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Nonlinear Waves in Low-dimensional Systems - Part II

S. FLACH
New Zealand Institute for Advanced Study
Centre for Theoretical Chemistry & Physics Massey University Auckland
New Zealand

Nonlinear Waves in Low-Dimensional Systems: essentials, problems, perspectives

THE ENGINE OF THE NEW NEW ZEALAND

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- Fermi, Pasta, Ulam and the essentials of statistical physics
- discrete breathers – localizing waves on lattices
- destruction of Anderson localization

CTCP

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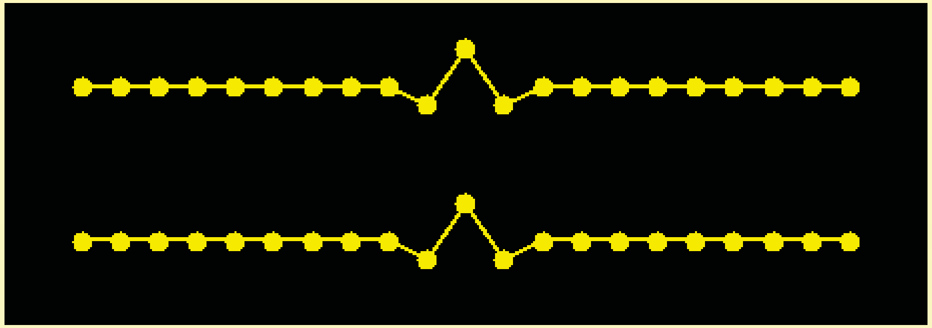
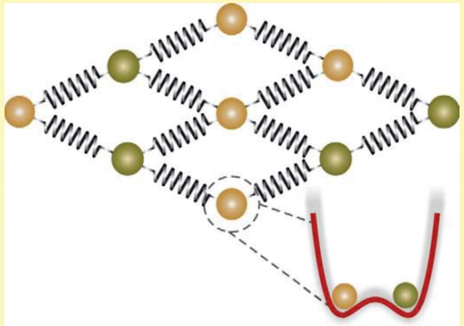
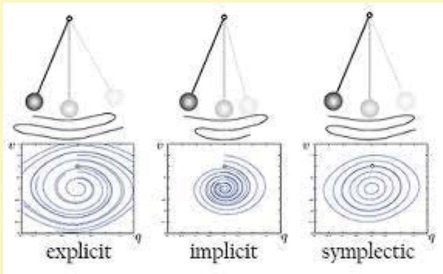


A few preliminaries

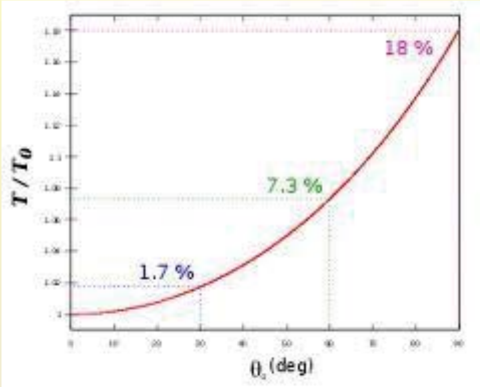
- waves on lattices = arrays of interacting oscillators
- lattice: crystals, layered structures
- nonlinearity: from nonlinear response of medium to waves, or approximative quantum many body dynamics

Lattice waves





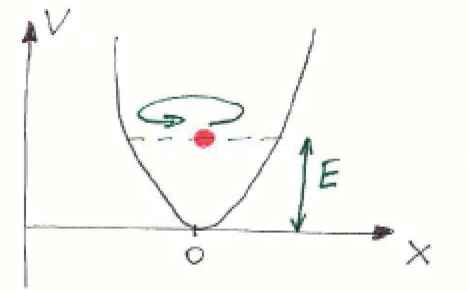
discretize space – introduce lattice
one oscillator per lattice point
oscillator state is defined by amplitude and phase
introduce interaction between oscillators



anharmonic potential = nonlinear wave equation
intensity increase changes frequency
in quantum world energy levels NOT equidistant

Typical excitations in condensed matter, optics, etc

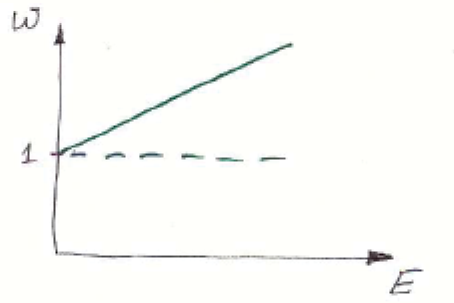
one classical anharmonic oscillator:



$$H_0(P,X) = \frac{1}{2}P^2 + \frac{1}{2}X^2 + \frac{v_4}{4}X^4$$

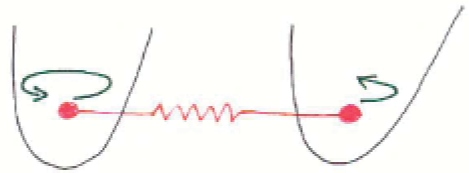
The frequency of oscillations is depending on the energy:

$$\omega \approx 1 + \frac{3}{2}v_4 E$$



Two interacting oscillators:

$$H(1,2) = H_0(1) + H_0(2) + \frac{1}{2}C(X_1 - X_2)^2$$

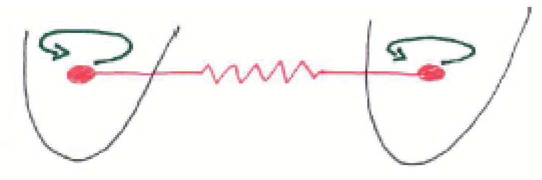


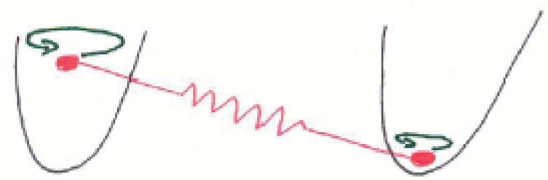
H is permutationally invariant: $H(1,2) = H(2,1)$

And the solutions?

Small amplitudes:
linear equations, beating
(p-invariant).

Large amplitudes:
no p-invariance, 'localization'!





Integrable example:

$$-i\dot{\Psi}_{1,2} = |\Psi_{1,2}|^2\Psi_{1,2} + C\Psi_{2,1}$$

Periodic solutions:

$$\Psi_{1,2} = A_{1,2}\mathrm{e}^{i\omega t+\Delta_{1,2}}$$

Phase space contains separatrix which separates p-invariant regions with periodic solutions
$A_1 = A_2$, $\Delta_2 - \Delta_1 = 0, \pi$
from non-p-invariant regions with periodic solutions
$A_1 \neq A_2$

$$H = \frac{1}{2}|\psi_1|^4 + \frac{1}{2}|\psi_2|^4 + C\cdot(\psi_1^* \psi_2 + cc) \,, \quad \dot{\psi}_{1,2} = i\,\frac{\partial H}{\partial \psi_{1,2}^*}$$

$$B = |\psi_1|^2 + |\psi_2|^2 \,, \quad \dot{B} = 0$$

$$\psi_{1,2} = A_{1,2}\cdot e^{i\varphi_{1,2}} \,, \quad \Delta\varphi = \varphi_2 - \varphi_1 \,, \quad s\varphi = \varphi_1 + \varphi_2$$

$\Downarrow$

$$H = \frac{1}{2}(A_1^4 + A_2^4) + 2C A_1 A_2 \cdot \cos\Delta\varphi \,, \quad B = A_1^2 + A_2^2$$

<u>Isolated Periodic Orbits</u>: grad $H \parallel$ grad B , $\vec{R} = (A_1, A_2, \Delta\varphi, s\varphi)$

$$\text{grad}\, H = \begin{pmatrix} 2A_1^3 + 2C A_2 \cos\Delta\varphi \\ 2A_2^3 + 2C A_1 \cos\Delta\varphi \\ -2C A_1 A_2 \sin\Delta\varphi \\ 0 \end{pmatrix} , \quad \text{grad}\, B = \begin{pmatrix} 2A_1 \\ 2A_2 \\ 0 \\ 0 \end{pmatrix}$$

$\Downarrow$

$\sin\Delta\varphi = 0 \Rightarrow \Delta\varphi = 0$ ($A_1/A_2 < 0$ takes care of π)

$A_{1,2}^3 + C A_{2,1} = \varkappa A_{1,2}$ ($\varkappa$ is some constant)

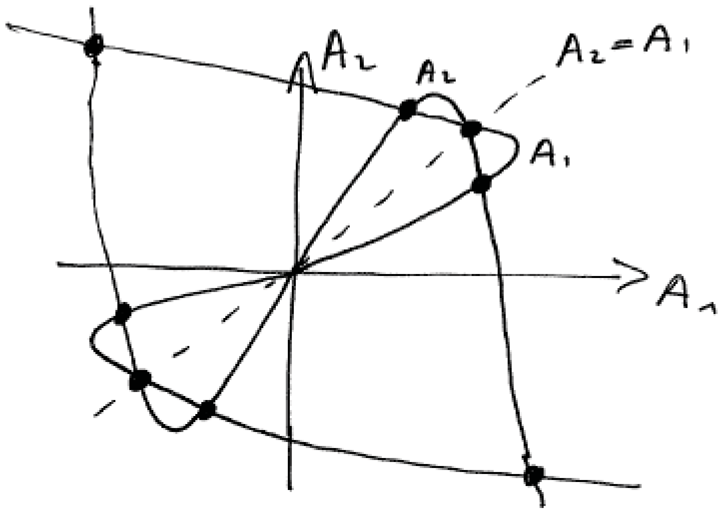
$$\psi_{1,2}(t) = A_{1,2}(t)\cdot e^{i\varphi(t)} \,, \quad \frac{d}{dt}|\psi_1|^2 \sim \sin\Delta\varphi = 0 \Rightarrow \begin{cases} A_{1,2} = \text{const} \\ \dot{\varphi} = \omega = \varkappa \end{cases}$$

Solutions :

a) $A_1 = A_2 \Rightarrow \omega = A^2 + c$ ↑↑ in phase

b) $A_1 = -A_2 \Rightarrow \omega = A^2 - c$ ↑↓ out of phase

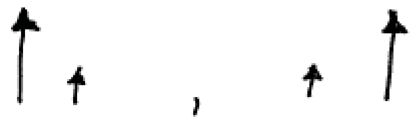
c) $A_2 = \frac{\omega}{c} A_1 - \frac{1}{c} A_1^3$, $A_1 = \frac{\omega}{c} A_2 - \frac{1}{c} A_2^3$



Bifurcation:

$B_b = 2c, \; E_b = 3c, \; \omega_b = 2c$

$$\begin{cases} A_{1,2}^2 = \frac{1}{2}\left[\omega \pm \sqrt{\omega^2 - 4c^2}\right] \\ \omega = 1 + B \end{cases}$$



