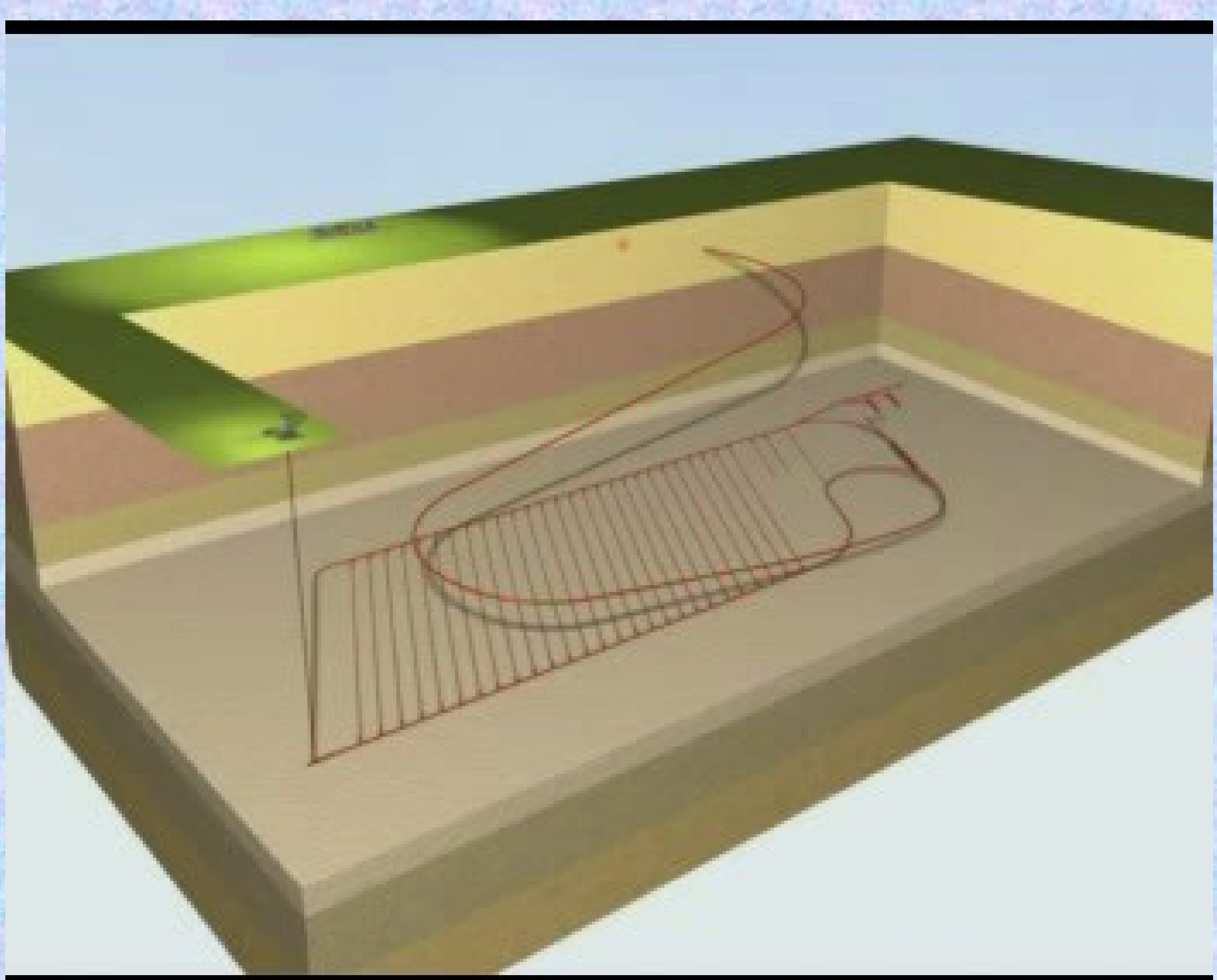


300° C, 3 days

About 36% of muscovite is transformed

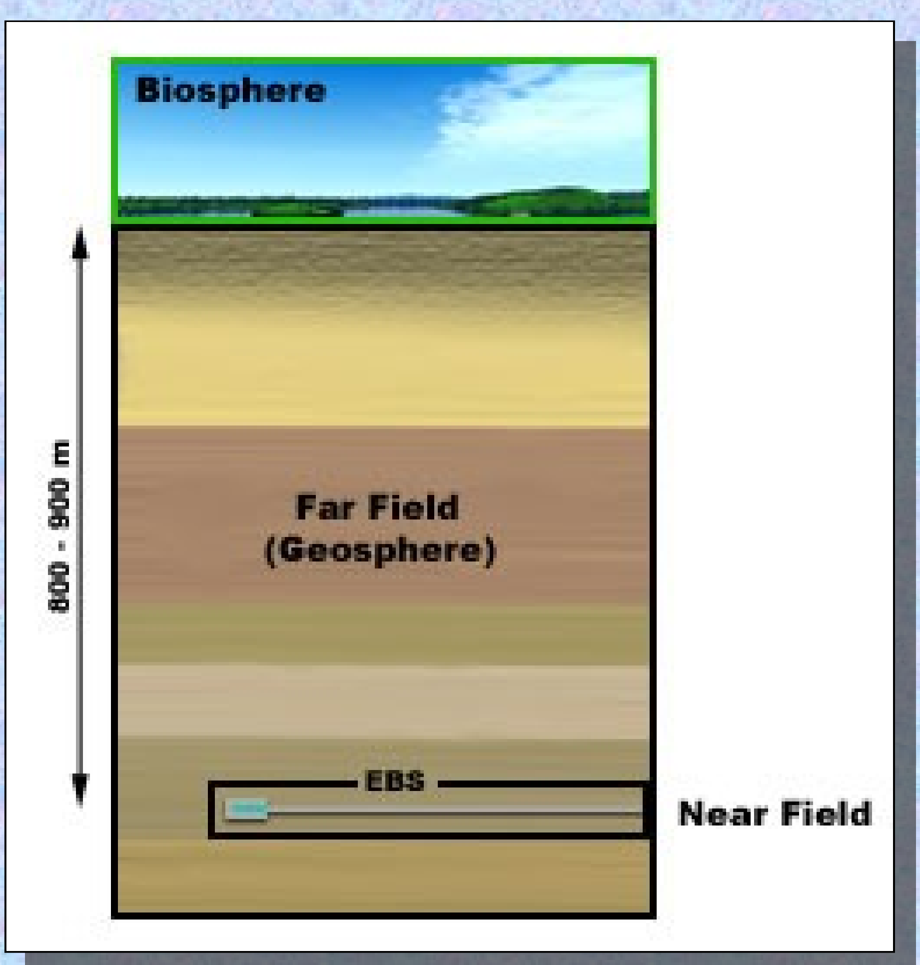
K^+

Why LTRT can be interesting?



Deeep geological depositories for nuclear waste.

Reconstructive transformations trap the radionuclides



EBS:
Engineered barrier system

- In laboratory lutetium substitutes to heavy radionuclides

Reconstructive transformation of muscovite

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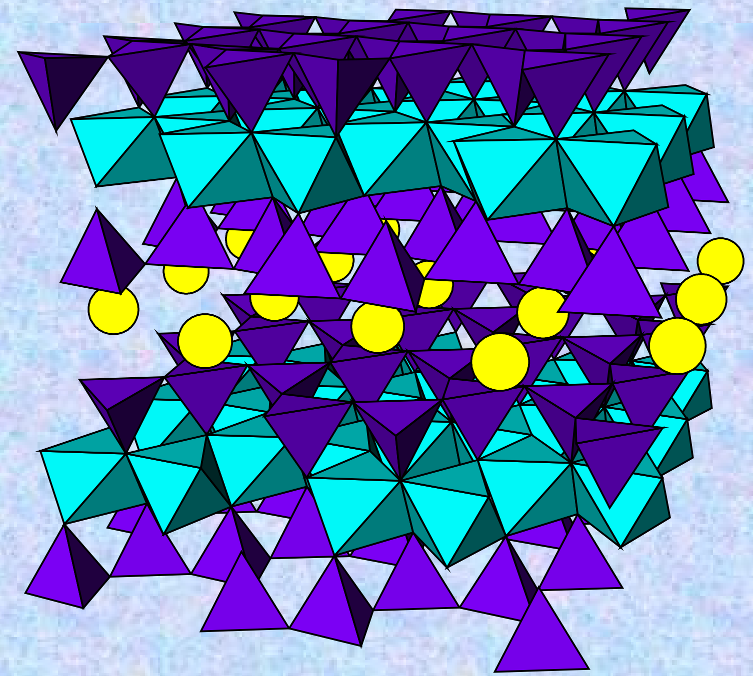
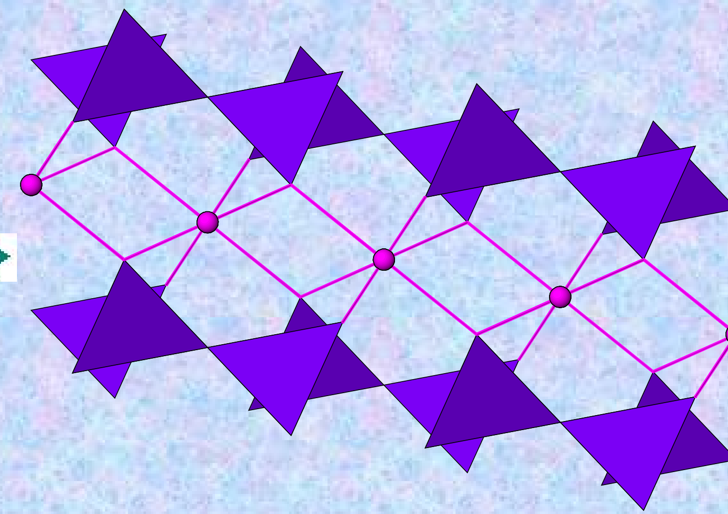


Lu^{3+}



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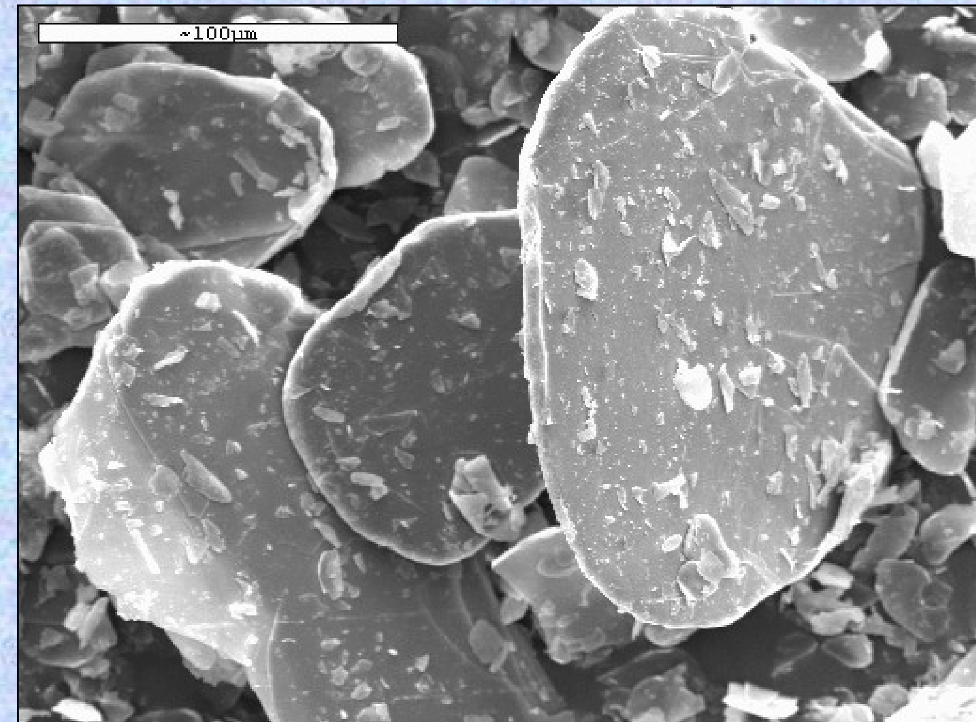
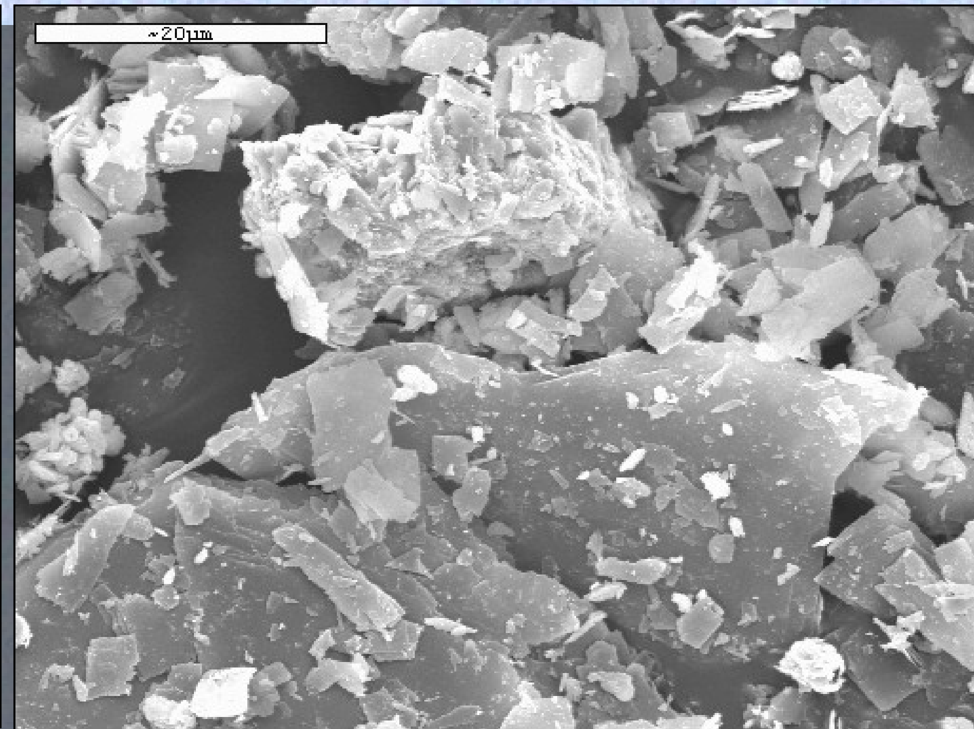
Scanning electron microscopy with energy dispersive X-ray (EDX) analysis

Untreated muscovite



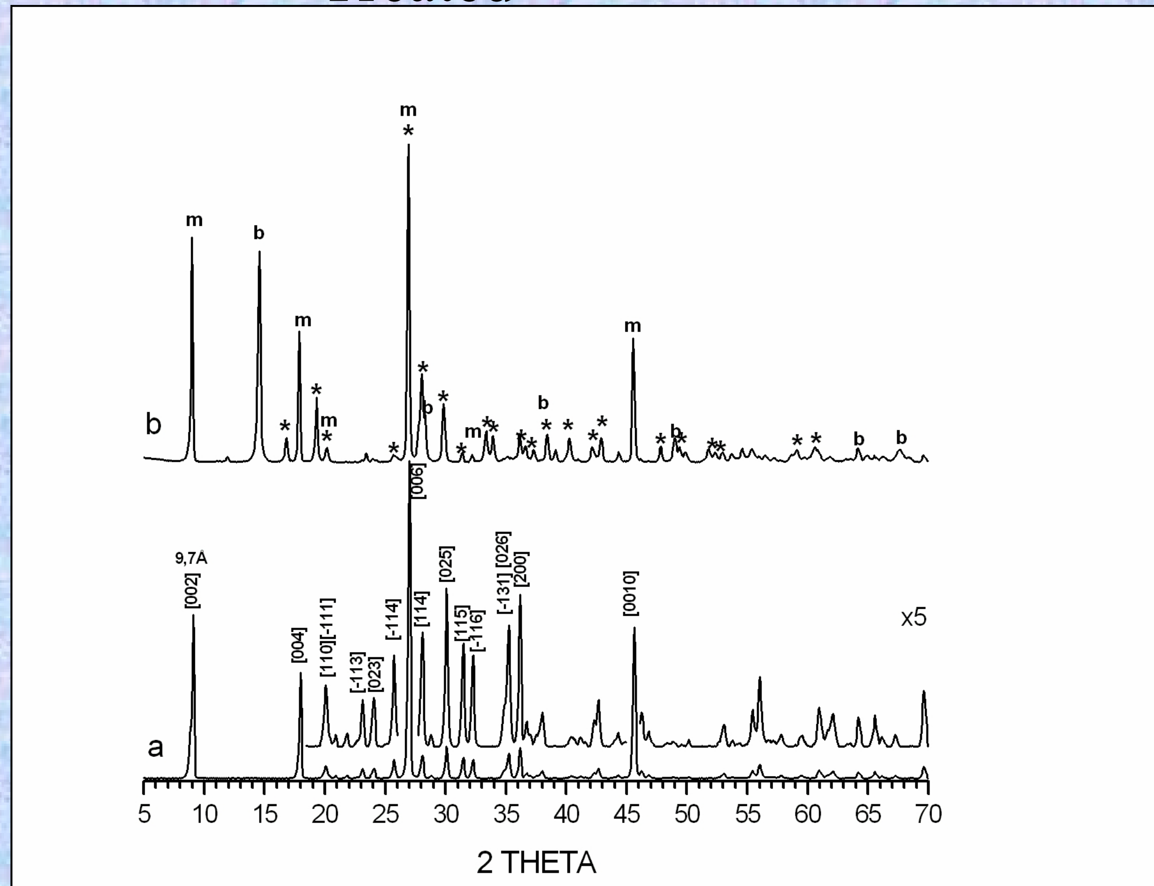
Treated muscovite



Three different types of particles: muscovite, $Lu_2Si_2O_7$ and bohemite

X-Ray powder diffraction

Treated



Untreated

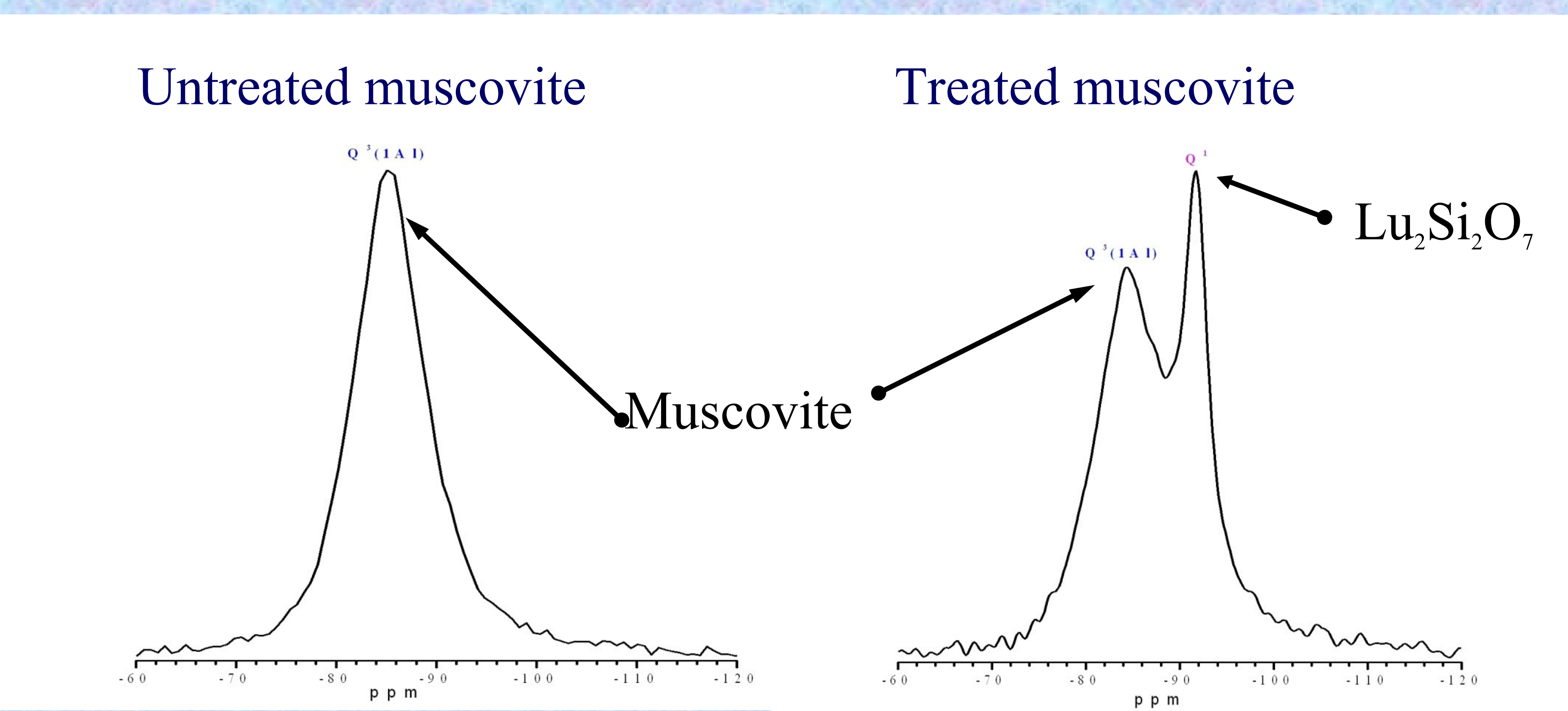
m=muscovite, b=bohemite, *$Lu_2Si_2O_7$

Consistent with:

- Untreated:
  - Perfect ordering
- Treated
  - Two new phases:
    - $Lu_2Si_2O_7$
    - Bohemite
- Uncomplete transformation

[Alba and Chain, Clays Clay Min. **53**. 39 (2005)]

Nuclear Magnetic Resonance
Magic Angle Spinning for silicon



36.6% of Si has changed to the $Lu_2Si_2O_7$ phase

Reconstructive transformations in layered silicates

- In the laboratory the long times of ageing are simulated with higher temperatures
- Activation energies range typically about 200-400 kJ/mol
- They involve the breaking of the Si-O bond, stronger than that between any other element and oxygen and are observed in silicates only above 1000 C
- A condition for the transformation to take place is that sufficient atoms have enough energy to achieve a transition *activated state*.
- **Low temperature reconstructive transformations (LTRT) in layered silicates was achieved by MSG at temperatures 500 C lower than the lowest temperature reported before** [Becerro et al, J. Mater. Chem **13**, (2003)]
- LTRT take place in the presence of the cation layer
- Possible application in engineered barriers for nuclear waste in deep geological repositories.

Some facts about LTRT

LTRT can be described by:
- Breaking of the Arrhenius law
- An increase of the reaction speed
- A diminution of the activation energy

No explanation had been provided for LTRT

Could breathers be?

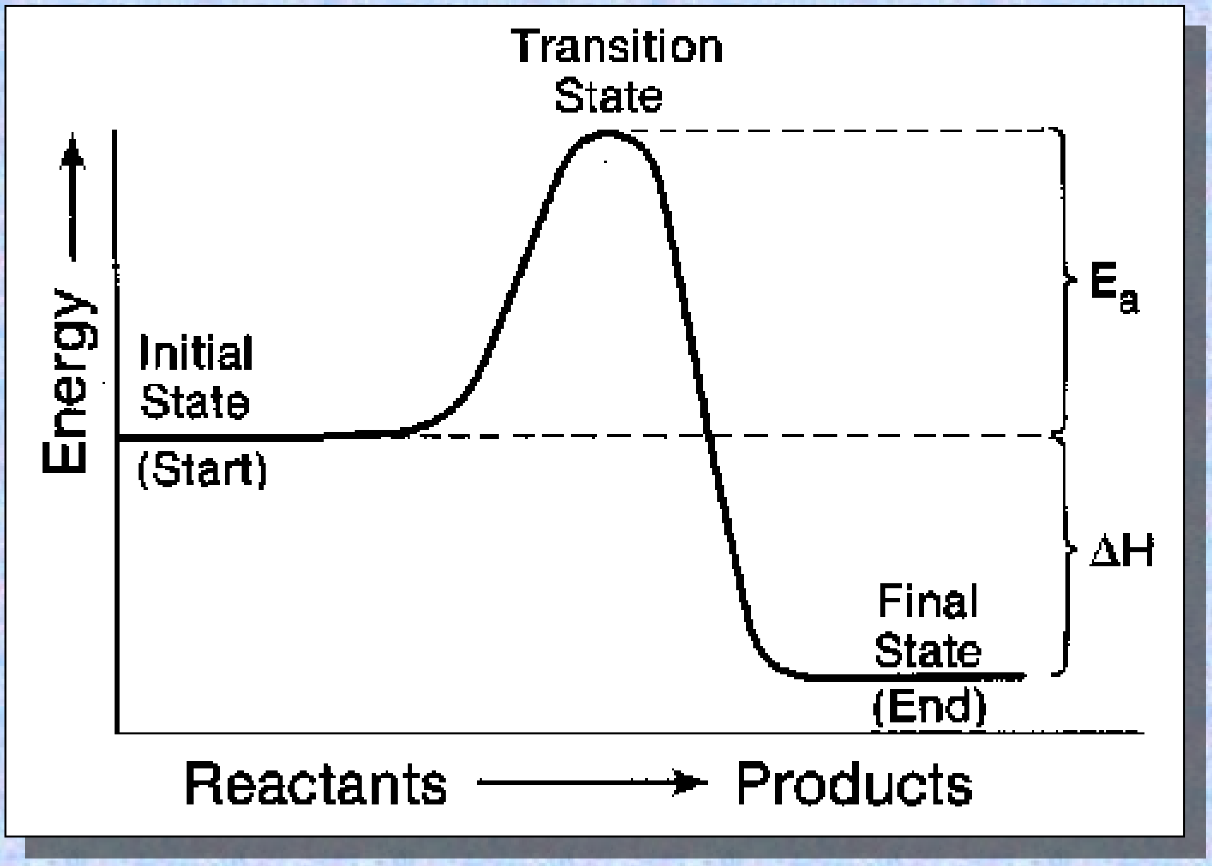
Mackay and Aubry [Nonlinearity, 7, 1623 (1994)] suggested the breaking of Arrhenius law as a consequence of discrete breathers.

Reaction speed and statistics

Arrhenius law: $\kappa = A \exp(-E_a/RT)$

Transition state theory

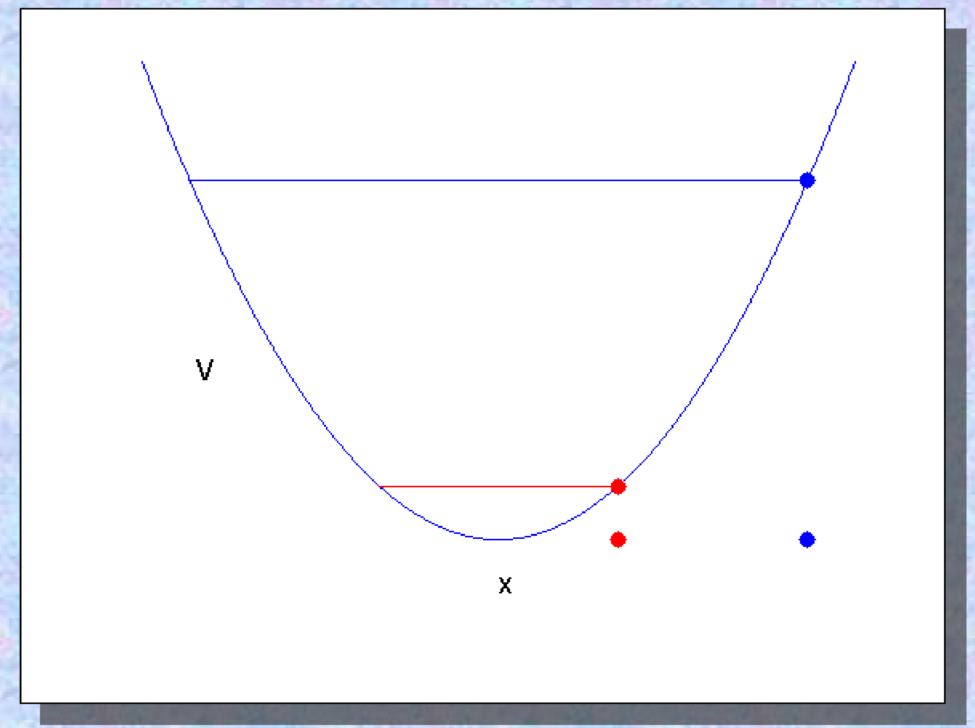
$E_{\mathbf{a}}$~100-200 KJ/mol



Outline of what follows:

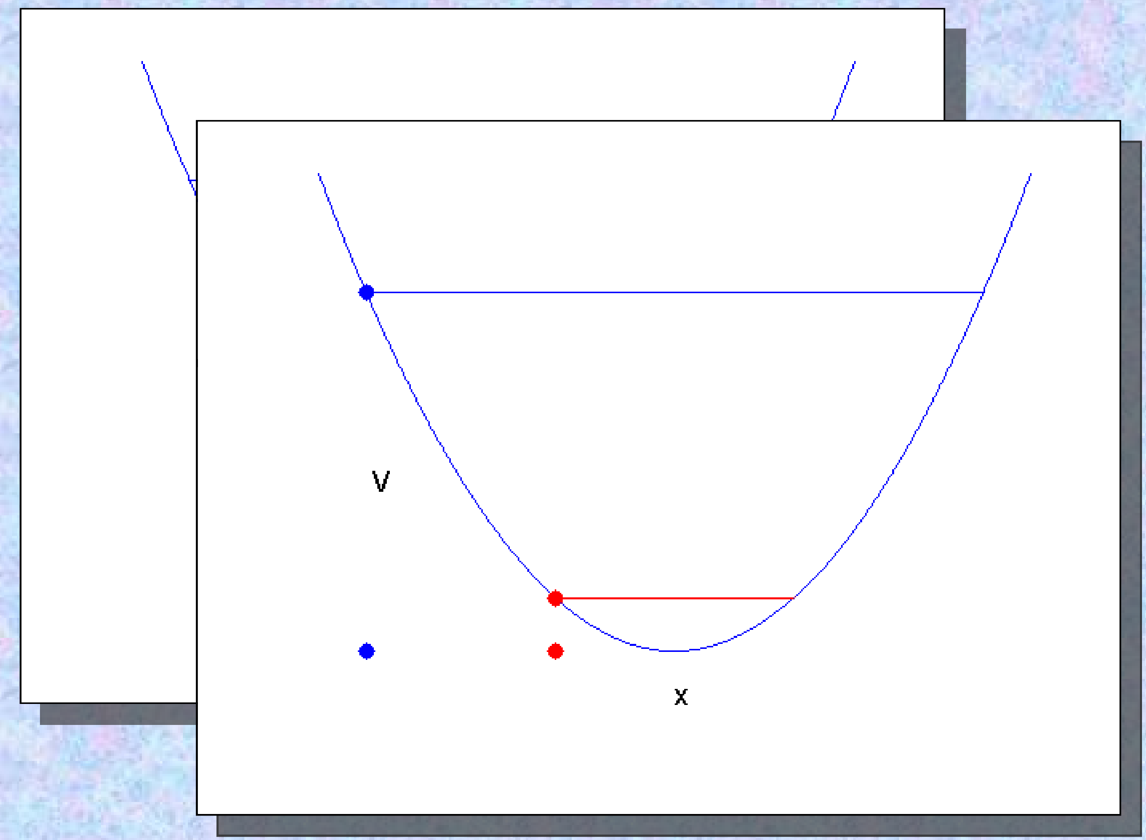
Breather review with application to mica
Breathers in mica.
Breather statistics with modification
Effect of breathers on the reaction rate
Effect of breathers on the reaction rate theory

Linear oscillator: $F=-k\,x$, $V=\frac{1}{2}\,k\,x^2$



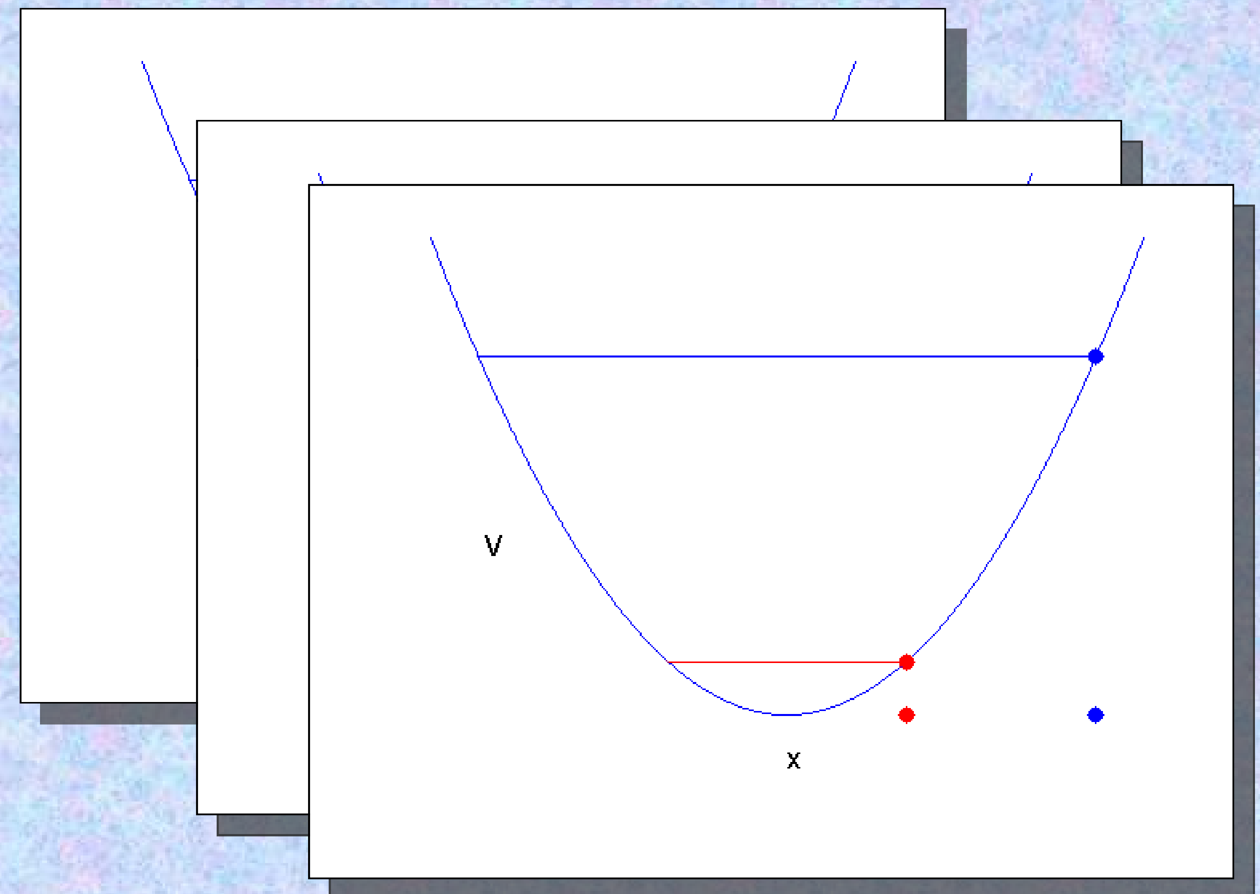
$$x = A\cos(\omega_0\,t + \varphi_0)\ ,$$

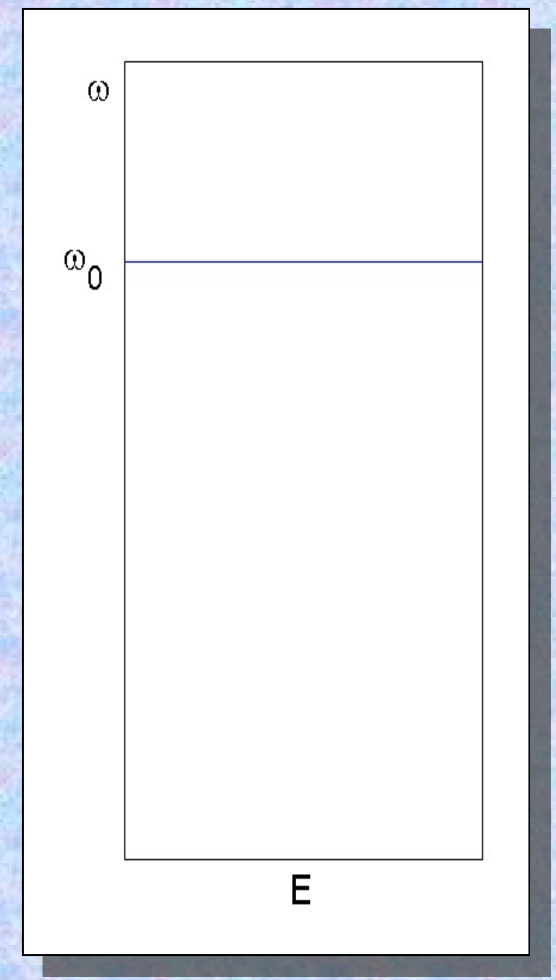
Linear oscillator: $F=-k\,x$, $V=\frac{1}{2}k\,x^2$



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

Linear oscillator: F=-k x, V= ½ k x^2

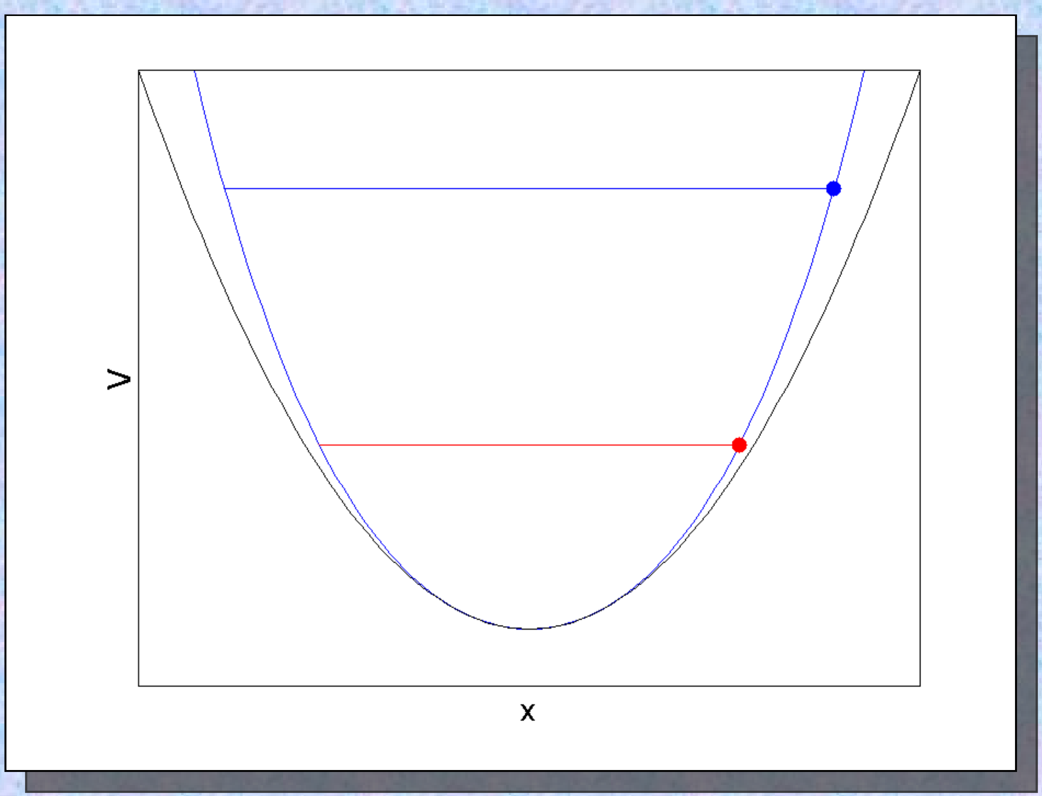




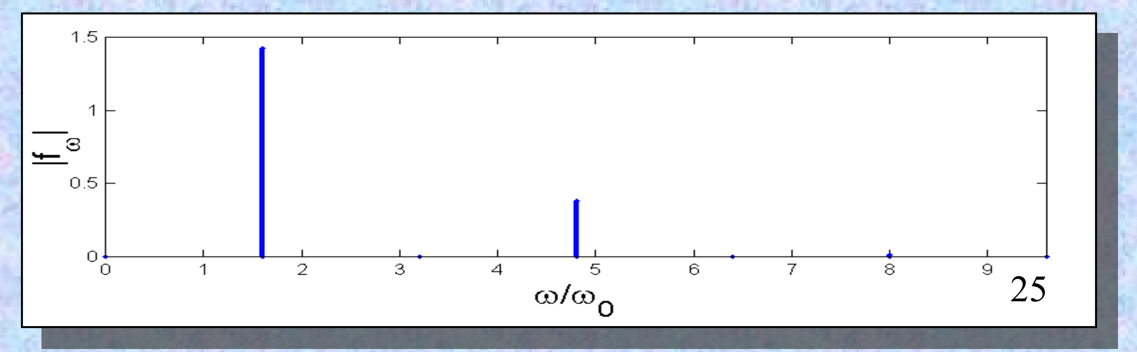
The blue and red balls come back at the same time