Integrating the dimer

$$y = A_1^2 - \frac{B}{2}, \quad H = \frac{1}{4}B^2 + y^2 + 2C\sqrt{\frac{B^2}{4} - y^2}\cdot\cos\Delta\varphi$$

$$\Downarrow$$

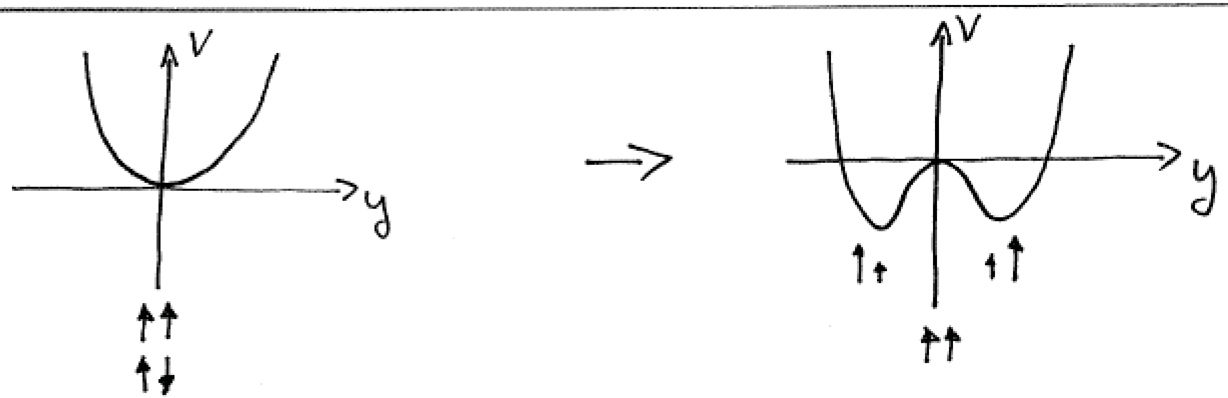
$$\dot{y} = \frac{\partial H}{\partial \Delta\varphi}, \quad \Delta\dot{\varphi} = -\frac{\partial H}{\partial y}; \quad s\dot{\varphi} = \frac{\partial H}{\partial B}, \quad \dot{B} = -\frac{\partial H}{\partial s\varphi}$$

$$\Downarrow$$

$$\begin{cases} \dot{B} = 0, \quad s\dot{\varphi} = \frac{1}{2}B + B\cdot C\cdot\frac{\cos\Delta\varphi}{\sqrt{B^2/4 - y^2}} \\ \dot{y} = -2\cdot C\cdot\sqrt{B^2/4 - y^2}\cdot\sin\Delta\varphi, \quad \Delta\dot{\varphi} = -2y + \frac{2Cy}{\sqrt{B^2/4 - y^2}}\cos\Delta\varphi \end{cases}$$

$$\Downarrow$$

$$\boxed{\ddot{y} = -\frac{\partial V}{\partial y}, \quad V(y;E,B) = \left(-E + \frac{B^2}{4} + 2C^2\right)y^2 + \frac{1}{2}y^4}$$



collecting evidence

Table experiments with coupled magnetic pendula

Two magnetic pendula, small amplitudes

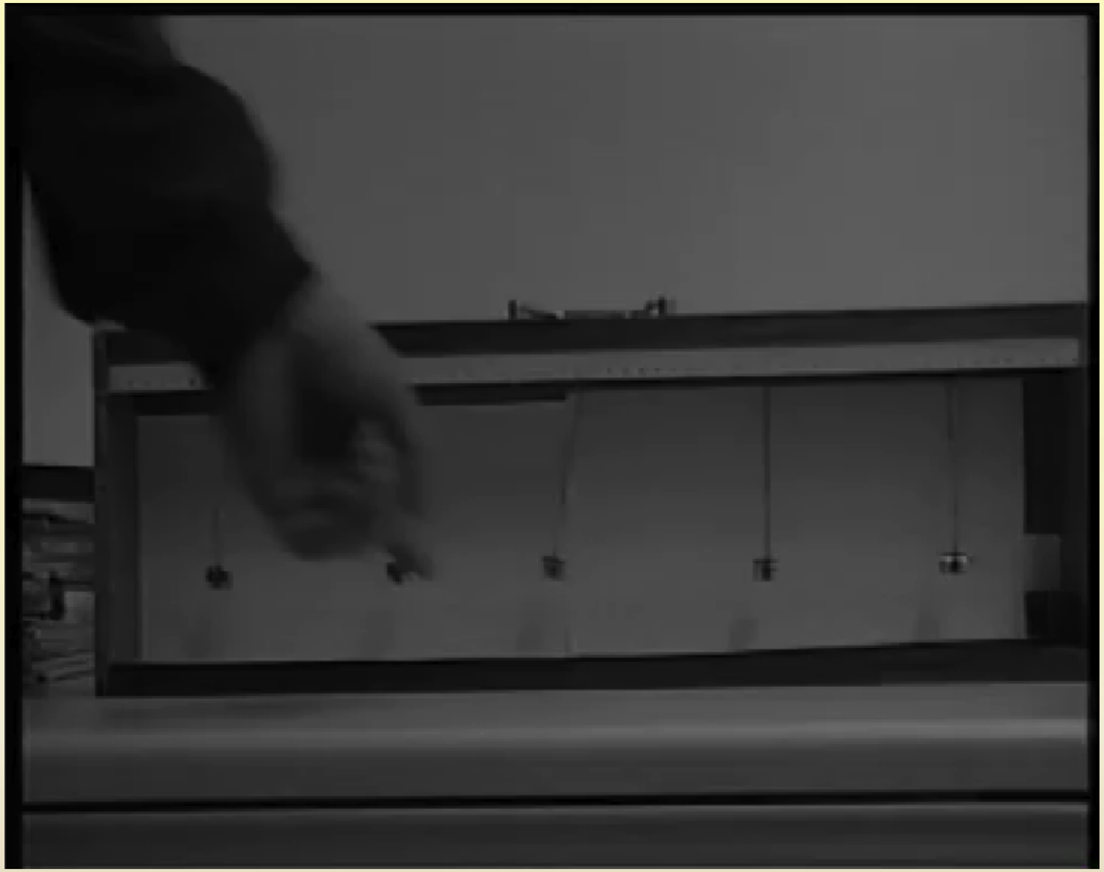
Gravitational potential: -cos(x) , anharmonic!

Linear regime, beating, no localization

Two magnetic pendula, large amplitudes

Nonlinear regime, no beating, localization

Chain of magnetic pendula, small amplitudes



Linear regime, wave spreading, delocalization

Chain of magnetic pendula, large amplitudes

Nonlinear regime, no wave spreading, localization

Cooling a two-dimensional lattice at the boundaries

- **a thermalized 2d lattice**
- **delocalized excitations are removed at the boundaries**
- **localized excitations will stay untouched**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Discrete breathers in transient processes and thermal equilibrium

M.V. Ivanchenko[a], O.I. Kanakov[a], V.D. Shalfeev[a], S. Flach[b,*]

[a] Department of Radiophysics, Nizhny Novgorod University, Gagarin Avenue 23, 603950 Nizhny Novgorod, Russia
[b] Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

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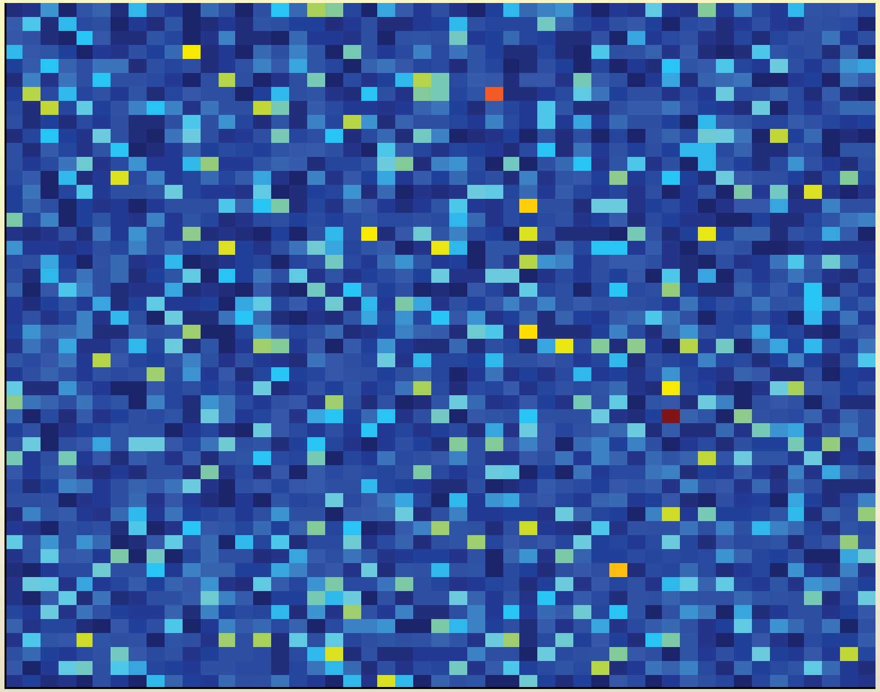
Cooling a two-dimensional lattice at the boundaries



Originally designed by Bikaki et al (1999) to study slow energy relaxation of the remaining excitations

Exciting a plane wave in a two-dimensional lattice

- **periodic boundary conditions**
- **plane wave is modulationally unstable**
- **what will it decay into?**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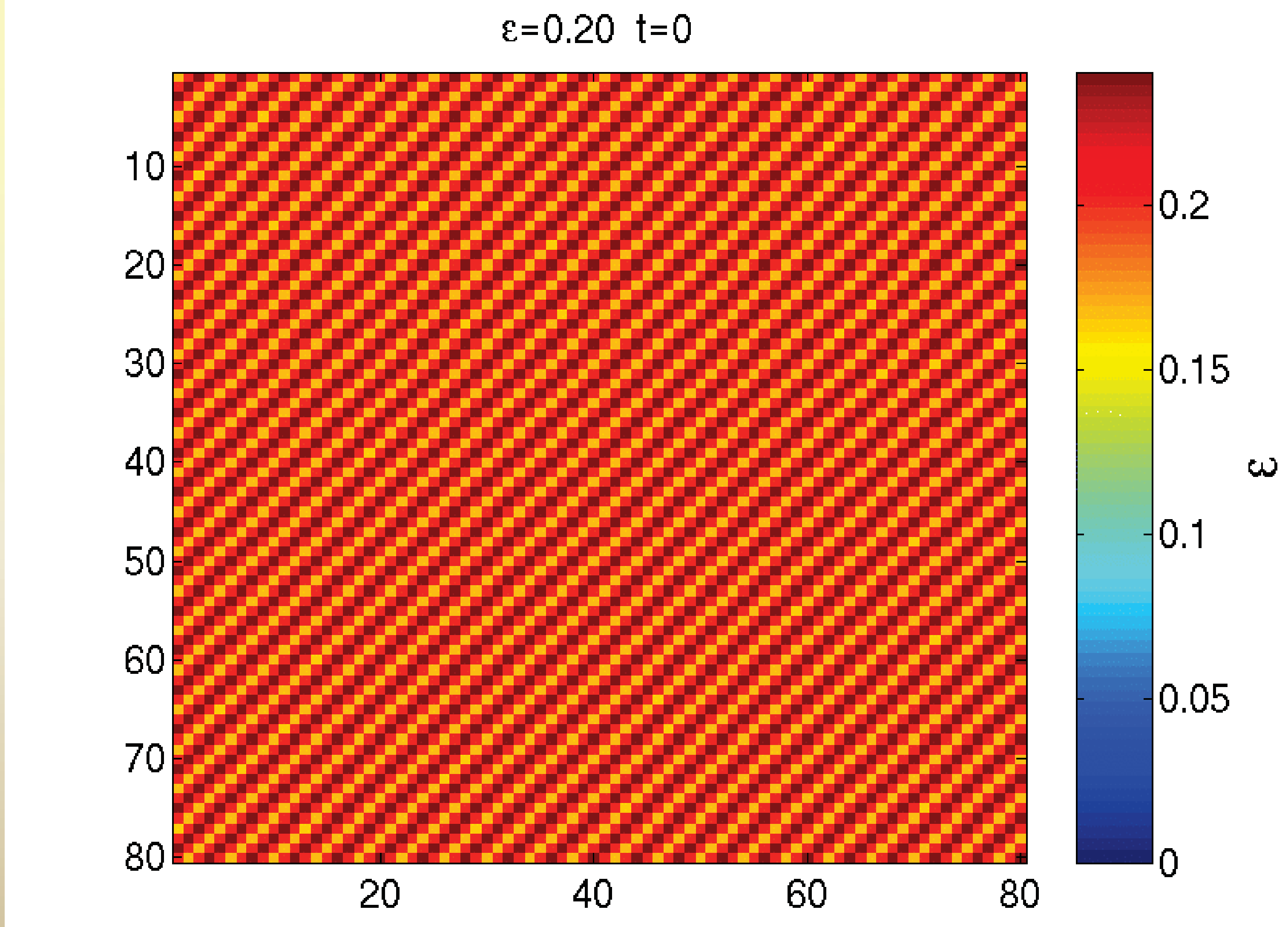
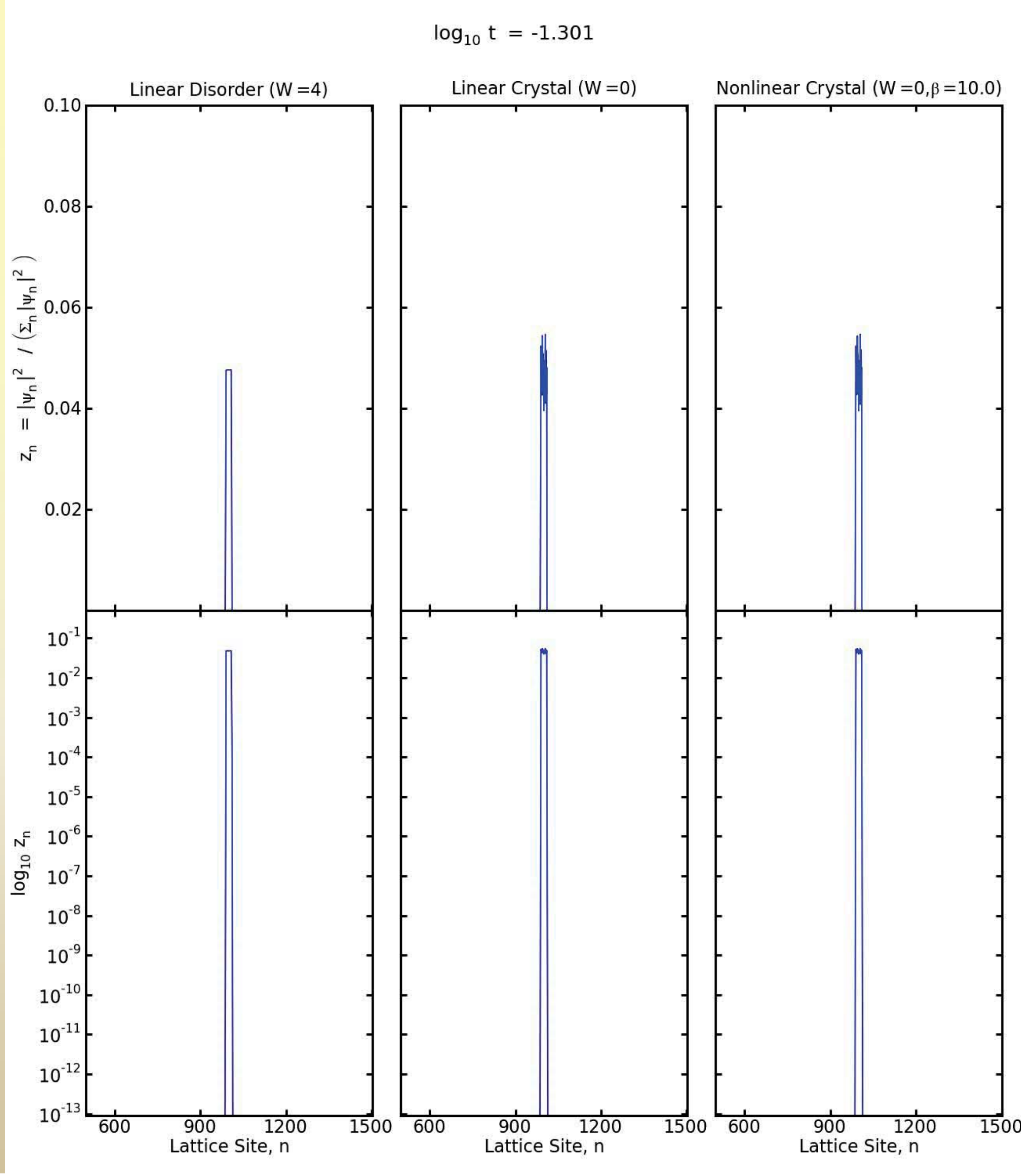
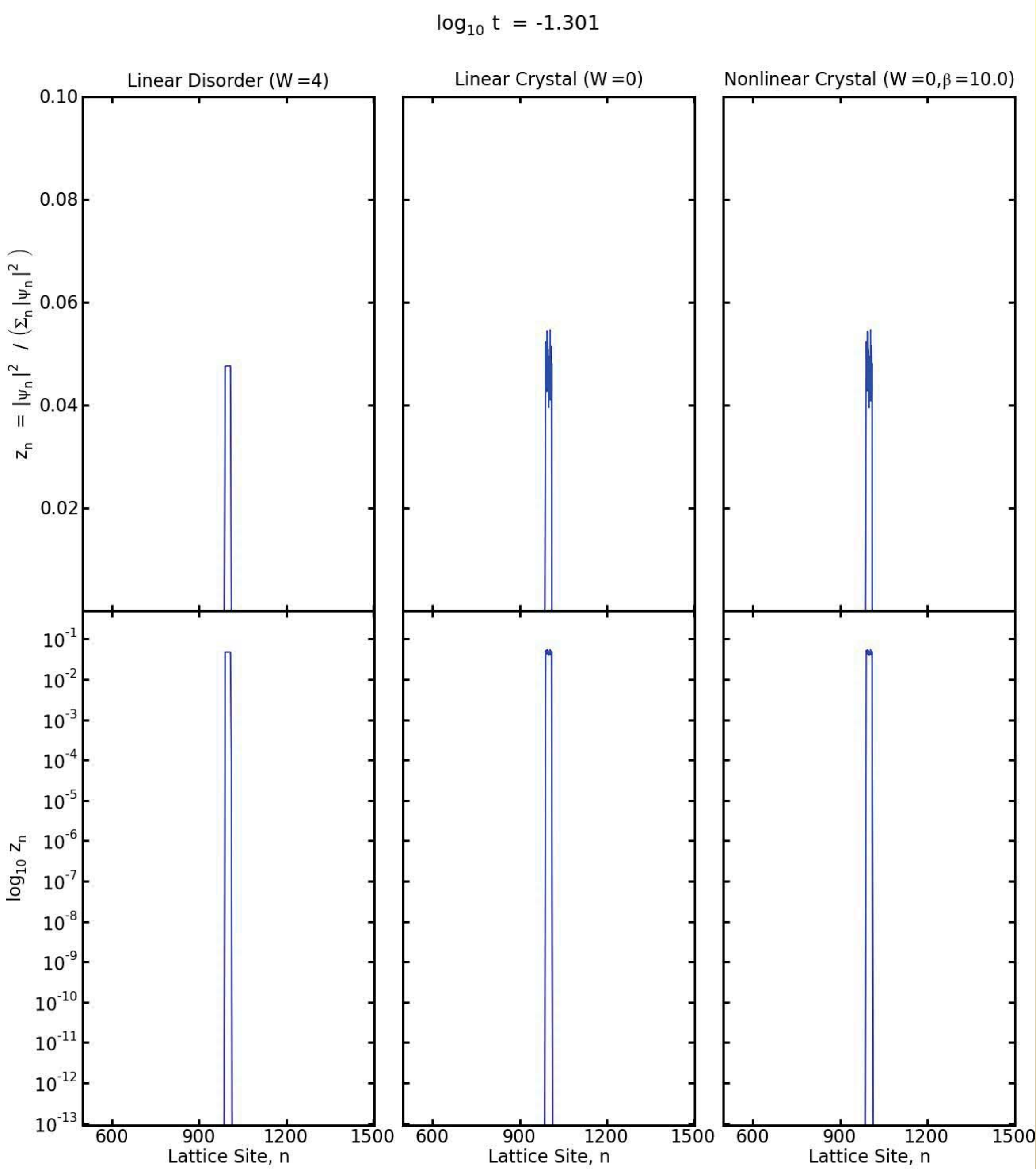




$\log_{10} t = -1.301$
Linear Disorder (W =4)
Linear Crystal (W =0)
Nonlinear Crystal (W =0,β =10.0)
$z_n = |\psi_n|^2 / (\Sigma_n |\psi_n|^2)$
0.10
0.08
0.06
0.04
0.02
$\log_{10} z_n$
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
600
900
1200
1500
Lattice Site, n



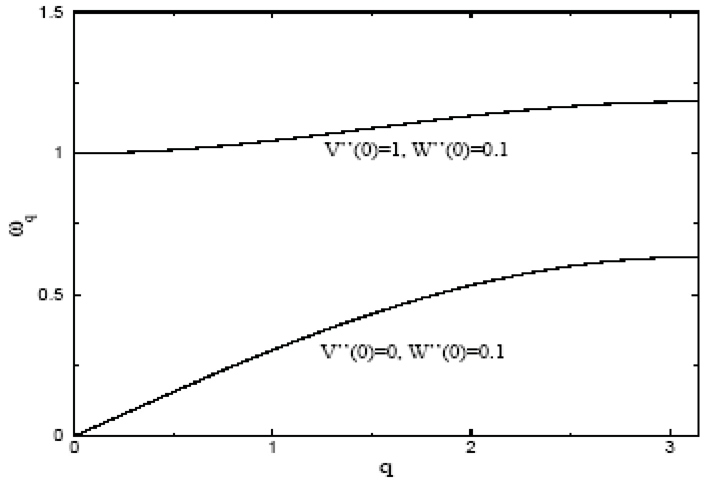
$\log_{10} t = -1.301$
Linear Disorder (W =4)
Linear Crystal (W =0)
Nonlinear Crystal (W =0,β =10.0)
$z_n = |\psi_n|^2 / (\Sigma_n |\psi_n|^2)$
$\log_{10} z_n$
Lattice Site, n

discrete breathers

A few more definitions first, using a simple model class

$$H = \sum_l \left[\frac{1}{2}p_l^2 + V(x_l) + W(x_l - x_{l-1})\right]$$

$$V(0) = W(0) = V'(0) = W'(0) = 0$$
$$V"(0), W"(0) \geq 0$$



Equations of motion:

$$\dot{x}_l = p_l \; , \; \dot{p}_l = -V'(x_l) - W'_{l,l-1} + W'_{l+1,l}$$

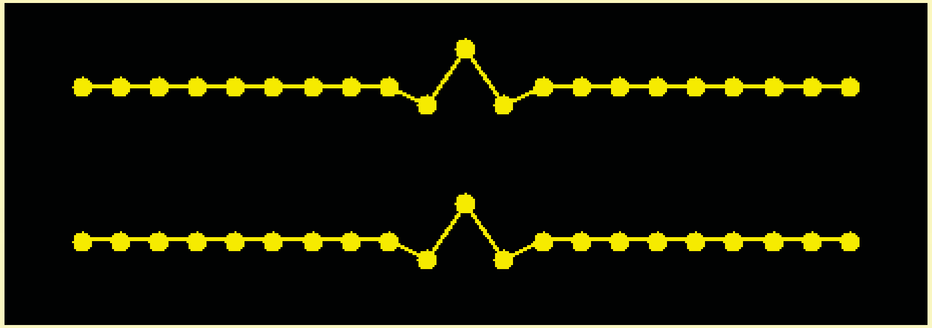
Small amplitude plane waves:

$$x_l(t) \sim \mathrm{e}^{\mathrm{i}(\omega_q t - ql)} \; , \; \omega_q^2 = V"(0) + 4W"(0)\sin(\frac{q}{2})$$

Group velocity $v_g(q)$:

$$v_g(q) = \frac{\mathrm{d}\omega_q}{\mathrm{d}q}$$

For N sites trajectories evolve in a $2N$-dimensional phase space!