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

Hard nonlinear oscillator



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



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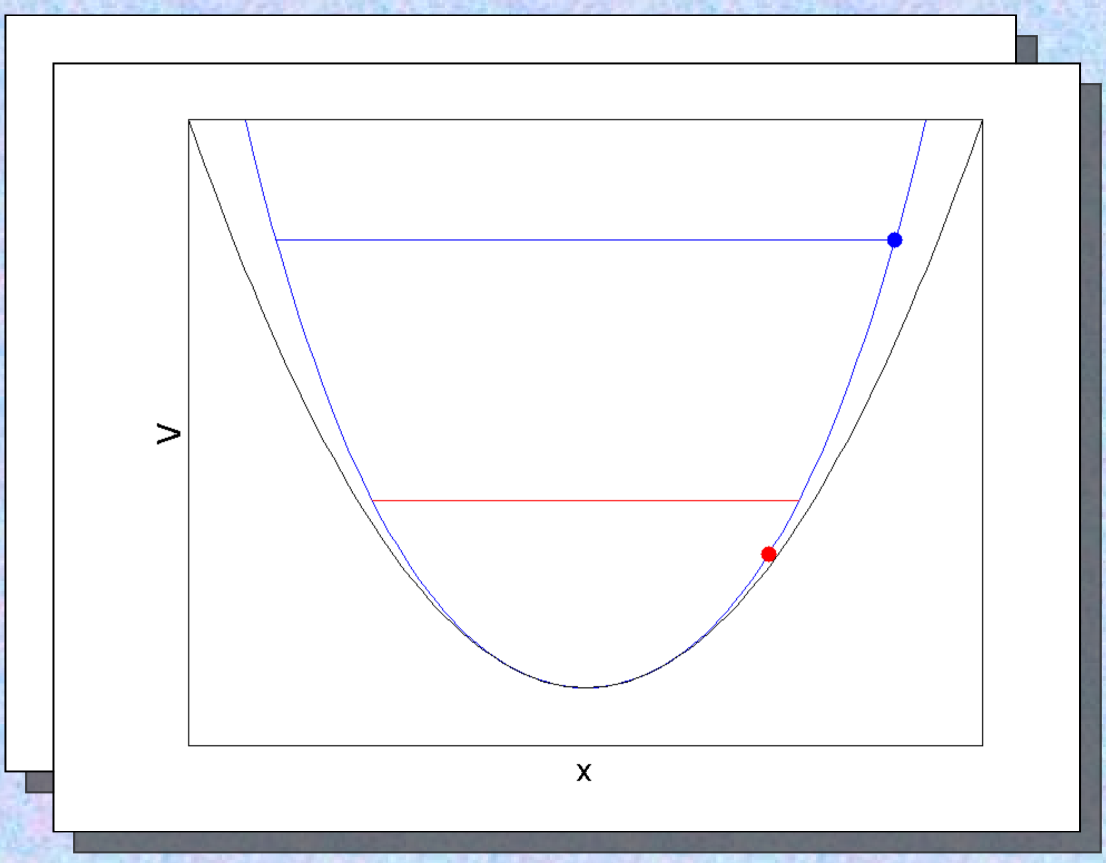
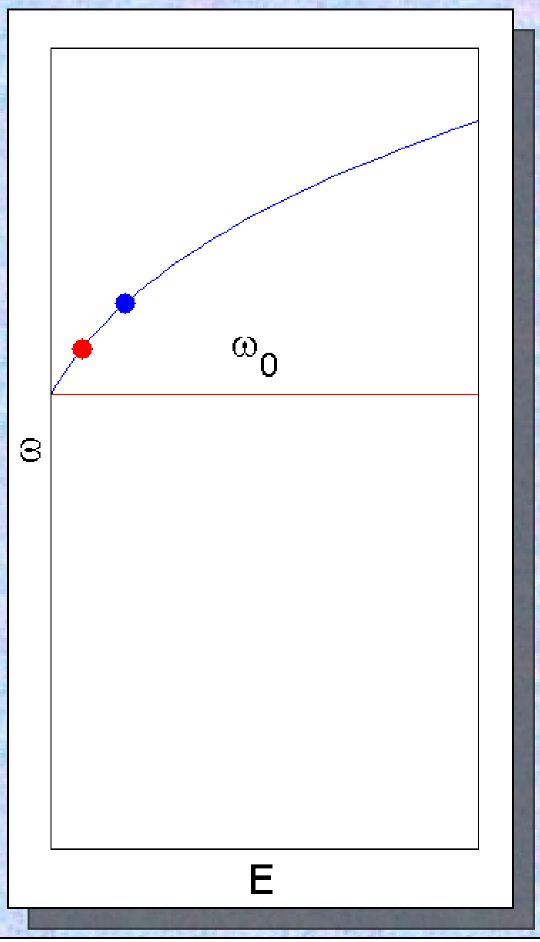
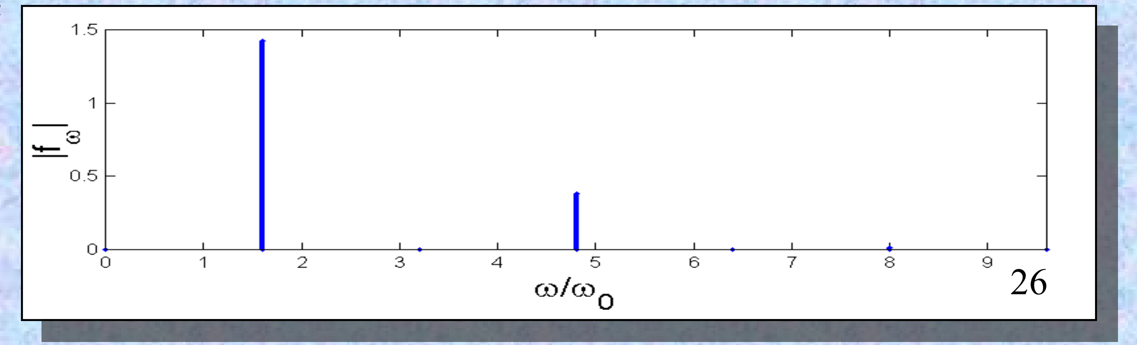


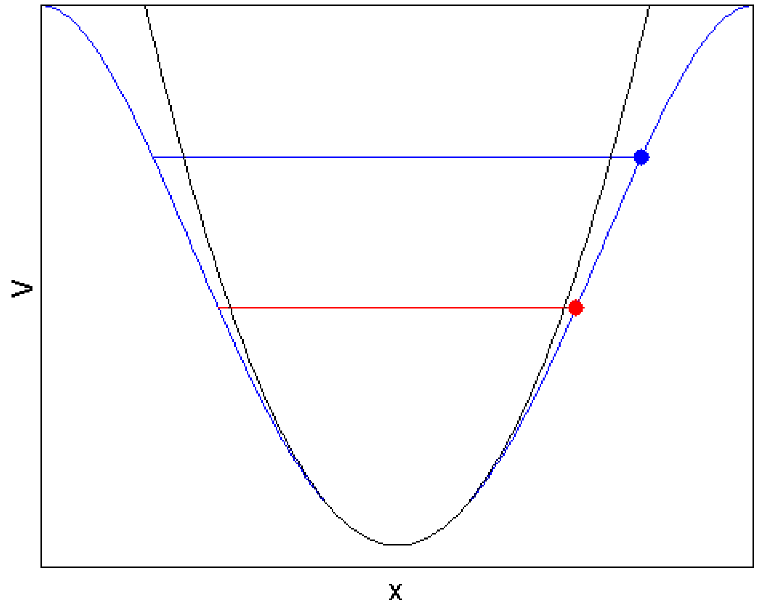


The blue ball has done a complete oscillation but the red one has not

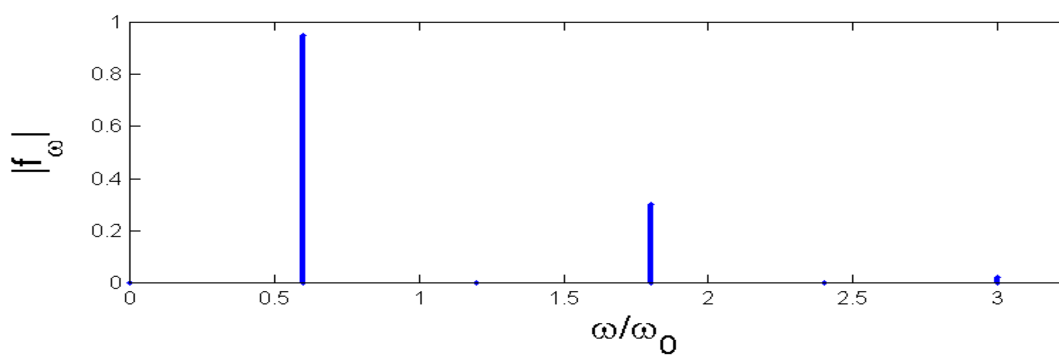
$$V=\frac{1}{2}(\omega_0)^2x^2+\frac{1}{4}x^4$$



Soft nonlinear oscillator



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



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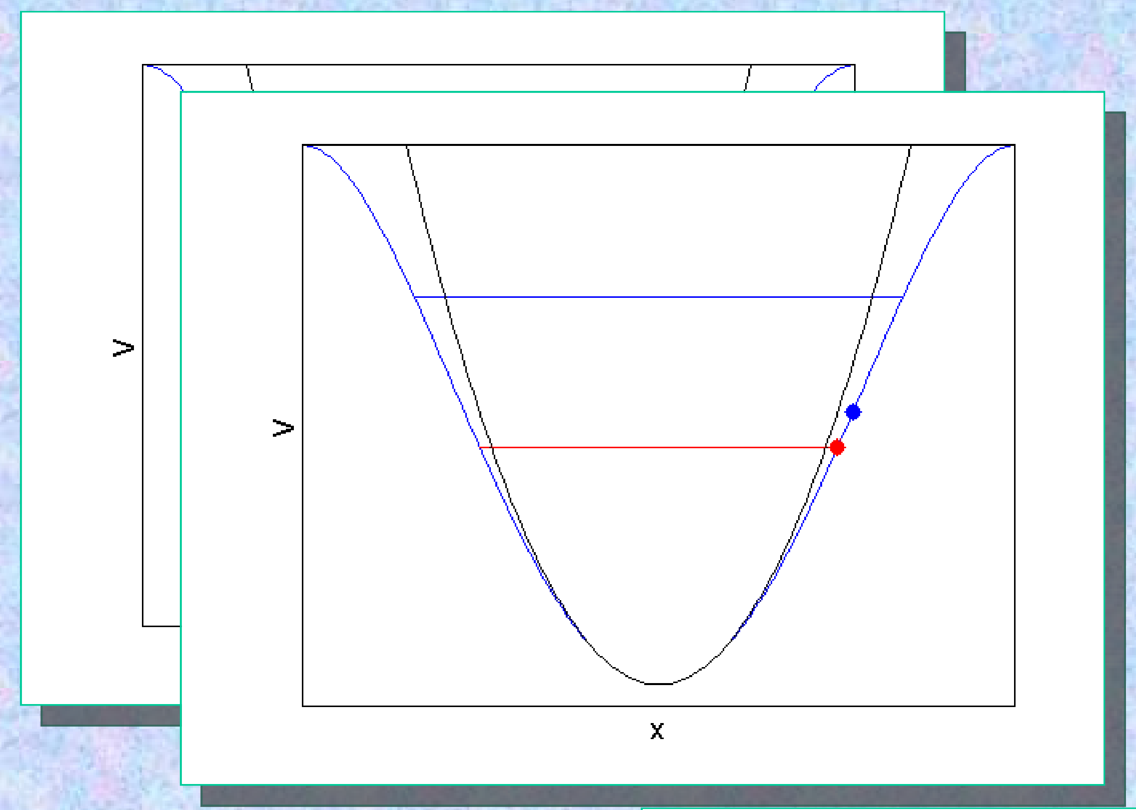

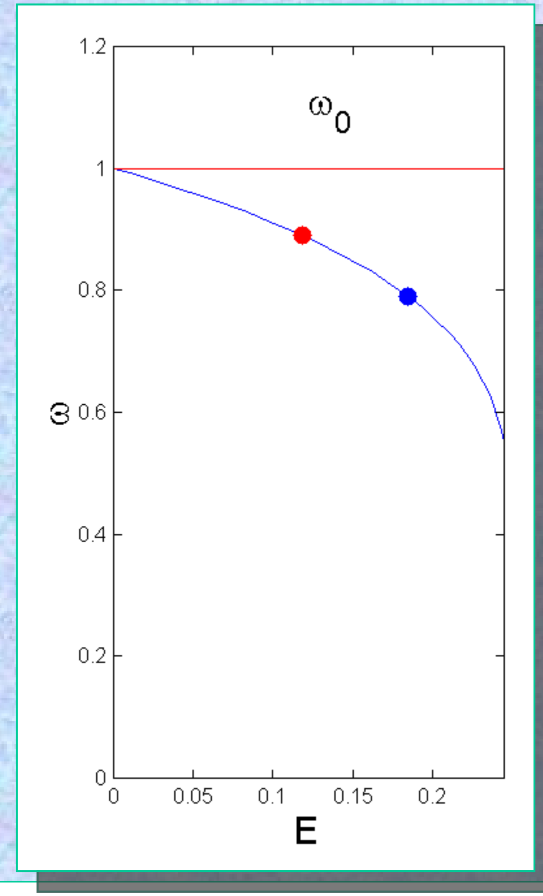

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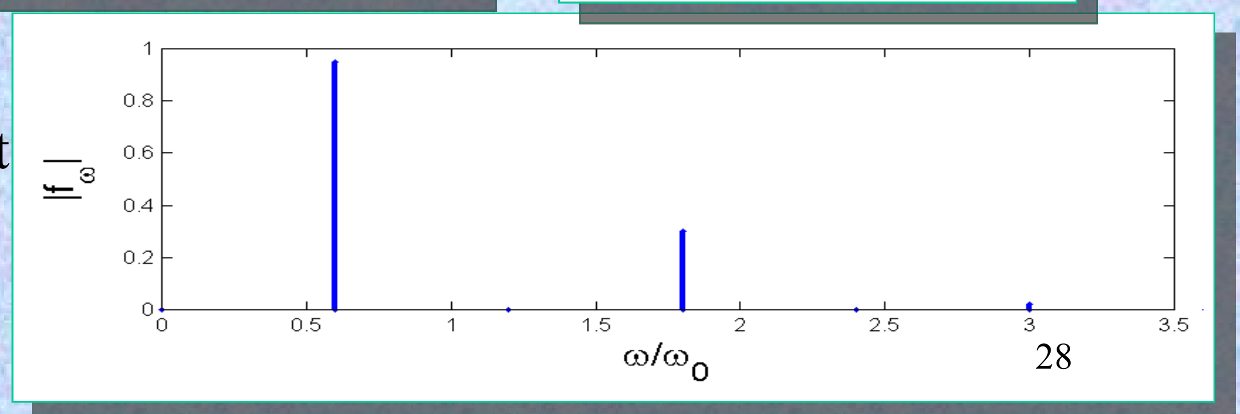
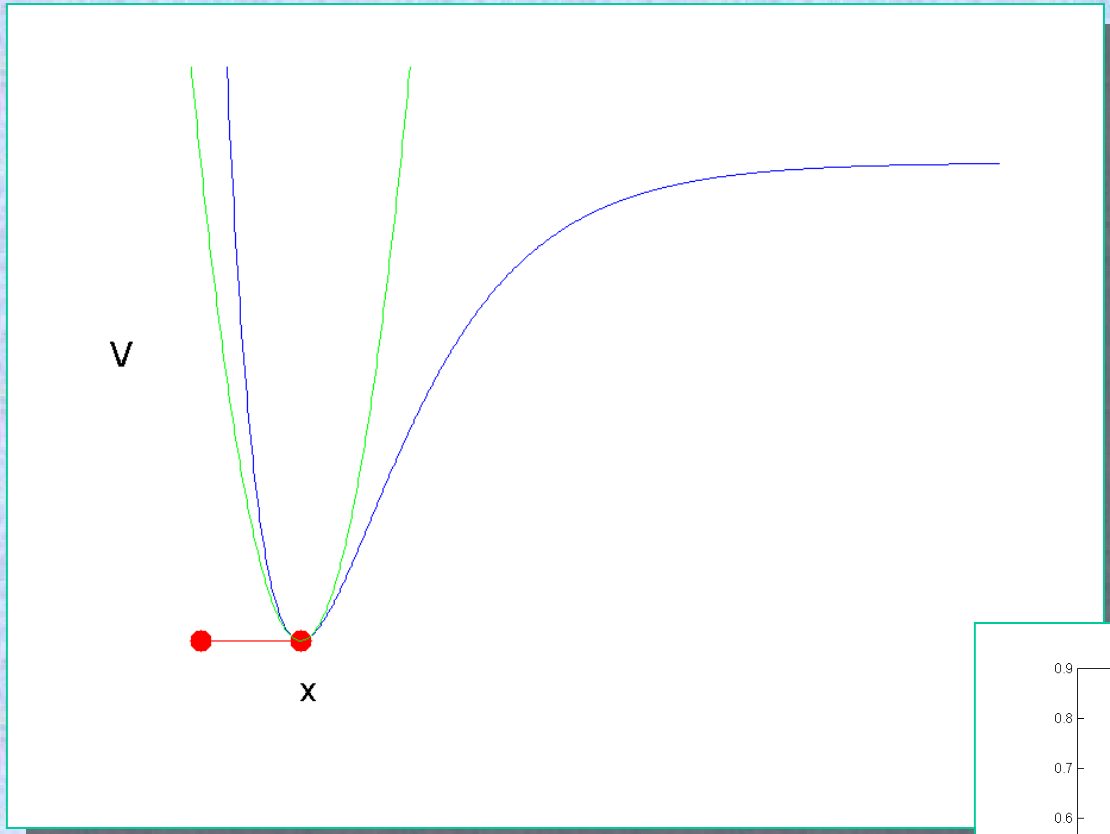
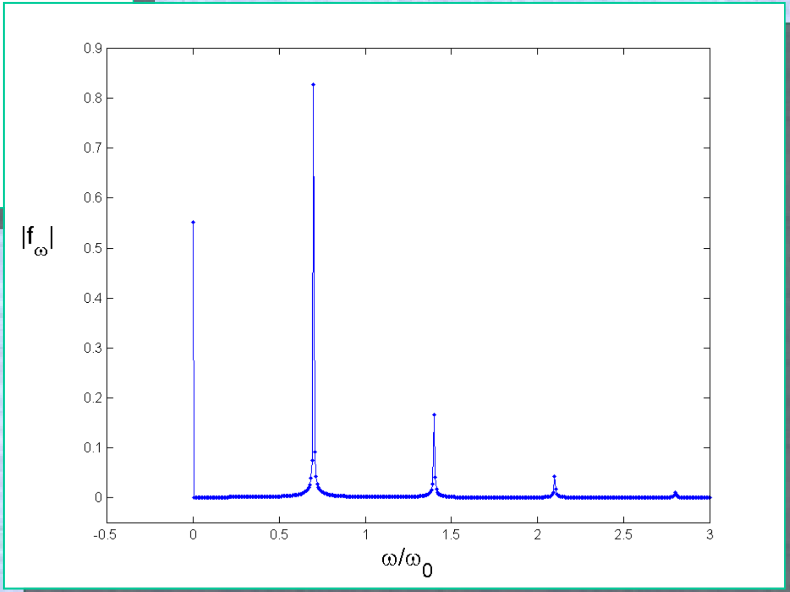


Asymmetric soft nonlinear oscillator





Morse potential

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

The nonlinear oscillator

Potential: $V(x) \sim 1/2\ m\ (\omega_0)^2\ x^2 + a\ x^3 + b\ x^4 + \cdots$

Fuerza: $F = -V'(x) = -m\ (\omega_0)^2\ x + 3a\ x^2 + 4\ b\ x^3\ \neq -k\ x$

Solution: $x = g(\omega_b\ t + \varphi_0)$; g: 2π periodic

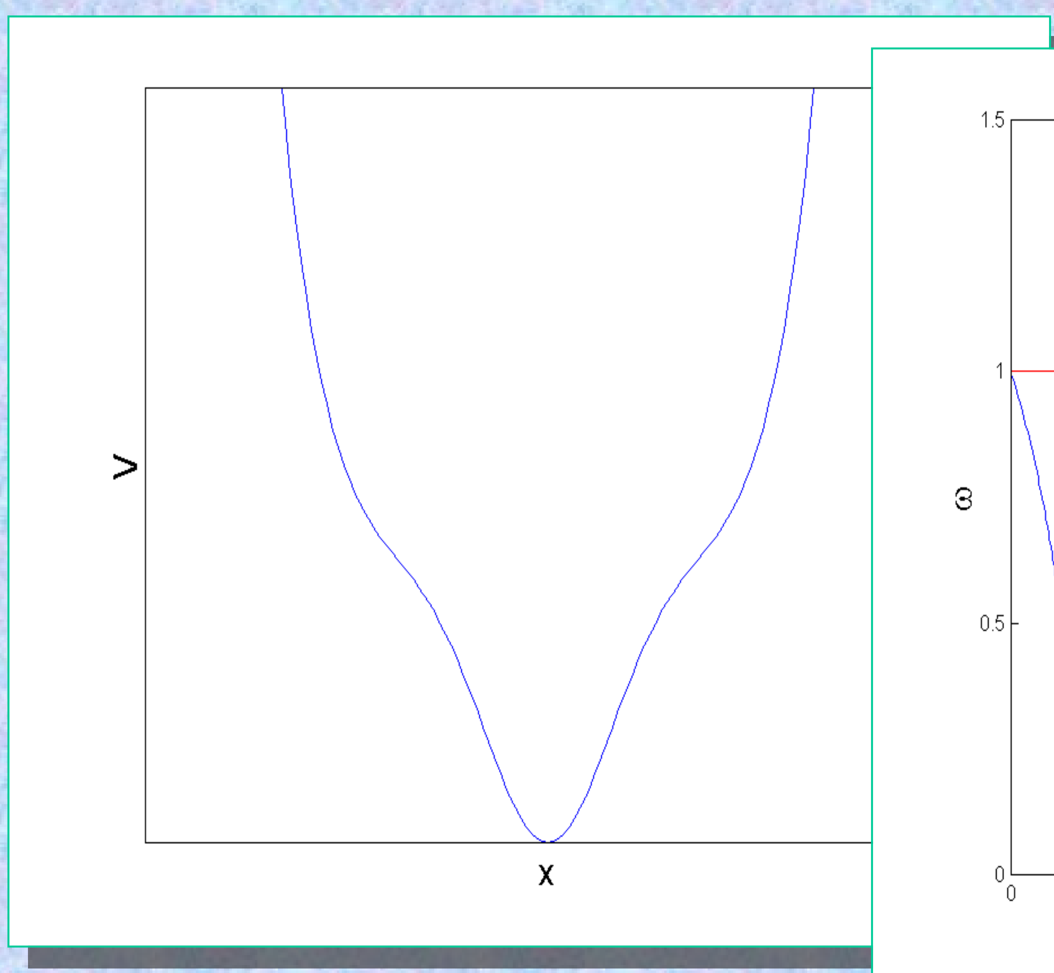
$x = a_0 + a_1 \cos(\omega_b\ t + \varphi_1) + a_2 \cos(2\omega_b\ t + \varphi_2) + \cdots$

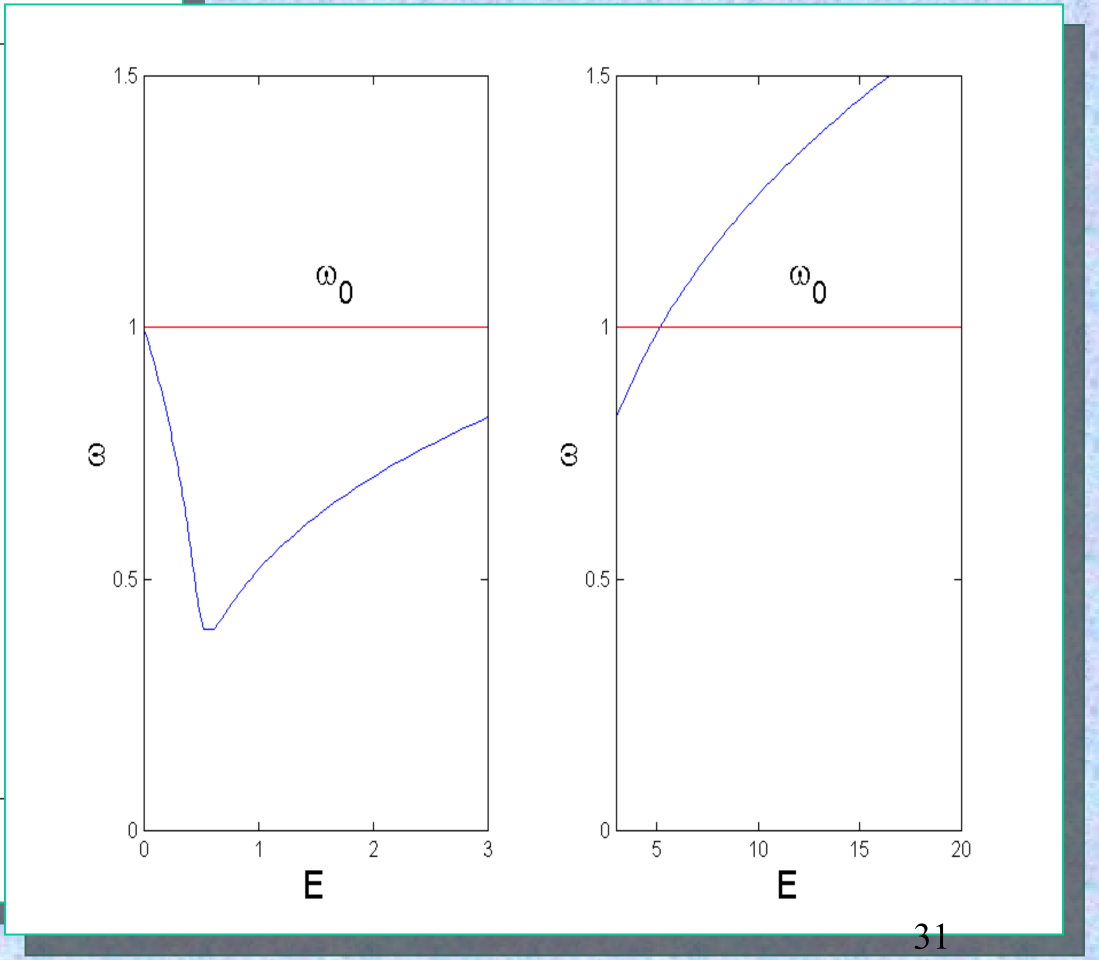
Breather frequency ω_b depends on E: $\omega_b = \omega_b(E)$

- Hard: $\omega_b'(E) > 0$, $\omega_b > \omega_0$
- Soft: $\omega_b'(E) < 0$, $\omega_b < \omega_0$

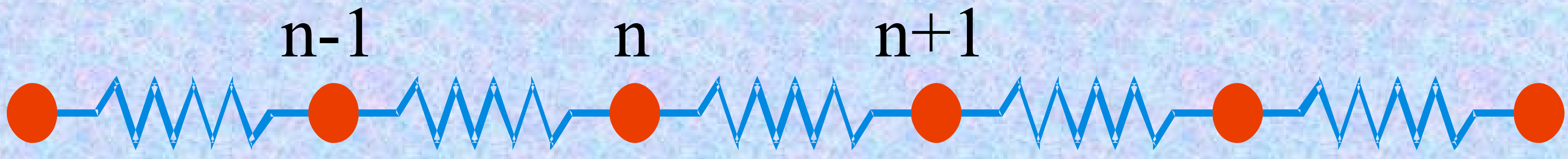
Nonlinear oscillator: soft-hard potential

Potential $V(x)=D(1-e^{-bx^2})+\gamma x^6$





Lattice of coupled nonlinear oscillators



Equation:

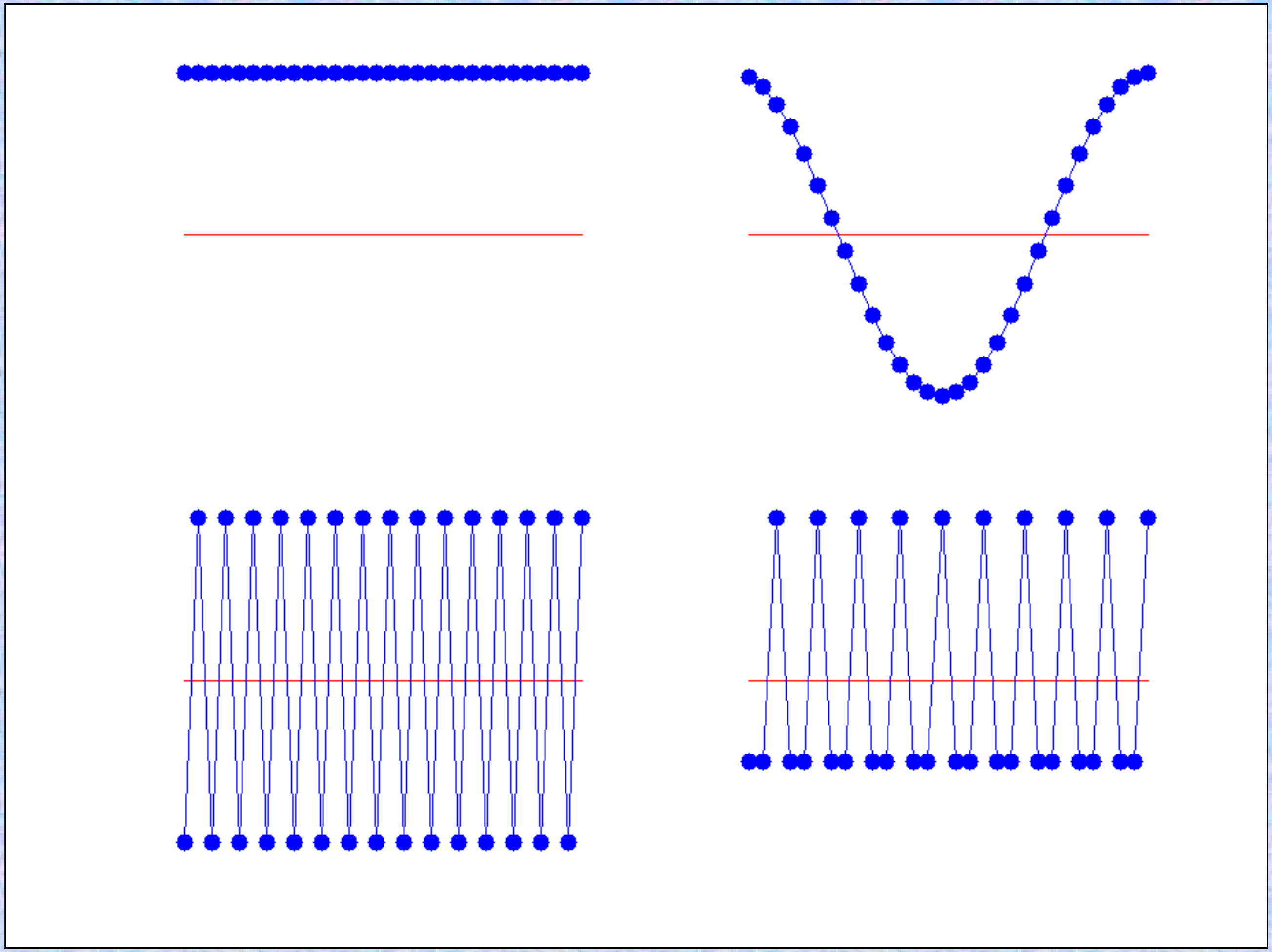
$$x_n''(t) = -V''(x_n) + \varepsilon\,(x_{n+1} - x_n) - \varepsilon\,(x_n - x_{n-1})$$

For small oscillations or linear potentials:

$$x_n''(t) = -\,\omega_0^2 x_n^2 + \varepsilon\,(x_{n+1} - x_n) - \varepsilon\,(x_n - x_{n-1})$$

Well known solutions: **phonons**

Phonons: $x_n = A\cos(q\,n - \omega_q t)$



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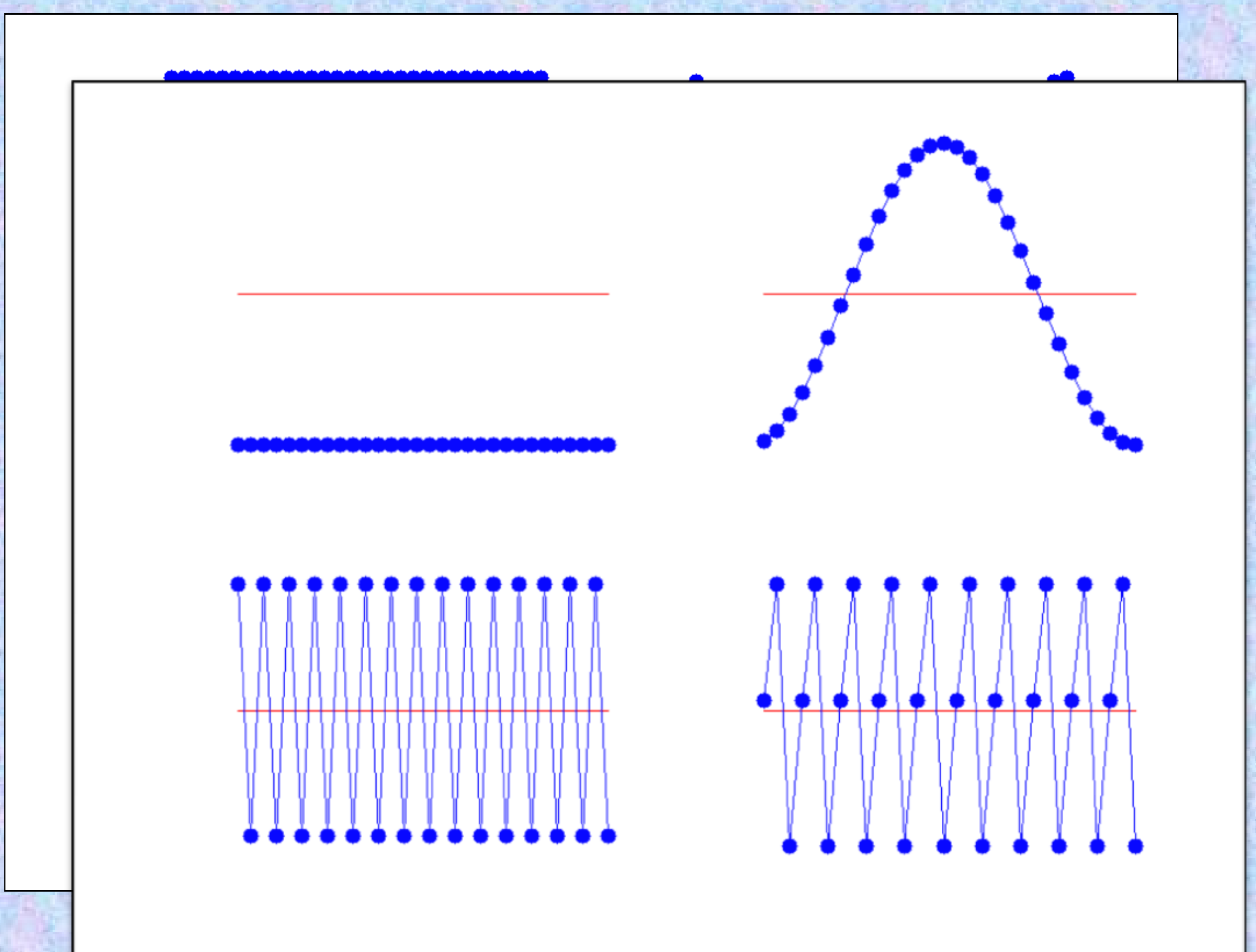

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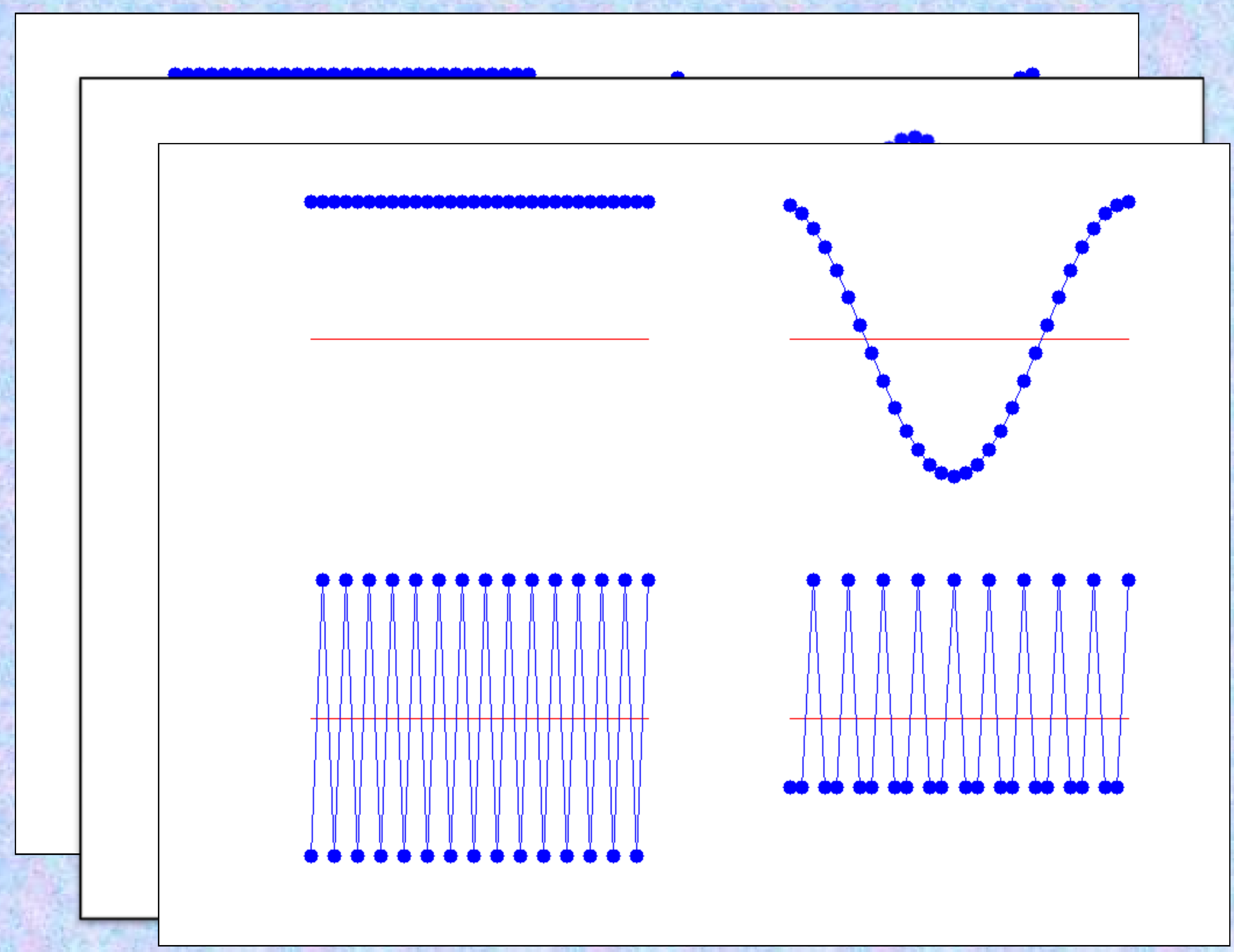
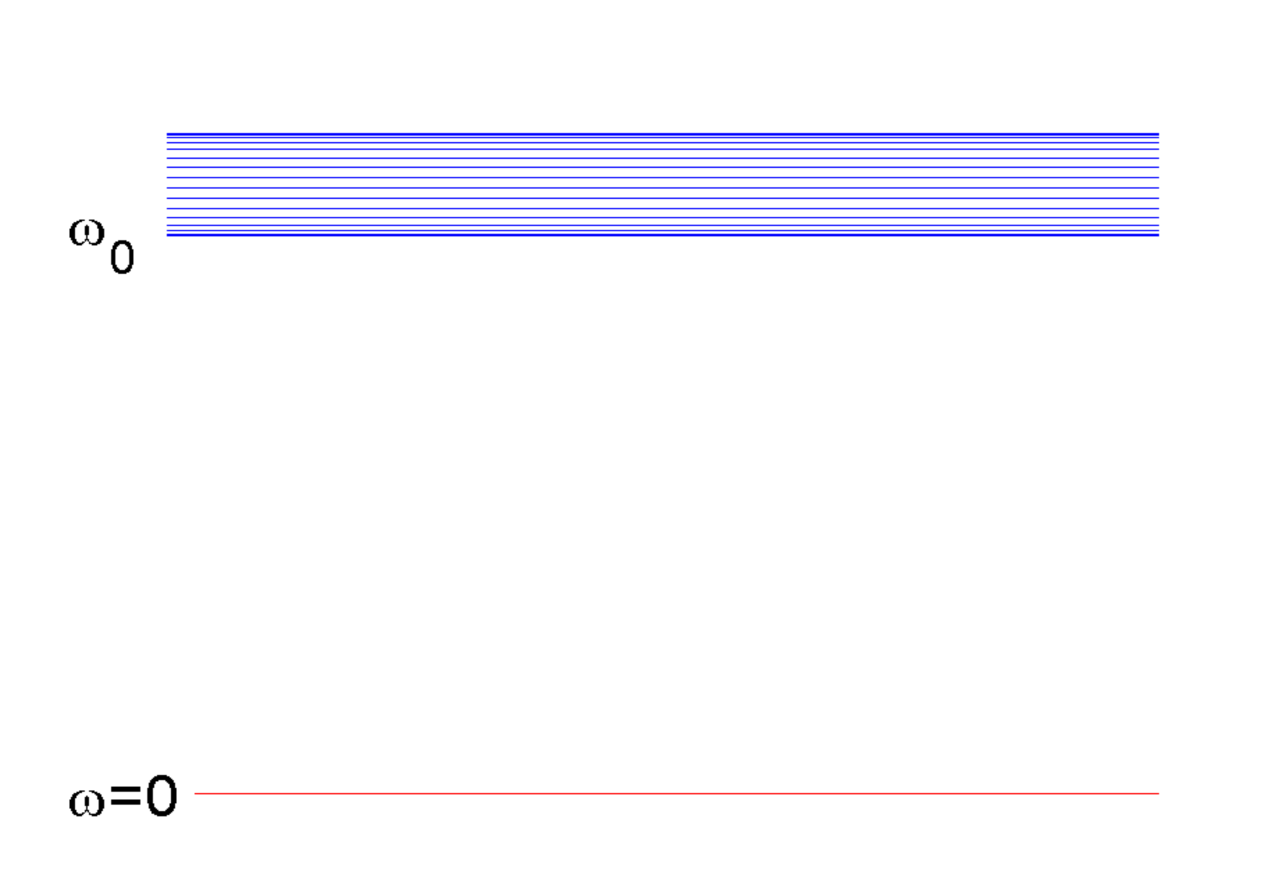