- linearized equations of motion
- translational invariance
- symmetry is kept in the eigenvectors
- any initial condition is a superposition of eigenvectors

And therefore any initial localized excitation will spread 'ballistically' into infinities, nothing will remain at the site of original excitation. We will observe complete DELOCALIZATION

AND FOR NONLINEAR EQUATIONS OF MOTION?

Exact solutions?

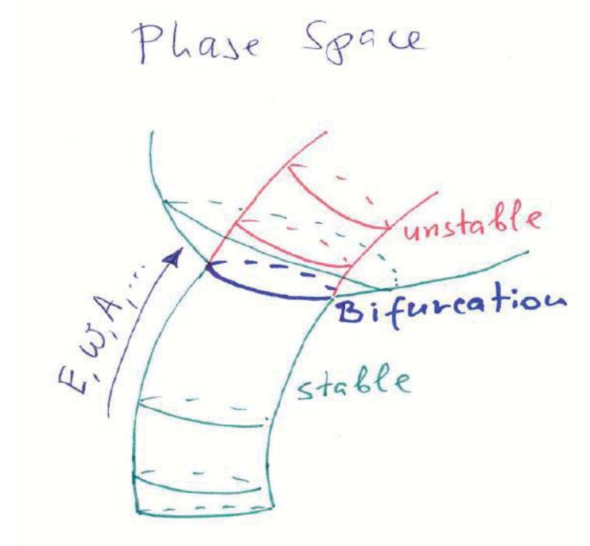
Discrete Breathers:

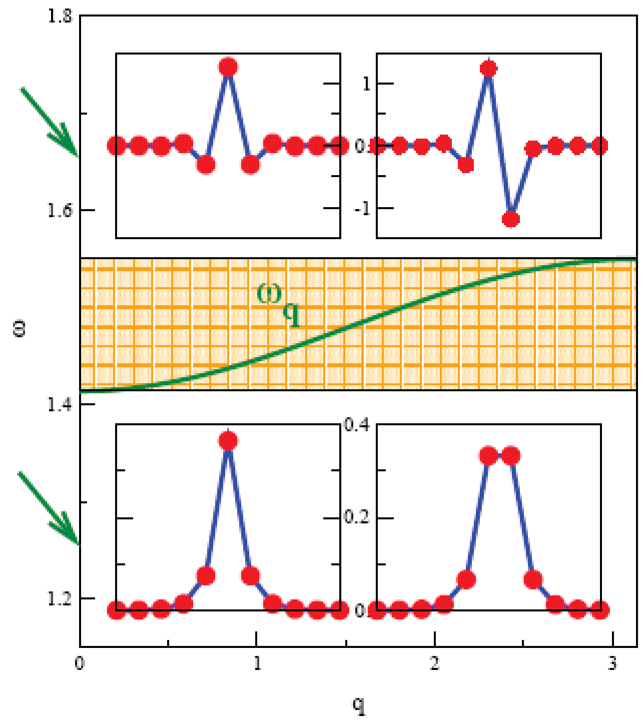
time-periodic, spatially localized solutions of the equations of motion with finite energy (action) with frequency Ω_b

Breathers exist in
$d = 1, 2, 3, ...$-dimensional lattice models

Existence proofs: MacKay/Aubry, Flach, James, Sepulchre, ...

Are dynamically and structurally stable, form one-parameter families of solutions





Necessary ingredients:

nonlinear equations of motion and bounded spectrum ω_q of small amplitude oscillations (phonons, magnons, whateverons)

Necessary condition for existence (Flach 1994):

$$k\Omega_b \neq \omega_q \quad , \quad k = 0, 1, 2, 3, ...$$

Thus:
in general no localized exciations with quasiperiodic time dependence (Flach 1994)

Ansatz: $x_l(t) = \sum_k A_{kl} \mathrm{e}^{ik\omega_b t}$
Insert into EoM, assume localization, go into tails, linearize w.r.t. A_{kl}

$$k^2 \omega_b^2 A_{kl} = v_2 A_{kl} + w_2 (2A_{kl} - A_{k,l-1} - A_{k,l+1})$$

Proof of existence of breathers for time-reversible or Hamiltonian networks of weakly coupled oscillators

R S MacKay†§ and S Aubry‡

Nonlinearity **7** (1994) 1623–1643

Abstract. Existence of 'breathers', that is, time-periodic, spatially localized solutions, is proved for a broad range of time-reversible or Hamiltonian networks of weakly coupled oscillators. Some of their properties are discussed, some generalizations suggested, and several open questions raised.

$$H((x_n, p_n)_{n\in\mathbb{Z}}) = \sum_{n\in\mathbb{Z}} \tfrac{1}{2}p_n^2 + V(x_n) + \tfrac{1}{2}\alpha(x_{n+1} - x_n)^2.$$

Our proof of existence of discrete breathers for weak coupling is in two steps. The first step is to prove persistence of solutions in a space of symmetric time-periodic solutions of fixed period. The second step is to prove that these solutions decay exponentially in space.

The operator $F: SL_{T,1} \times \mathbb{R} \to SM_{T,0}$ is defined by

$$F(z, \alpha) = w$$

where, denoting $z = (x_n, p_n)_{n\in\mathbb{Z}}$, $w = (u_n, v_n)_{n\in\mathbb{Z}}$, we have

$$u_n(t) = \partial H/\partial x_n + \dot{p}_n(t) = V'(x_n(t)) - \alpha(x_{n+1}(t) - 2x_n(t) + x_{n-1}(t)) + \dot{p}_n(t)$$

$$v_n(t) = \partial H/\partial p_n - \dot{x}_n(t) = p_n(t) - \dot{x}_n(t).$$

Weakly coupled anharmonic oscillators

$W \to \varepsilon \cdot W$, $\varepsilon = 0$: noninteracting oscillators

$\vec{R}_0 = \{ x_{n\neq 0} = \dot{x}_{n\neq 0} = 0,\ x_0 = A,\ \dot{x}_0 = 0 \}$

↳ periodic orbit with period $T(A)$ $\quad (\Omega = \frac{2\pi}{T})$

Map of phase space (integrating over time T):

$M(\vec{R};\varepsilon) = \vec{R}'$, $\quad \vec{G}(\vec{R};\varepsilon) = M(\vec{R}) - \vec{R}$

↳ $\vec{G}(\vec{R}_0, 0) = 0$. $\quad \frac{\partial \vec{G}}{\partial \vec{R}} \cdot d\vec{R} + \frac{\partial \vec{G}}{\partial \varepsilon} \cdot d\varepsilon \overset{?}{=} 0$

zero of $\vec{G}$ continuable if $\hat{N} = \left.\frac{\partial \vec{G}}{\partial \vec{R}}\right|_{\vec{R}_0, \varepsilon = 0}$ invertible

$n \neq 0$: $\quad \ddot{x} = -\omega_0^2 x$, $\quad x = c_1 \cdot \cos\omega_0 t + c_2 \cdot \sin\omega_0 t$

$x(0) = 1,\ \dot{x}(0) = 0 \implies x(T) = \cos\omega_0 T,\ \dot{x}(T) = -\omega_0 \sin\omega_0 T$

$x(0) = 0,\ \dot{x}(0) = 1 \implies x(T) = \frac{1}{\omega_0}\sin\omega_0 T,\ \dot{x}(T) = \cos\omega_0 T$

$$\hat{F}_1 = \begin{pmatrix} \cos\omega_0 T & -\omega_0 \sin\omega_0 T \\ \frac{1}{\omega_0}\sin\omega_0 T & \cos\omega_0 T \end{pmatrix}, \qquad \lambda = \cos\omega_0 T \pm i\,|\sin\omega_0 T|$$

$$\lambda = 1 \Rightarrow \omega_0 T = 2\pi n$$

$$\hat{N} = \begin{pmatrix} \left(\frac{dT}{dA}\right)^2 dA & 0 & 0 & \cdots \\ 0 & \boxed{\hat{F}_1 - I} & 0 & \\ 0 & & & \\ \vdots & 0 & \boxed{\hat{F}_2 - I} & \\ & & & \ddots \end{pmatrix}$$

$\hat{N}$ invertible if $\frac{dT}{dA} \neq 0$, $\omega_0 \neq n \cdot \Omega$

Periodic orbit stable if $\omega_0 \neq \frac{n}{2}\Omega$

computing discrete breathers

Obtaining breathers up to machine precision

Time-periodic localized excitations persist
quasi-periodic excitations radiate
Reason: resonances with ω_q!

Ansatz: $x_l(t) = \sum_k A_{kl} \mathrm{e}^{ik\omega_b t}$
Insert into EoM, assume localization, go into tails, linearize w.r.t. A_{kl}

$$H = \sum_l \left[\frac{1}{2}p_l^2 + V(x_l) + W(x_l - x_{l-1})\right]$$

$$V(z) = \sum_{\alpha=2,3,\ldots} \frac{v_\alpha}{\alpha} z^\alpha \ , \ W(z) = \sum_{\alpha=2,3,\ldots} \frac{w_\alpha}{\alpha} z^\alpha$$

$$\ddot{x}_l = -v_2 x_l - w_2(2x_l - x_{l-1} - x_{l+1}) + F_l^{nl}(x_{l'})$$

$$F_l^{(nl)}(t) = \sum_{k=-\infty}^{+\infty} F_{kl}^{(nl)} \mathrm{e}^{ik\omega_b t}$$

$$= - \sum_{\alpha=3,4,\ldots} \left[v_\alpha x_l^{\alpha-1} + w_\alpha((x_l - x_{l-1})^{\alpha-1} - (x_{l+1} - x_l)^{\alpha-1})\right]$$

$$k^2 \omega_b^2 A_{kl} = v_2 A_{kl} + w_2(2A_{kl} - A_{k,l-1} - A_{k,l+1}) + F_{kl}^{(nl)}$$

Designing a map Nr.1 to find solutions

$$A_{kl}^{(i+1)} = \frac{1}{k^2\omega_b^2}\left[(v_2 + 2w_2)A_{kl}^{(i)} - w_2(A_{k,l-1}^{(i)} + A_{k,l+1}^{(i)}) + F_{kl}^{(nl)}(A_{k'l'}^{(i)})\right] \;,\; \lambda_{kl} = \frac{v_2}{k^2\omega_b^2}$$

$$A_{kl}^{(i+1)} = \frac{1}{v_2}\left[(k^2\omega_b^2 - 2w_2)A_{kl}^{(i)} + w_2(A_{k,l-1}^{(i)} + A_{k,l+1}^{(i)}) - F_{kl}^{(nl)}(A_{k'l'}^{(i)})\right] \;,\; \lambda_{kl} = \frac{k^2\omega_b^2}{v_2}$$

So choose $\lambda > 1$ for $l = 0, k = \pm 1$ and $\lambda < 1$ otherwise!