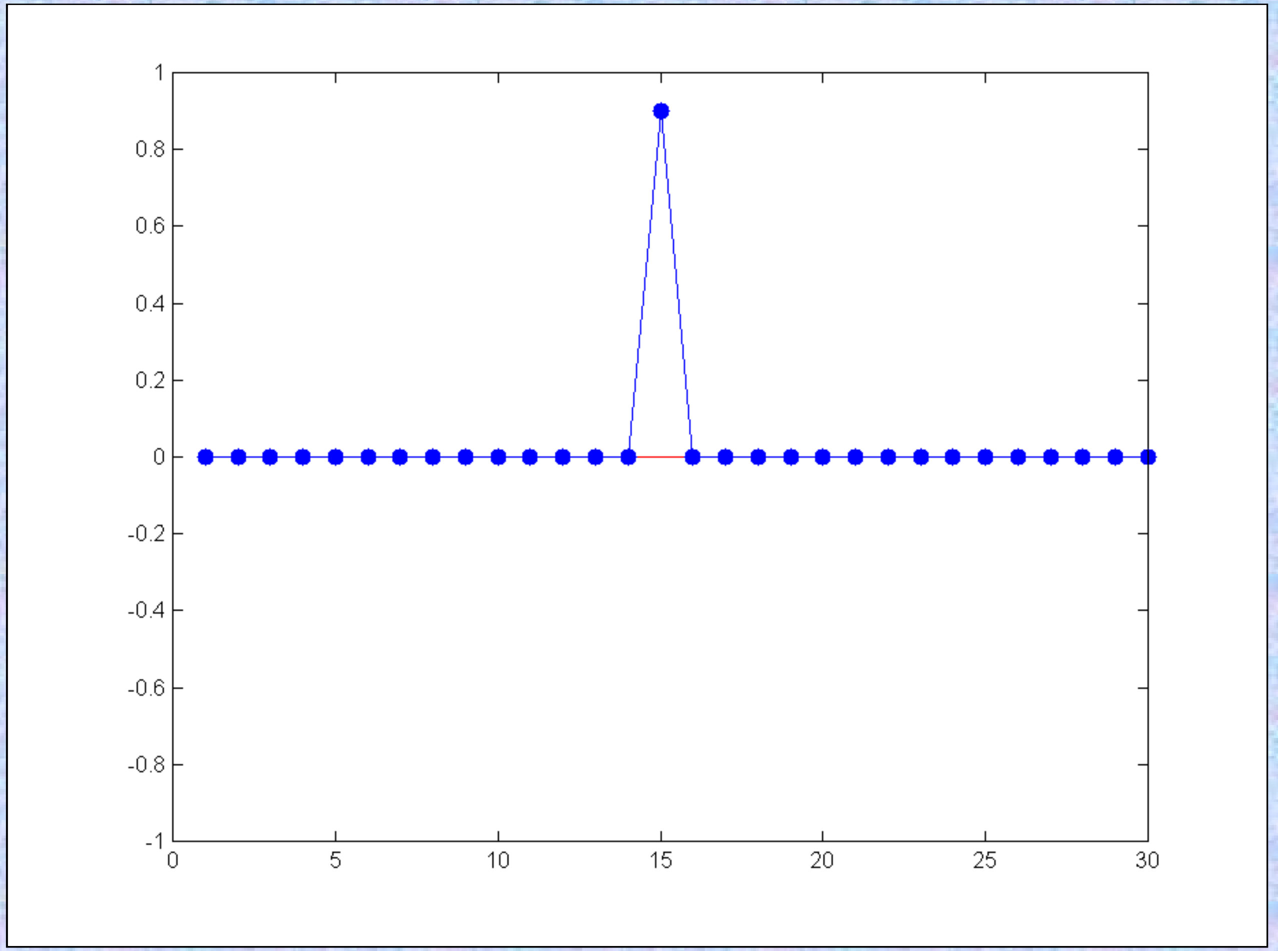
Phonon characteristics

- Extended with uniform amplitude
- Frquency band:



Perturbation of a linear network or small pertubation of a nonlinear one

- The energy is dispersed on phonons



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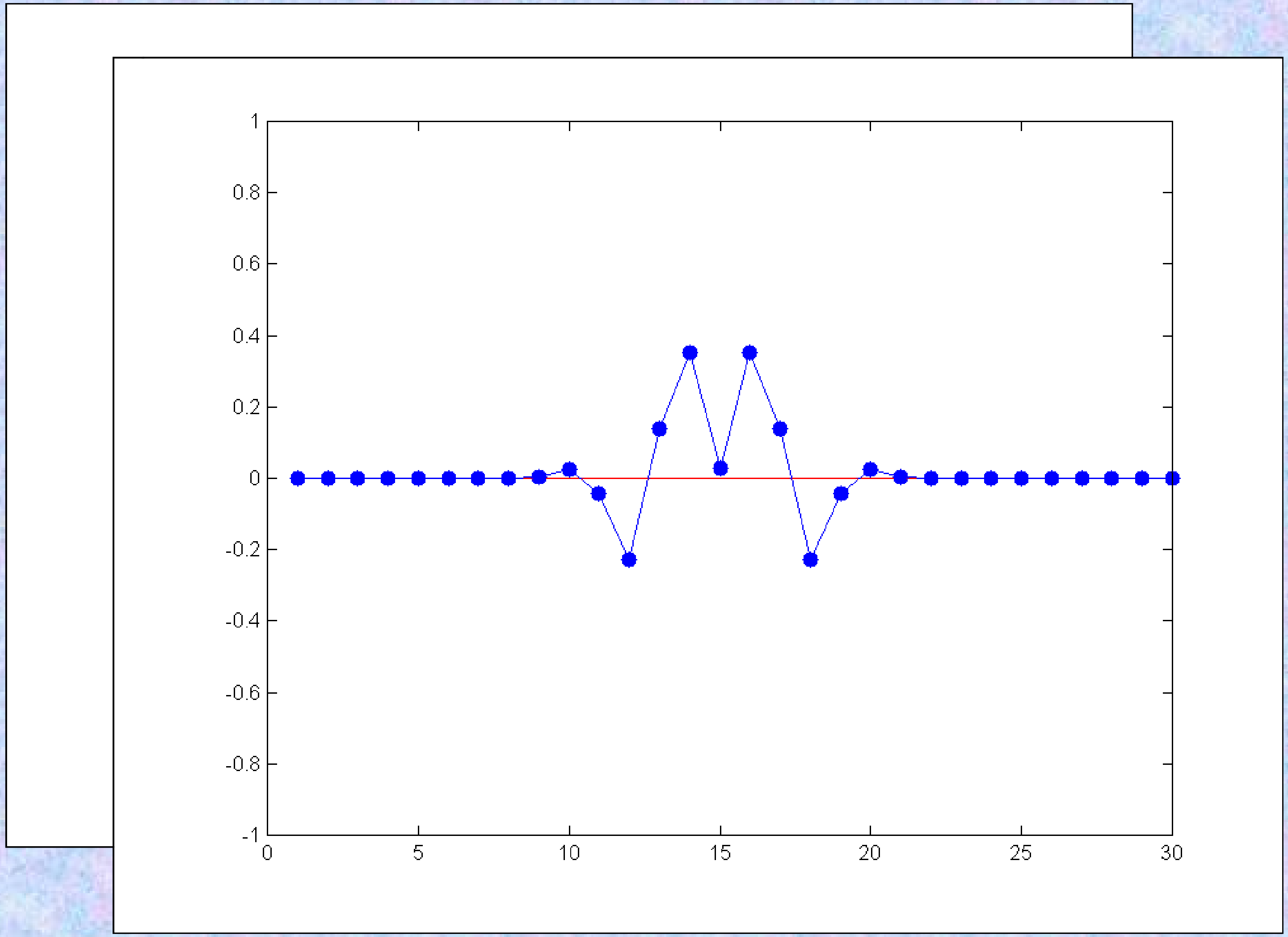

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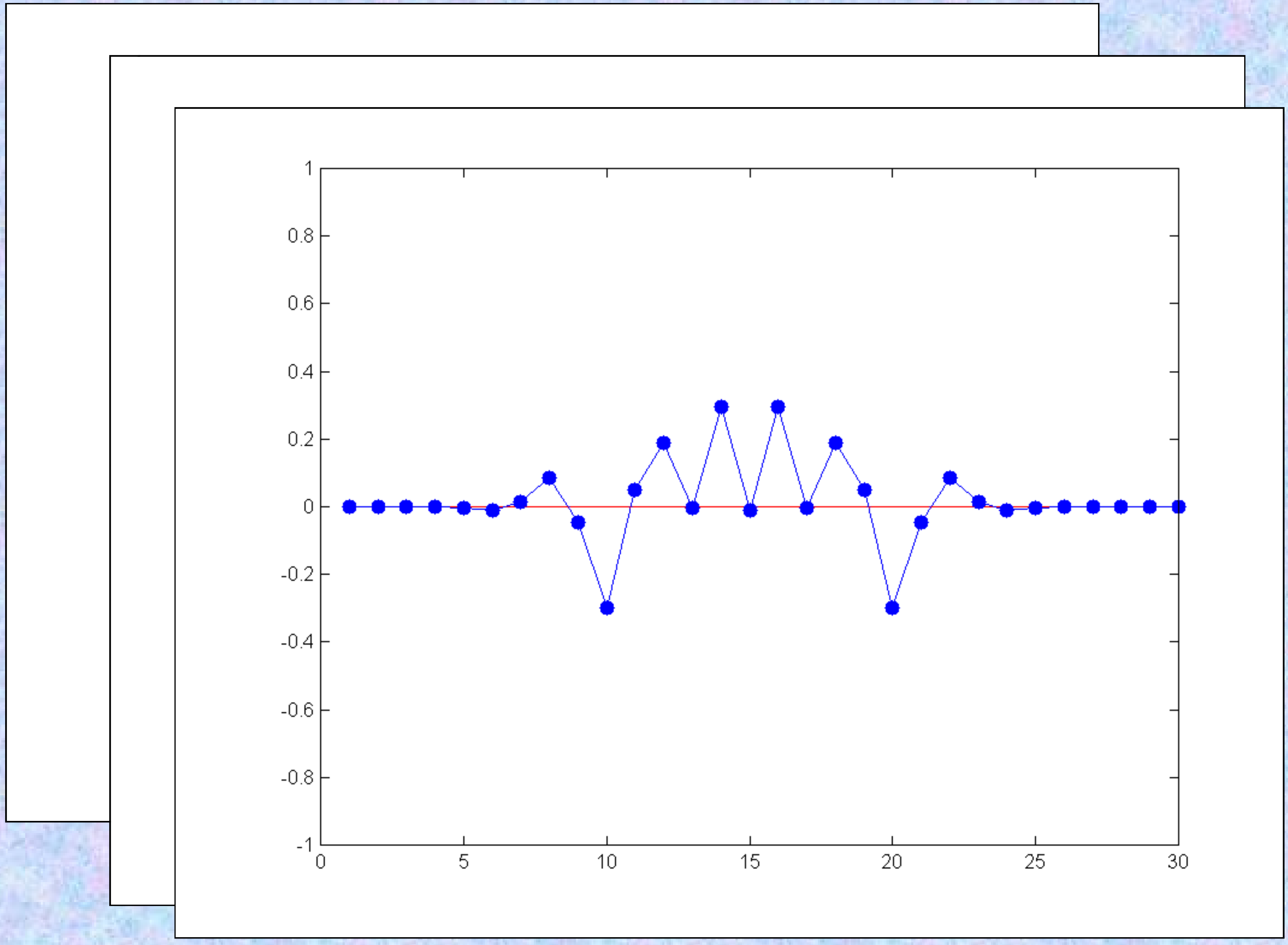

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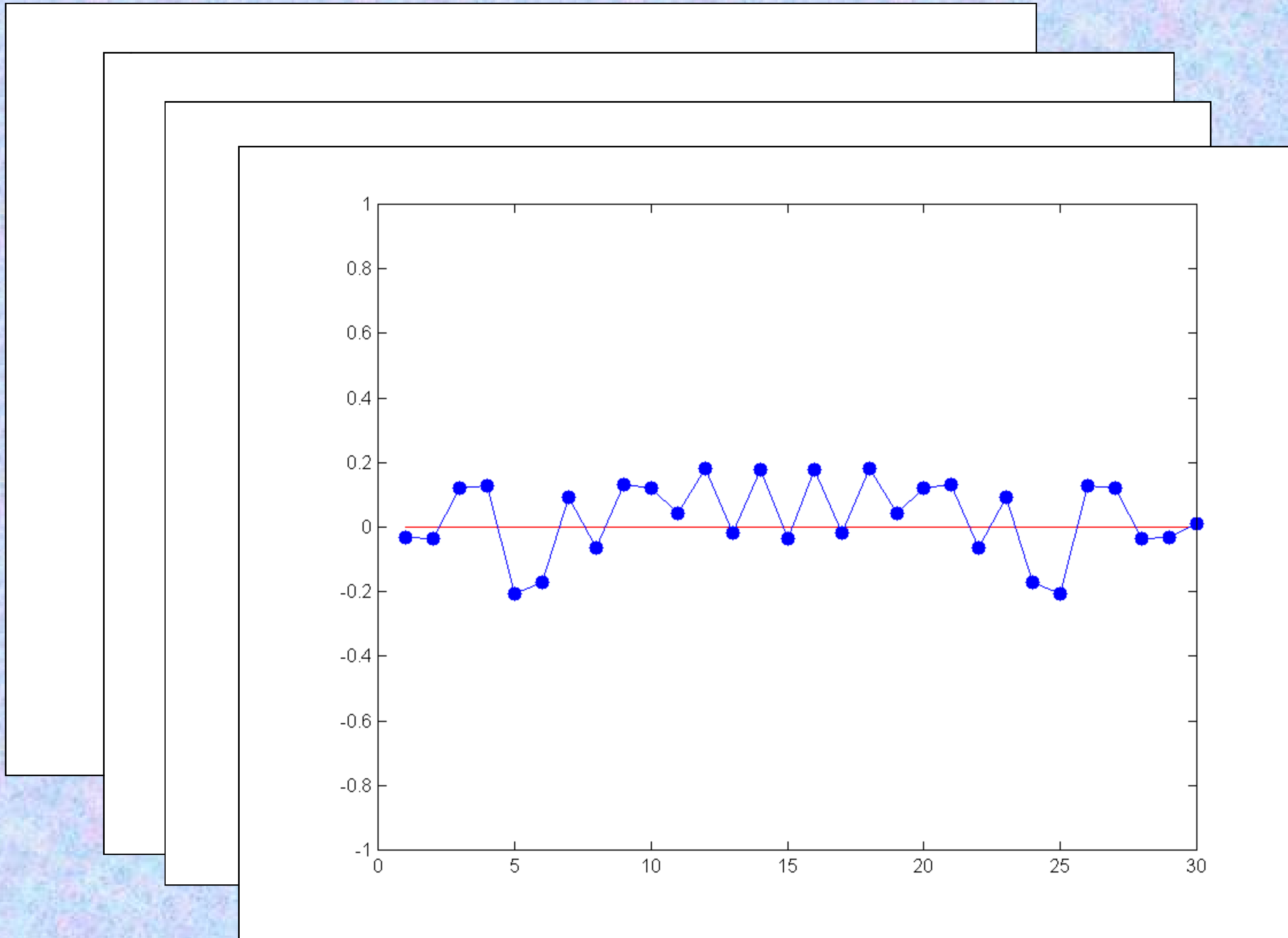
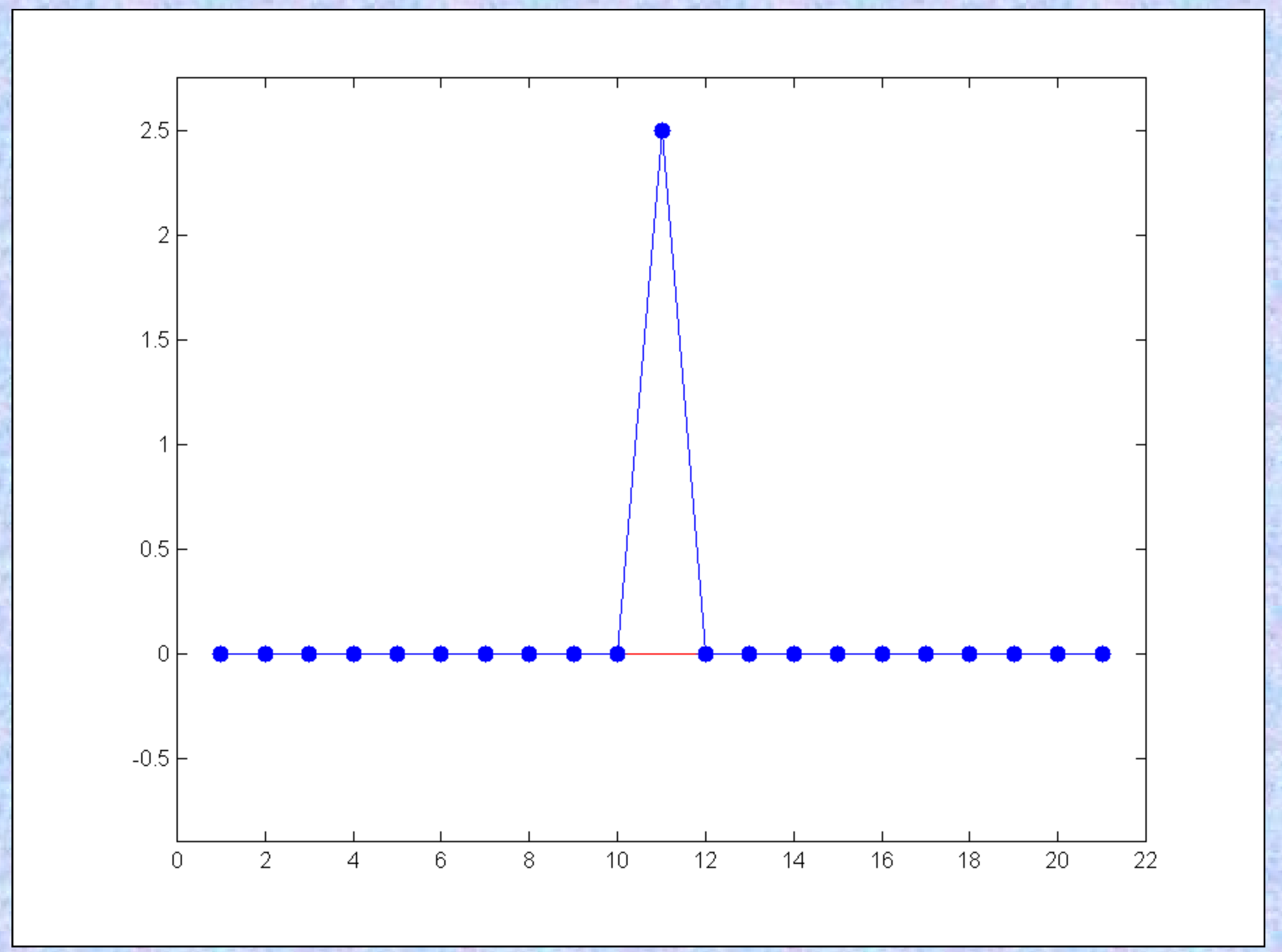


Large perturbation of a nonlinear network

- Energy remains localized



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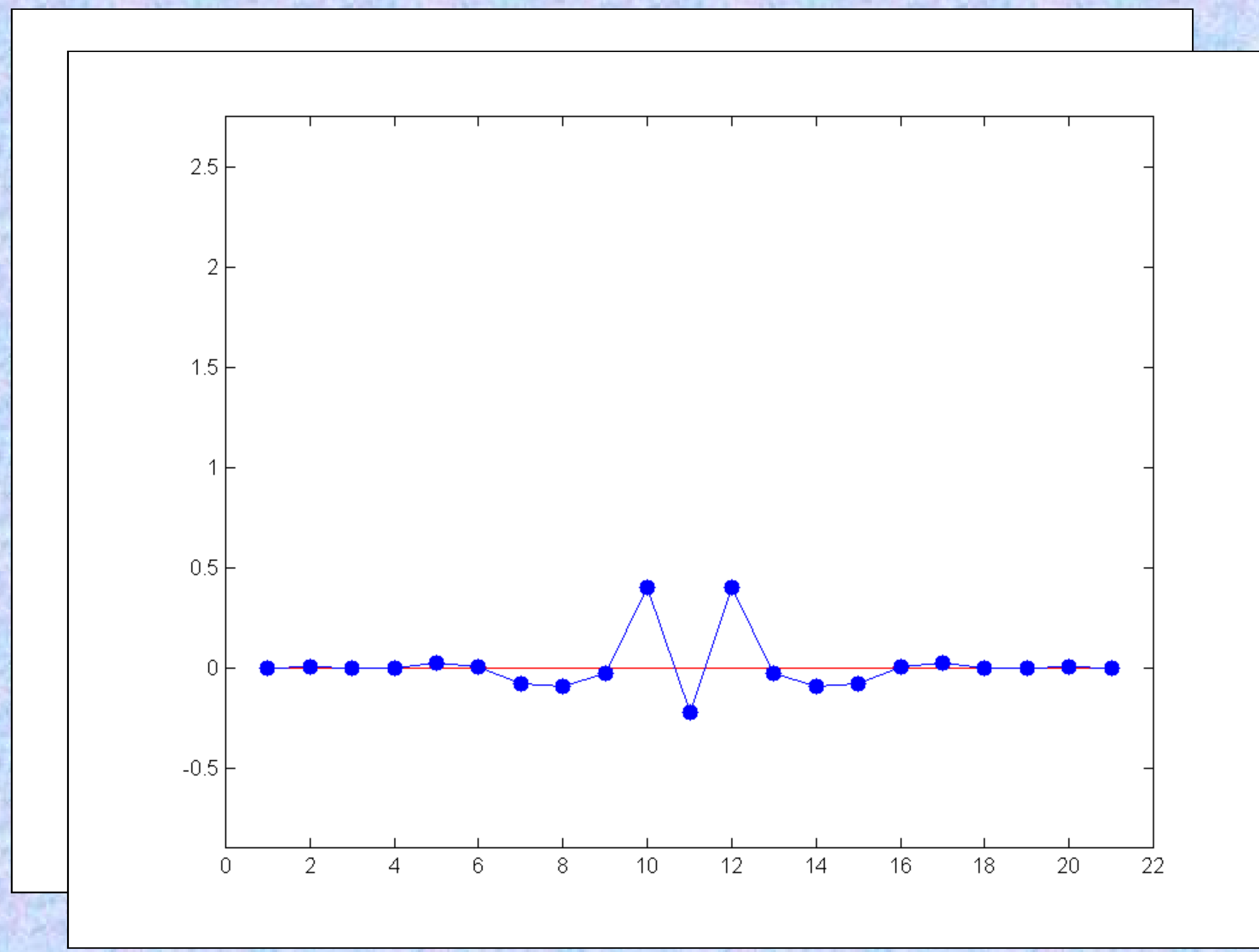

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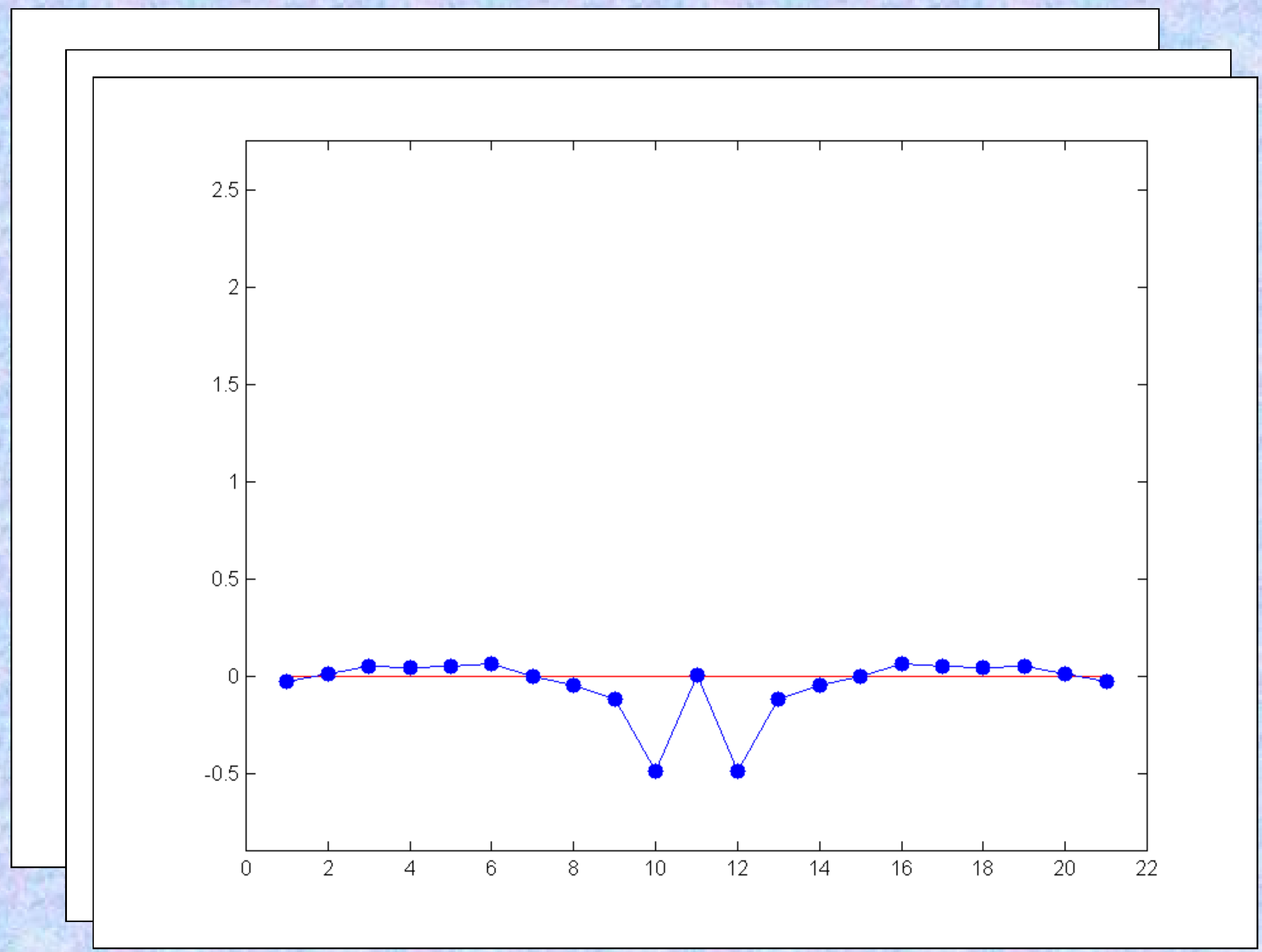

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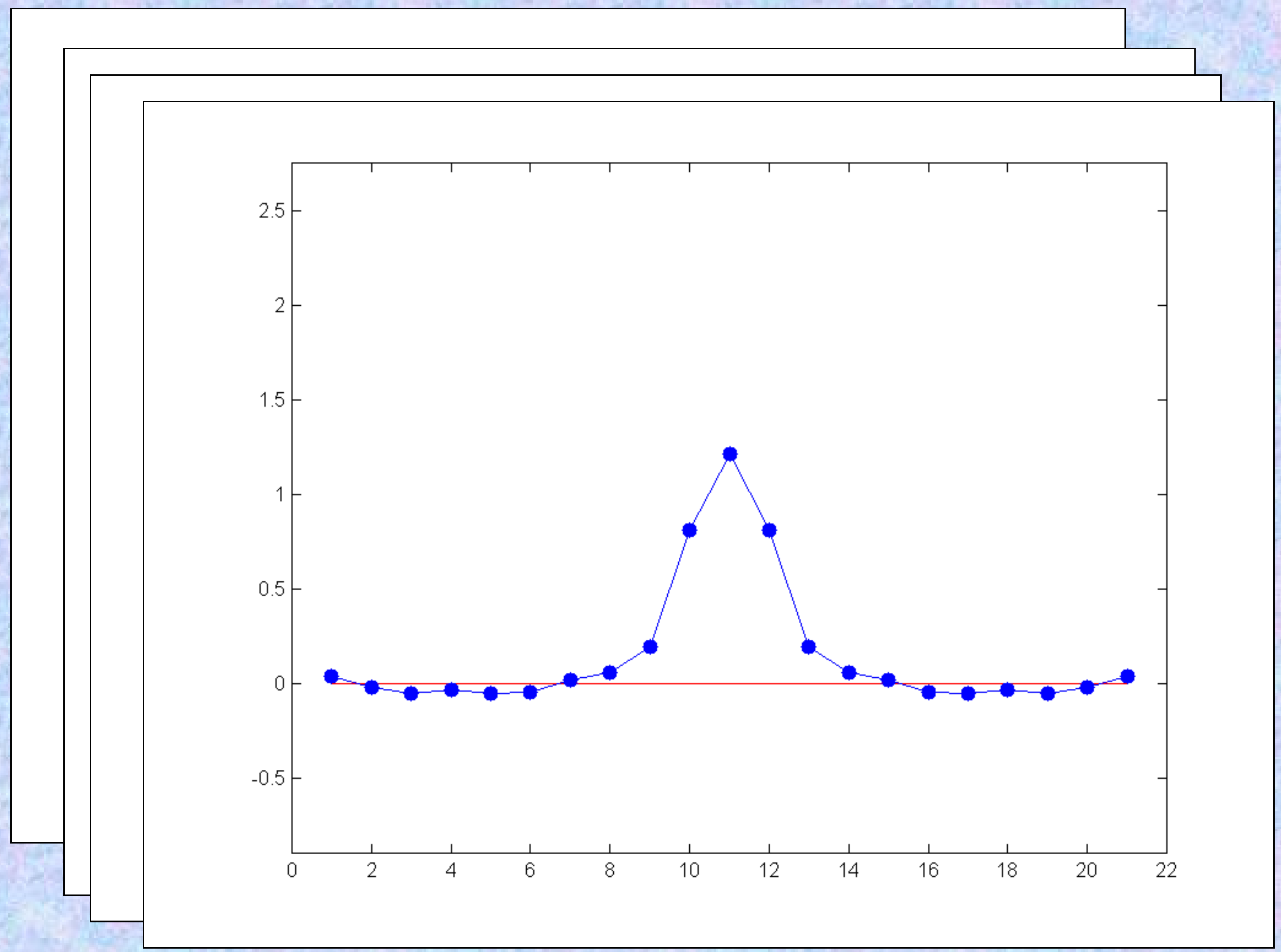
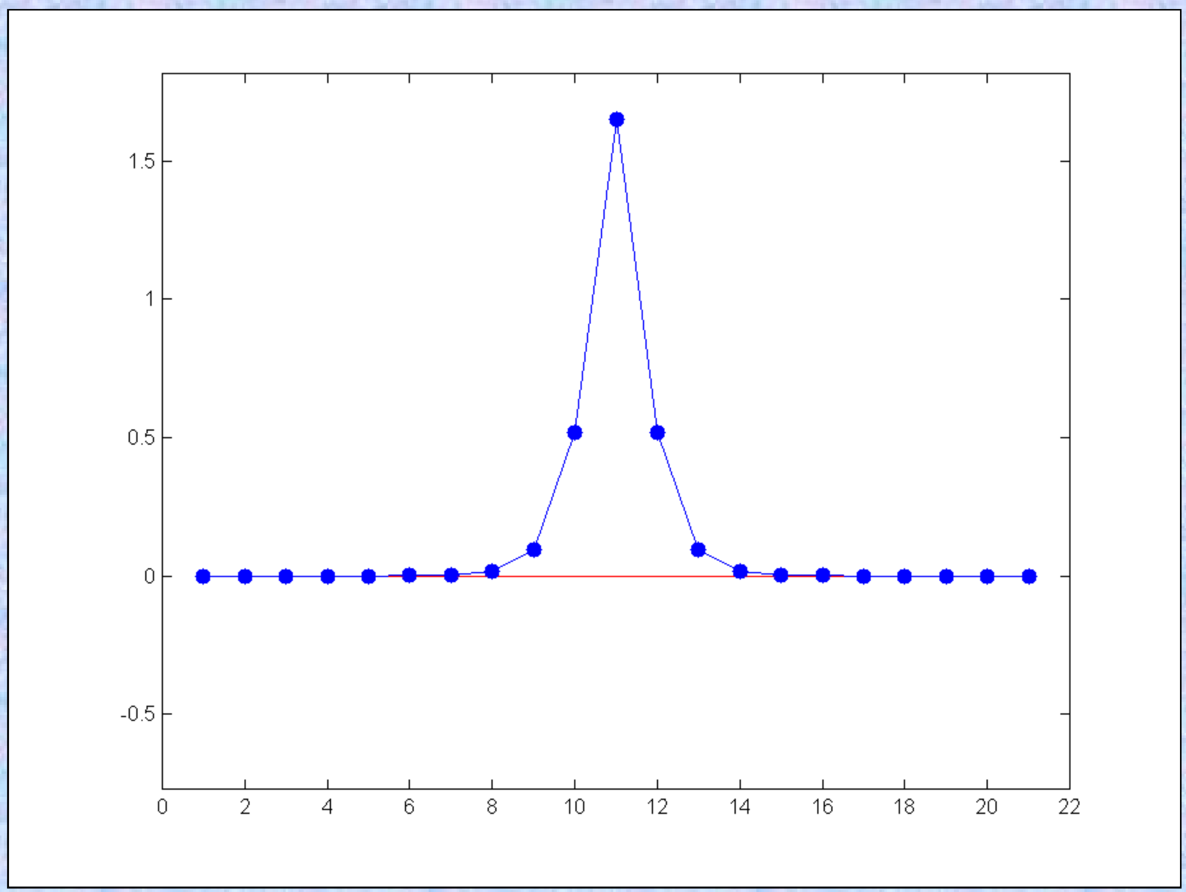


Breather

- Exact, periodic, localized solution



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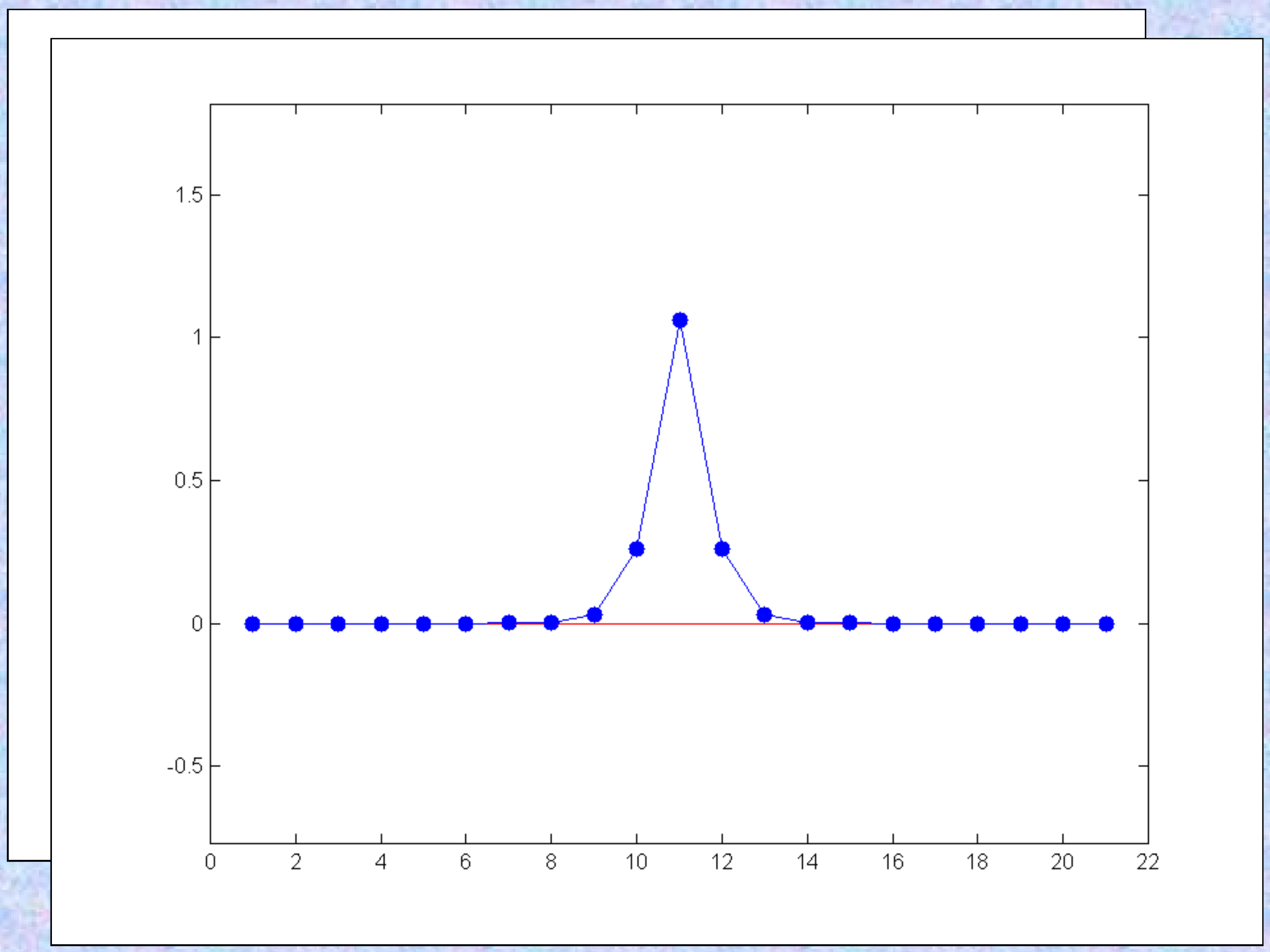

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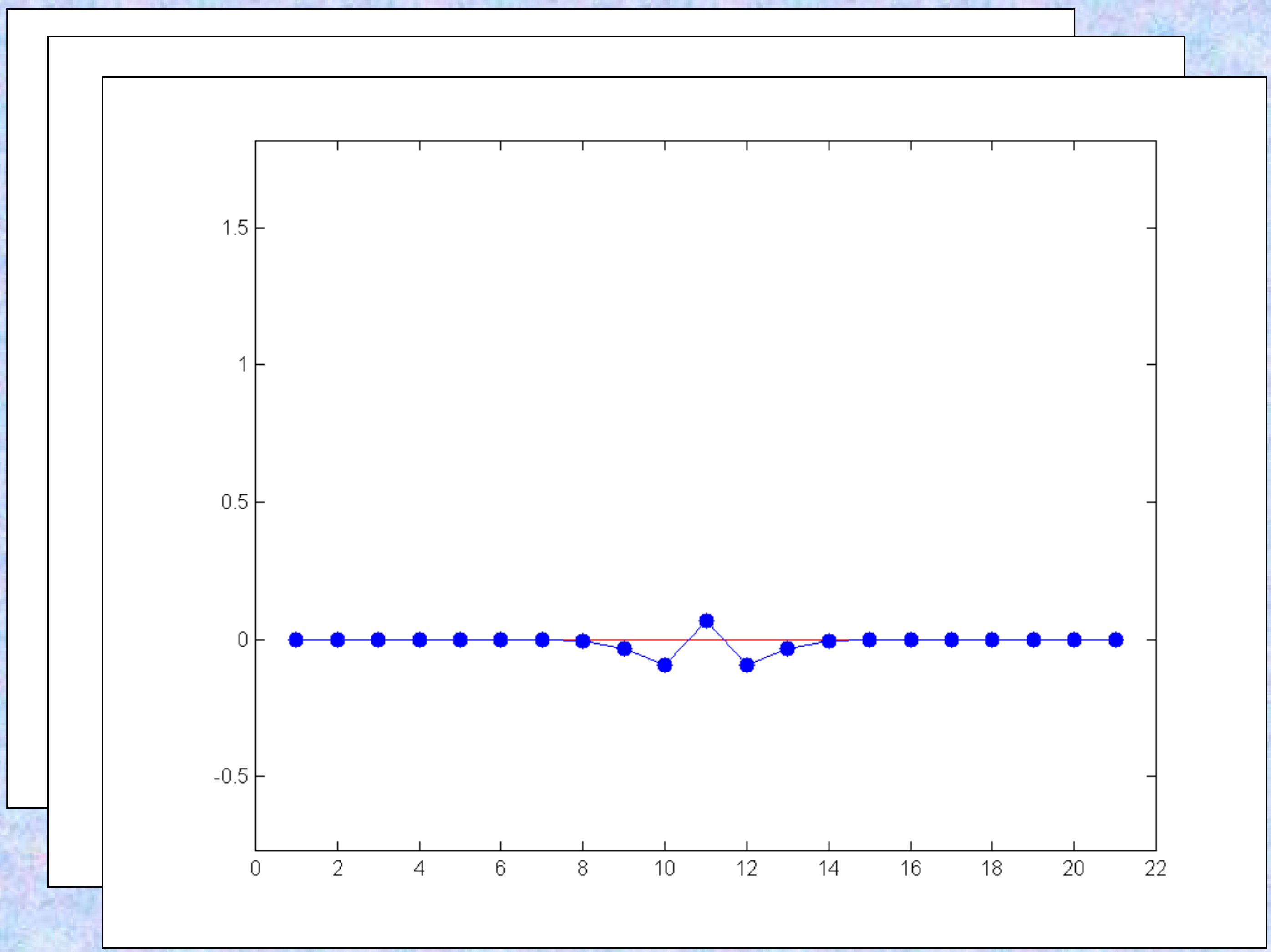