For low order polynomial potential functions e.g.:

$$F_{kl}^{(nl)} = \sum_{\alpha=3,4,\ldots} v_\alpha \sum_{k_1,k_2,\ldots,k_{\alpha-1}=-\infty}^{+\infty} A_{k_1 l} A_{k_2 l} \ldots A_{k_{\alpha-1} l} \delta_{k,(k_1+k_2+\ldots+k_{\alpha-1})}$$

Otherwise integrate numerically at each step:

$$F_{kl}^{(nl)} = \frac{1}{T_1}\int_{-T/2}^{T_2} F_l^{(nl)}(t) \mathrm{e}^{-ik\omega_1 t} \mathrm{d}t$$

Stop the iteration when e.g.

$$\sum_{k,l} |A_{kl}^{(i)} - A_{kl}^{(i-1)}| < 10^{-10}$$

A special case of (nearly) homogeneous potential functions

$$I = \sum_l \left[\frac{1}{2}p_l^2 + \frac{v_2}{2}x_l^2\right] + POT \ , \ POT = \sum_l \left[\frac{v_{2m}}{2m}x_l^{2m} + \frac{w_{2m}}{2m}(x_l - x_{l-1})^{2m}\right] \ , \ m = 2, 3, 4, \ldots$$

$$\ddot{x}_l + v_2 x_l = -v_{2m}x_l^{2m-1} - w_{2m}(x_l - x_{l-1})^{2m-1} + w_{2m}(x_{l+1} - x_l)^{2m-1}$$

Time space separation: $x_l(t) = A_l G(t)$

$$\frac{\ddot{G} + v_2 G}{G^{2m-1}} = -\kappa = \frac{1}{A_l}\left[-v_{2m}A_l^{2m-1} - w_{2m}(A_l - A_{l-1})^{2m-1} + w_{2m}(A_{l+1} - A_l)^{2m-1}\right]$$

$\kappa > 0$ is a separation parameter, can be choosen freely.

Time dependence $\ddot{G} = -v_2 G - \kappa G^{2m-1}$: single anharmonic oscillator

Spatial profile:

$$\kappa A_l = \frac{\partial POT}{\partial x_l}|_{\{x_{l'} \equiv A_{l'}\}} \ , \ \frac{\partial S}{\partial A_l} = 0 \ , \ S = \frac{1}{2}\kappa \sum_l A_l^2 - POT(\{x_l' \equiv A_l'\})$$

Breathers are saddles of S!

Method Nr.2: Saddles on the rim!

choose direction in N-dimensional space of all A_l, e.g. $(\ldots 0001000\ldots)$, $(\ldots 0001001000\ldots)$

Start from space origin P0 $A_l = 0$, depart with small steps in chosen direction, compute S

It will first increase and then pass through a maximum P1

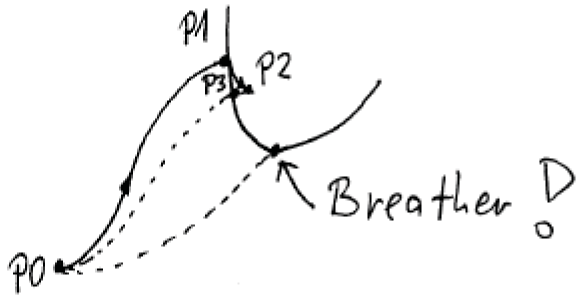
Now we are on the rim

Compute the gradient of S here and make a small step in opposite direction to P2

Maximise S on the line P0-P2 to be on the rim again.

Repeat until you reach a saddle!

A very simple and efficient way to compute different types of breathers, multibreathers etc in arbitrary dimensional lattices



Method Nr.3: Homoclinic orbits (only in $d = 1$ and with short range interaction)!

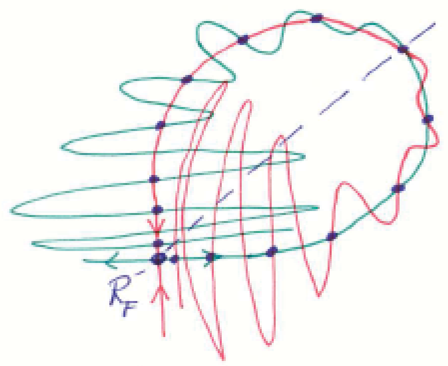
$$A_{l+1} =$$

$$A_l + \left[v_{2m} A_l^{2m-1} + w_{2m}(A_l - A_{l-1})^{2m-1} - \kappa A_l\right]^{\frac{1}{2m-1}}$$

2d map with $\vec{R}_l = (x_l, y_l) = (A_{l-1}, A_l)$:

$$x_{l+1} = y_l$$

$$y_{l+1} = y_l + \left[v_{2m} y_l^{2m-1} + w_{2m}(y_l - x_l)^{2m-1} - \kappa y_l\right]^{\frac{1}{2m-1}}$$



Fixpoint: $\vec{R}_F = (0, 0)$
(un)stable 1d manifold:
(backward) iteration converges to $\vec{R}_F$
Manifold intersections:
homoclinic points!
Iterated for- or backward yield
homoclinic orbits. i.e. breathers!
Reflection symmetry:
one homoclinic point on $x = y$
depends parametrically on κ
Simple numerical search by e.g. fixing
$x_0 = y_0$ and varying κ
Can be used for a formal
existence proof!
Existence of multibreathers follows from
generic intersection structure

Using the phase space

So far: periodic orbits as solutions of algebraic equations
Variables: Fourier coefficients or simply amplitudes

Of course we can use more general methods of solving algebraic equations, e.g. various gradient methods or Newton routines

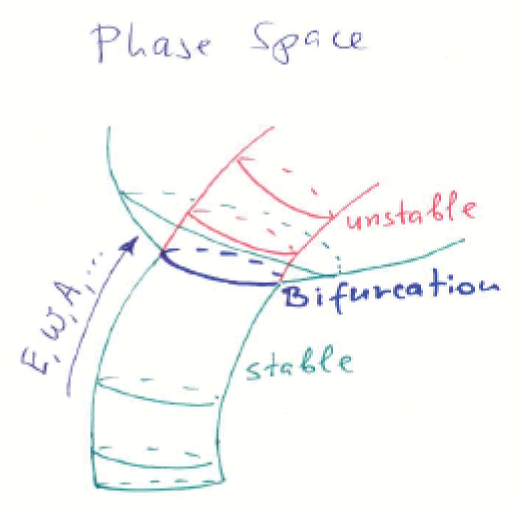
We need always a good initial guess (start close to a case where you know the solution!)

Gradient methods: more sophisticated in programming
Newton routines: may suffer from long times needed to invert matrices, danger when close to a noninvertable case (bifurcations!)
(recall: $f(x = s) = 0$, $f(x) = f(x_0) + f'(x_0)(x - x_0) + hot$
$x_{n+1} = x_n - f(x_n)/f'(x_n)$)

If besides the Hamiltonian H we have another conserved quantity B, then the manifolds of some isolated periodic orbits may satisfy the parallelity of gradients, i.e. $grad(H) \parallel grad(B)$

Periodic orbit:
loop in phase space

Isolated periodic orbit (PO):
neighbourhood in phase space free of POs with identical conserved quantities (as opposed to POs on resonant tori)



Method Nr.4: NEWTON in phase space

Integrate a given initial condition $\vec{\tilde{R}}$ with $x_l(t=0) \equiv X_l$, $p_l(t=0) \equiv P_l$ over a certain time T:

$$x_l(T) \equiv I_l^x(\{X_{l'}, P_{l'}\}, T)$$

$$p_l(T) \equiv I_l^p(\{X_{l'}, P_{l'}\}, T)$$

Consider the functions

$$F_l^x = I_l^x - X_l \ , \ F_l^p = I_l^p - P_l$$

If $\vec{\tilde{R}}$ belongs to a PO with period T then

$$F_l^x = F_l^p = 0$$

For a Newton routine to converge: remove all degeneracies!

If $\vec{\tilde{R}}$ belongs to the PO, then a 1d manifold of points belong to the PO

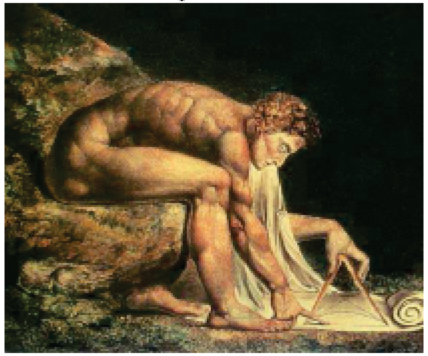
Degeneracy removed by one additional condition, e.g. $P_M = 0$

So for N degrees of freedom zeroes of $2N-1$ coupled equations of $2N-1$ variables!

Make sure that a zero of these $2N-1$ equations with the additional initial condition $P_M = 0$ uniqely fixes $p_M(T) = 0$, e.g. through energy conservation.

Advantages of Newton:
exponential convergence $|\vec{F}|_{n_{it}+1} \sim |\vec{F}|_{n_{it}}$
easy to program
we may use one Newton matrix for several iterations

Disadvantages of Newton:
computational time $\sim N^2$
matrix inversion sensitive to bifuractions
may need subtle routines (singular value decomposition, dealing with sparse matrices etc)
Blake's representation of Newton:



Method Nr.5:
STEEPEST DESCENT in phase space

$$g(\vec{\tilde{R}}) = \sum_l \left[F_l^x F_l^x + F_l^p F_l^p\right]$$

$$(\nabla g)_n = \frac{\partial g}{\partial \tilde{R}_n}$$

Start in phase space, go in direction opposite to the gradient!

Advantages of Descent
computational time $\sim N$
insensitive to bifurcations

Disadvantages of Descent
more clumsy to program
slower convergence
distinguish zero minimima from nearly zero minima?

localization properties

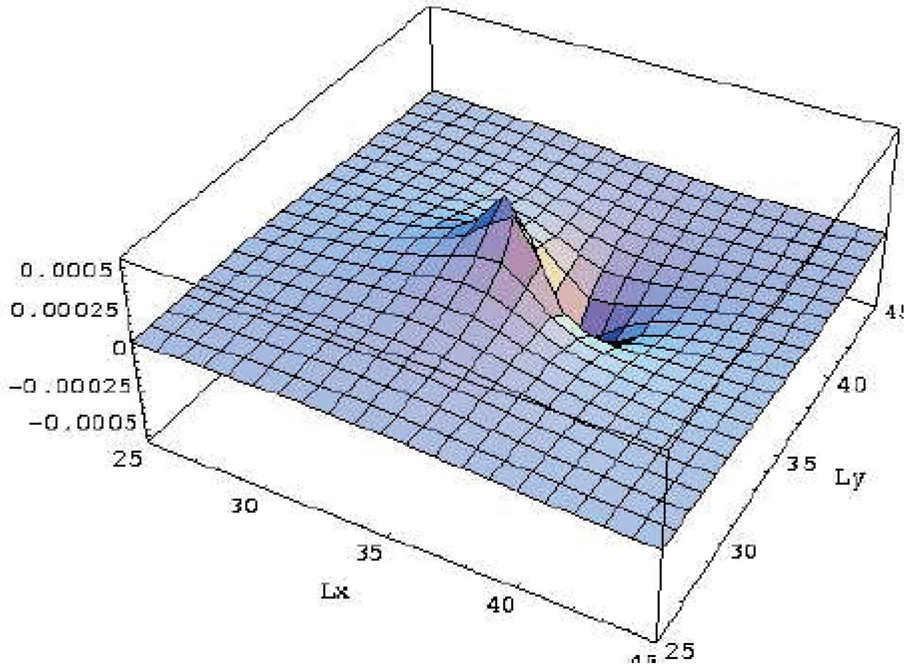
Localization in space?

exponential or algebraic for analytic or nonanalytic function $E(q) = \omega_q^2$ (MacKay,Aubry,Flach,Gaididei,...)

$$A_{kl} \sim A G_{k\Omega_b}(l)$$
$$G_{k\Omega_b}(l) = \int \frac{\cos(ql)}{-(k\Omega_b)^2 + \omega_q^2} \mathrm{d}^d q$$
$$r = \ln(|\lambda_k(\Omega_b)|) l \equiv \delta l$$
$$G(x) \sim \mathrm{e}^{-x} \quad , \quad d = 1$$
$$G(x) \sim \int \frac{\mathrm{e}^{-x\sqrt{1+\xi^2}}}{\sqrt{1+\xi^2}} \mathrm{d}\xi \quad , \quad d = 2$$
$$G(x) \sim \frac{1}{x} \mathrm{e}^{-x} \quad , \quad d = 3$$

'acoustic' breather: $\omega_{q=0} = 0$

static lattice deformation $\sim 1/r^{d-1}$ (Flach/Kladko/Takeno)



Dimension induced energy barriers:

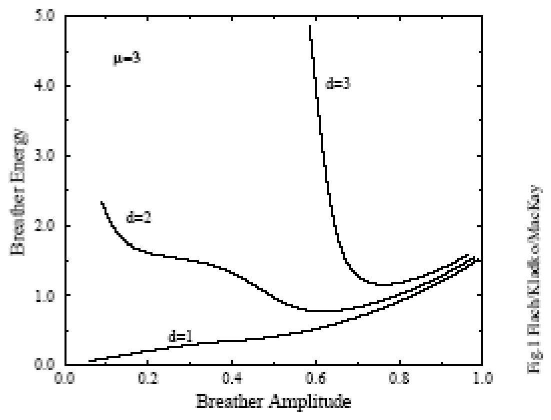
(Flach,Kladko,MacKay 1997), also Weinstein,Kastner,...

Breathers for small amplitudes:

$$|\Omega_b - \omega_{q_{BE}}| \sim \delta^2 \sim A^z$$

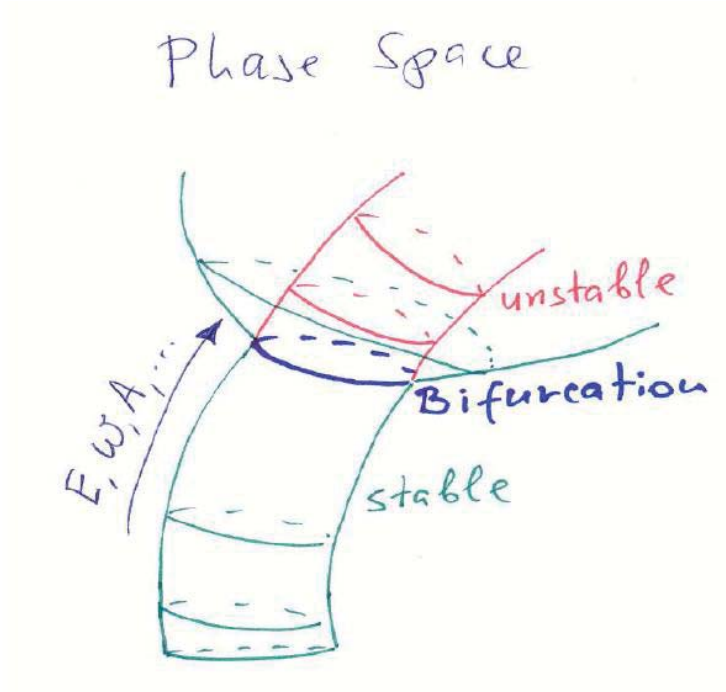
$$E_b \sim \frac{1}{2}A^2 \int r^{d-1}G^2(A^{z/2}r)\mathrm{d}r$$

$$E_b \sim A^{(4-zd)/2} \ , \ \ z=2$$



The breather zoo of localized:

vibrations
rotations
spin excitations
bound states with quasiparticles
...



stability and scattering

Perturbing breathers

Breather solution $x_l(t)$.
Now we add a small perturbation $\epsilon_l(t)$ to it and linearize the resulting equations for $\epsilon_l(t)$:

$$\ddot{\epsilon}_l = -\sum_m \frac{\partial^2 H}{\partial x_l \partial x_m}|_{\{x_{l'}(t)\}} \epsilon_m$$

This problem corresponds to a time-dependent Hamiltonian $\tilde{H}(t)$

$$\tilde{H}(t) = \sum_l \left[\frac{1}{2}\pi_l^2 + \frac{1}{2}\sum_m \frac{\partial^2 H}{\partial x_l \partial x_m}|_{\{x_{l'}(t)\}} \epsilon_l \epsilon_m \right]$$

$$\dot{\epsilon}_l = \frac{\partial \tilde{H}}{\partial \pi_l}\,,\ \dot{\pi}_l = -\frac{\partial \tilde{H}}{\partial \epsilon_l}$$

For simplicity we drop the lattice index here.
Define the matrix $\mathcal{J}$

$$\mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and the evolution matrix $\mathcal{U}(t)$

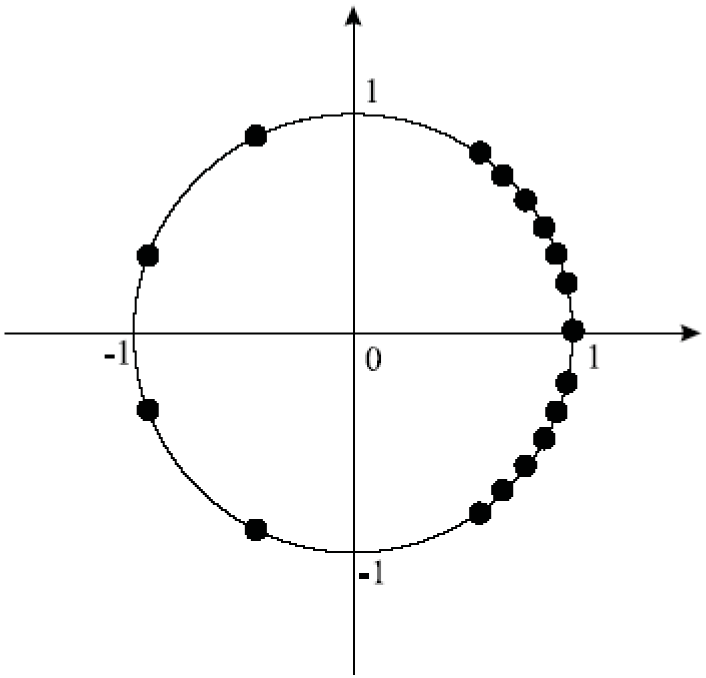
$$\begin{pmatrix} \pi(t) \\ \epsilon(t) \end{pmatrix} = \mathcal{U}(t) \begin{pmatrix} \pi(0) \\ \epsilon(0) \end{pmatrix}$$

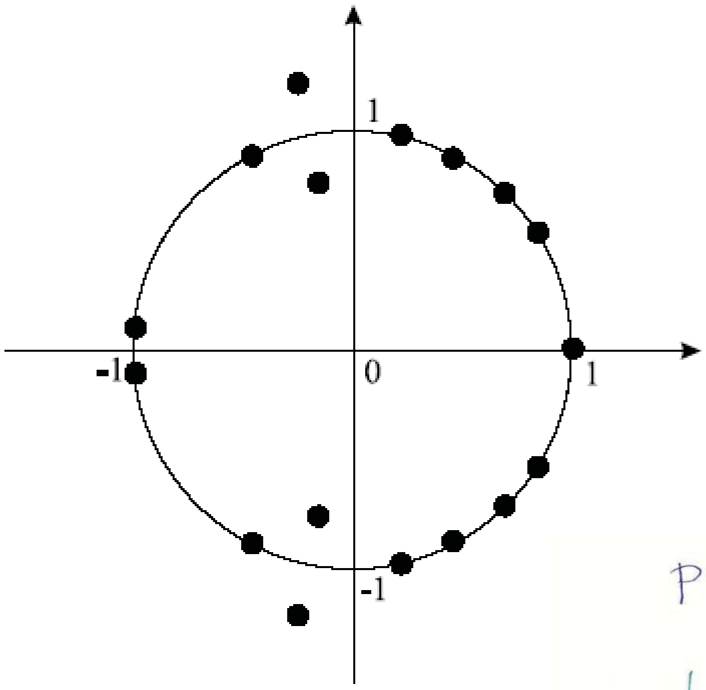
It follows

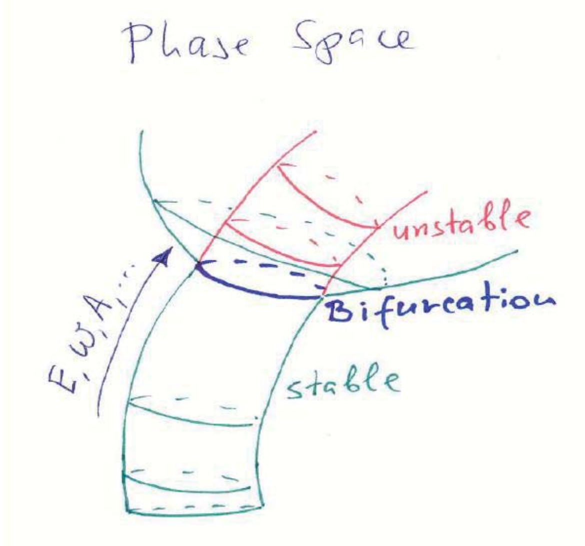
$$\to \mathcal{U}^T(t)\mathcal{J}\mathcal{U}(t) = \mathcal{J}$$

Thus $\mathcal{U}(t)$ is symplectic!

Schematic view of the Floquet eigenvalues



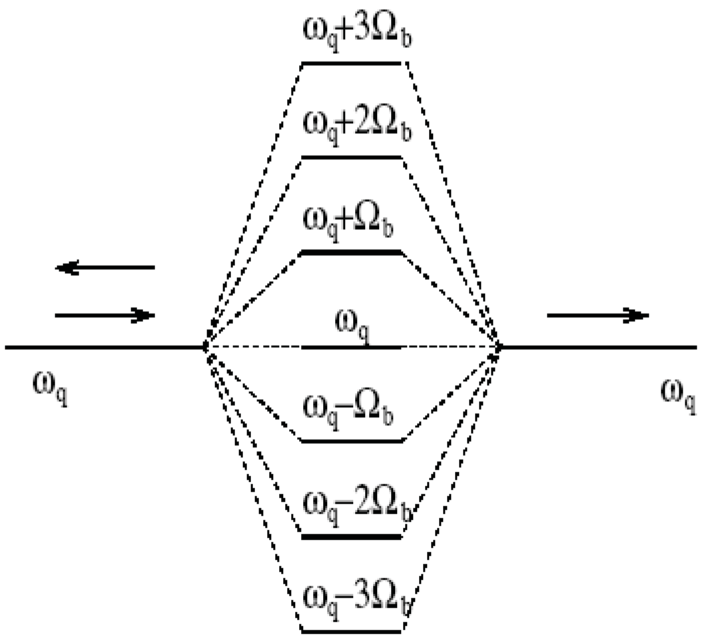




Computing transmission up to machine precision

Scattering goes through the extended Floquet states:

$$\epsilon_l(t) = \sum_{k=-\infty}^{\infty} e_{lk} \mathrm{e}^{\mathrm{i}(\omega_q + k\Omega_b)t}$$



Possibility to obtain Fano resonances due to destructive interference (perfect reflection)!