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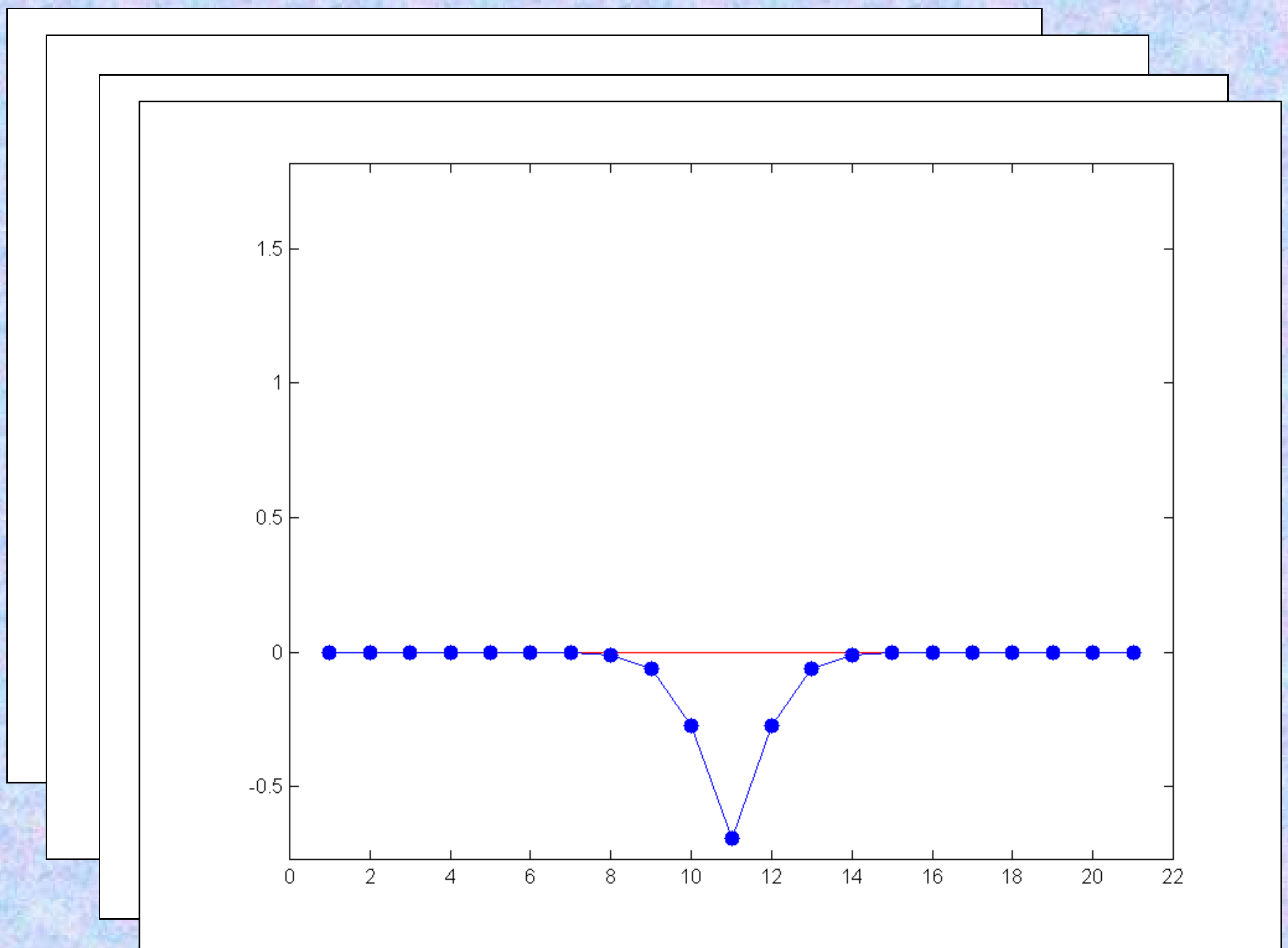
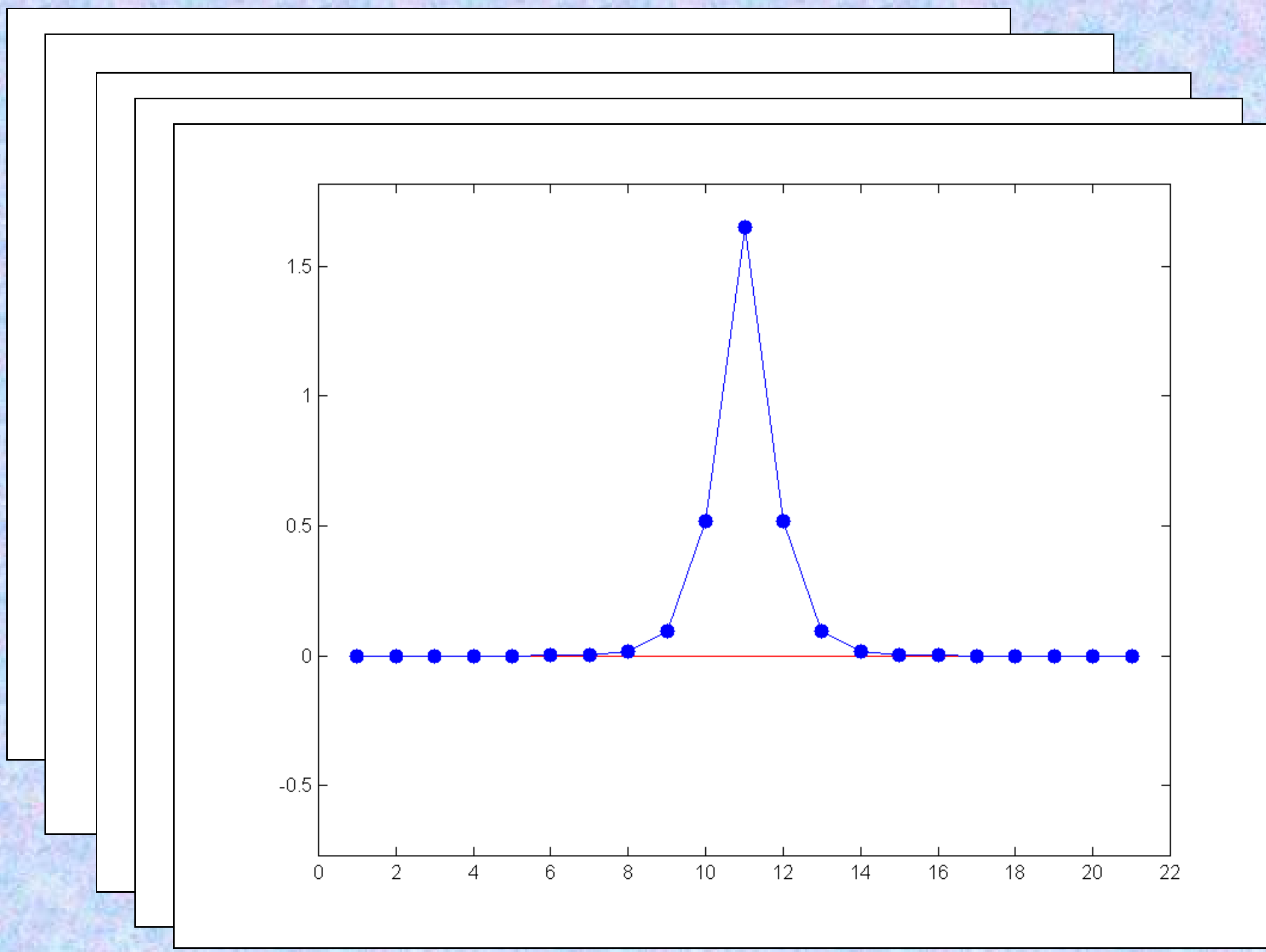
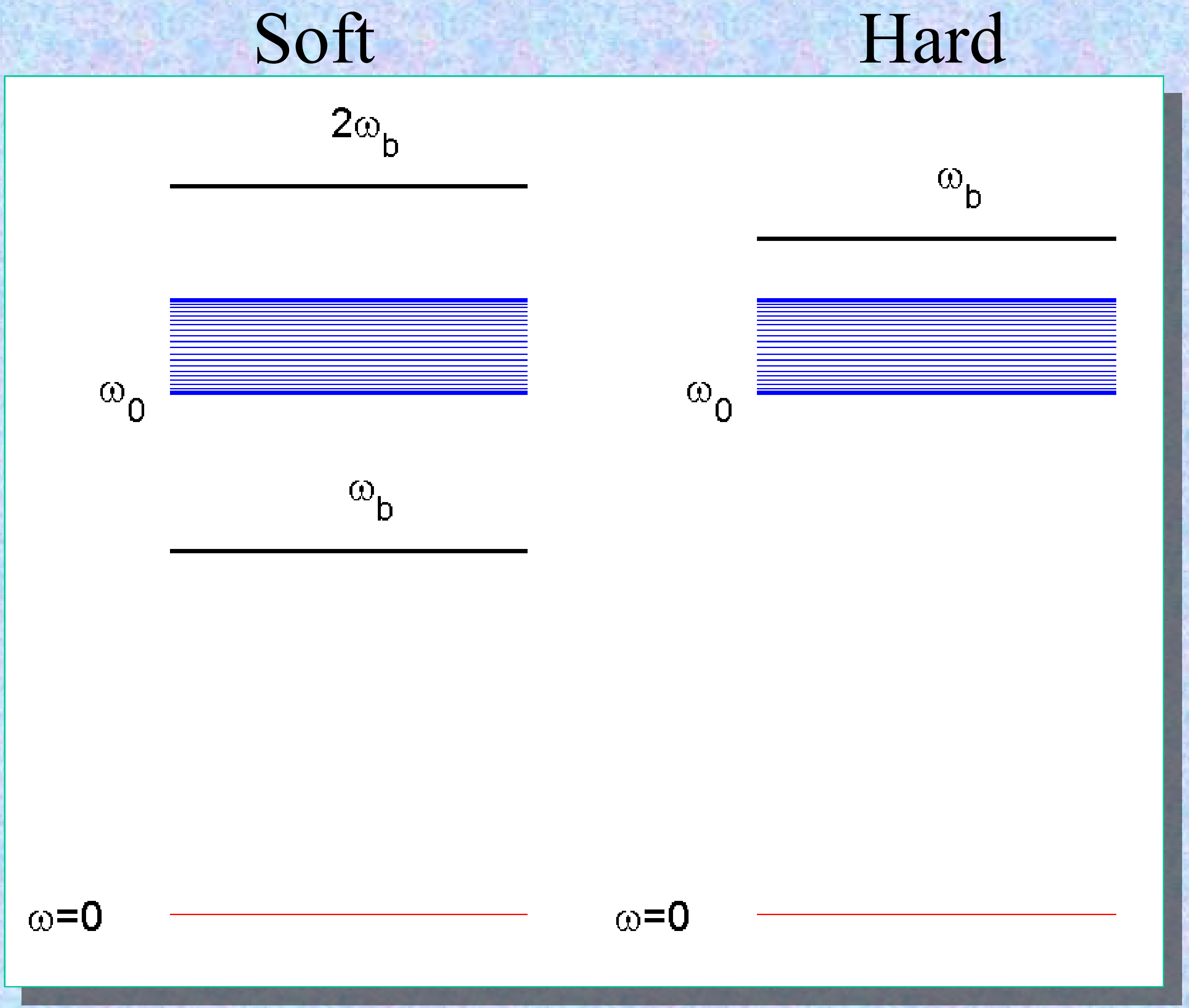


Breather

- Exact, periodic, localized solution



Breather frequency and phonon band



Conditions for breather existence

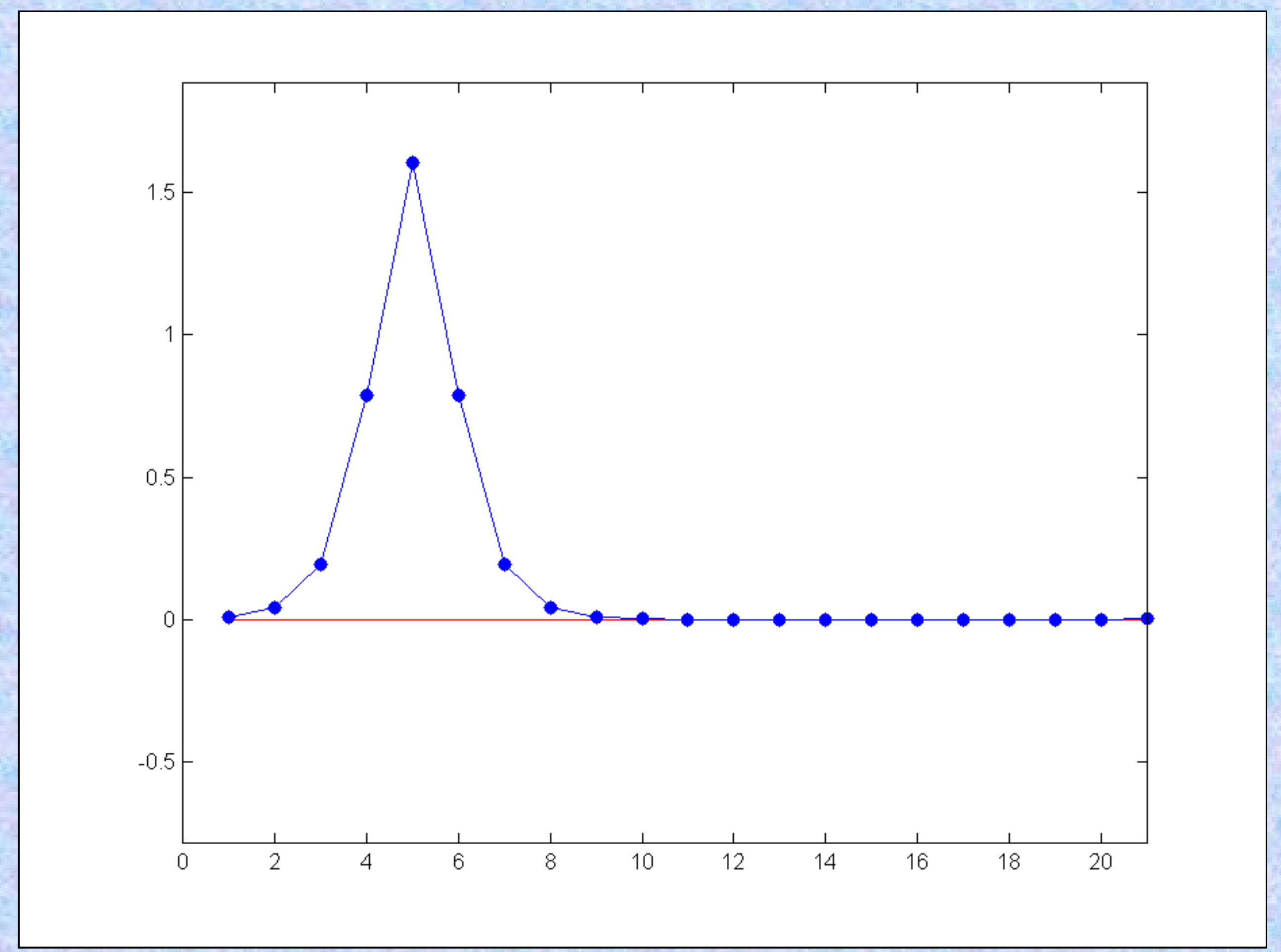
- The breather frequency and its harmonics have to be outside the phonon band.

$$n\,\omega_b \notin [\omega_0, \omega_{ph,max}]$$

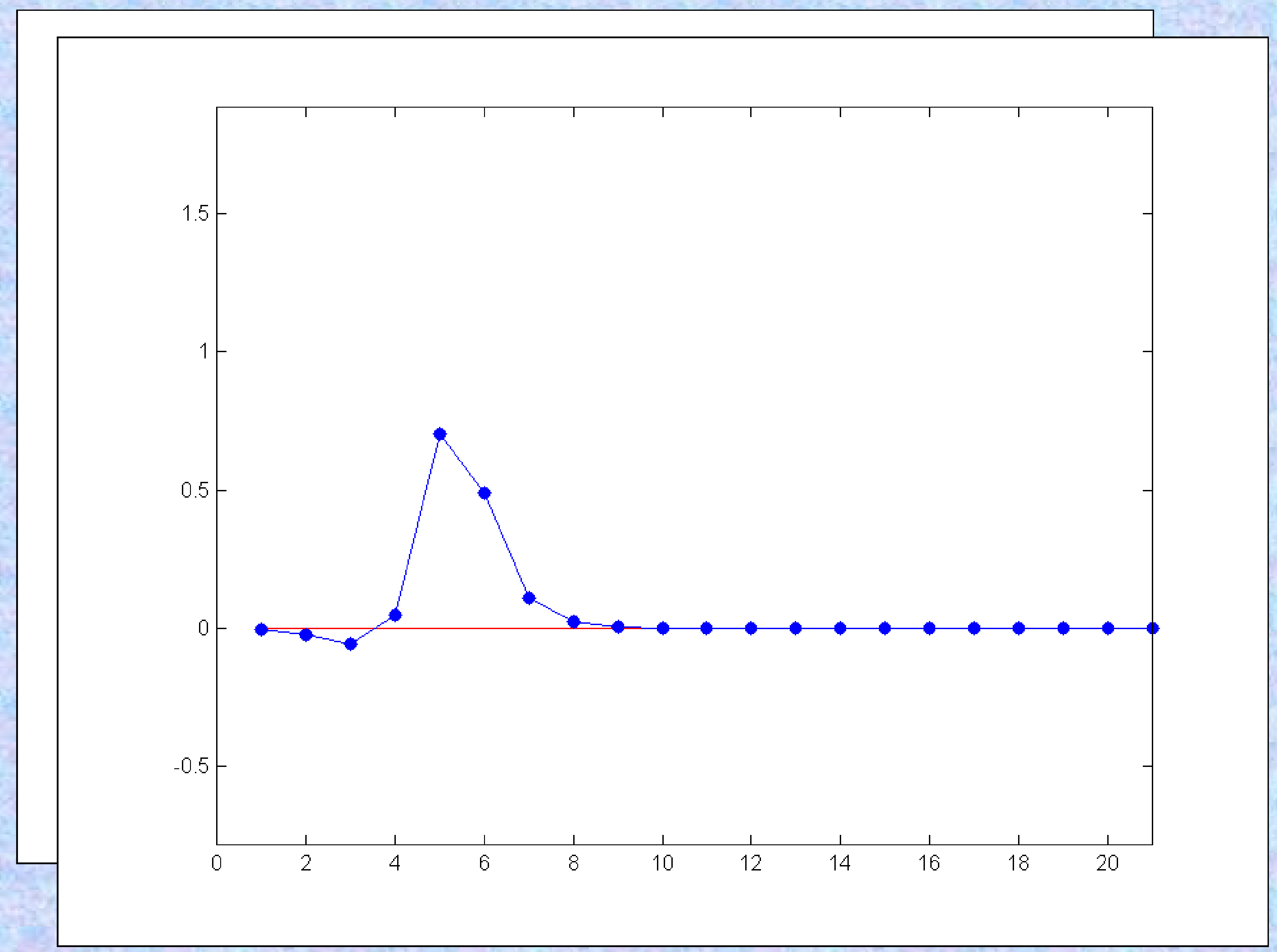
- The oscillator has to be nonlinear for the given amplitude or energy