Numerical Scheme for one-channel scattering: find the zeroes of $\mathbf{G}$:

$$\mathbf{G}(\vec{\epsilon}(0), \dot{\vec{\epsilon}}(0)) = \begin{pmatrix} \vec{\epsilon}(0) \\ \dot{\vec{\epsilon}}(0) \end{pmatrix} - e^{i\omega_q T_b} \begin{pmatrix} \vec{\epsilon}(T_b) \\ \dot{\vec{\epsilon}}(T_b) \end{pmatrix}$$

Boundary conditions:

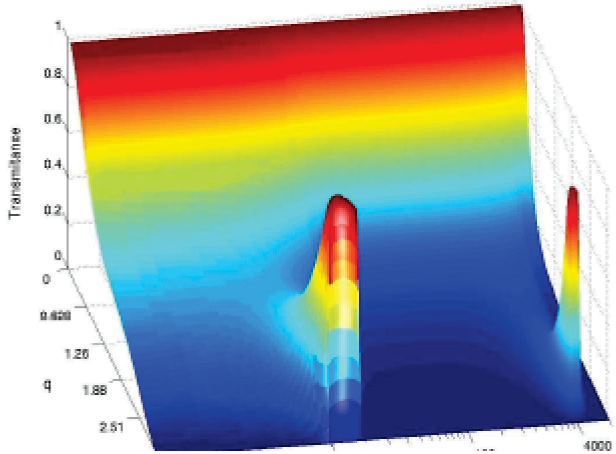
$$\epsilon_{N+1} = e^{-i\omega_q t}\ ,\ \epsilon_{-N-1} = (A+iB)e^{-i\omega_q t}$$

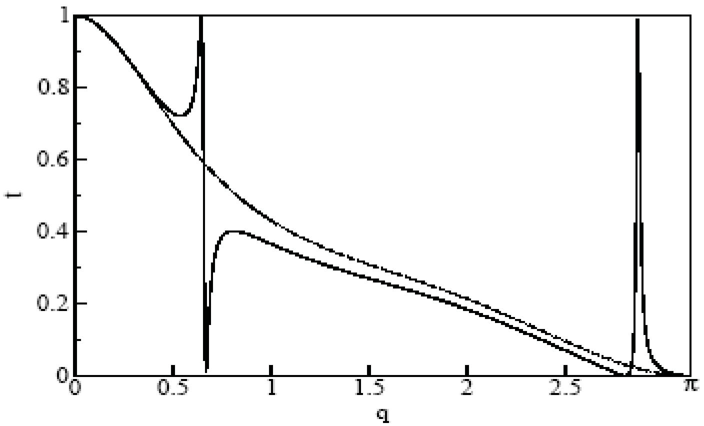
Fixing for the moment A, B, use standard Newton to find zeroes of $\mathbf{G}$.

Find values for A, B such that $\epsilon_N = e^{-iq-i\omega_q t}$
Use the notation $\epsilon_l(t) = \zeta_l(t)e^{-i\omega_q t}$.
Then the transmission coefficient is given by

$$t_q = \frac{4\sin^2 q}{|(A+iB)e^{-iq} - \zeta_{-N}|^2}$$

FPU chains:





- **So there is resonant transmission and reflection (same for KG chains)**

- **Resonant transmission: single channel resonances, no phase coherence required**

- **Resonant reflection: several channels needed, phase coherence required, here: effect of time-dependent scattering potential**

- **Mechanism?**

Start with DNLS as an example:

$$i\dot{\Psi}_n = C(\Psi_{n+1} + \Psi_{n-1}) + |\Psi_n|^2 \Psi_n$$

$$\omega_q = -2C \cos q$$

$$\hat{\Psi}_n(t) = \hat{A}_n e^{-i\Omega_b t} \, , \; \hat{A}_{|n| \to \infty} \to 0$$

Weak coupling:

$$\hat{A}_0 \approx \sqrt{|\Omega_b|} \, , \; \hat{A}_{n \neq 0} \approx 0$$

Linearize in small perturbations:

$$\Psi_n(t) = \hat{\Psi}_n(t) + \phi_n(t)$$

$$i\dot{\phi}_n = C(\phi_{n+1} + \phi_{n-1}) + \Omega_b \delta_{n,0}(2\phi_0 + e^{-2i\Omega_b t}\phi_0^*)$$
$$\phi_n(t) = X_n e^{i\omega_q t} + Y_n^* e^{-i(2\Omega_b + \omega_q)t}$$

$$-\omega_q X_n = C(X_{n+1} + X_{n-1}) + \Omega_b \delta_{n,0}(2X_0 + Y_0)$$
$$(2\Omega_b + \omega_q)Y_n = C(Y_{n+1} + Y_{n-1}) + \Omega_b \delta_{n,0}(2Y_0 + X_0)$$

$$\omega_L^{(y)} = 2(-\Omega_b + \sqrt{\Omega_b^2 + C^2}\,)$$

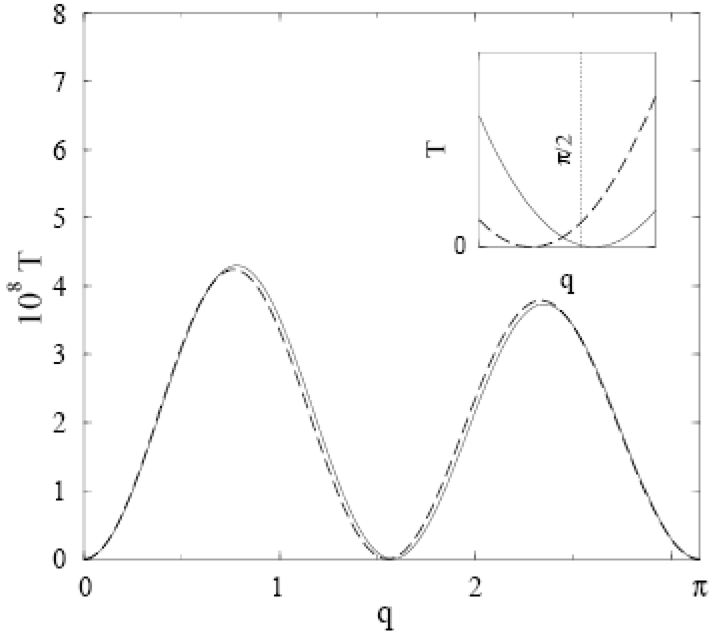
Localized mode in closed channel!

Solve for transmission using transfer matrix approach:

$$T = \frac{4\sin^2 q}{\left(\frac{2\Omega_b}{C} - \frac{\Omega_b^2}{2C^2}\frac{\kappa}{1+\kappa\cos q}\right)^2 + 4\sin^2 q}$$

$$1 + \kappa\cos q = 0 \leftrightarrow \omega_q = \omega_L^{(y)}$$

THIS IS A FANO RESONANCE!



Fano resonances in nanoscale structures
A. E. Miroshnichenko, S. Flach, Y. S. Kivshar
Rev. Mod. Phys. 82, 2257 (2010).

going beyond

Quantum breathers?

- Action quantization: E_n
- N-fold degeneracy?
- Degeneracy will be lifted
- Breathers start to tunnel

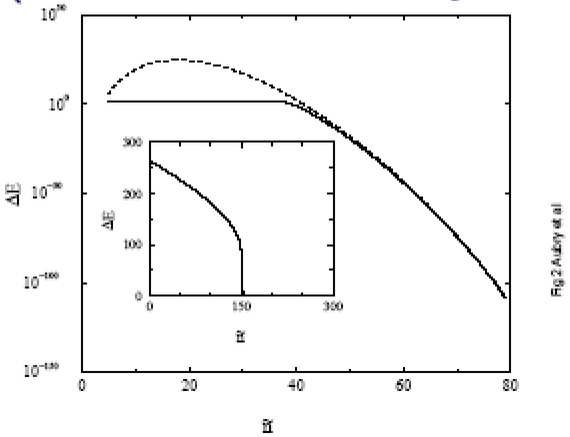
Bound states?

Numerical evidence for $N = 6$
(Bishop et al (1998))

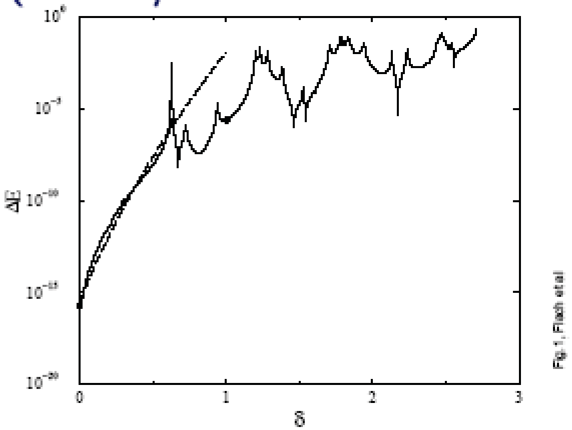
Back to $N = 2, 3$ (dimer, trimer)
Influence of nonintegrability and quantum corrections can be systematically traced

Results relevant for excitations of molecules

Level splittings for the dimer
(Flach,Kladko,Aubry et al 1996)



chaos assisted tunneling
(Flach/Fleurov 1997-2001)



experiments

Bound states of vibrational quanta:

local excitations in molecules and crystals,
i.e. bound N-phonon states, detectable
through red shift of excitation energies:

$N \leq 6$: Benzene, Naphtalene, Anthracene
(R. L. Swofford et al J Chem Phys (1976)

$N = 2$: Hydrogen vibration on auf H/Si(111) surface
P. Guyot-Sionnest PRL (1991)

$N = 3$: C-O vibration on CO/Ru(001)
P. Jakob PRL (1996)

$N = 3$: CO_2 crystal
R. Bini et al J Chem Phys (1993)

$N = 7$: PtCl complexes
B. I. Swanson et al PRL (1999)

VOLUME 82, NUMBER 16 PHYSICAL REVIEW LETTERS 19 APRIL 1999

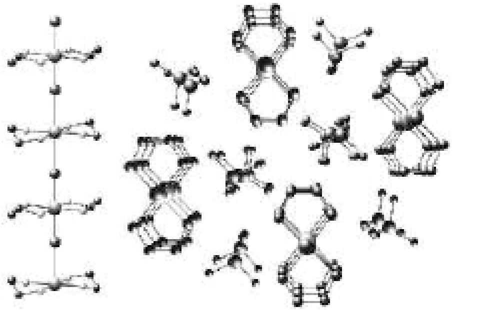
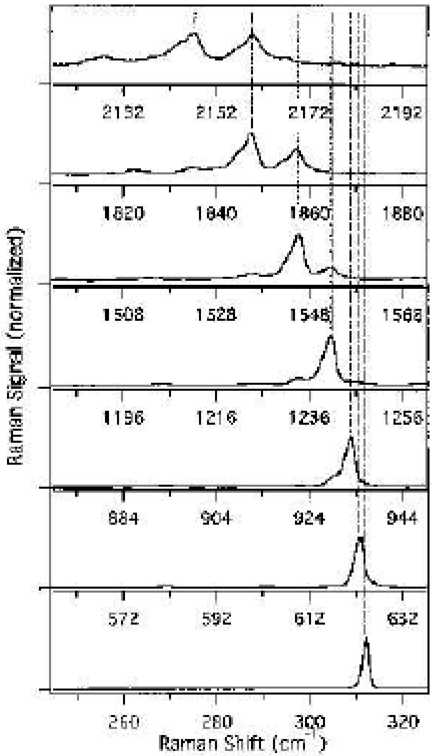