$$\omega_b'(E) \neq 0$$

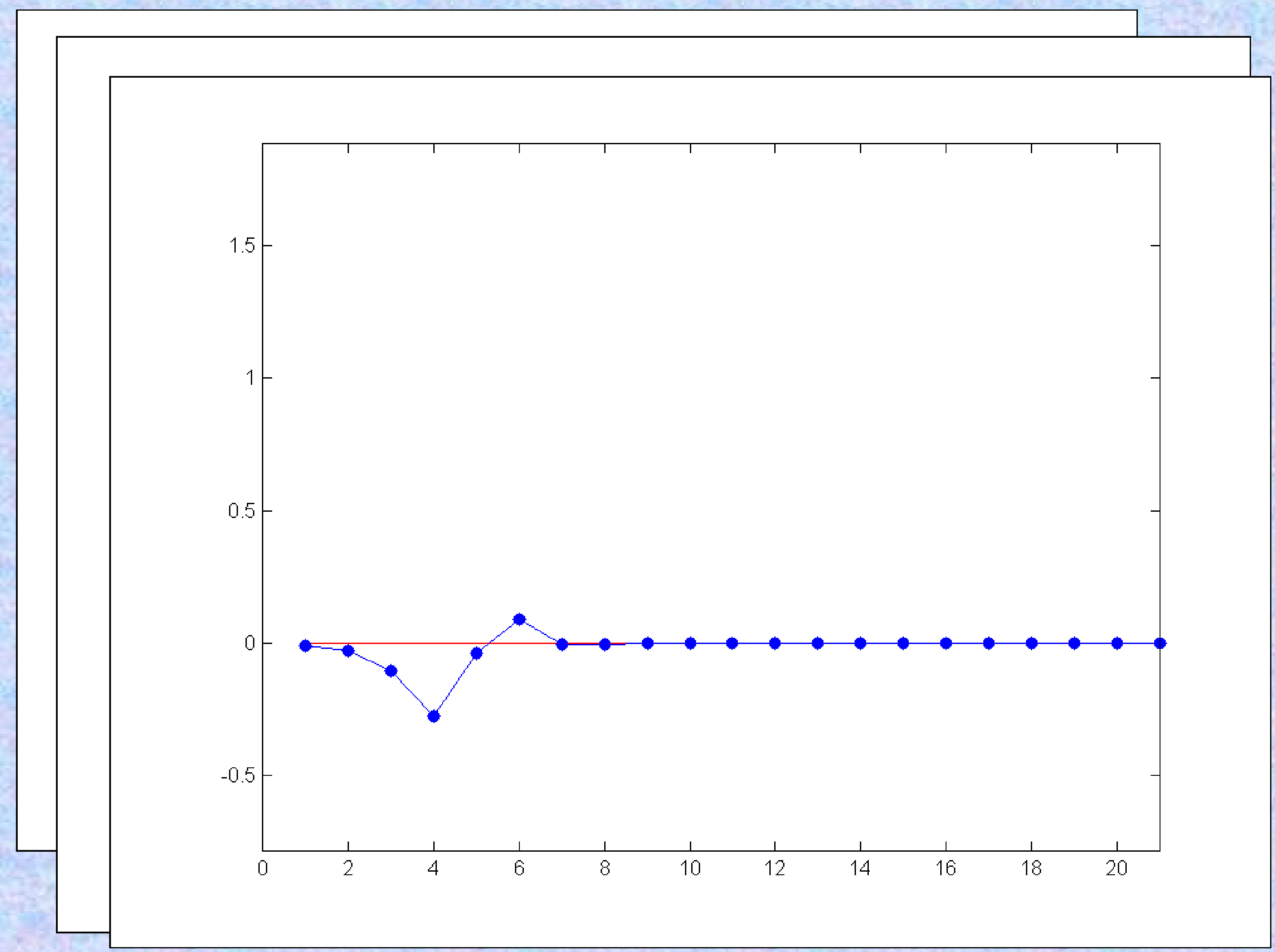
Moving breathers



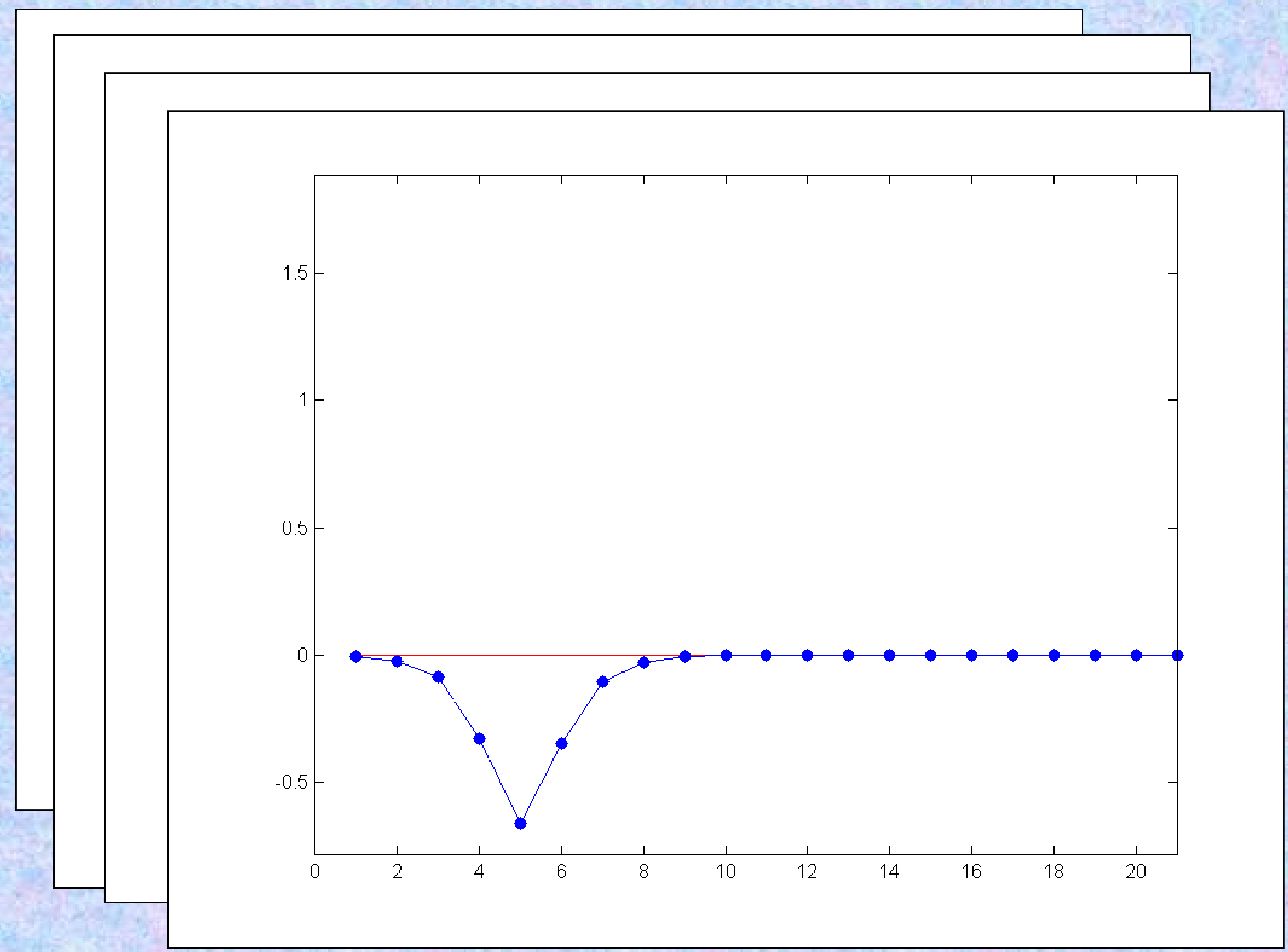
Moving breathers



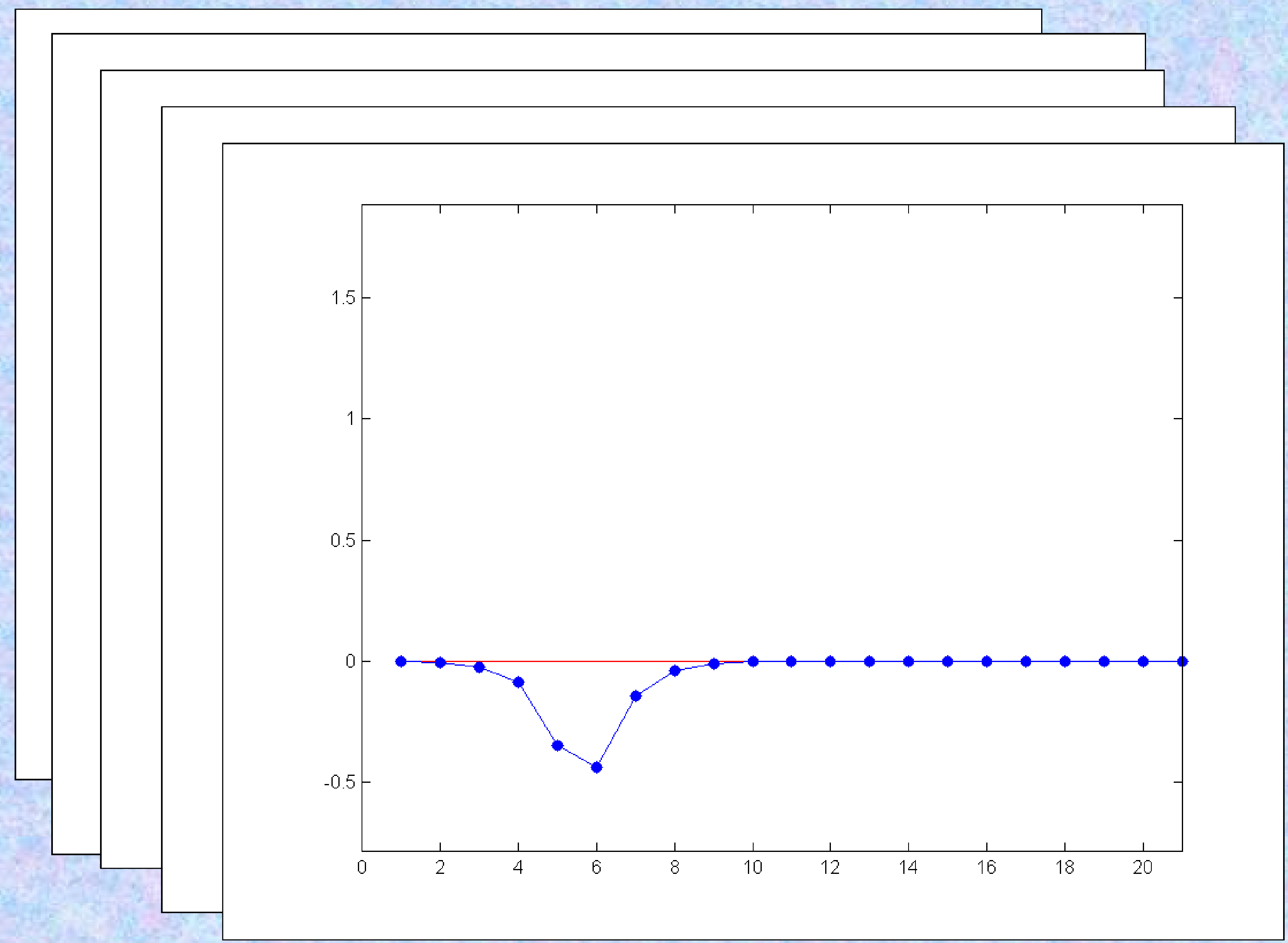
Moving breathers



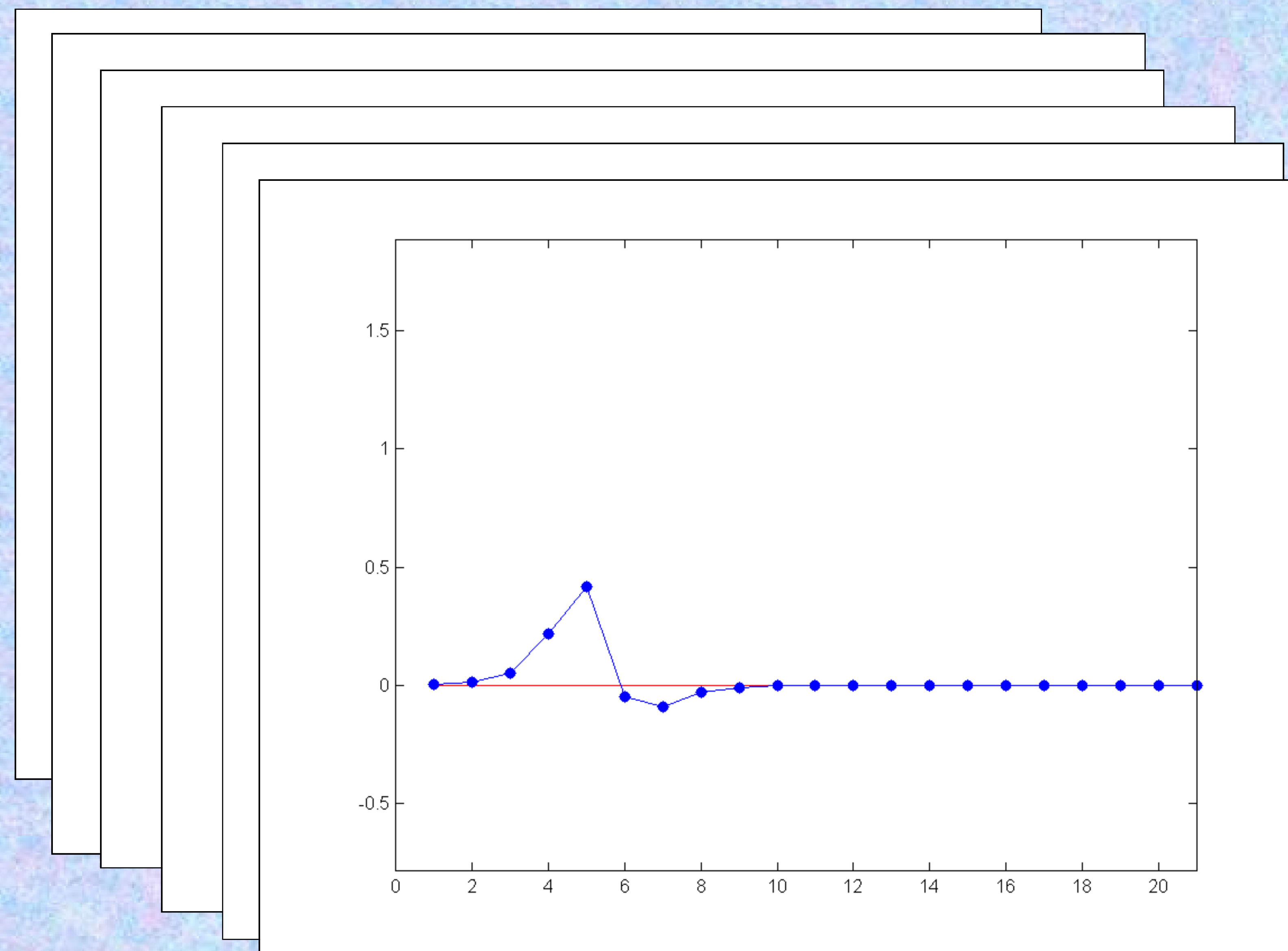
Moving breathers



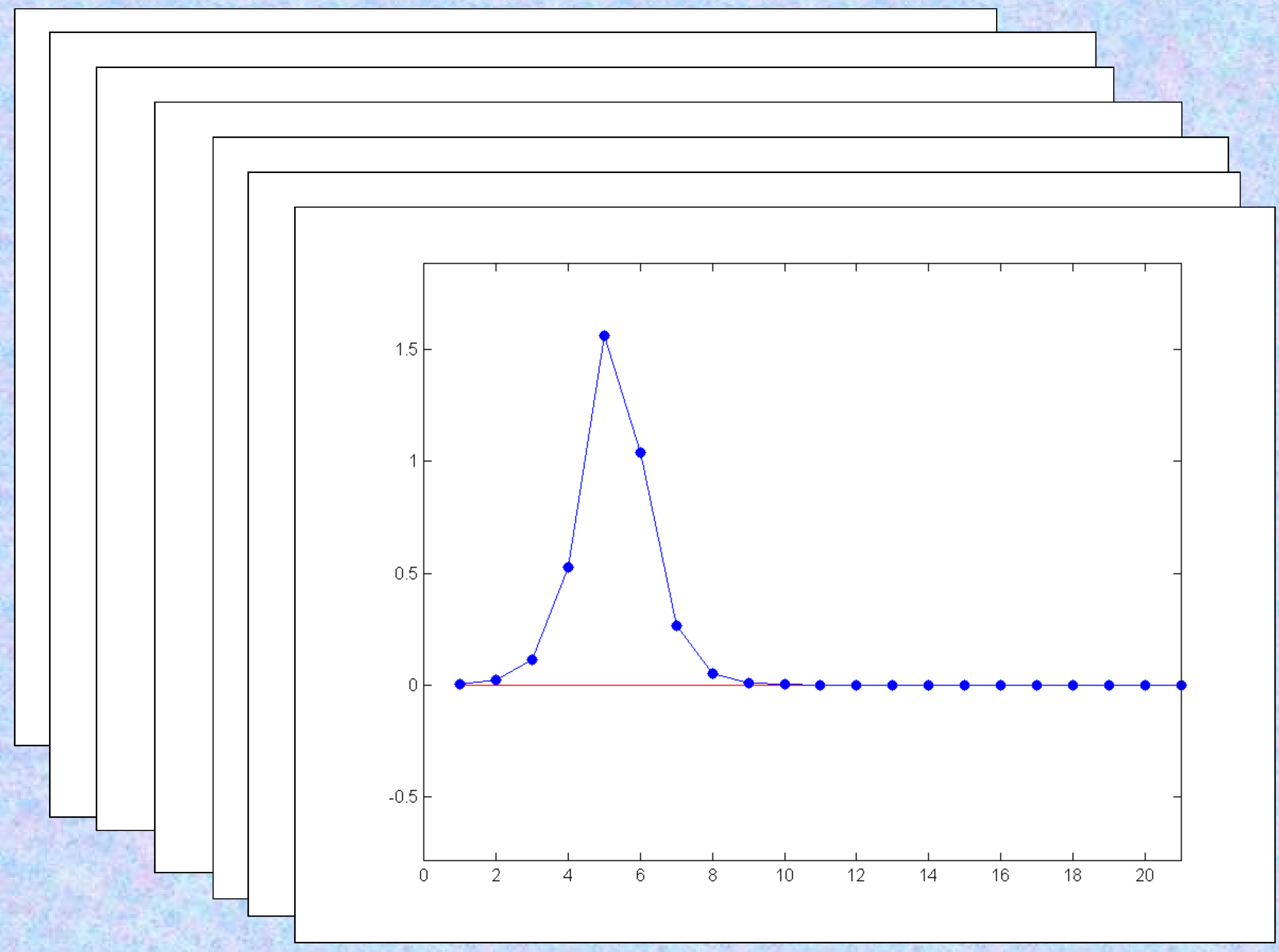
Moving breathers



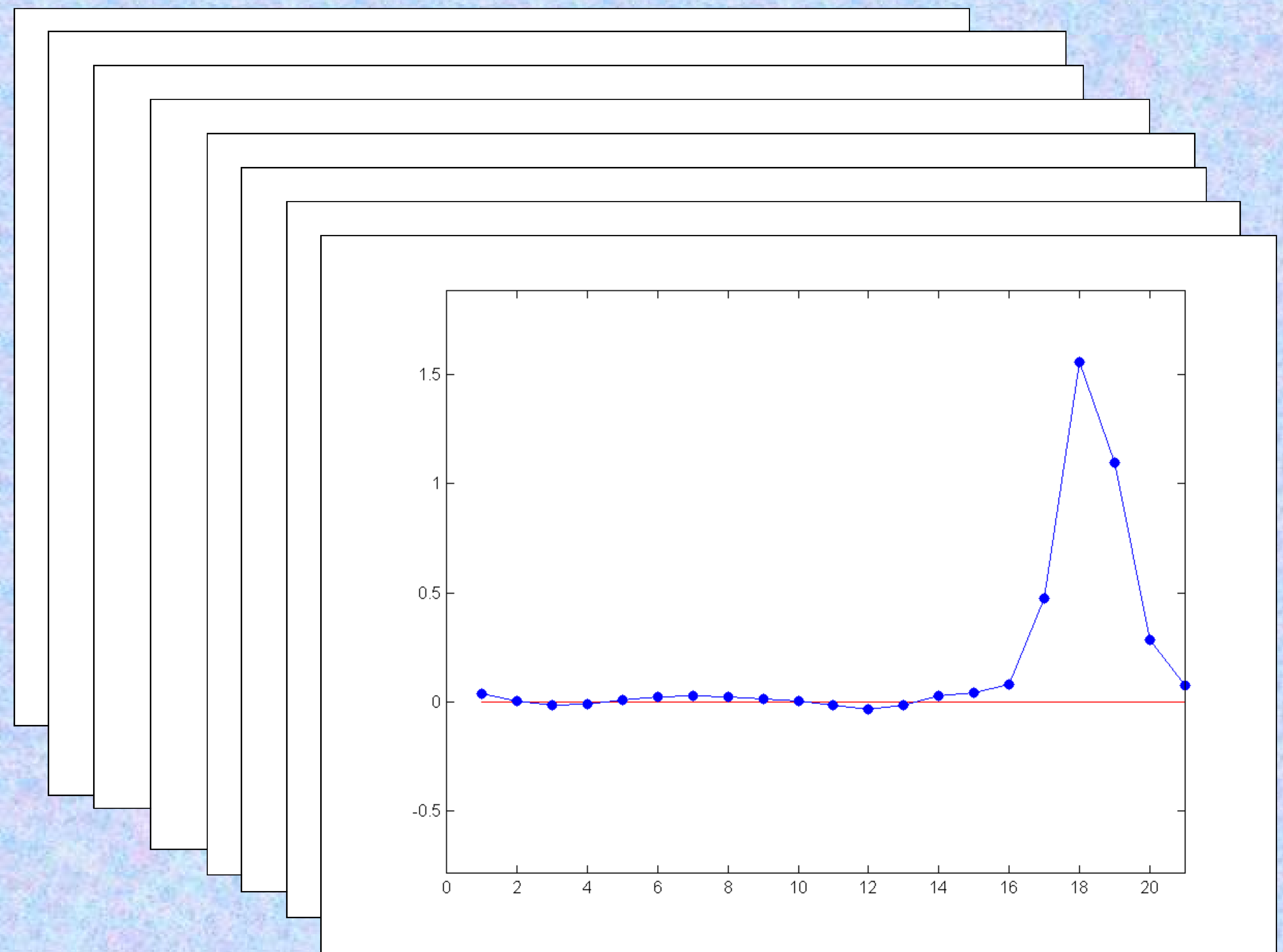
Moving breathers



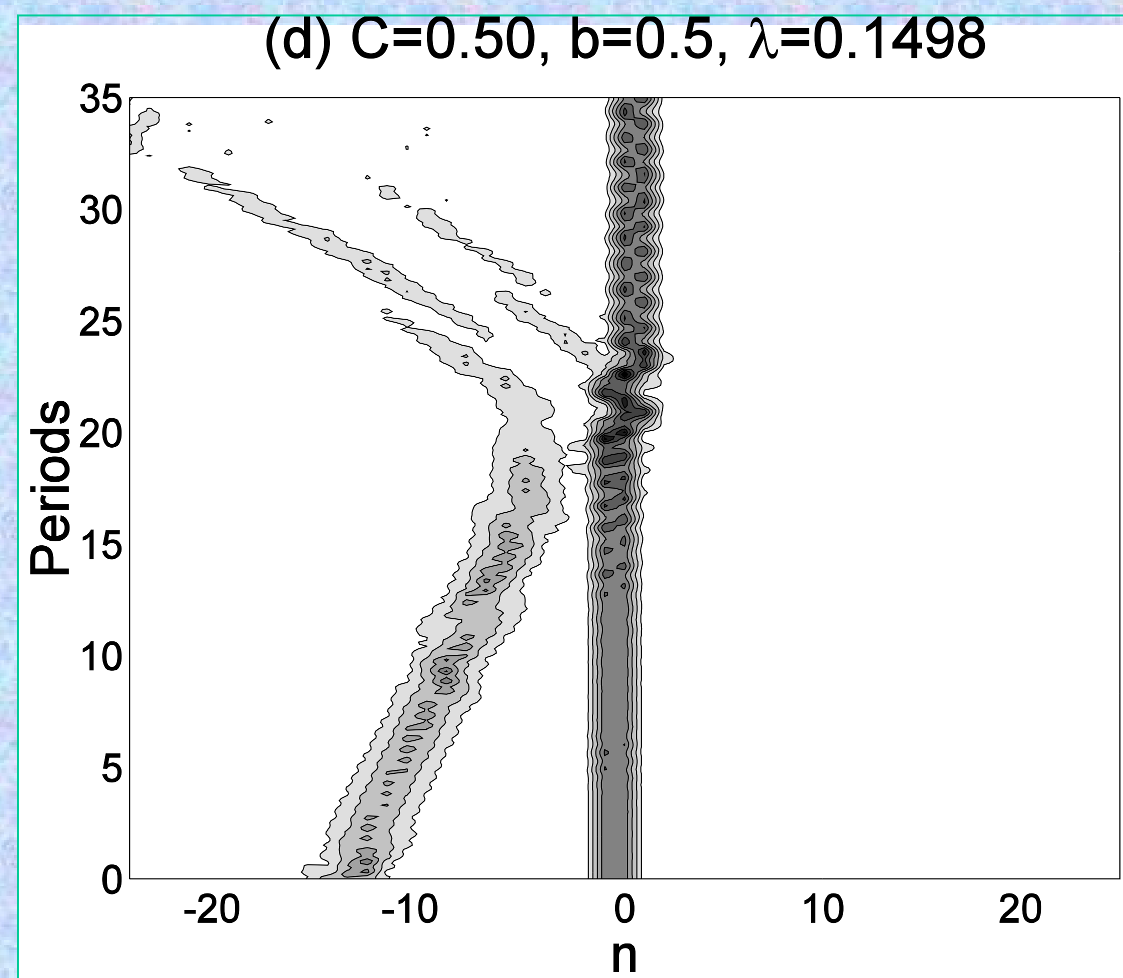
Moving breathers



Moving breathers



Moving breather sent against a vacancy



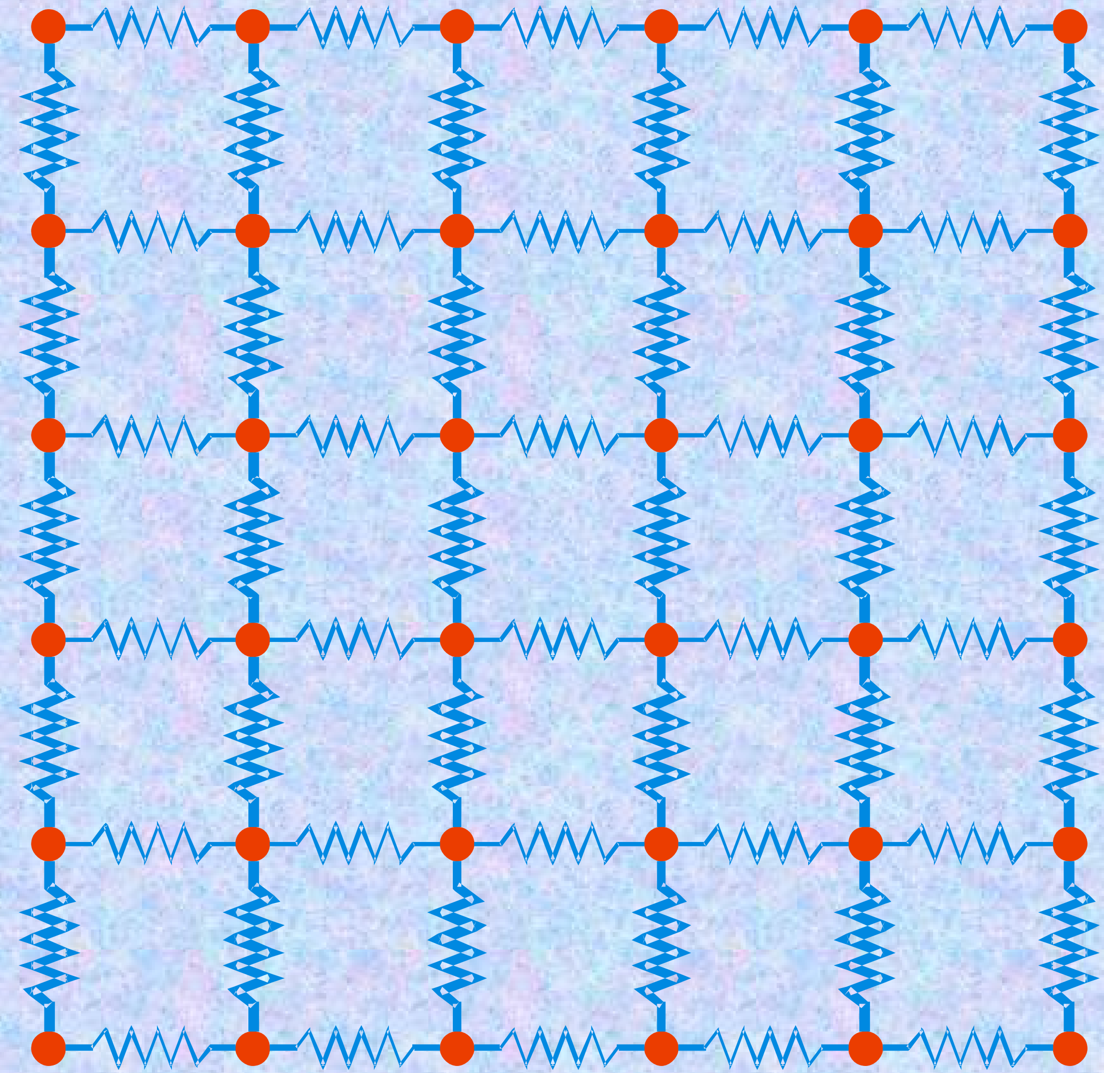
Interstitials and vacancies can:

1. move forward
2. move backwards
3. stay stationay

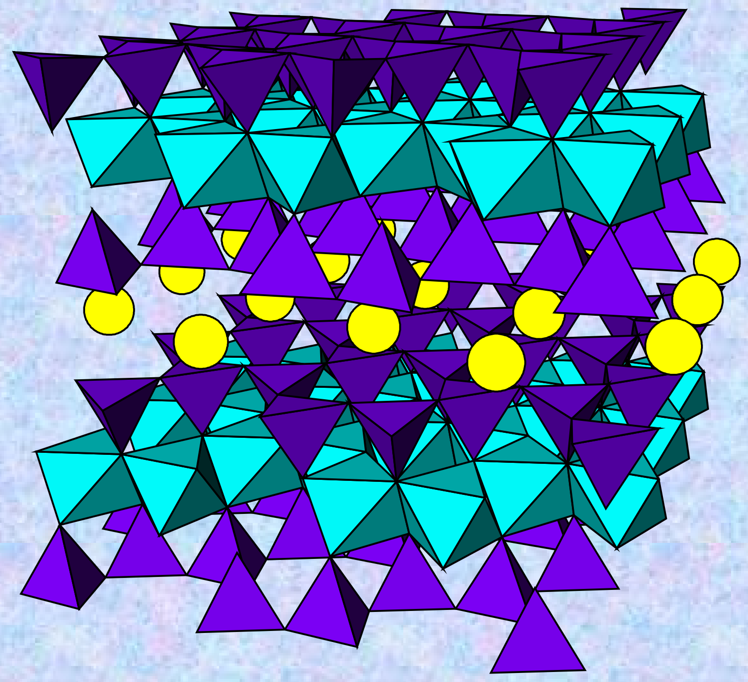
The behaviour is related with the defect breather

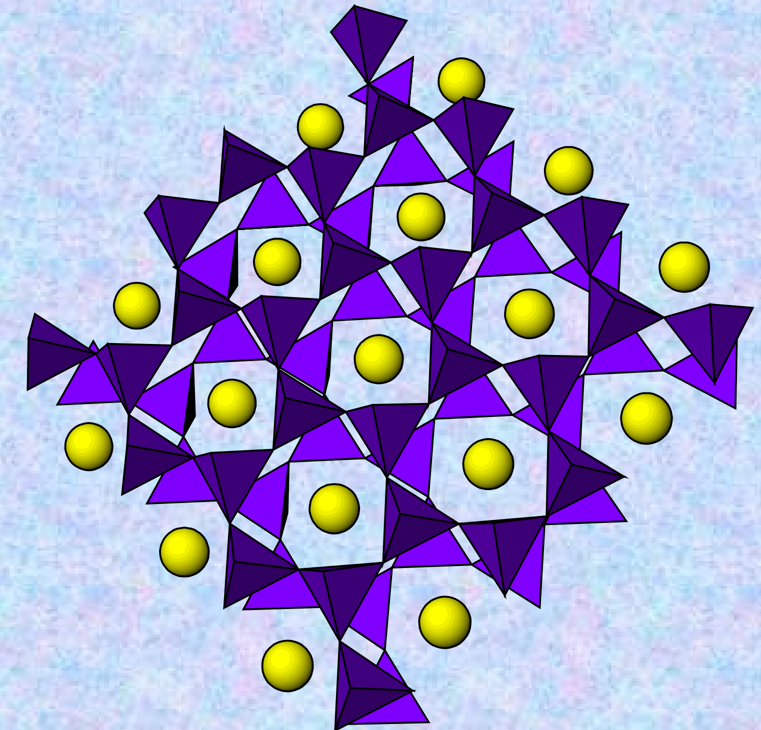
Influence of moving breathers on vacancies migration.
J Cuevas, C Katerji, JFR Archilla, JC Eilbeck and FM Russell
Phys. Lett. A 315(5):364-371, 2003

Two dimensional networks



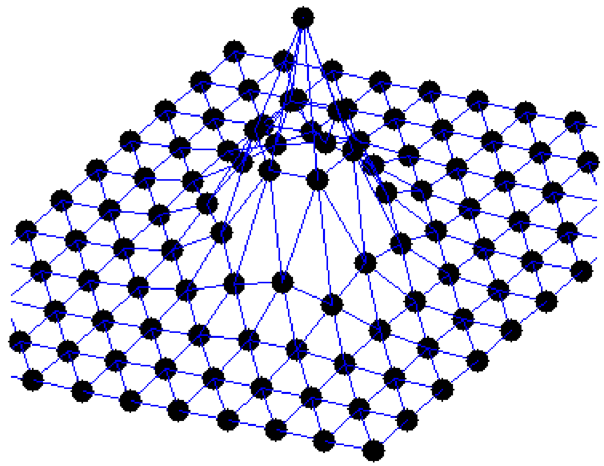
Example: moscovite mica



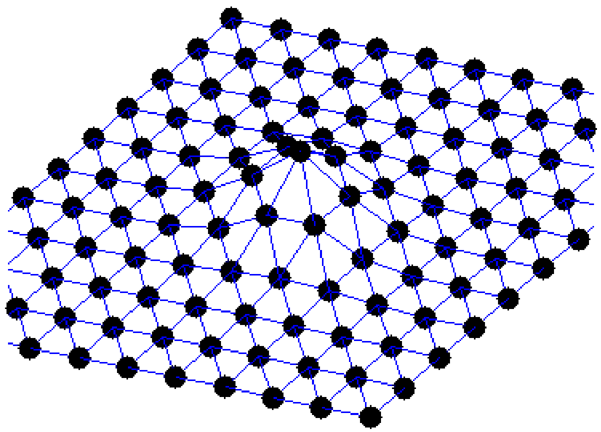


● K^+

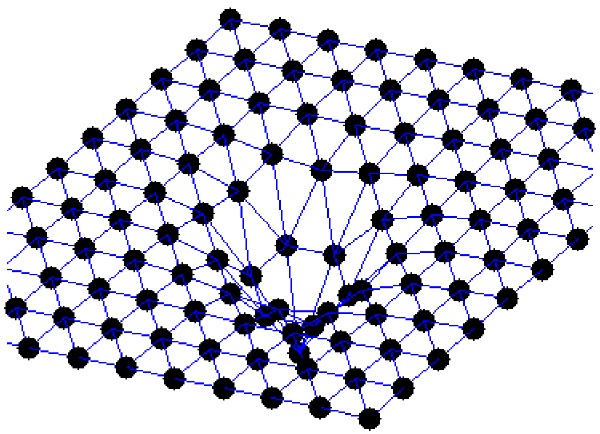
Breathers in mica



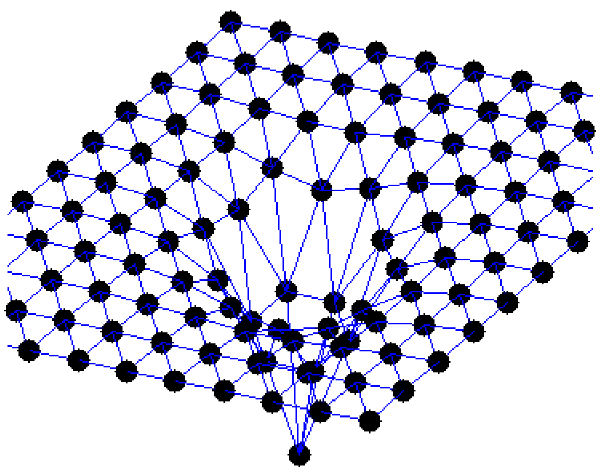
Breathers in mica



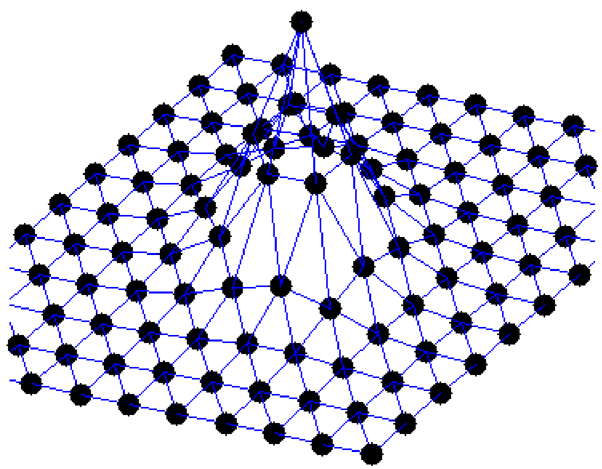
Breathers in mica



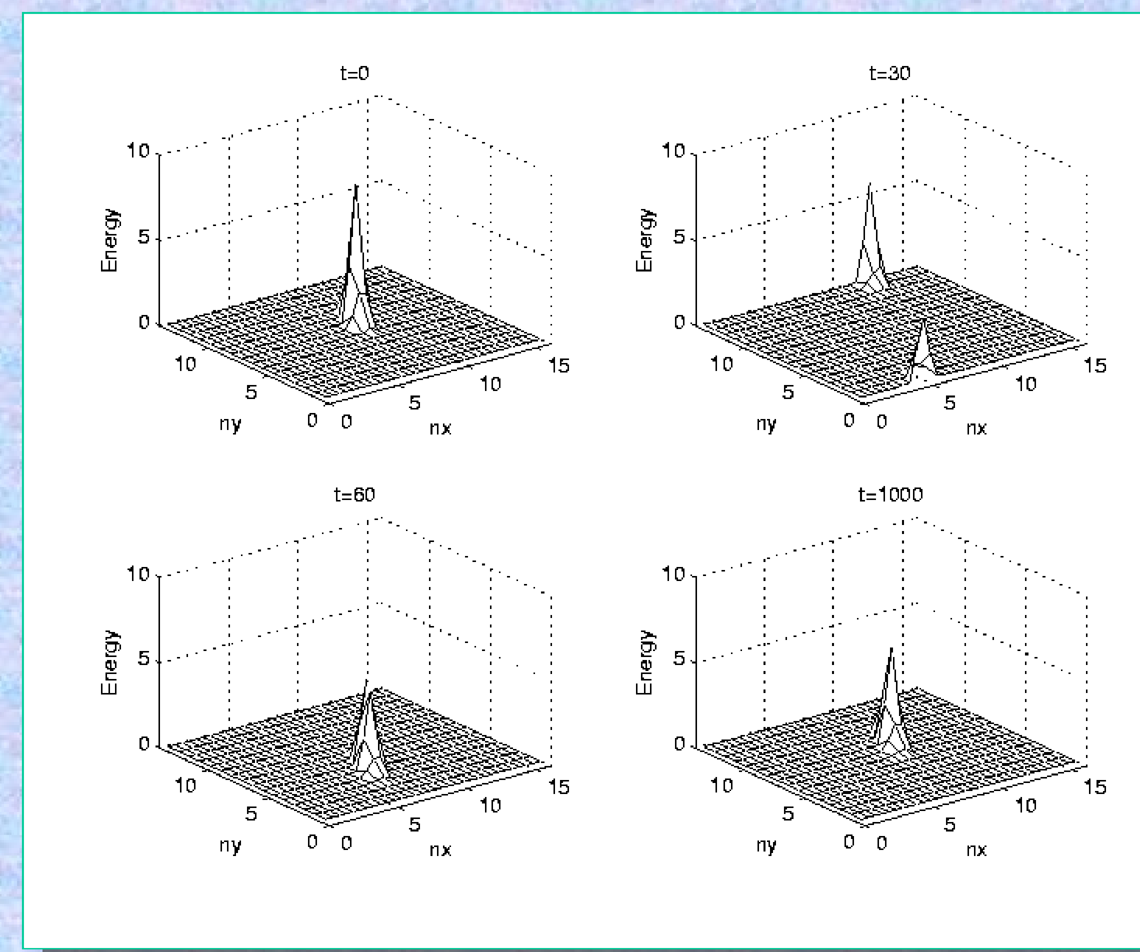
Breathers in mica



Breathers in mica



Moving breathers 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

Breathers in mica

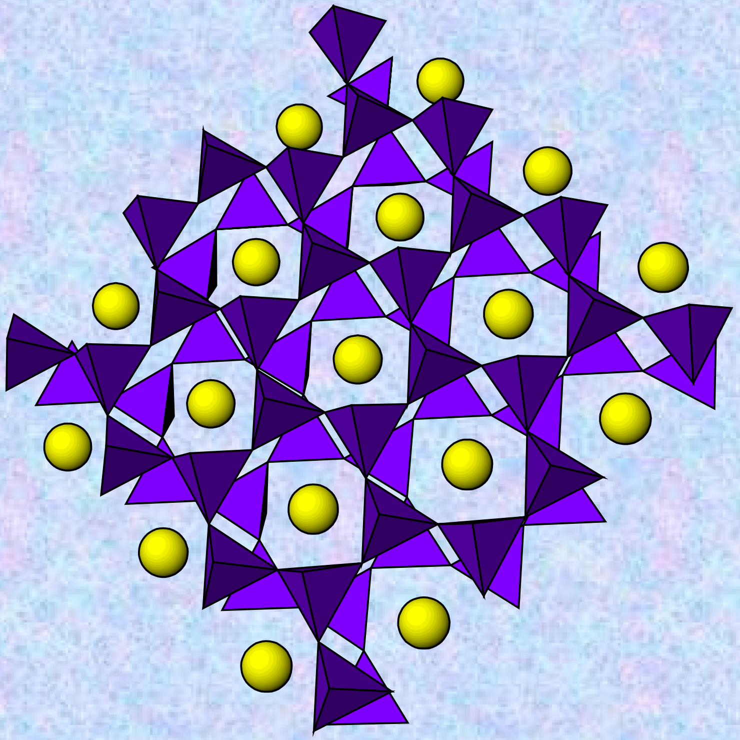
Steps:

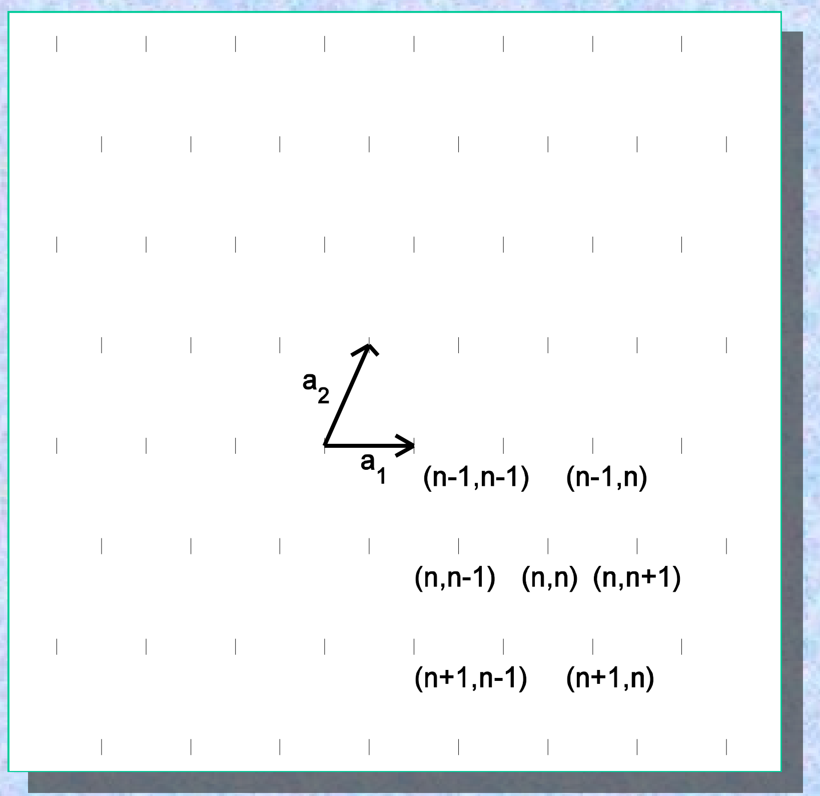
- Find the vibration mode
- Construct the model
- Obtain parameter values
- Obtain breather energies and frequencies

Later:

- Are their energies high enough to influence the reaction rate?
- Are there enough of them?

Mode: vibration of K^+ normal to the cation layer





Mathematical model

Hamiltonian

$$H = \sum_{\vec{n}} [\tfrac{1}{2} m \dot{u}_{\vec{n}}^2 + V(u_{\vec{n}}) + \tfrac{1}{2} k \sum_{\vec{n}'} (u_{\vec{n}} - u_{\vec{n}'})^2]$$

Harmonic coupling

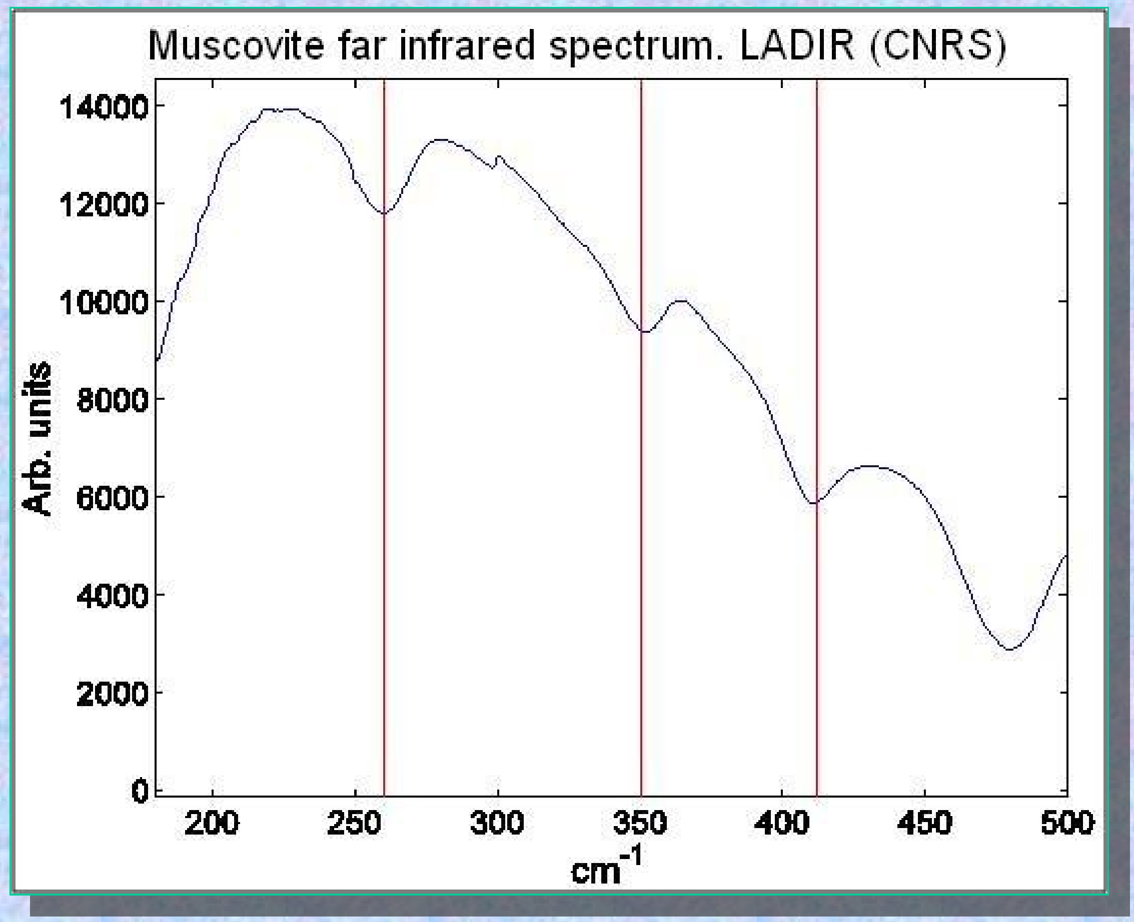
• k=10±1 N/m (D. R. Lide Ed., *Handbook of Chemistry and Physics,* CRC press 2003-2004)

Local potential *V*

• Assignement of far infrared absorption bands of K^+ in muscovite, [Diaz et al, *Clays Clay Miner.,* **48**, 433 (2000)] with a band at 143 cm^{-1}.

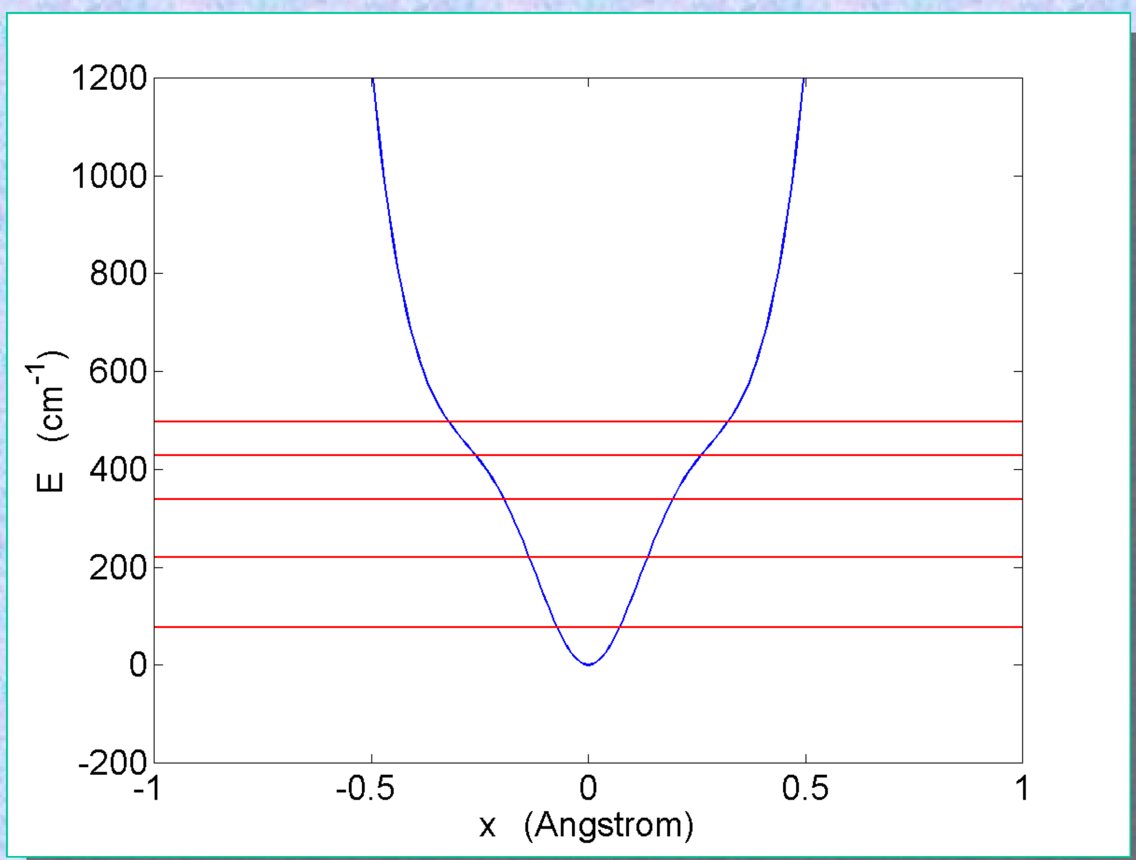
The nonlinear potential has to be obtained.

Mica far infrared spectrum obtained at LADIR-CNRS



Bands at 143, 260, 350 and 420 cm^{-1} are assigned to transitions of K^+ vibrations

Fitting the nonlinear potential $\hat{H}\Psi = E\Psi$



$V(x) =$
$D\left([1 - \exp(-b^2 x^2)] + \gamma x^6 \right)$

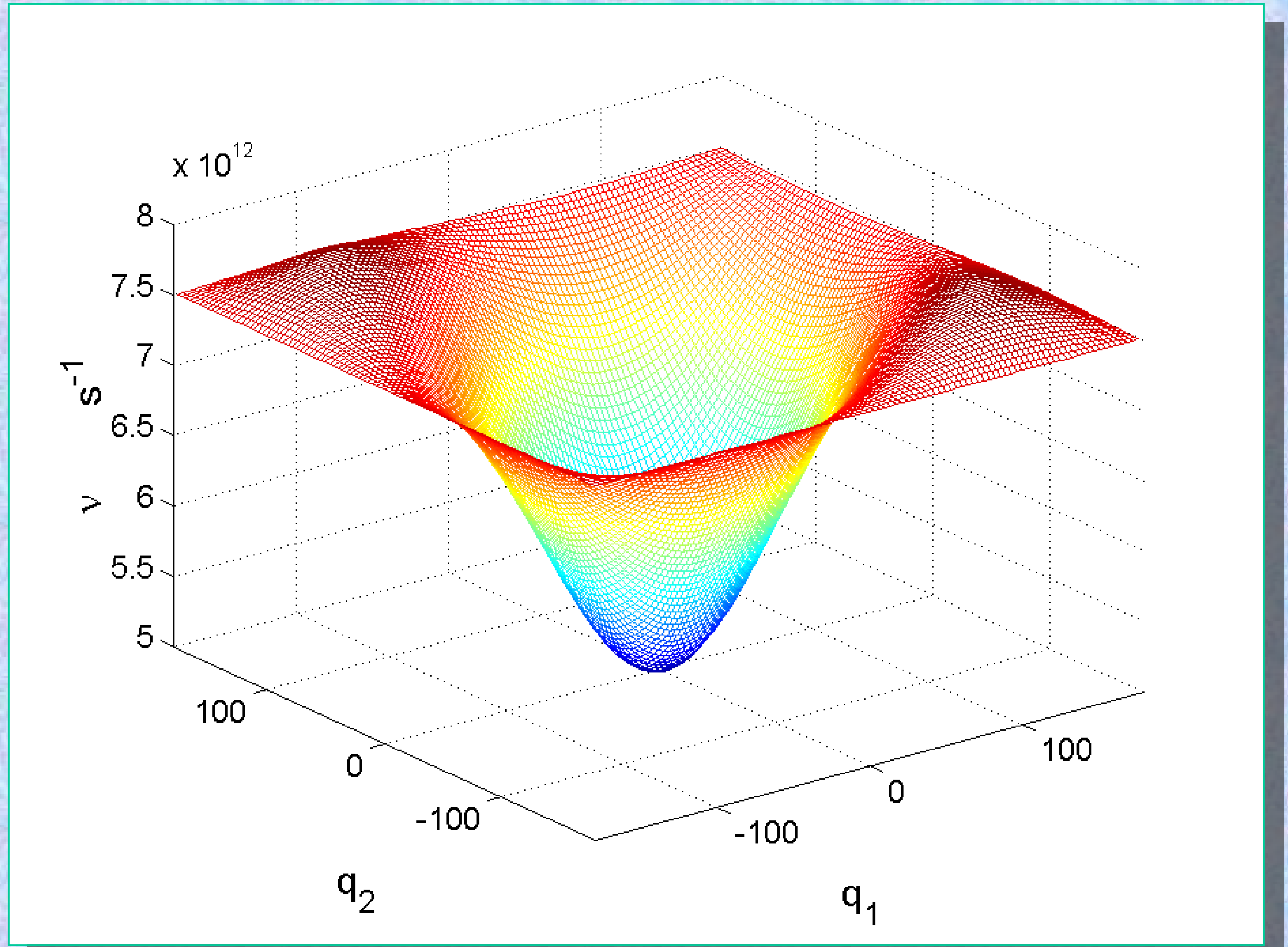
$D = 453\ cm^{-1}$
$b^2 = 36\ Å^{-2}$
$\gamma = 49884\ cm^{-1}\ Å^{-6}$

$cm^{-1} \sim 1.24 \times 10^{-4}$ eV
$1 eV \sim 8000\ cm^{-1}$

Consistent with the available space for K^+ 2x1.45 Å

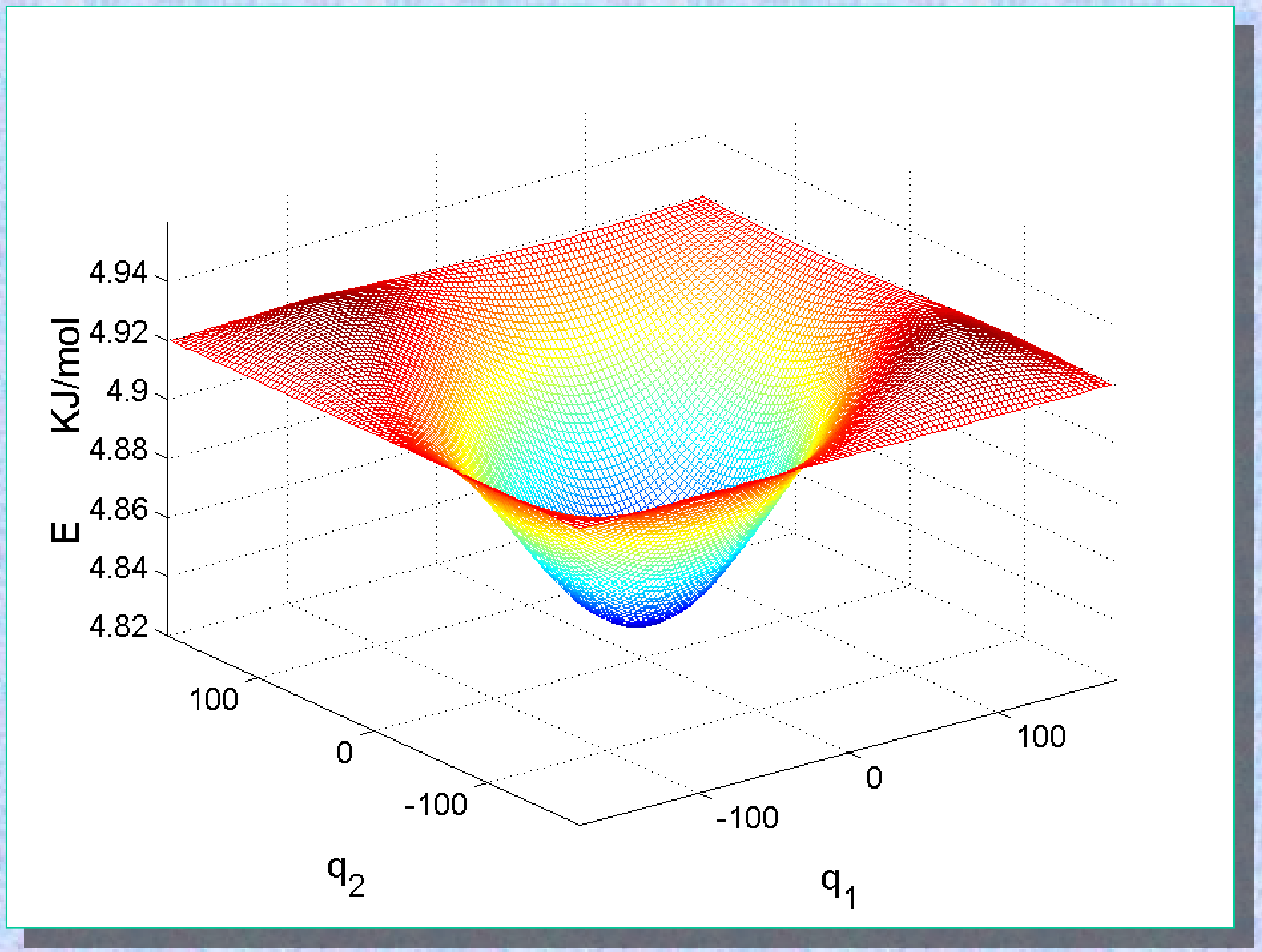
Phonon band

$\nu_f \in [5\ ,\ 7.8]$ THz



$\nu^2 = (\nu_0)^2[1+4\ \varepsilon(\text{sen}^2(q_1/2)+\text{sen}^2(q_1/2)+\text{sen}^2(q_2/2-q_1/2))]$

Mean energy of each phonon mode



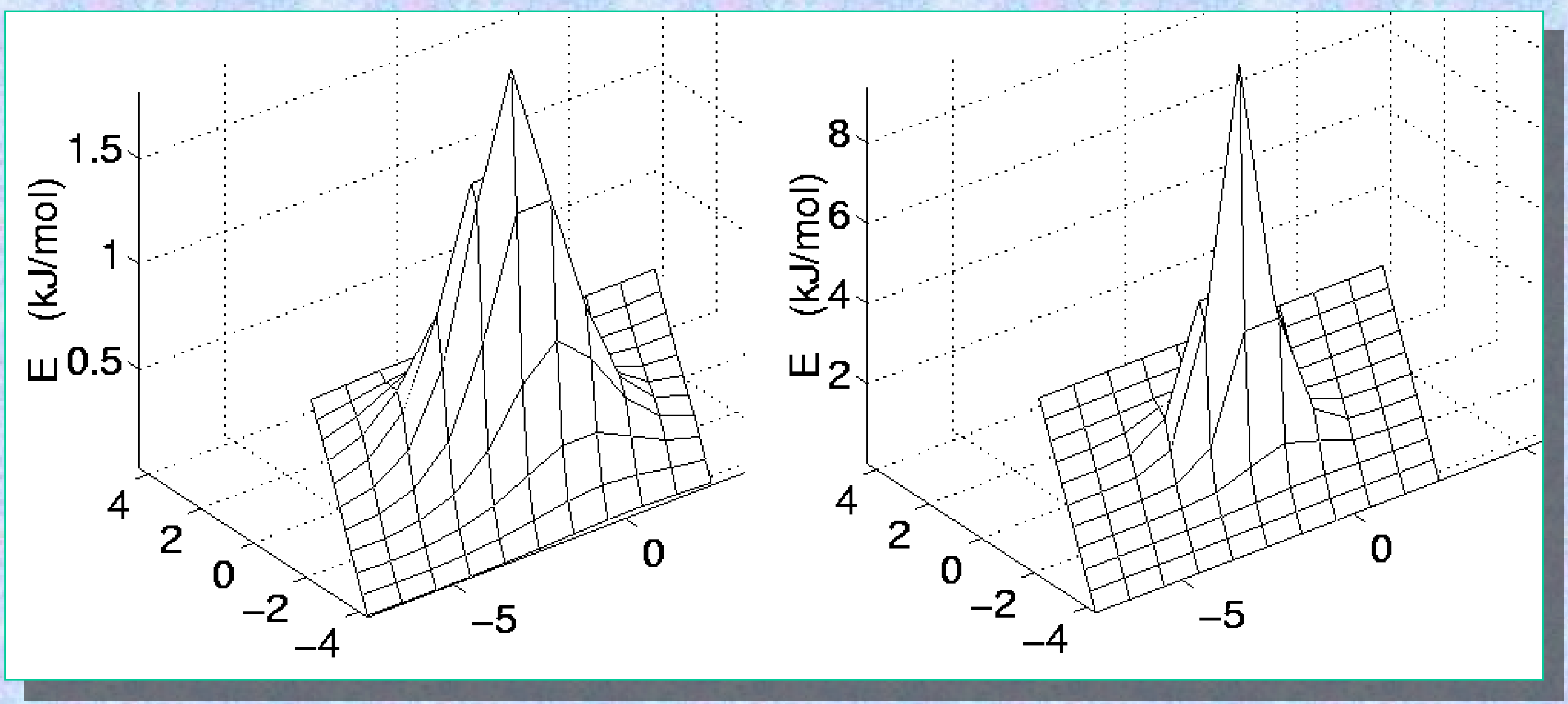
$<E_{ph}>=(n+0.5)\ h\nu$

$n=1/(e^{\beta h\nu} -1)$

T=573 K

1eV~100 KJ/mol

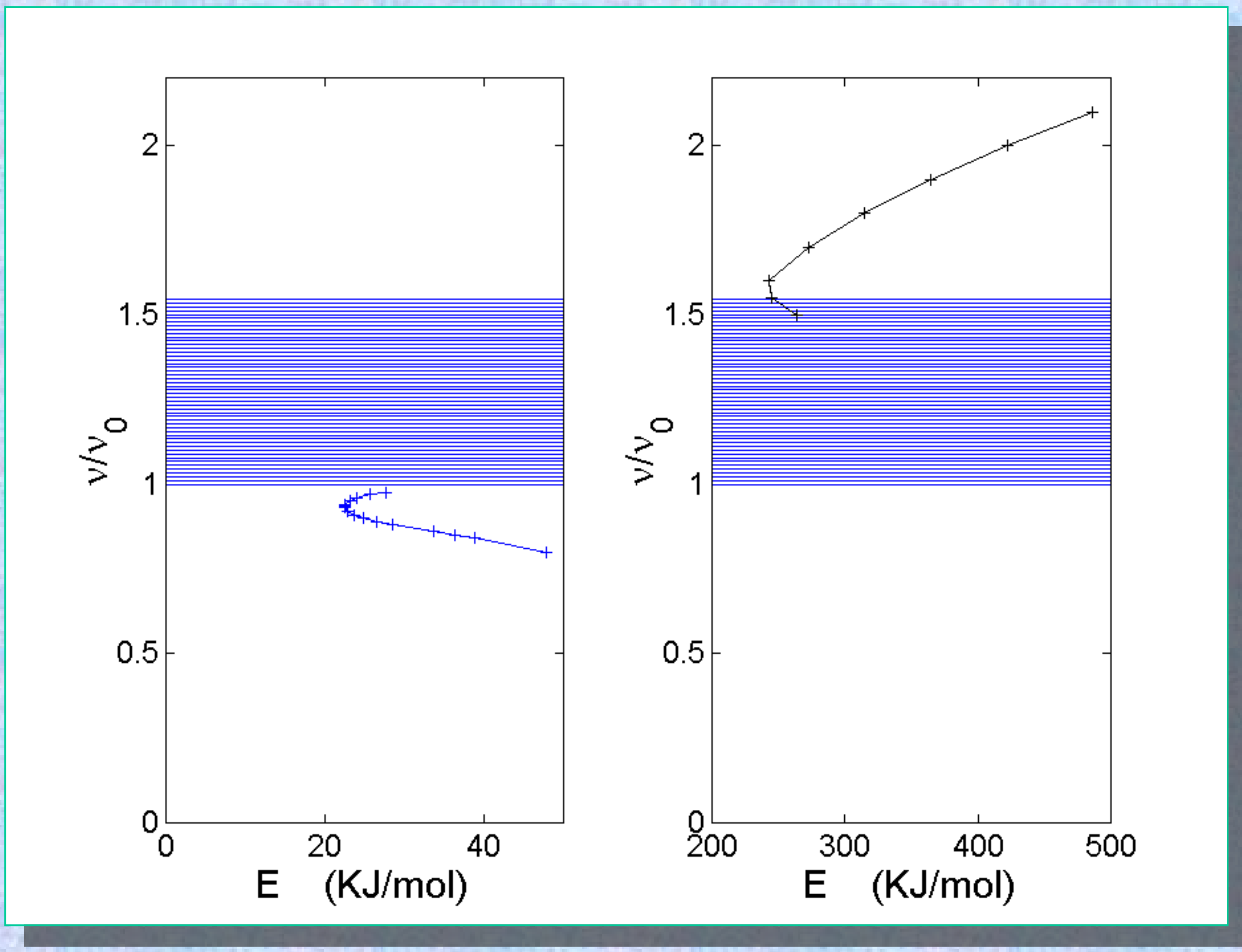
Energy density profiles for two soft breathers



ν_b=0.97ν_0, E =25.6 kJ/mol ν_b =0.85 ν_0, E =36.3 kJ/mol

ν_0= 167.5 cm^{-1} ~ 5·10^{12} Hz

Breather frequency versus energy



$\nu_0 = 167.5 cm^{-1}$
$\sim 5 \cdot 10^{12}$ Hz

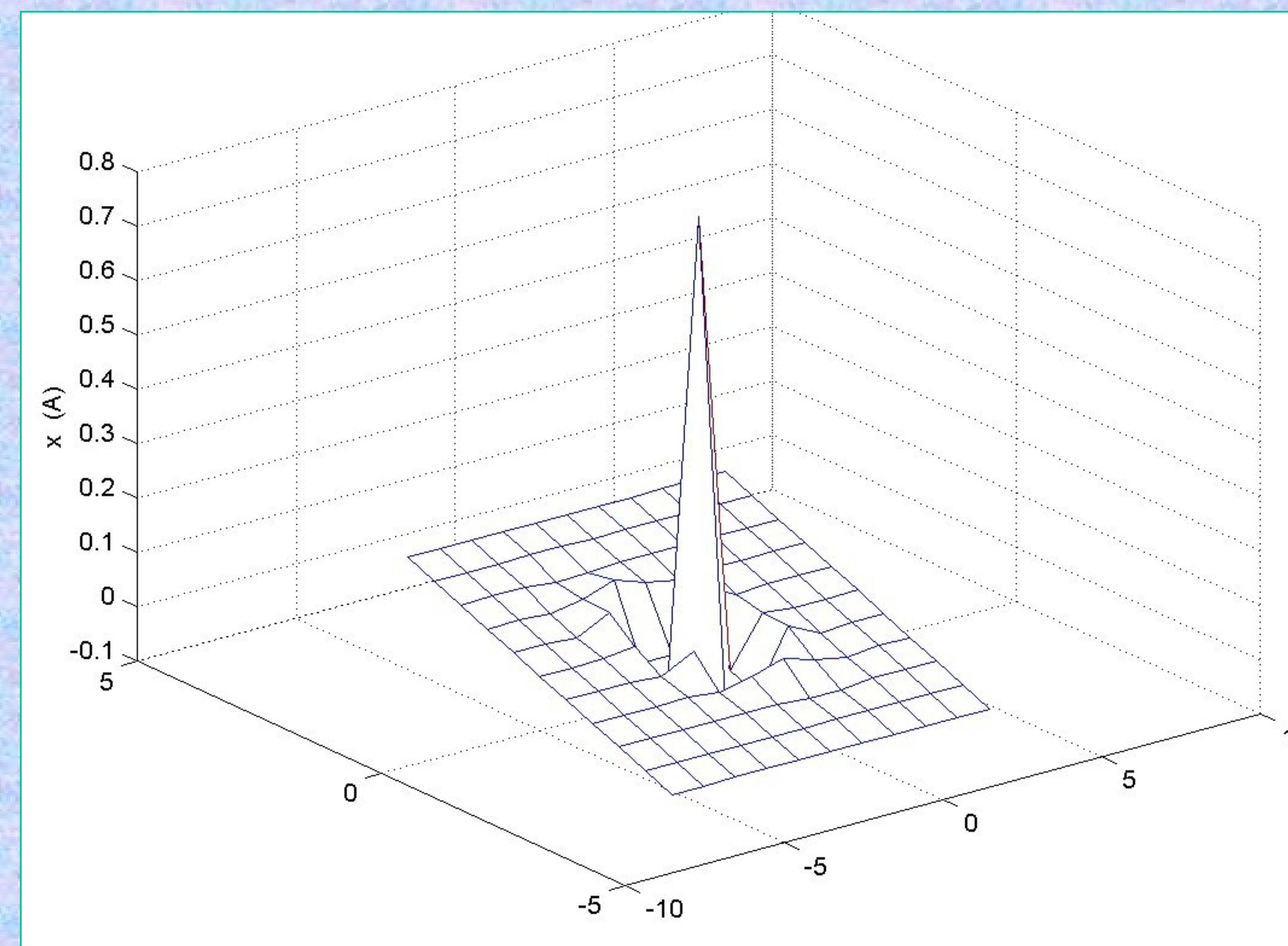
Mimimum energies
Δ_s = 22.4 kJ/mol

Δ_h = 240 kJ/mol

Activation energy
estimated in
100-200 kJ/mol

BREATHERS HAVE LARGER ENERGIES THAN THE ACTIVATION ENERGY

Profile of a hard breather



$\nu = 1.7\ \nu_0 =$ 8.54 THz

E=272 KJ/mol

¿How many phonons? ¿How many breathers? ¿With which energies?

Phonons: fraction of phonons per site with energy larger than Ea : $C_{ph}(E_a) = \exp(-E_a/RT)$

Breathers:

•Numerically: $\langle n_B \rangle \sim 10^{-3}$ por K^+

•Theory: Piazza et al, Chaos **13,** 589 (2003)]

2D breather statistics: Piazza et al, 2003

1.- They have a minimum energy: Δ

2.- Rate of breather creation: $B(E) \propto \exp(-\beta E)$, $\beta = 1/k_B T$

3.- Rate of breather destruction: $D(E) \propto 1/(E-\Delta)^z$

Large breathers live longer.

4.- Thermal equilibrium: if $P_b(E)\,dE$ is the probability that a breather energy is between E and E+dE:

$$D(E)\, P_b(E)\, dE = A\, B(E) dE, \qquad A \neq A(E)$$

5.- Normalization: $\int_0^\infty P_b(E)\, dE = 1$

Breathers statistics. Results.

1.-$P_b(E)=\beta^{z+1}(E-\Delta)^z\exp[-\beta(E-\Delta)]/\Gamma(z+1)$

2.- $\langle E\rangle=\Delta+(z+1)\,k_BT$

3.- Most probable energy: $E_p=\Delta+z\,k_BT$

3.-Fraction of breathers with energy above *E*:

$$C_b(E)=\Gamma(z+1)^{-1}\,\Gamma(z+1,\beta[E-\Delta])$$

4.- Mean number of breathers per site with energy above E:

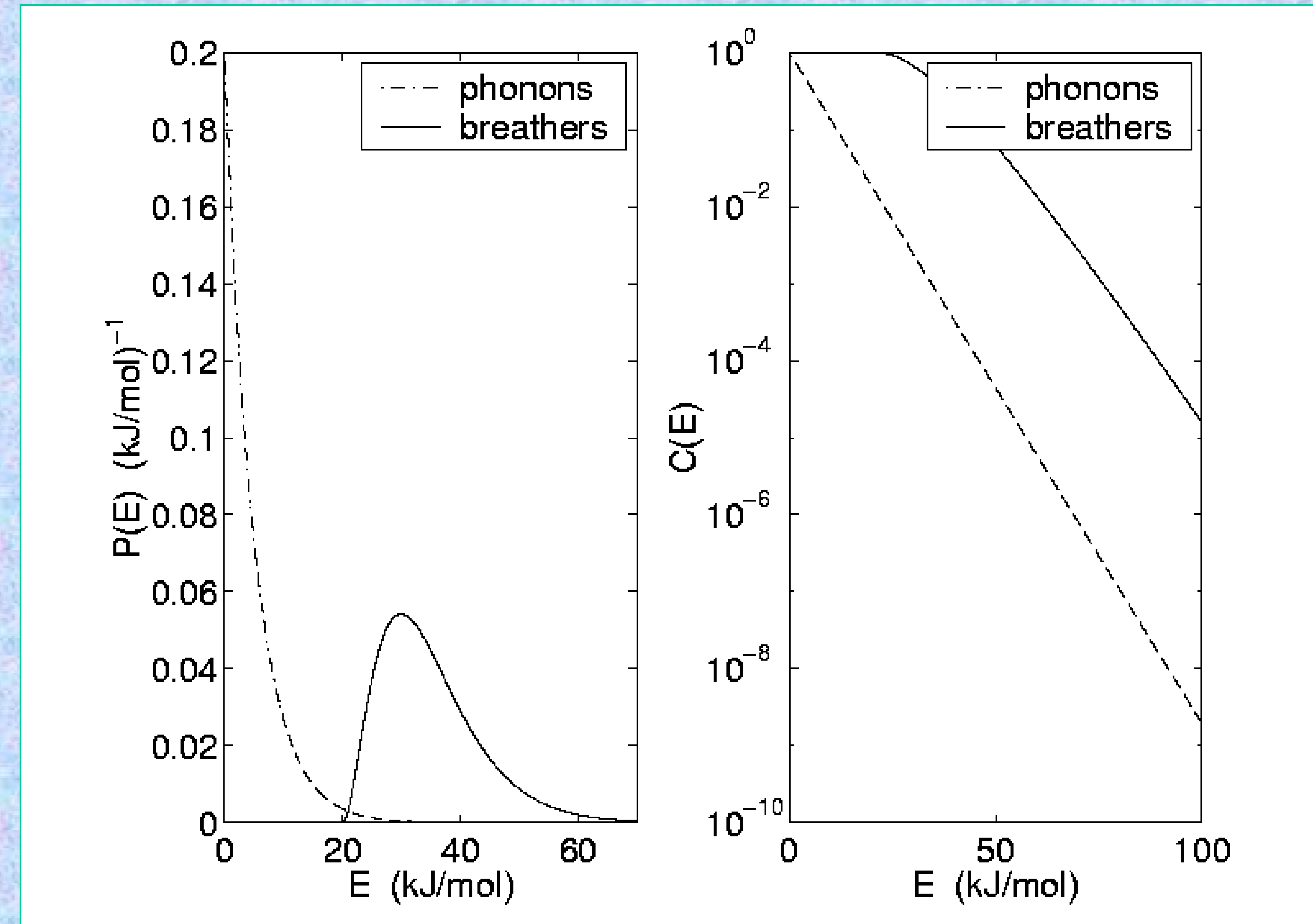
$$n_b(E)=\langle n_b\rangle C_b(E)$$

$\langle n_b\rangle$=mean number of breathers per site $\sim 10^{-3}$

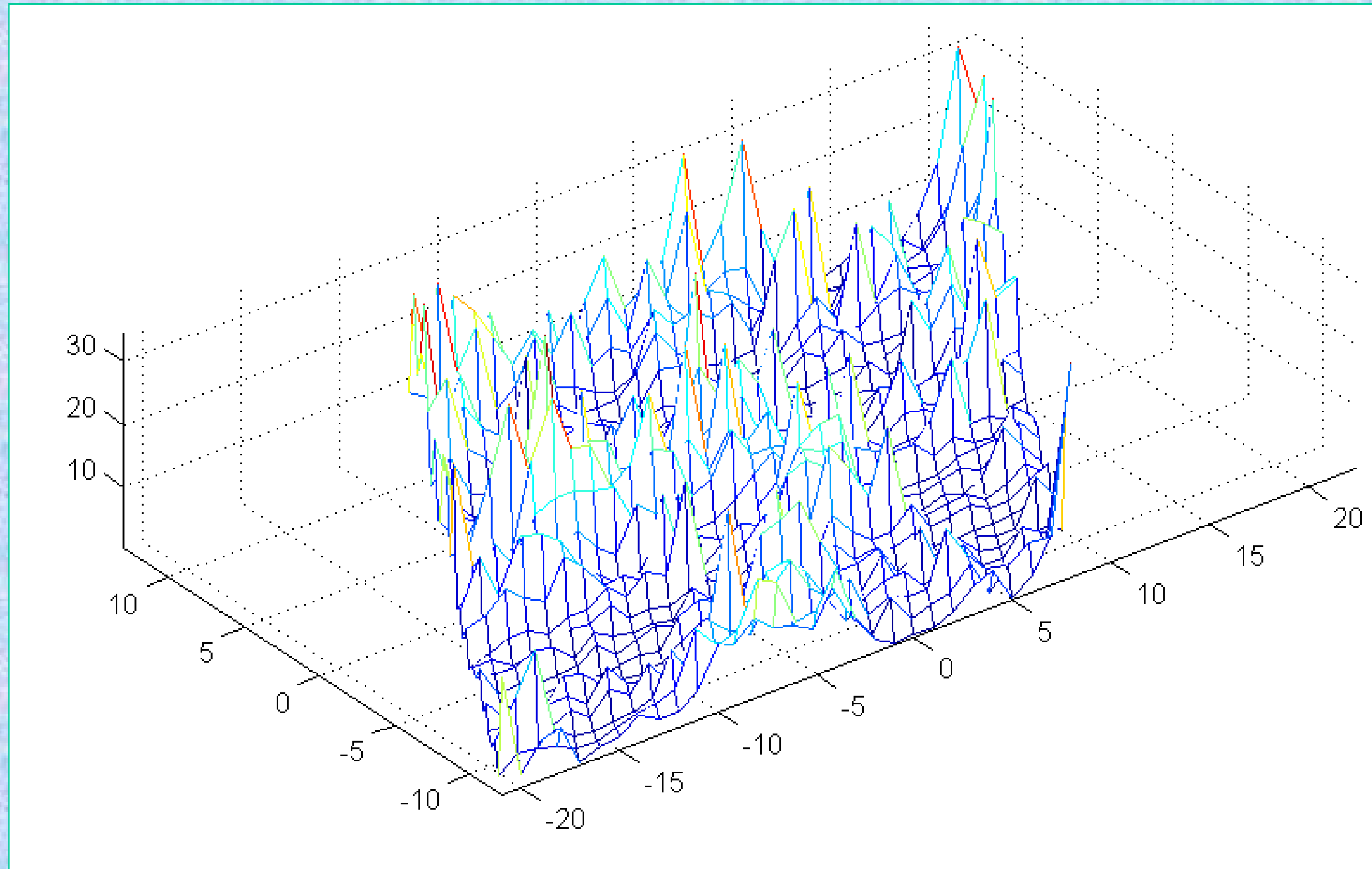
-Function gamma and first incomplete gamma function:

$$\Gamma(z+1)=\int_0^\infty y^z\exp(-y)dy,\quad \Gamma(z+1,x)=\int_x^\infty y^z\exp(-y)dy$$

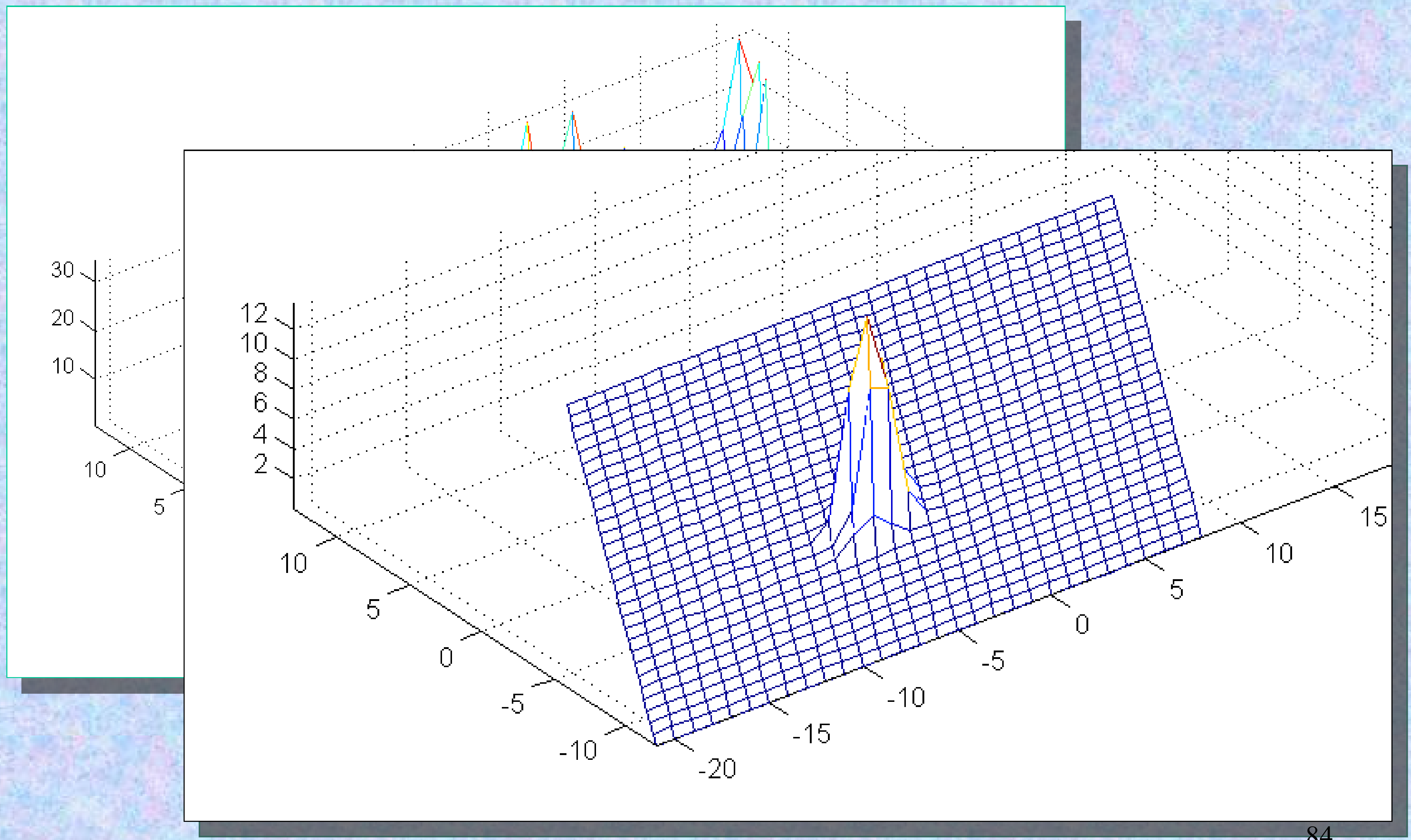
Probability density and cumulative probability. Breathers accumulate at higher energies



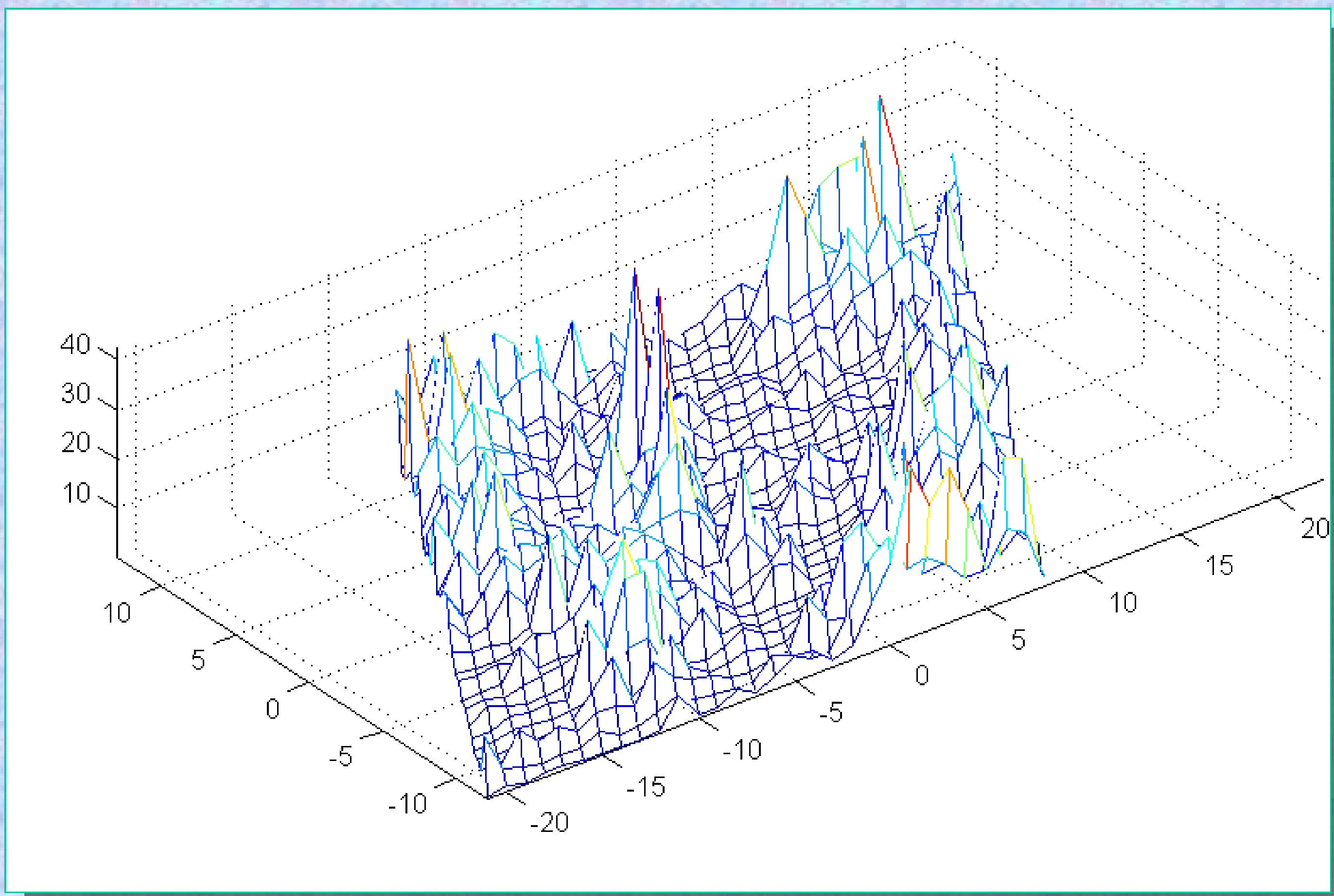
Numerical simulations in mica (1)



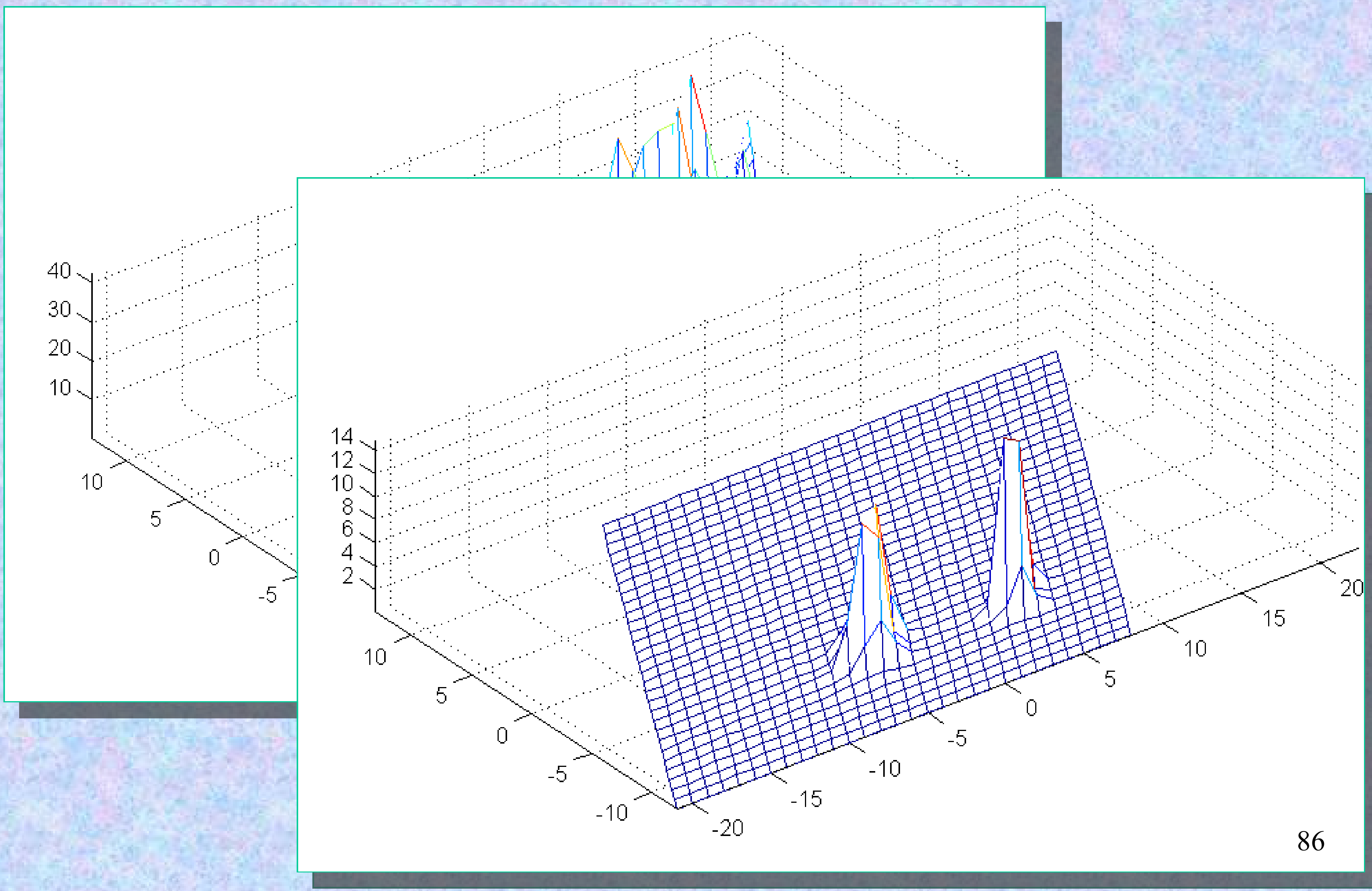
Numerical simulations in mica (1)



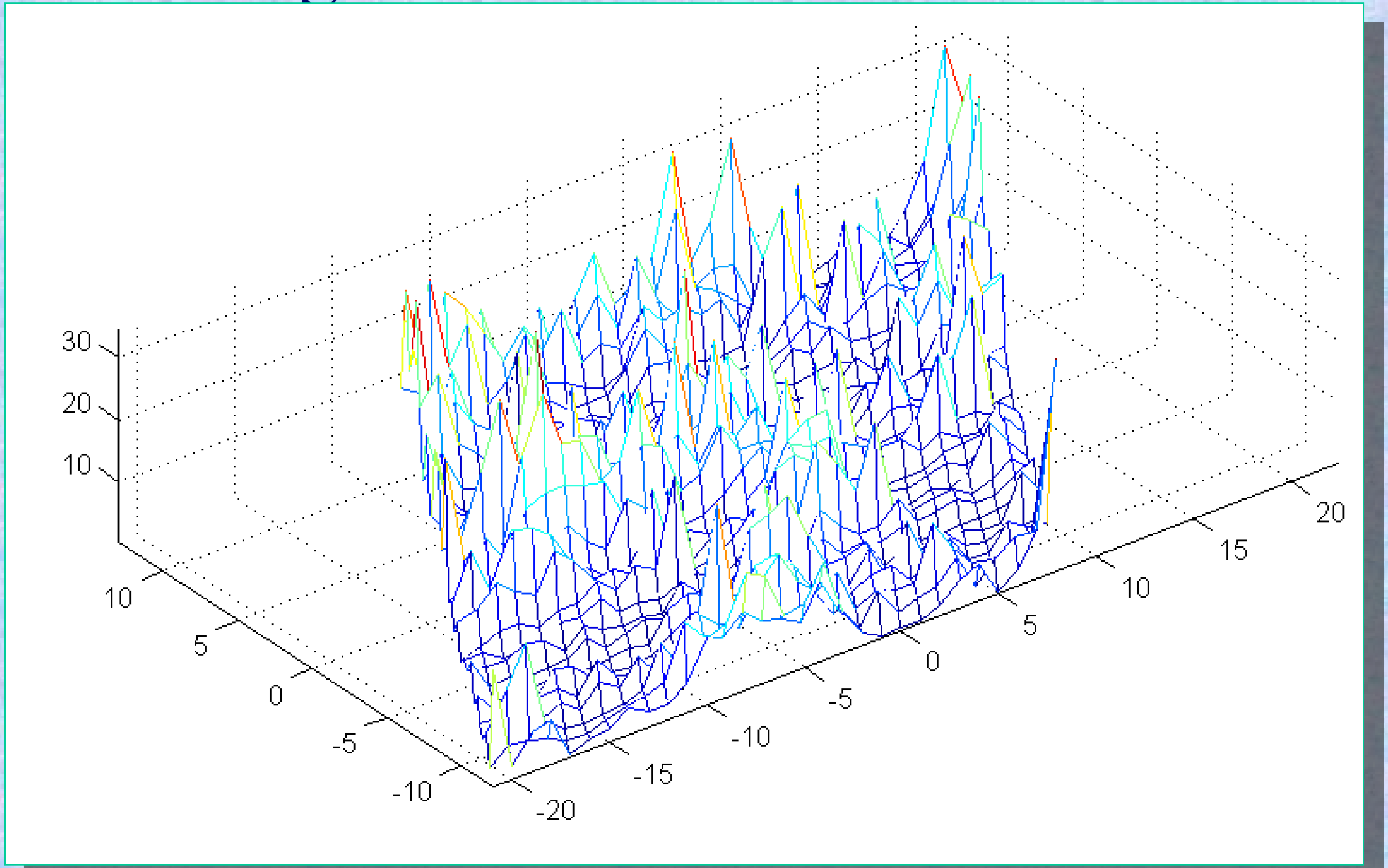
Numerical simulations in mica (2)



Numerical simulations in mica (2)

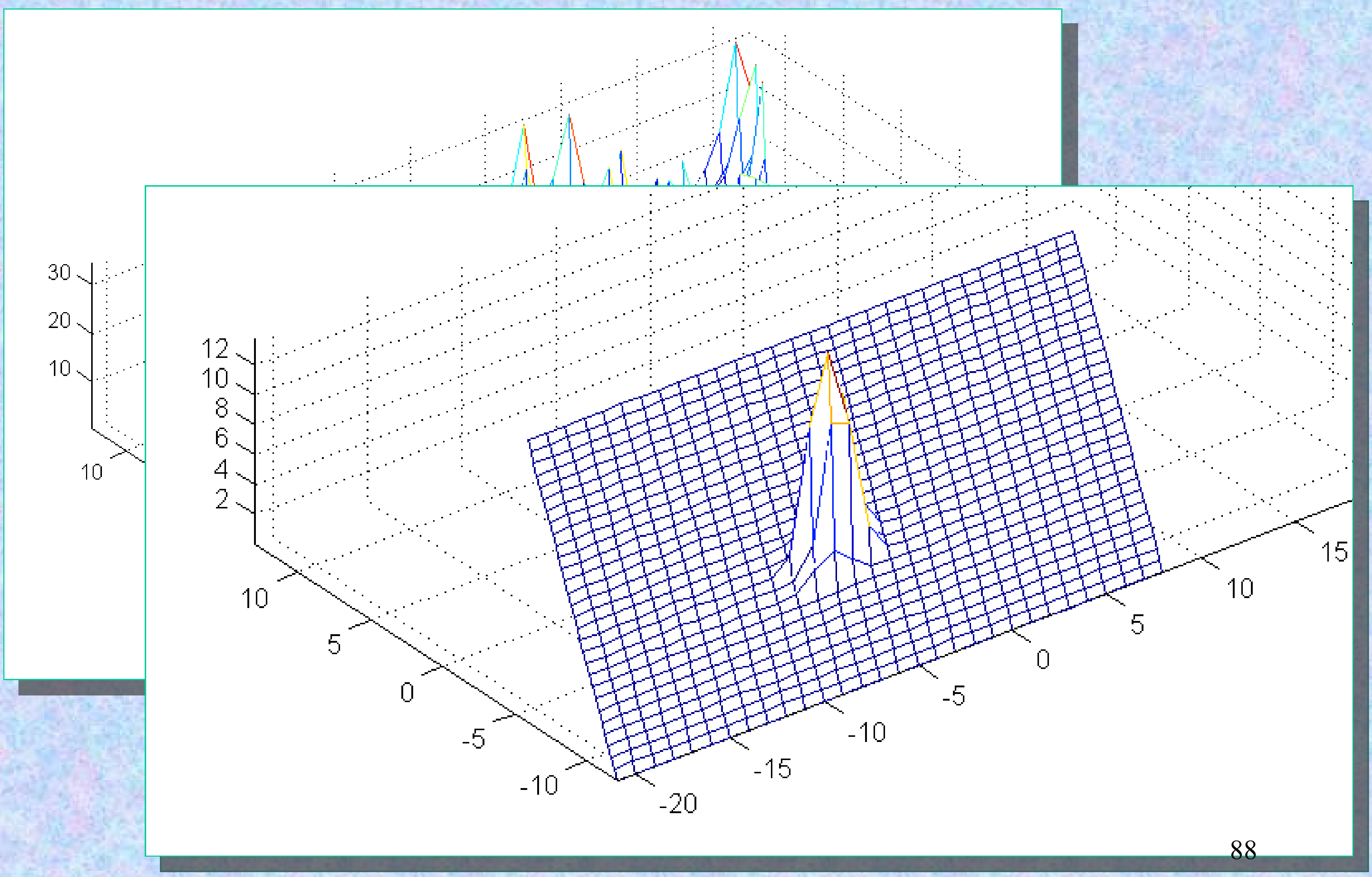


Comparison with numerical simulations in mica. Before cooling.

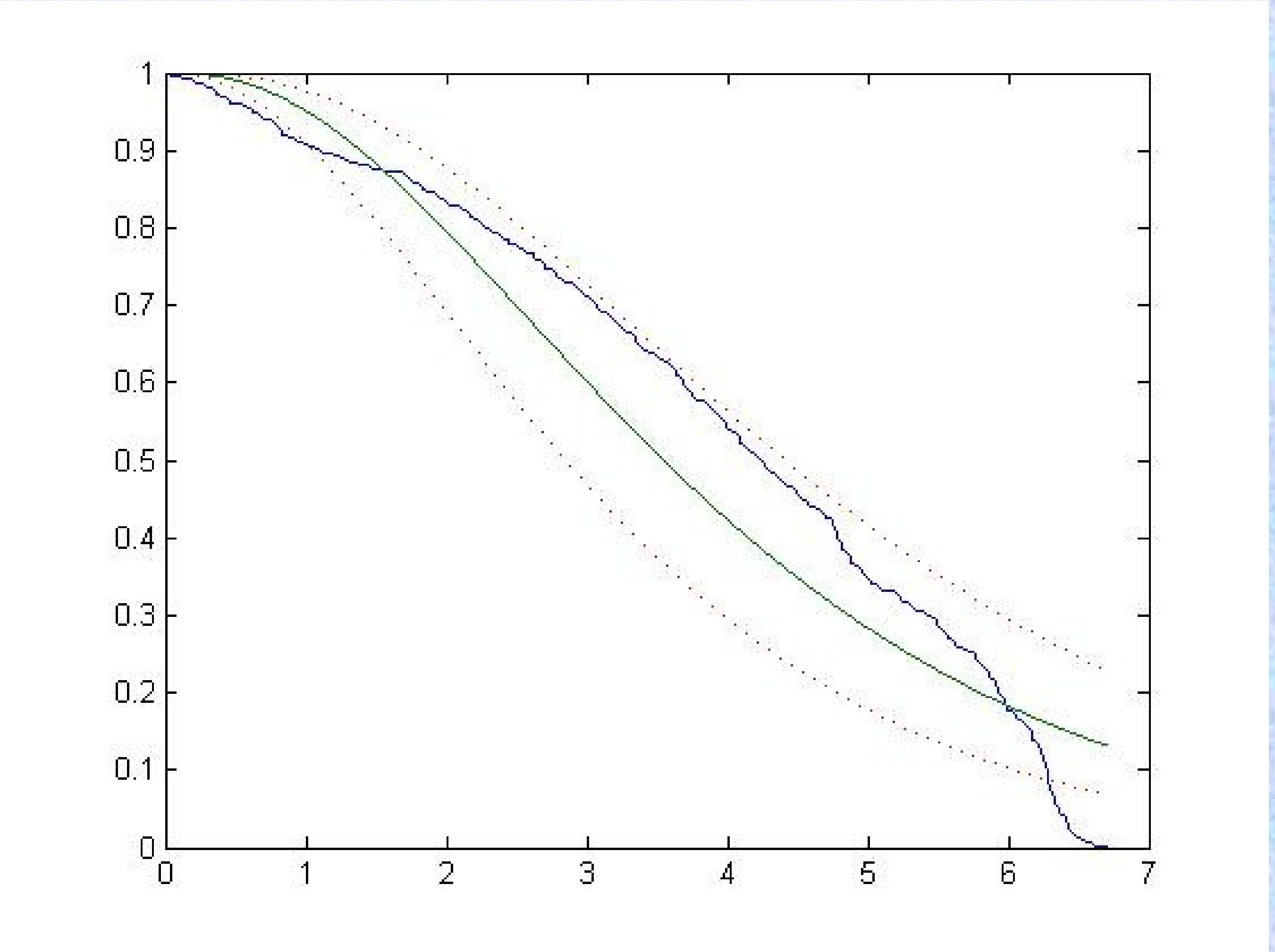


Random velocities and positions. Thermal equilibrium.
Cooling at the borders.

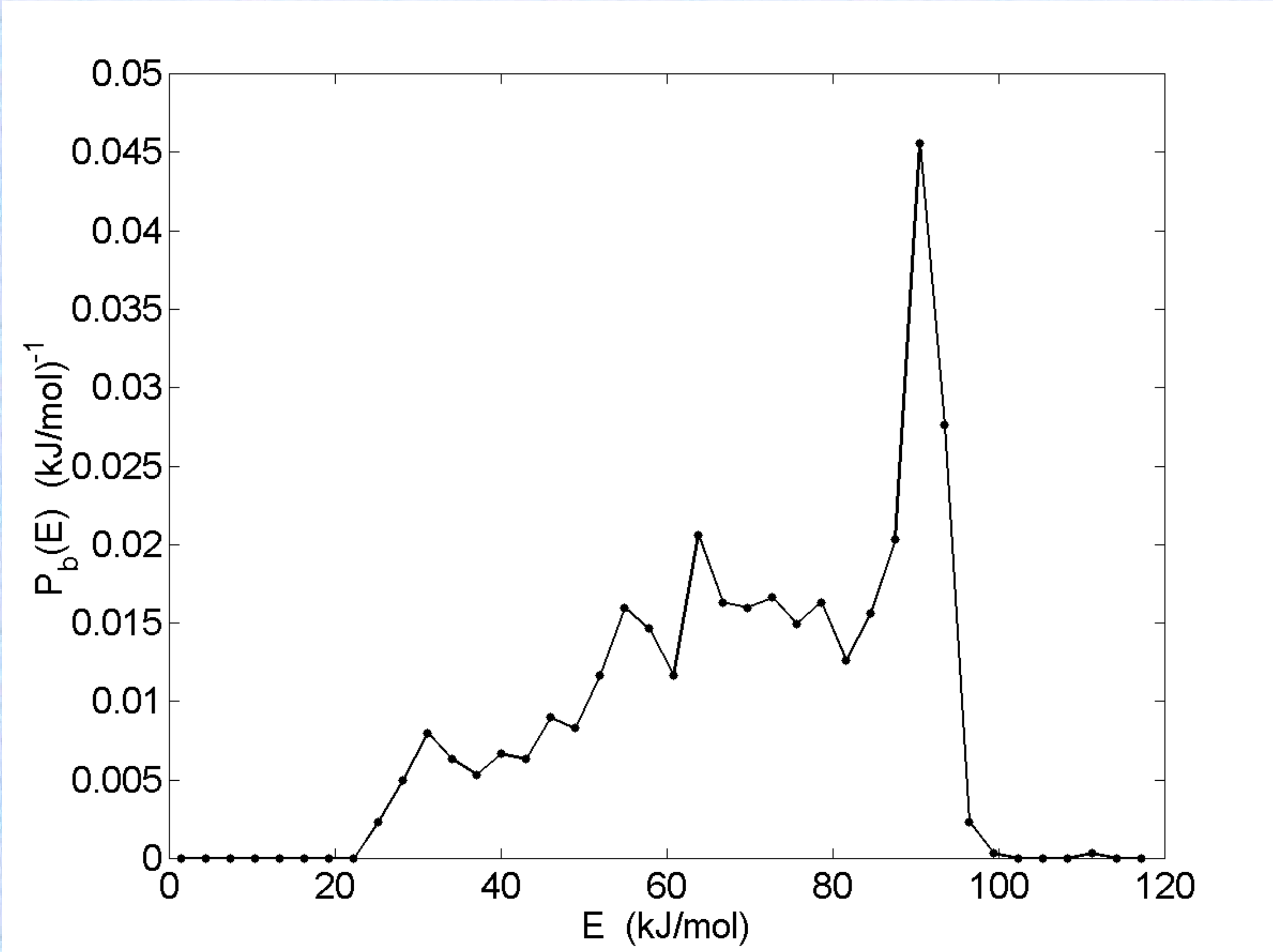
Numerical simulations in mica. After cooling.



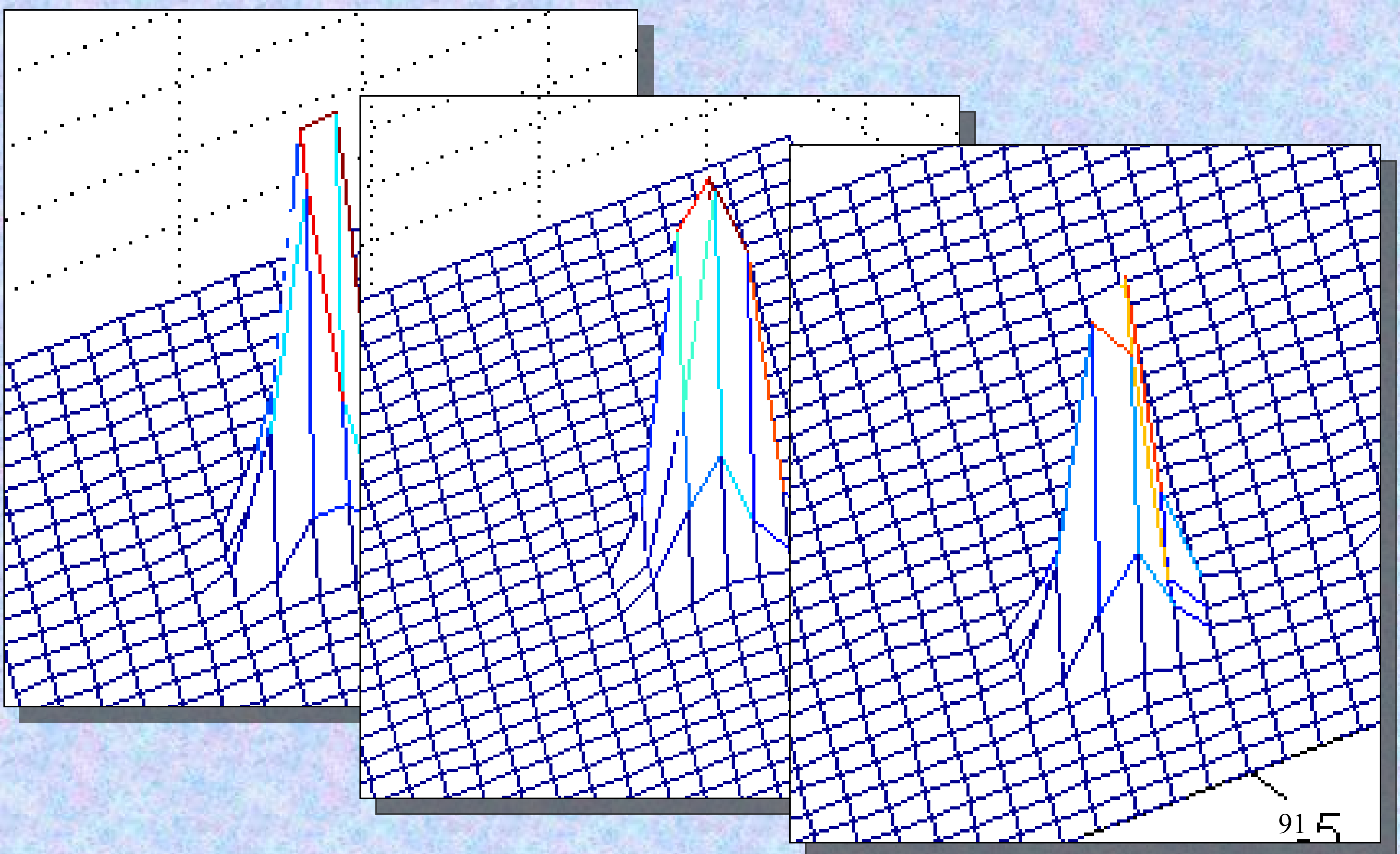
Attemp to fit $C_B(E)$: failure.



Total failure: $P_b(E)$



Reason: different breathers and multibreathers



Modification of the theory. Breathers with maximum energy

1.- Multiple breather types

2.- Differences:

- Minimum energy Δ
- Parameter z
- Maximum energy E_M !! :
  - Normalization: $\int_{\Delta}^{E_M} P_b(E)\, dE = 1$

- Different probability for each type of breather:

$$P(\Delta, z, E_M, ?)$$

Breathers with maximum energy. Results.

1.- Probability density:

$$P_b(E)= \beta^{z+1} (E- \Delta)^z \exp[- \beta(E- \Delta)]/ \gamma(z+1, \beta[E_M- \Delta])$$

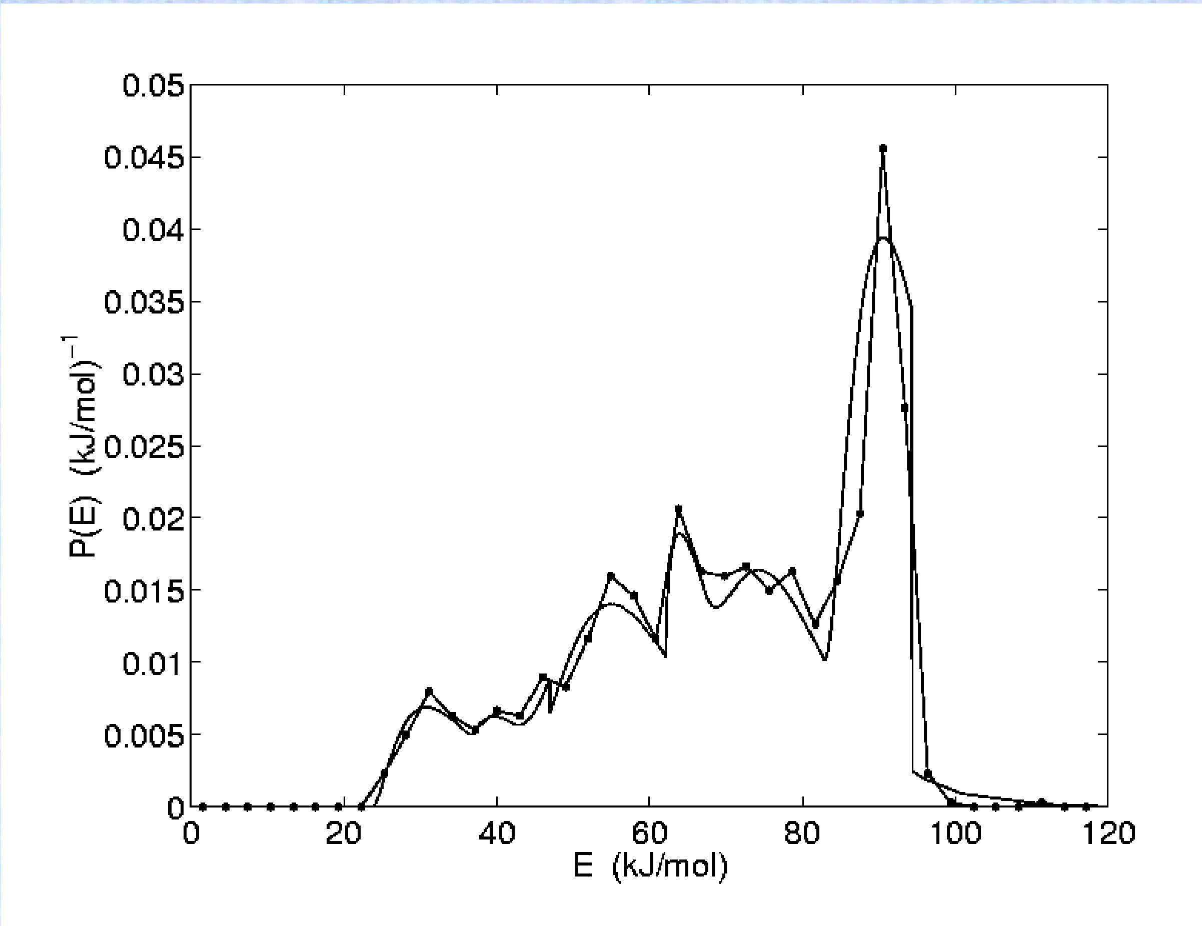
3.- Fraction of breathers with energy above *E*:

$$C_b(E)=1- \gamma(z+1, \beta[E-\Delta])/ \gamma(z+1, \beta[E_M-\Delta])$$

- Second incomplete gamma function:

$$\gamma(z+1,x)= \int_0^x y^z \exp(-y)dy$$

Density probability for breathers in mica

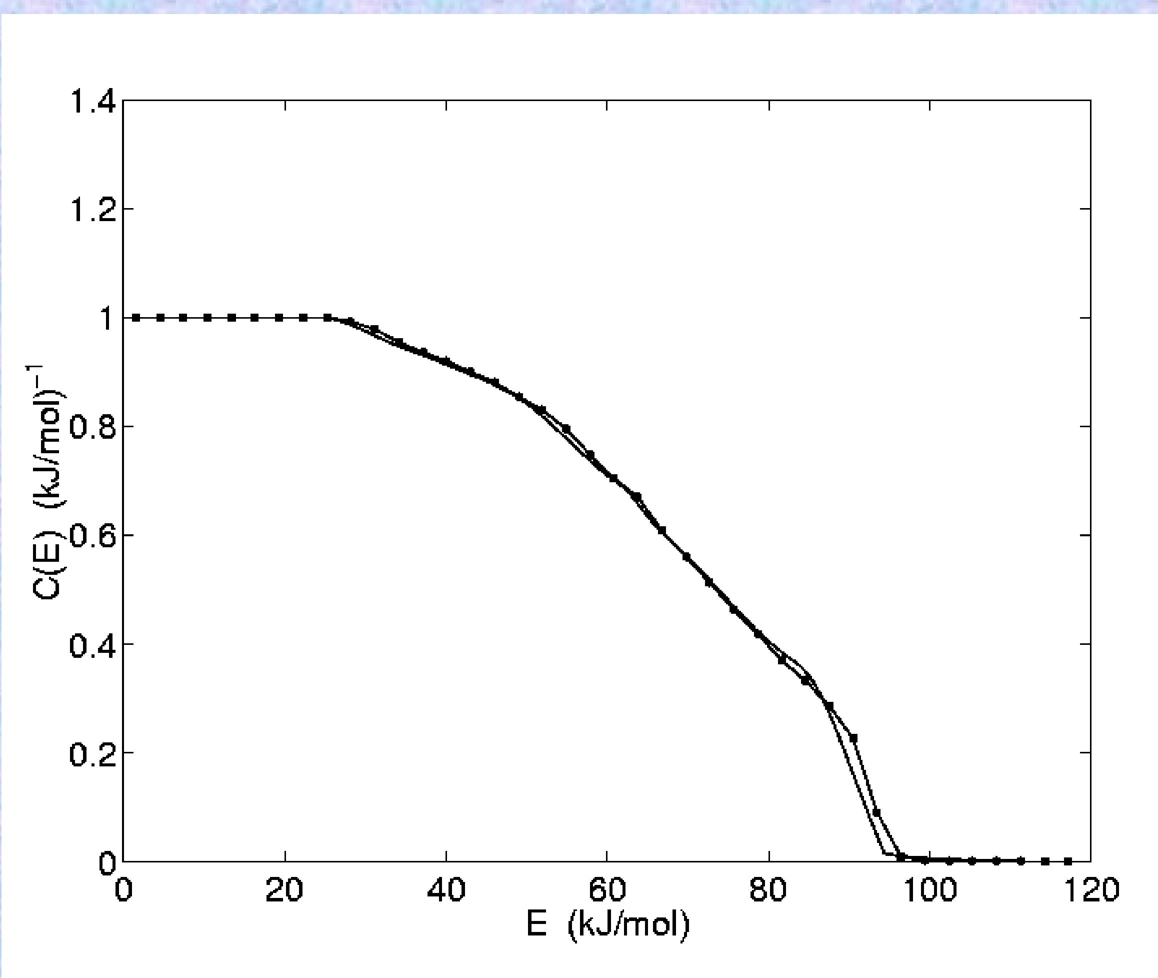


•-- Numerical

— Theoretical

Cumulative probability:

Fraction of breathers with energy equal or larger than E



--•-- Numerical

— Theoretical

Breather energy spectrum

Δ (kJ/mol)	23.9	36.6	41.4	62.2	67.3	82.9
z	1.50	1.17	3.00	0.52	2.07	1.80
E_M (kJ/mol))	-	46.9	-	-	-	94.4
probability	0.103	0.026	0.281	0.097	0.202	0.290

Estimations

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

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

Reaction time without breathers: 80 a 800 años,

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

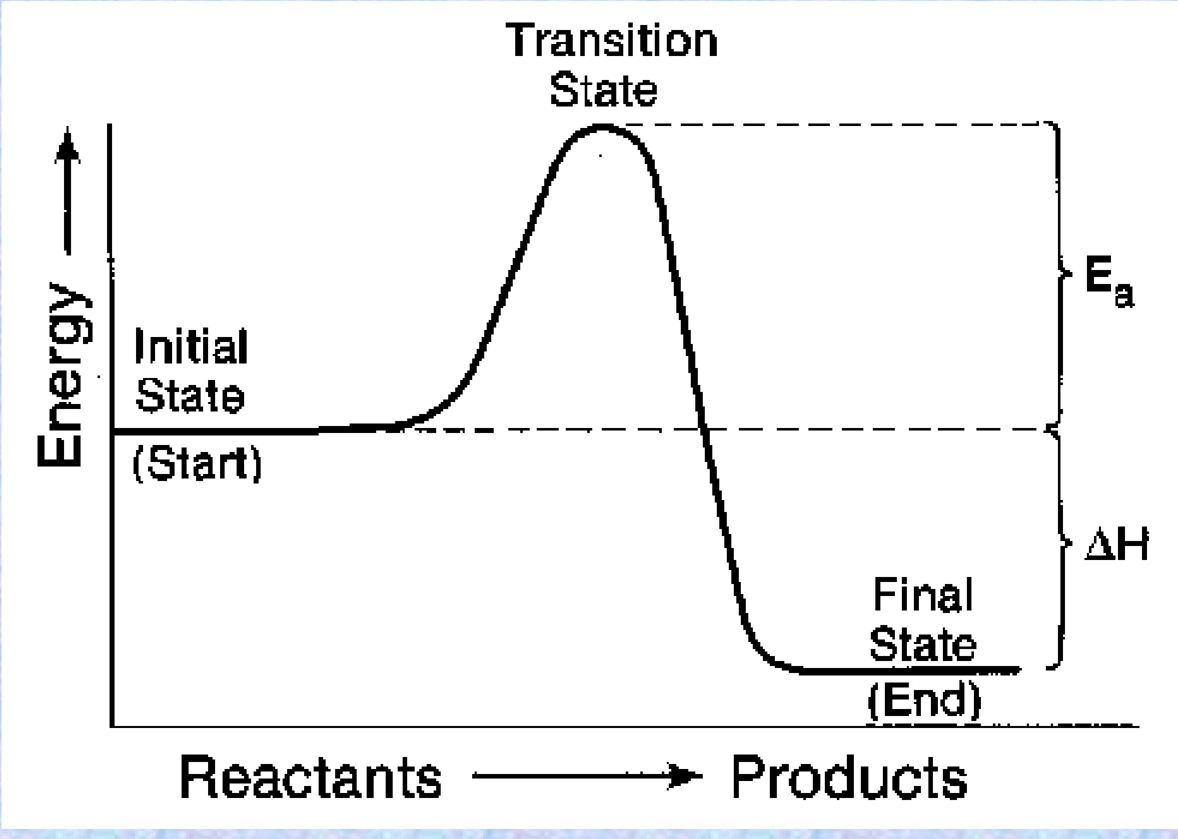
Discrete breathers for understanding reconstructive mineral processes at low temperatures
JFR Archilla, J Cuevas, MD Alba, M Naranjo and JM Trillo,
J. Phys. Chem. B 110 (47): 24112-24120 (2006) DOI:10.1021/jp0631228.

Kramer’s theory revisited

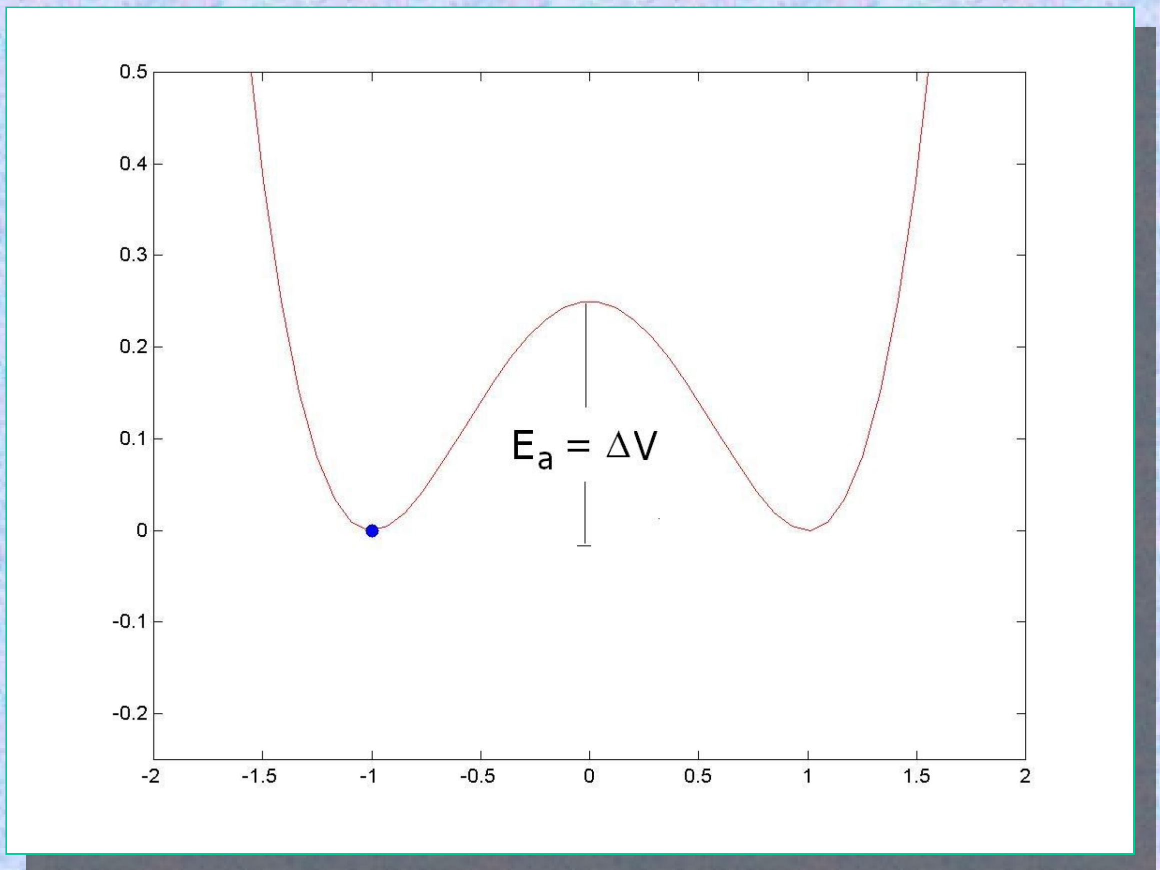
Arrhenius law: $\kappa = A \exp(-E_a/RT)$

Transition state theory

$E\mathbf{a}$~100-200 KJ/mol

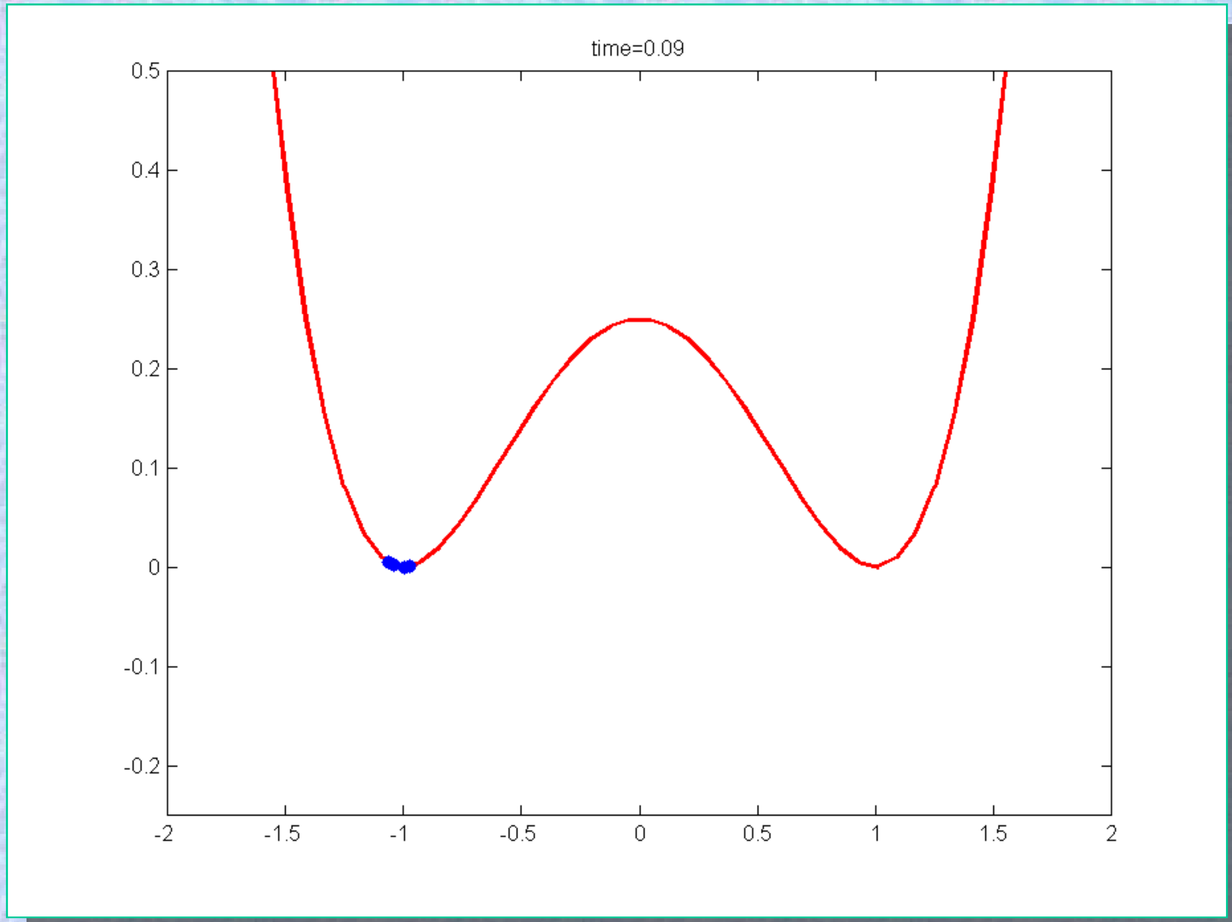


Kramers theory of reaction rate (1)



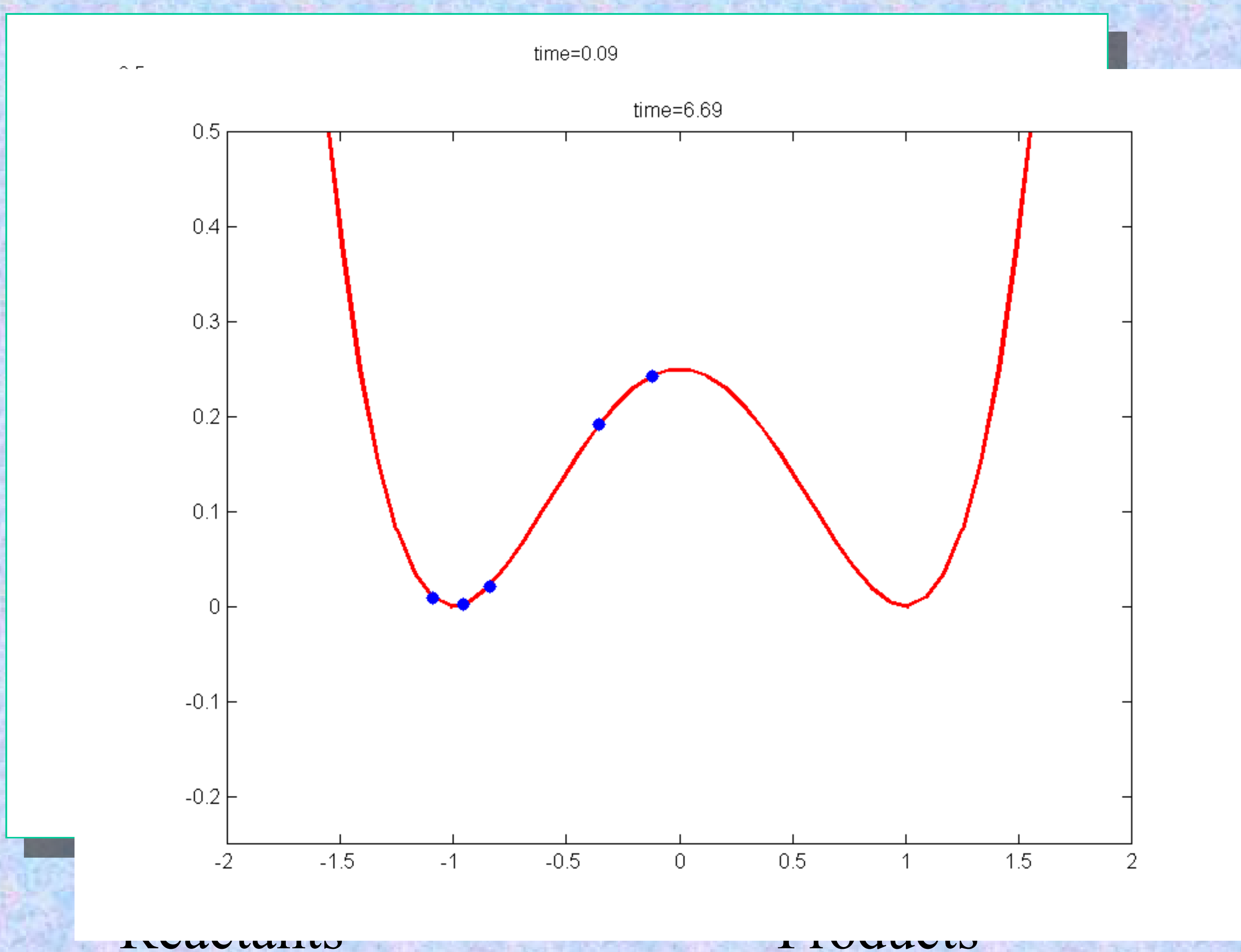
Reactants Products

Kramers theory of reaction rate (2)

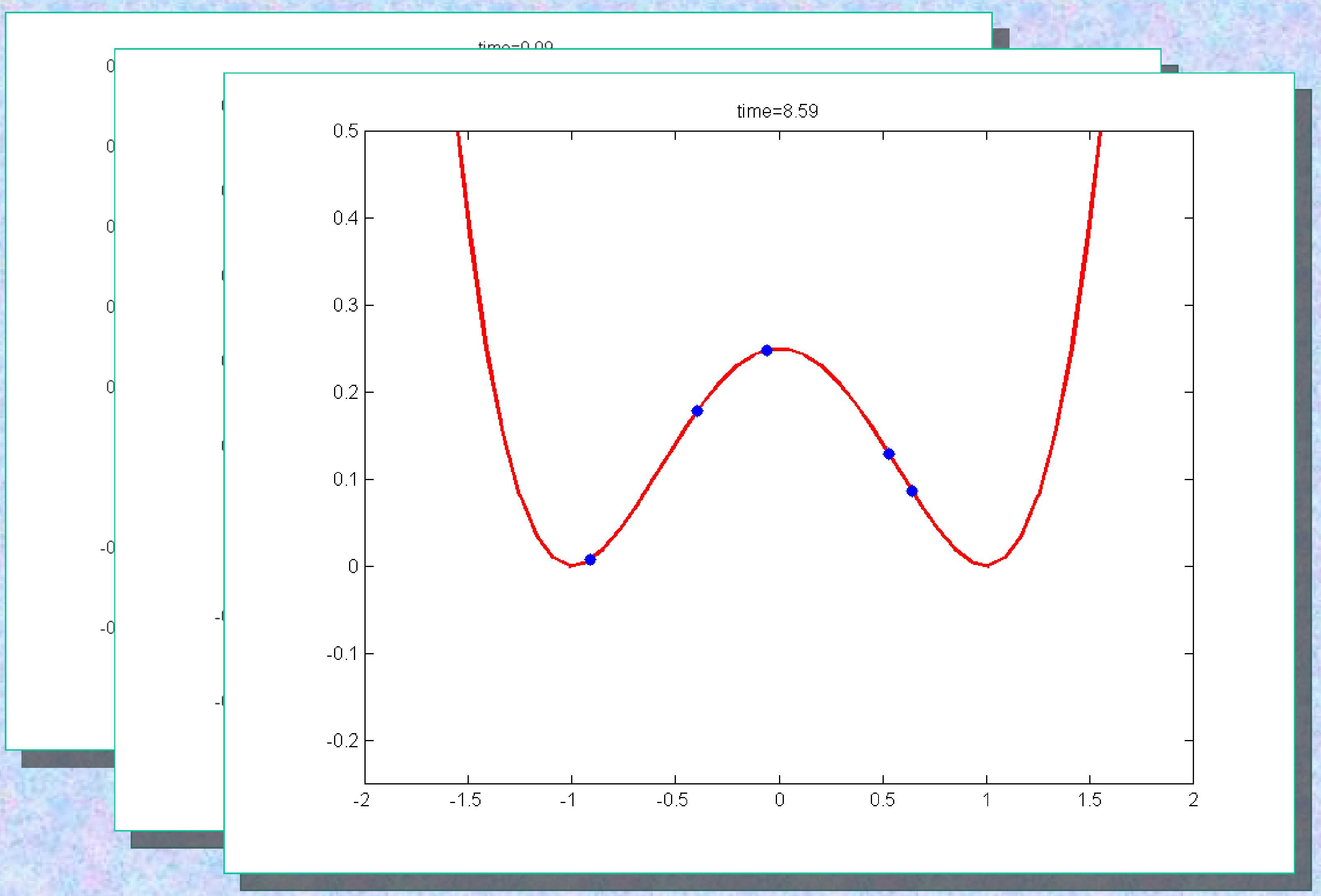


Reactants Products

Kramers theory of reaction rate (2)

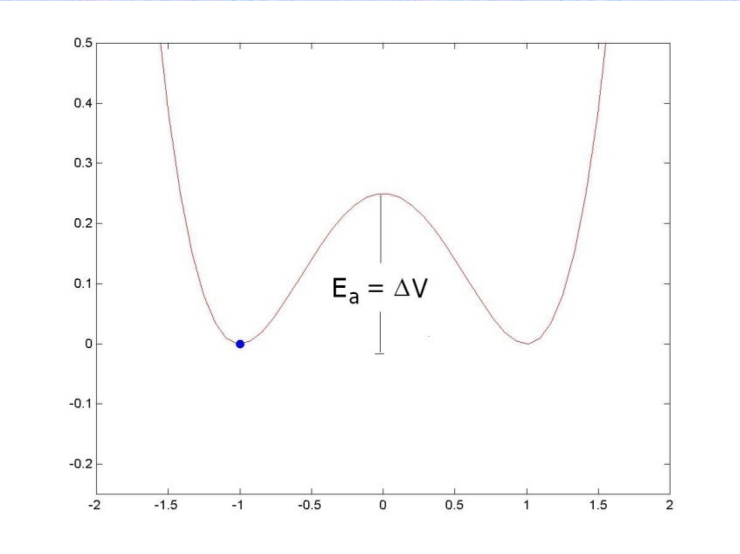


Kramers theory of reaction rate (2)



Reactants Products

Kramers theory of reaction rate (3)



$$V(x) = (1/4)bx^4 - (1/2)ax^2$$

Minima at $\pm x_m = \pm (a/b)^{1/2}$

Barrier height=activation energy:

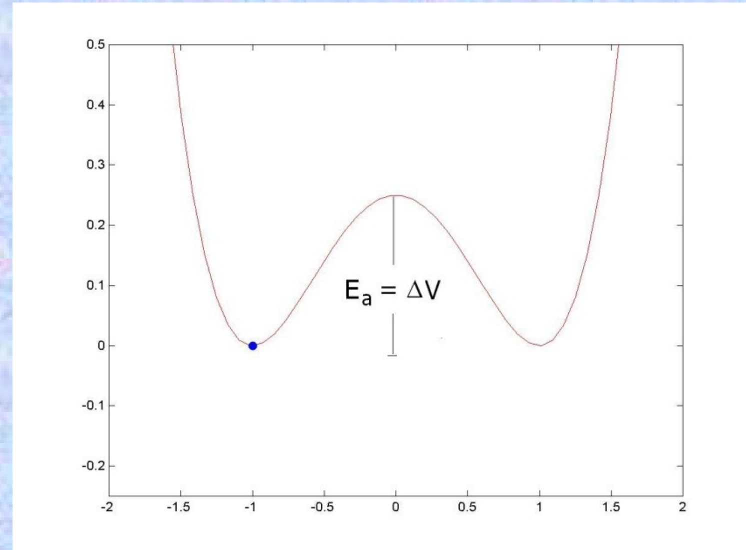
$$E_a \equiv \Delta V = a^2/4b$$

Frequencies: $\omega_0^2 = V''(x_m)/m \qquad \omega_b^2 = |V''(x_b)/m|$

Stochastic equation: $\ddot{x} = -V''(x) - \gamma\dot{x} + F(t)$

Stochastic force: $\langle F(t)\rangle = 0 \qquad \langle F(t)F(t')\rangle = 2\pi\gamma k_B T\delta(t'-t)$

Kramers theory of reaction rate (4)



Reaction $A + B \rightarrow C$

Reaction rate constant: k_R

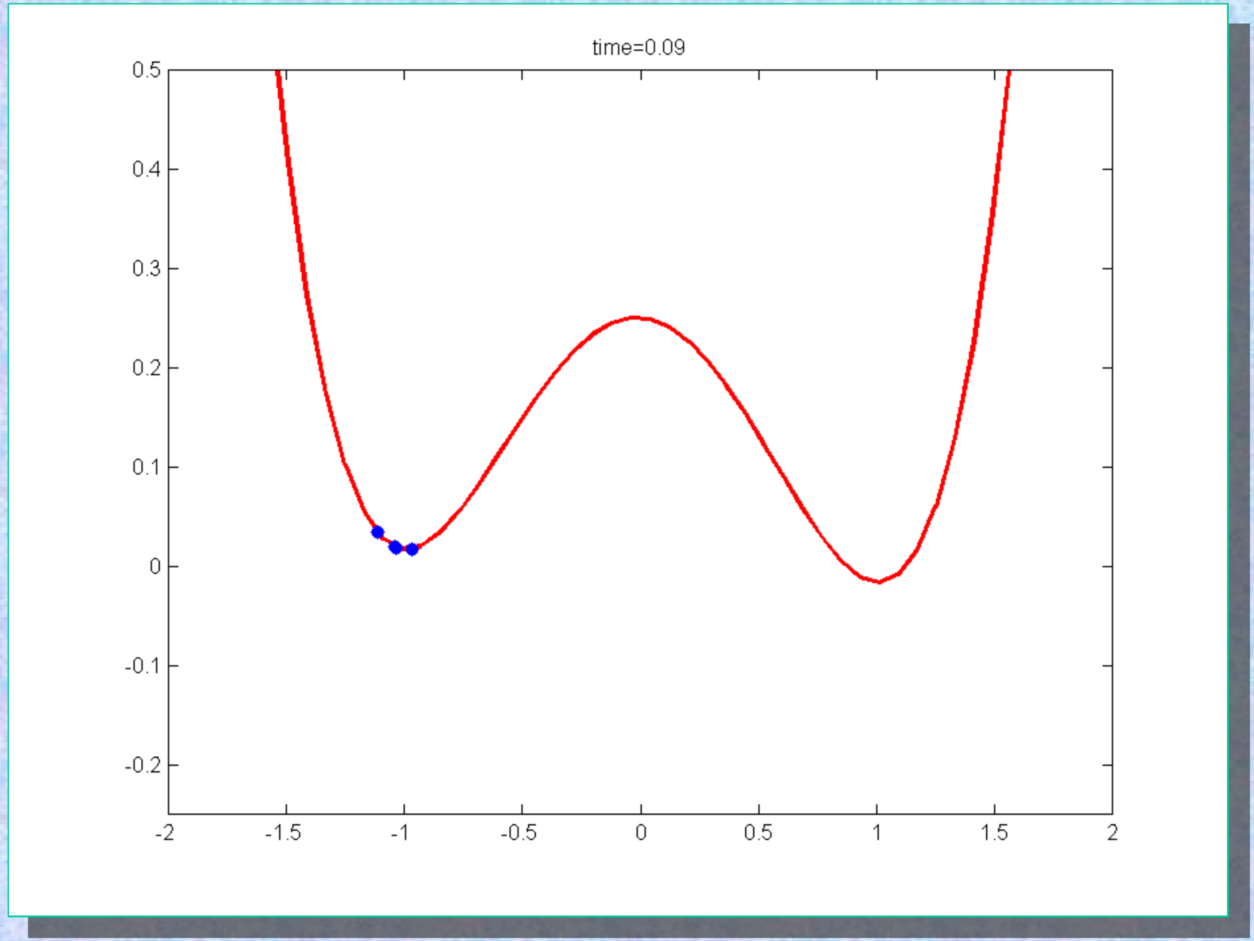
$$\frac{\mathrm{d}\,C}{\mathrm{d}\,t} = k_R [A]^n [B]^m$$

Arrhenius' law:

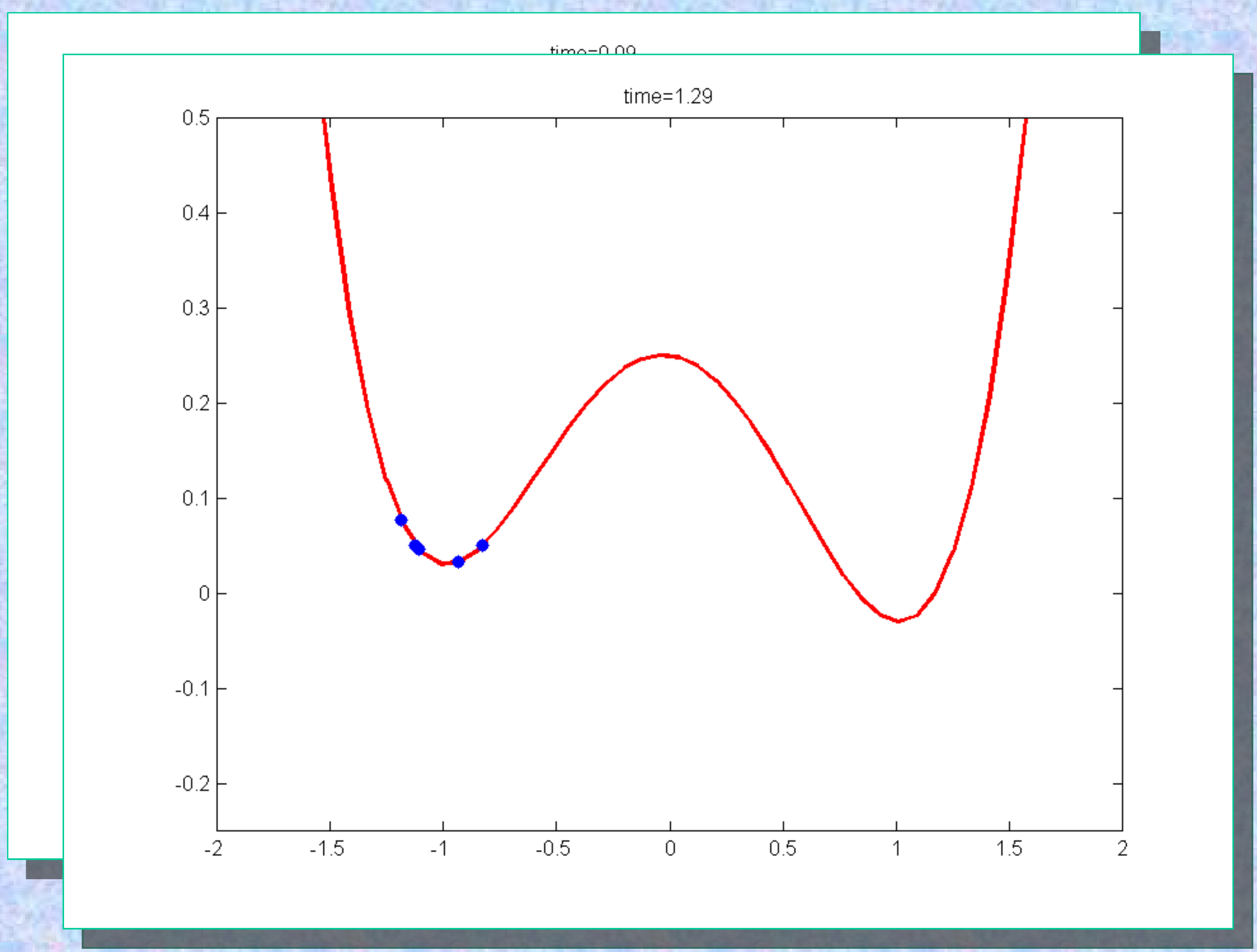
$$k_R = A \exp\left(-E_a / k_\mathrm{B} T\right)$$

Kramers reaction rate constant: $$k_R = \frac{\omega_b \omega_0}{2\pi\gamma} \exp\left(-E_a / k_\mathrm{B} T\right)$$

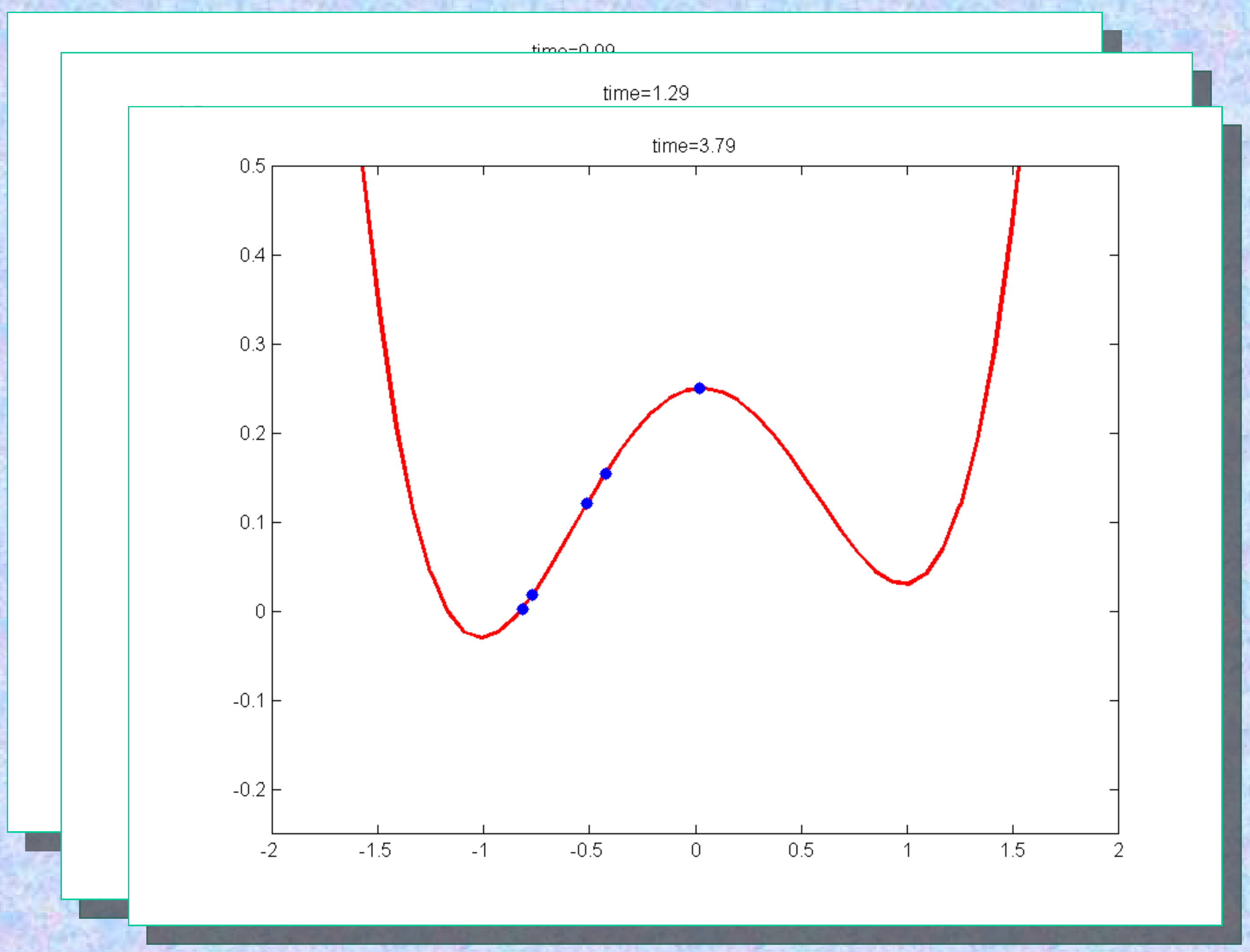
Breather effect: modulation of the potential barrier (1)



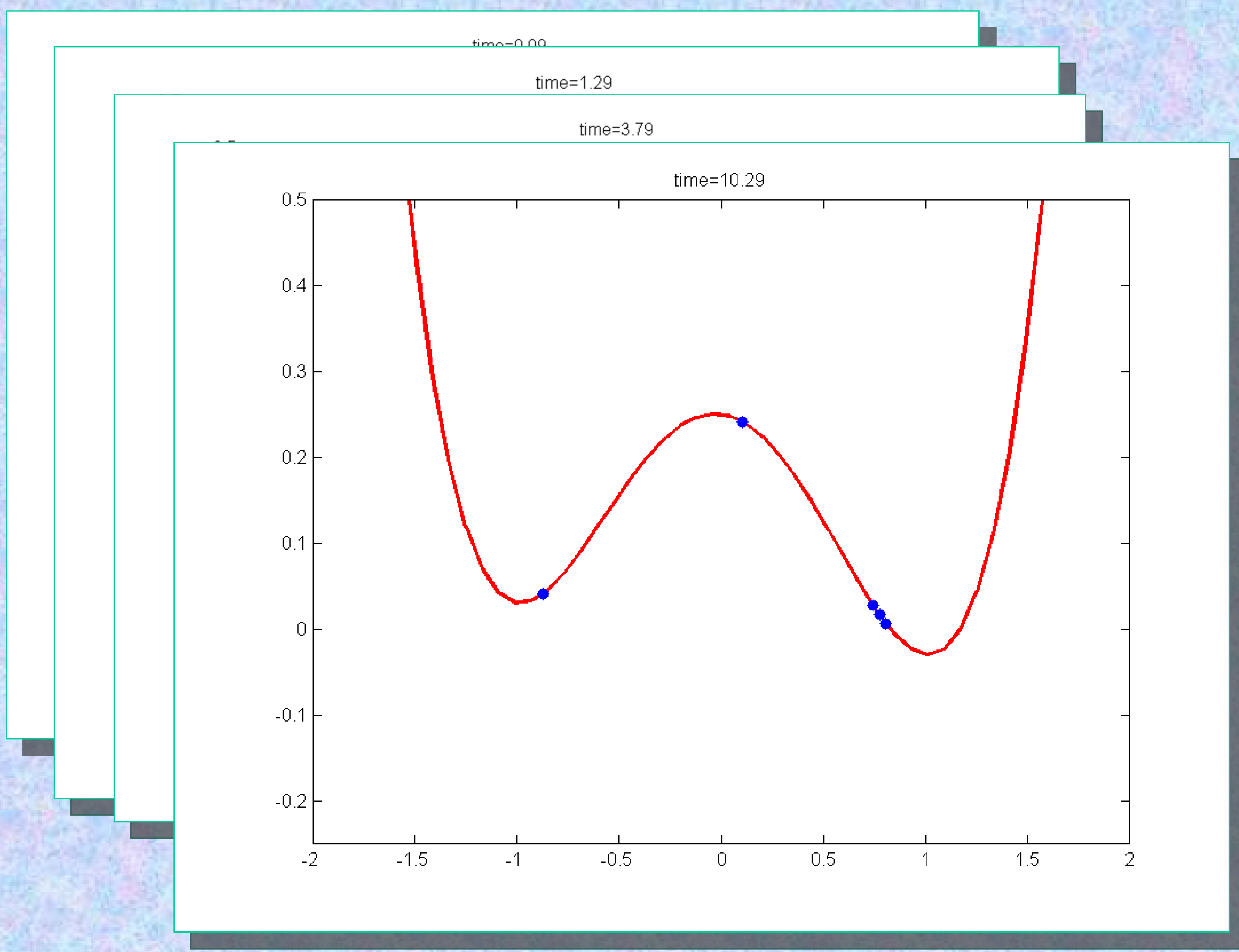
Breather effect: modulation of the potential barrier (1)



Breather effect: modulation of the potential barrier (1)



Breather effect: modulation of the potential barrier (1)



Breather effect: modulation of the potential barrier (2)

$$V(x,t) = V(x) - (x/x_m)V_m \cos(\Omega\, t)$$

If $\Omega << \omega_0$ (adiabatic assumption):

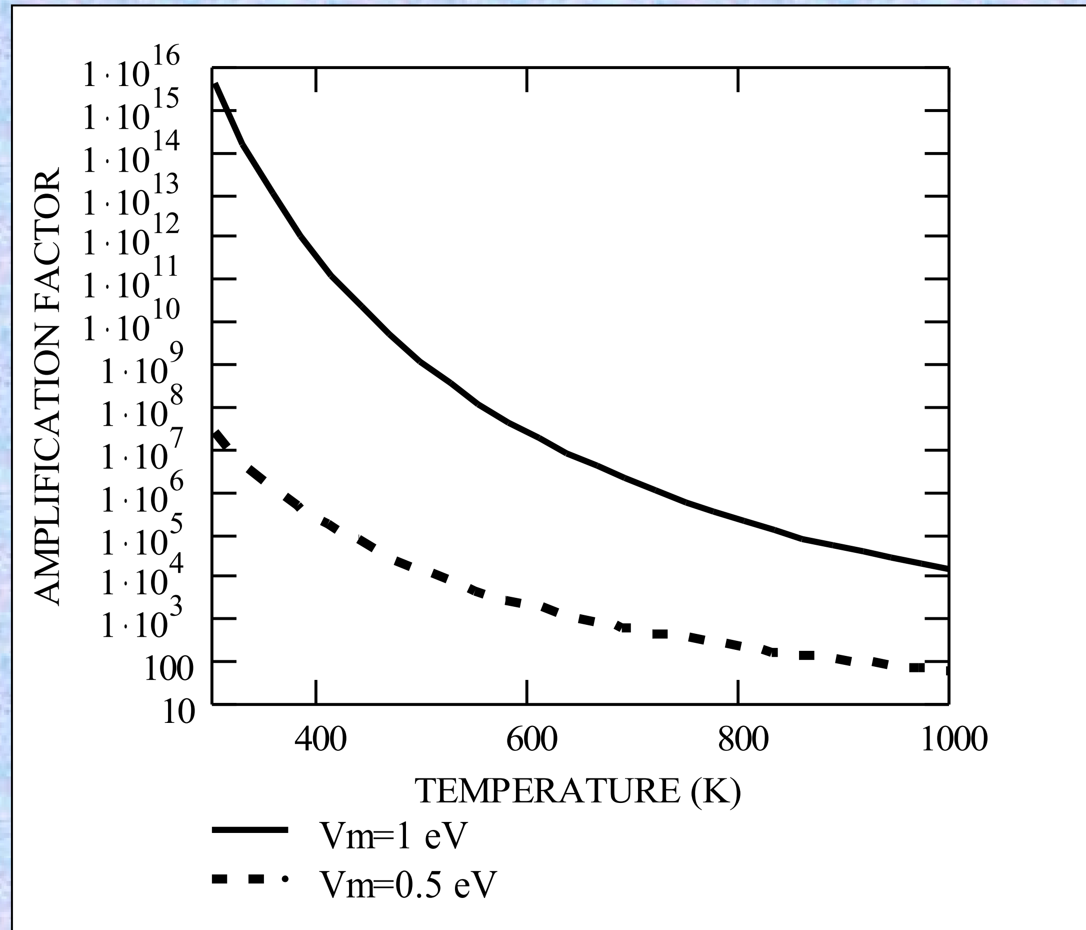
$$\dot{R}(t) = \dot{R}_K \exp\left(\frac{V_m \cos(\Omega\, t)}{k_B T}\right),$$ with mean value:

$$\left\langle \dot{R}(t) \right\rangle = \dot{R}_K \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} \exp\left(\frac{V_m \cos(\Omega\, t)}{k_B T}\right) dt = \dot{R}_K I_0\left(\frac{V_m}{k_B T}\right)$$

I_0 is the modified Bessel function of the first kind

Breather effect: modulation amplification factor

Amplification factor: $I_0\,(V_m/k_BT)$



Breather effect: random modulation

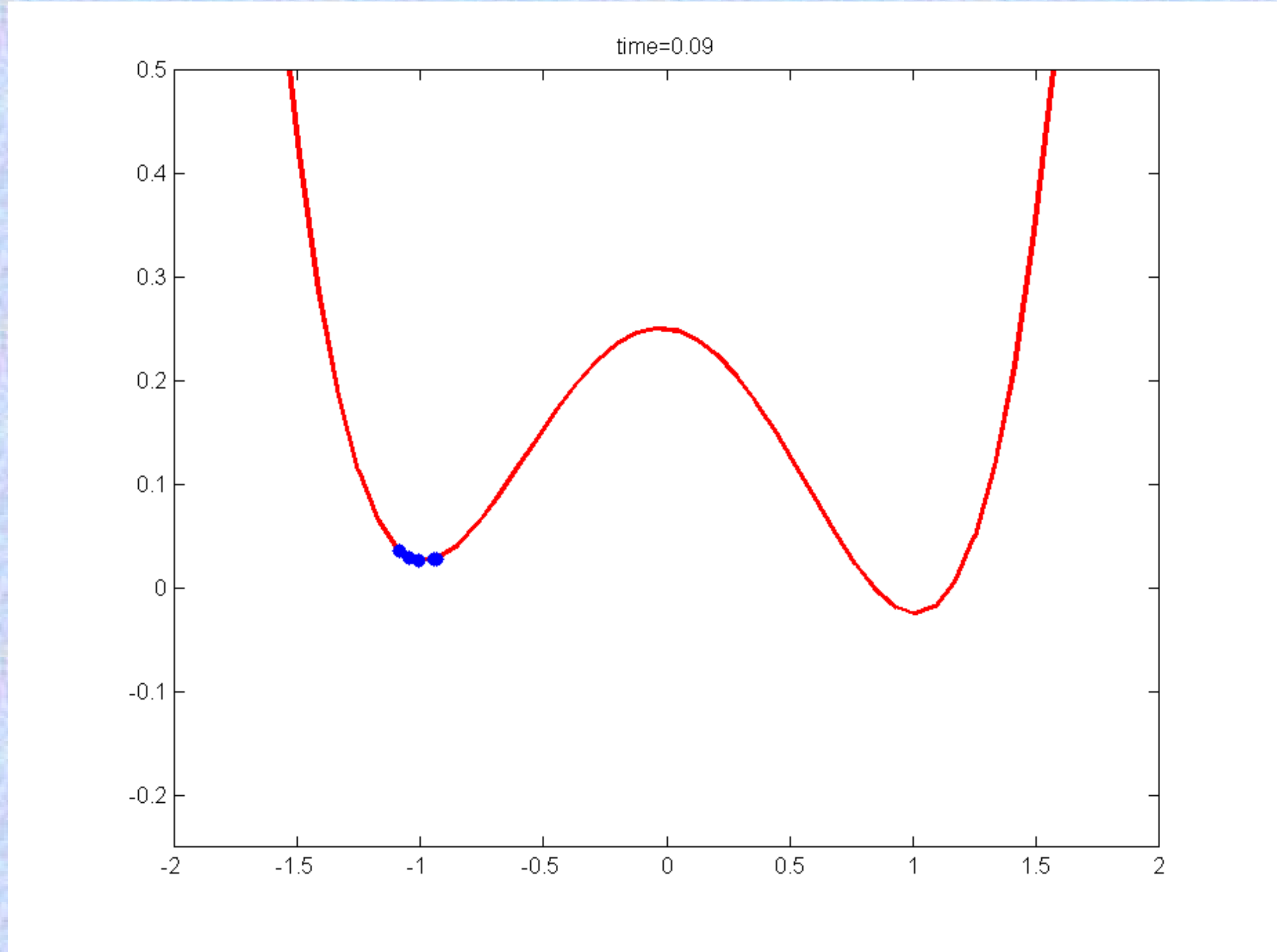
Probability of escape from the reactants well: $\exp(-\tilde{V} / k_B T)$

with $\tilde{V} = E_a + V_m \cos(\tilde{\varphi})$

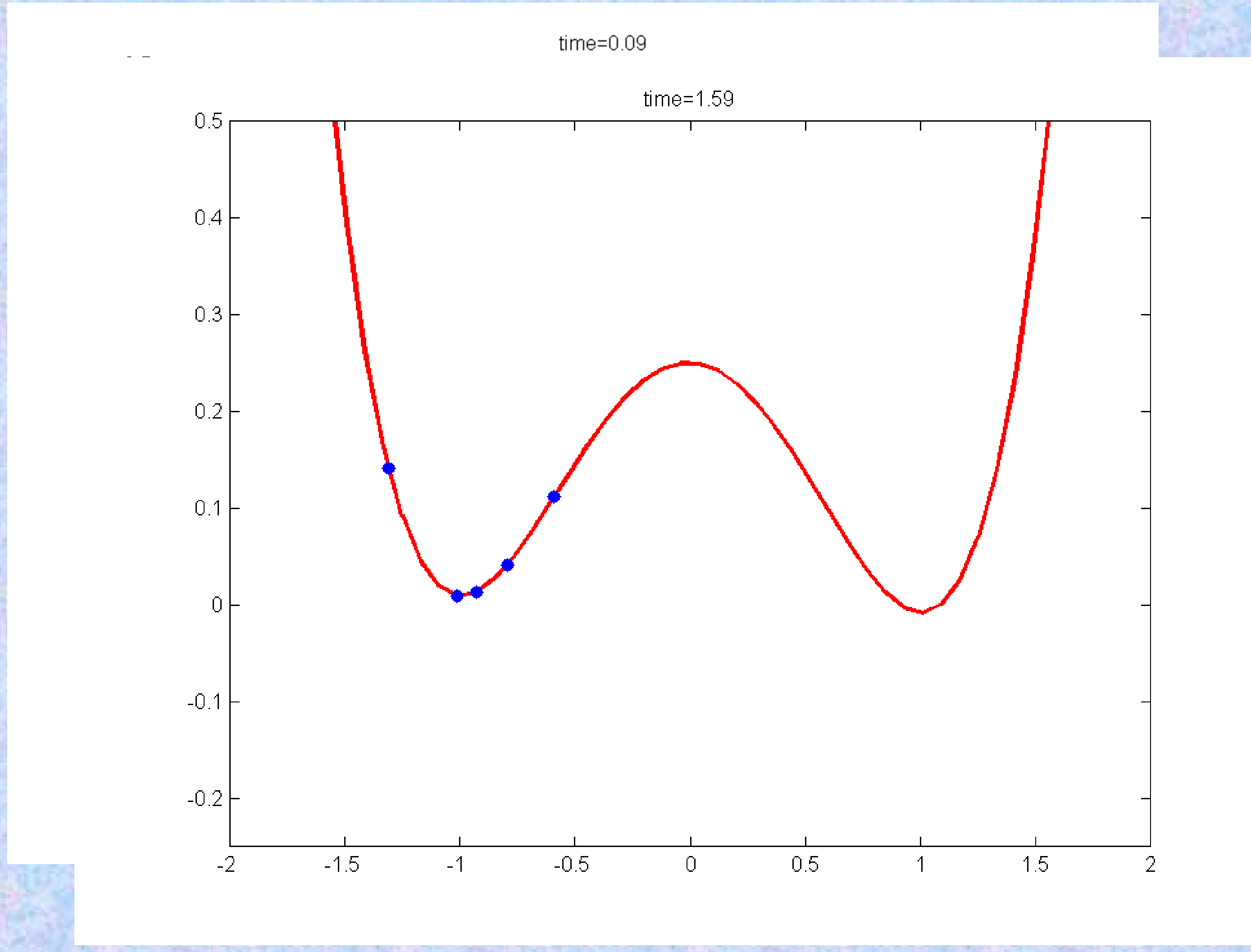
and $\tilde{\varphi}$ a random variable with probability density 1/2π, leads to

$$\left\langle \dot{R}(\tilde{\varphi}) \right\rangle = \dot{R}_K \frac{1}{2\pi} \int_0^{2\pi} \exp\left(\frac{V_m \cos(\tilde{\varphi})}{k_B T} \right) d\tilde{\varphi} = \dot{R}_K I_0\left(\frac{V_m}{k_B T} \right)$$

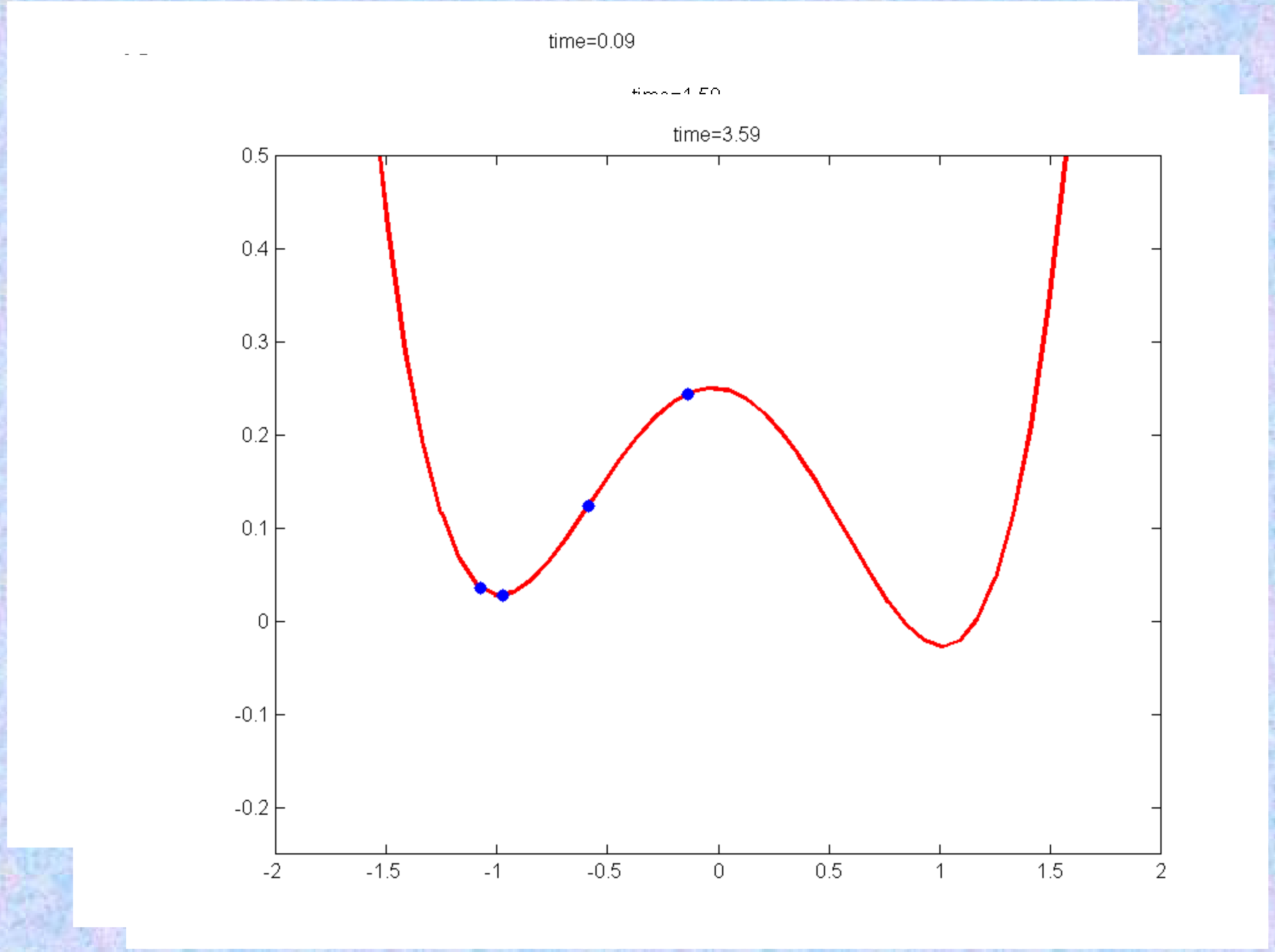
Breather effect: random modulation (2)



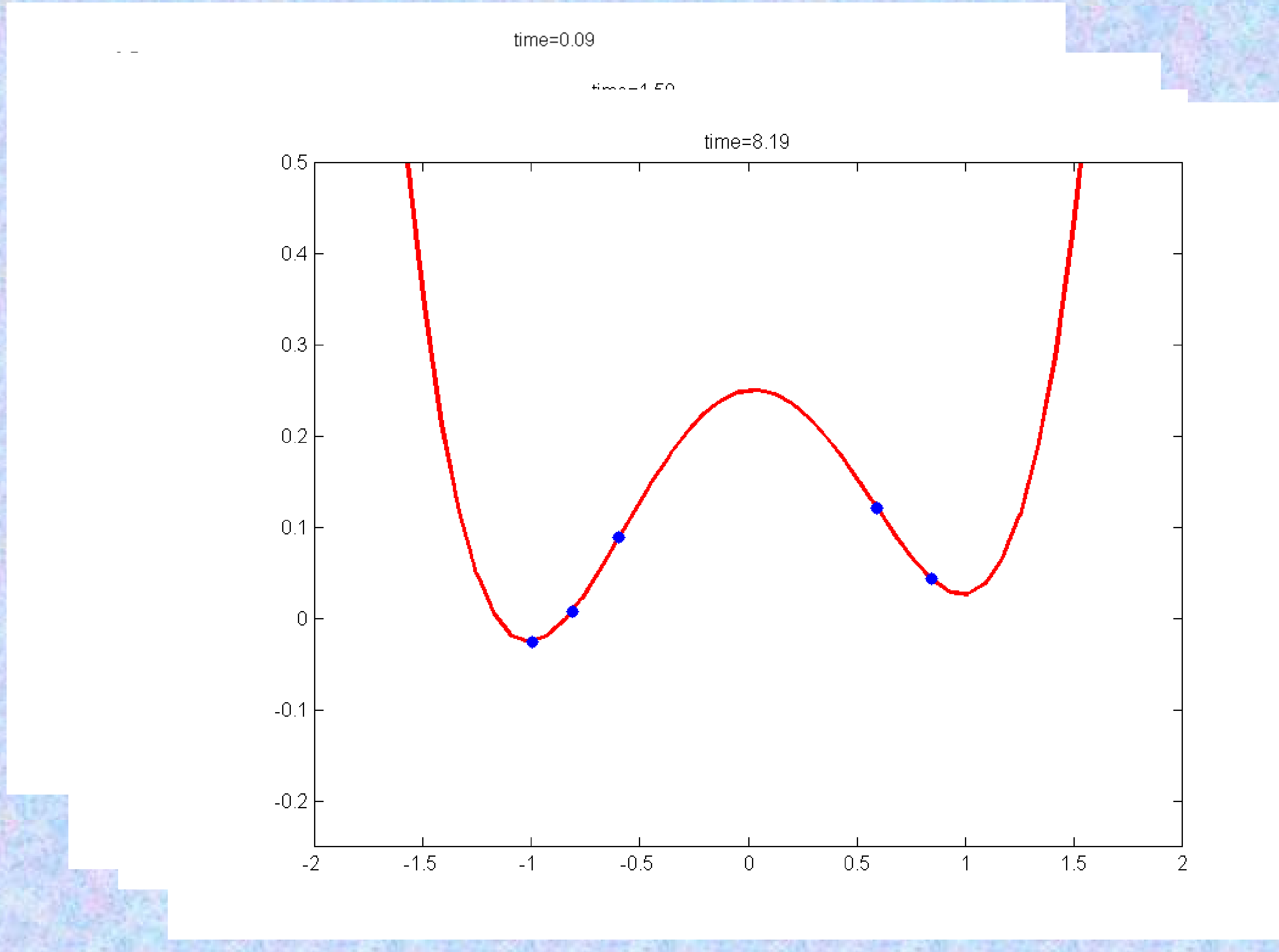
Breather effect: random modulation (2)



Breather effect: random modulation (2)

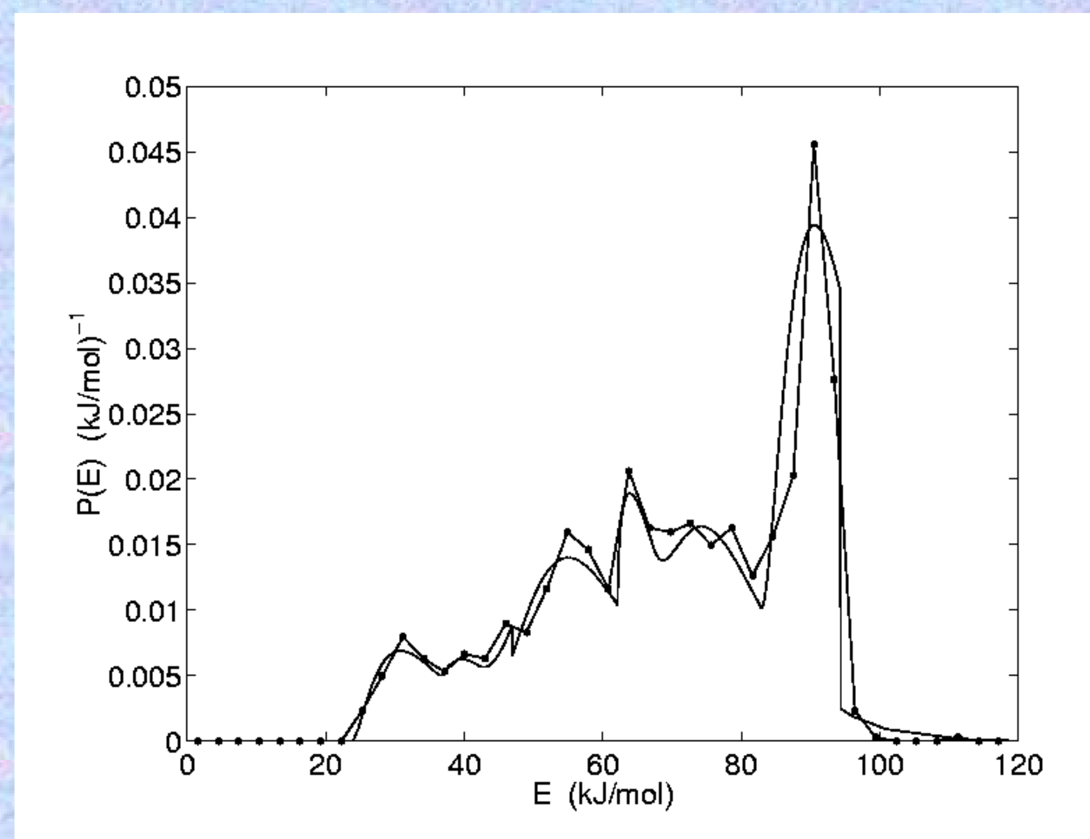


Breather effect: random modulation (2)

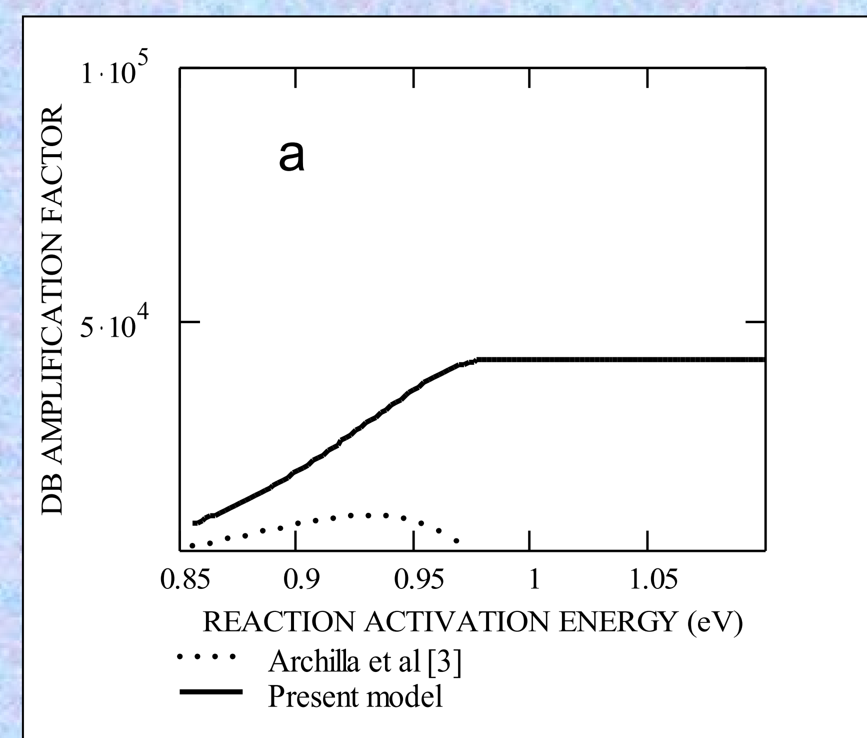


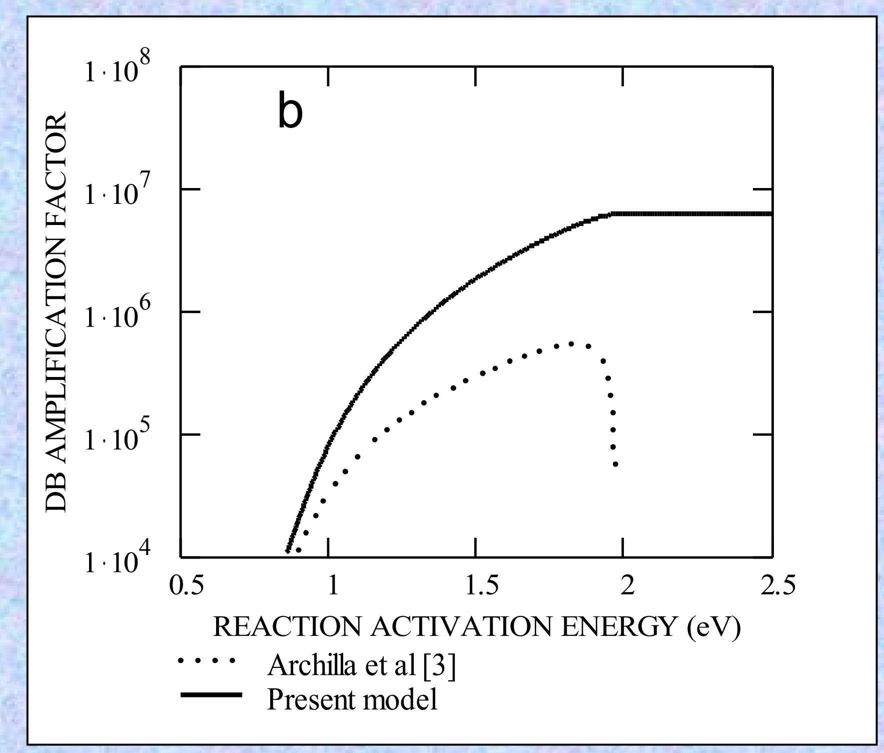
Amplification factor for breathers in the mica model

$$\langle \dot{R}_B \rangle = \dot{R}_K \int_{E_{\min}}^{\infty} f_B(E) I_0(E/k_B T) dE$$



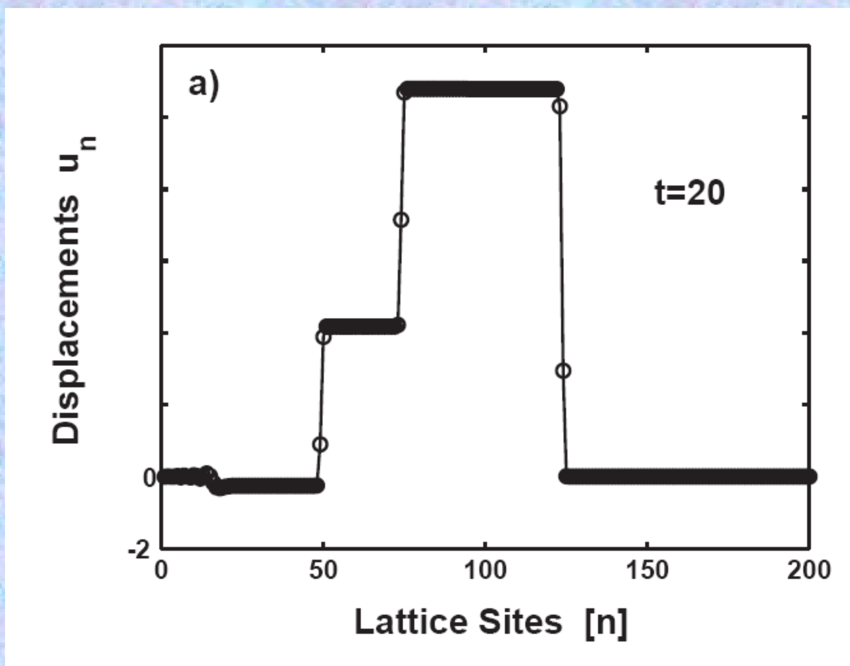
Amplification factor for breathers in the mica model

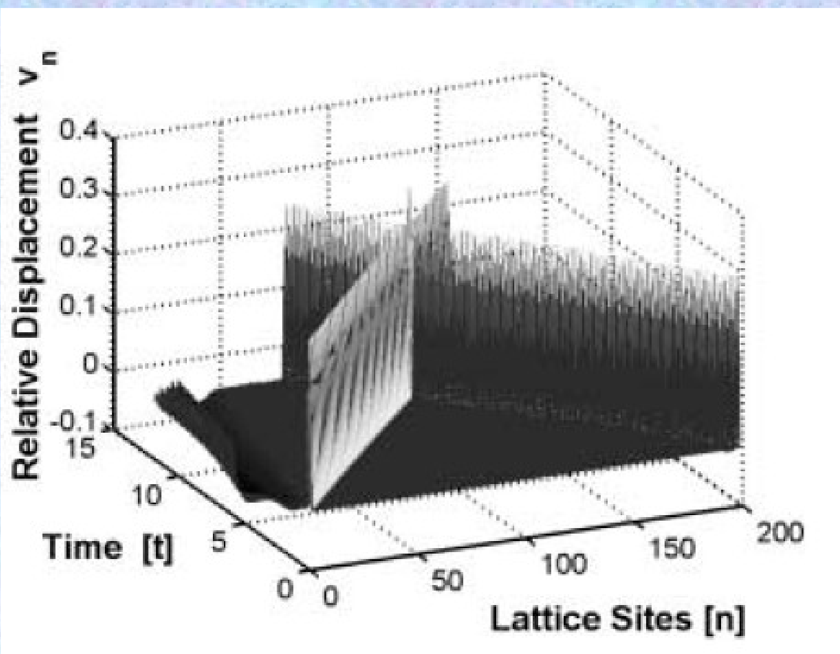




Reaction rate theory with account of the crystal anharmonicity
VI Dubinko, PA Selyshchev and JFR Archilla
Phys Rev E 83, 041124 (2011)

Transversal breathers move slowly but we pan to study supersonics kinks along the lattice directions





Supersonic discrete kink-solitons and sinusoidal patterns with "magic" wave number in anharmonic lattices. Yu A Kosevich, R Khomeriki and S Ruffo.
Europhys. Lett., 66 (1), pp. 21–27 (2004)

SUMMARY

1. Breathers do not need to have an energy larger that the activation energy to influence reconstructive transformations

2. A breather modulates the potential barrier in Kramers theory which introduces an amplification factor in the reaction rate.

3. Different types of breathers appear in simulations for the cation layer in muscovite

4. The amplification factor increases several order of magnitude the reaction rate according with the observed low temperature reconstructive transformations

5. They move slowly, then probably longitudinal kinks are more appropriate for quodons.