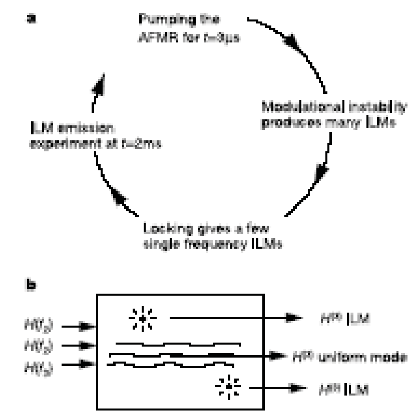
FIG. 1. Structure of $\{[Pt(en)_2][Pt(en)_2Cl_2](ClO_4)_4\}$ (en = ethylenediamine; H atoms are omitted) [11]. One PtCl chain is shown on the left. Each Pt atom is coordinated by two ethylenediamine units in a near square planar geometry, while Cl^- ions connect the Pt sites along the chain. The packing arrangement of the 1D chains and their ClO_4^- counterions is shown on the right.

peak pattern with an approximate 9.6:6.2:1 ratio (data not shown), as expected for localization of vibrational energy onto a single oxidized $PtCl_2$ unit with statistical distribution of Cl isotopes [15]. This suggests that in the natural abundance material, by the second overtone the resonance Raman process creates states with localization of vibrational energy onto nearly a single $PtCl_2$ unit, indicating an *increase in localization from the already somewhat localized fundamental.* These observations strongly indicate the usefulness of examining high overtones in the isotopically pure materials, which are free of isotopic disorder,



Direct observation of discrete breathers in antiferromagnets

Sato, Sievers, Nature 2004



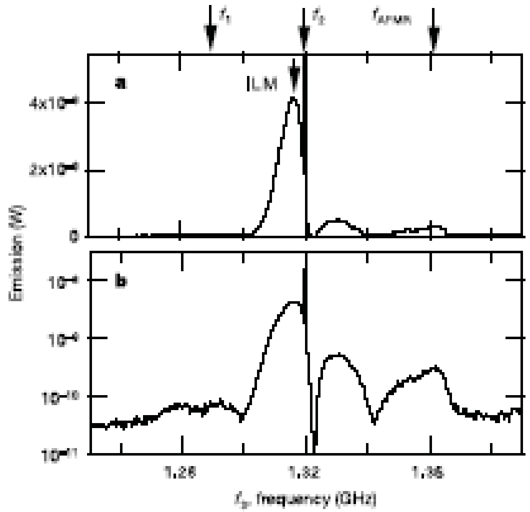
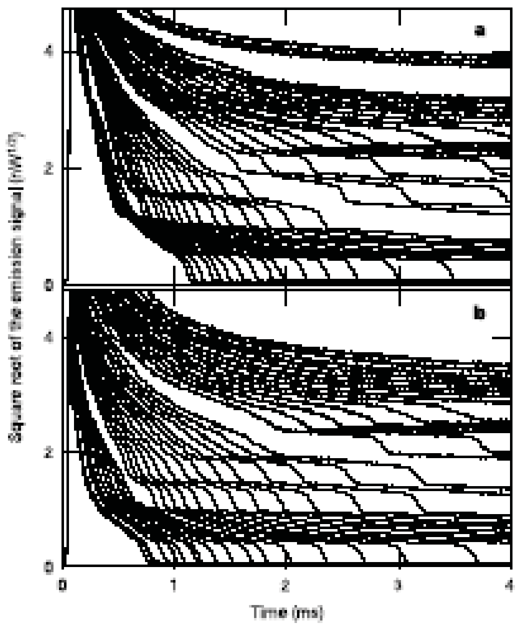


Figure 2 Snapshot of the mixing spectrum versus the probe oscillator frequency. **a**, Mixing data taken at 2 ms after the 3-μs-long, 52 W pulse at $f_1 = 1.29$ GHz. Here $f_2 = 1.32$ GHz at a c.w. power of 240 mW. The weak (~1 mW) probe oscillator of variable frequency f_3 is scanned. A number of features are seen in the $H^{(3)}$ emission. The



Light localization in photonic crystals: $\epsilon(\mathbf{r})$, Maxwell, Kerr-medium $n(E)$ AlGaAs (Silberberg et al 1998)

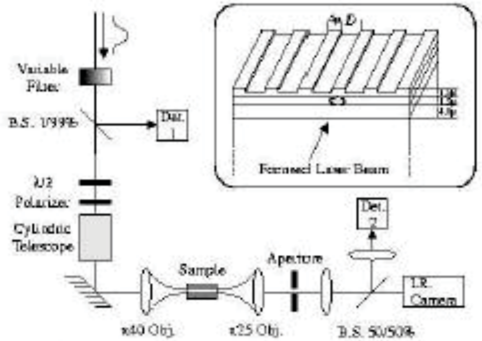
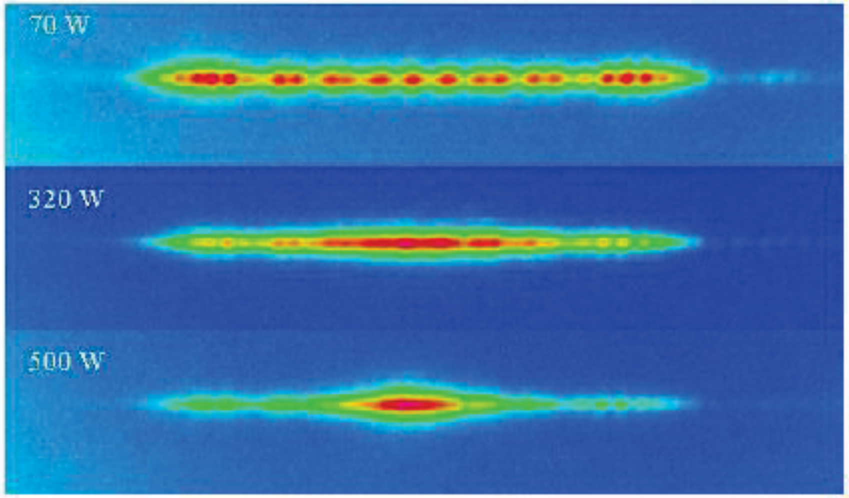


FIG. 2. The experimental setup. Inset: Schematic drawing of the sample. The sample consists of a $Al_{0.18}Ga_{0.82}As$ core layer and $Al_{0.24}Ga_{0.76}As$ cladding layers grown on top of a GaAs substrate. A few samples were tested with different separations D between the waveguides.



Nonlinear silica waveguides Cheskis et al 2003

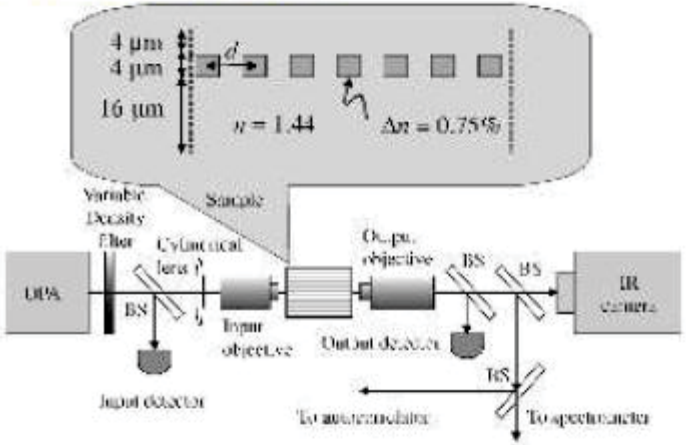


FIG. 1. Experimental setup and sample cross section.

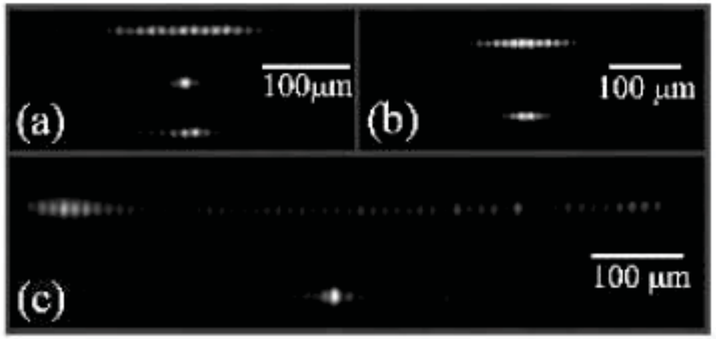
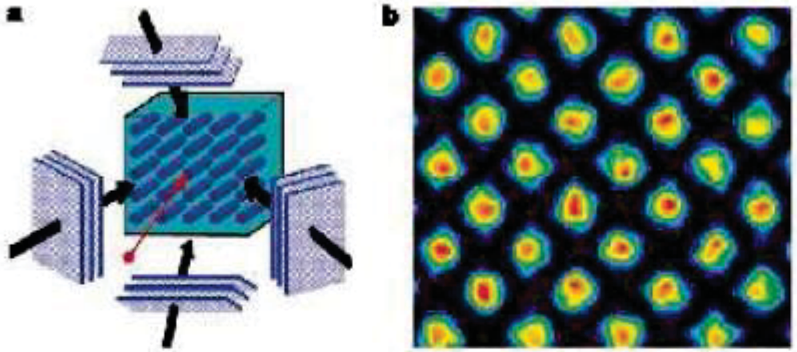
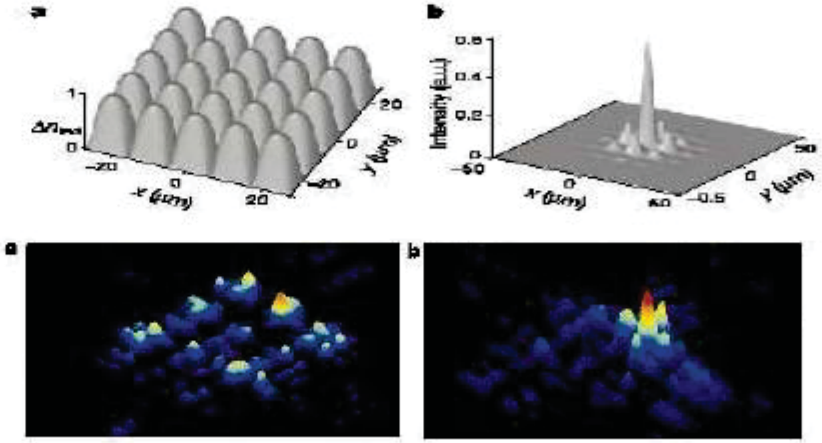


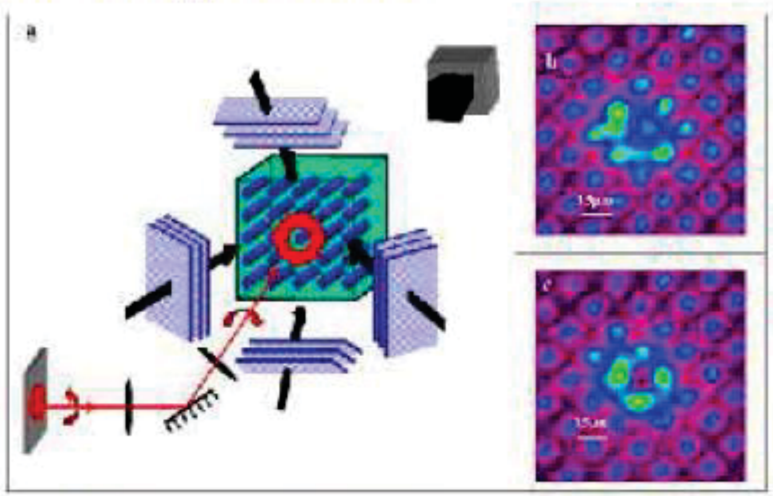
FIG. 2. Images of the sample's output facet under different excitation conditions. (a) Broad input beam (equal dispersion and diffraction lengths): top to bottom, 0.09, 0.45, and 0.74 MW. (b) The unstable mode is excited with the broad input beam: top, low power; bottom, high power. (c) Single waveguide excitation: top, 0.07 MW; bottom, 0.44 MW.

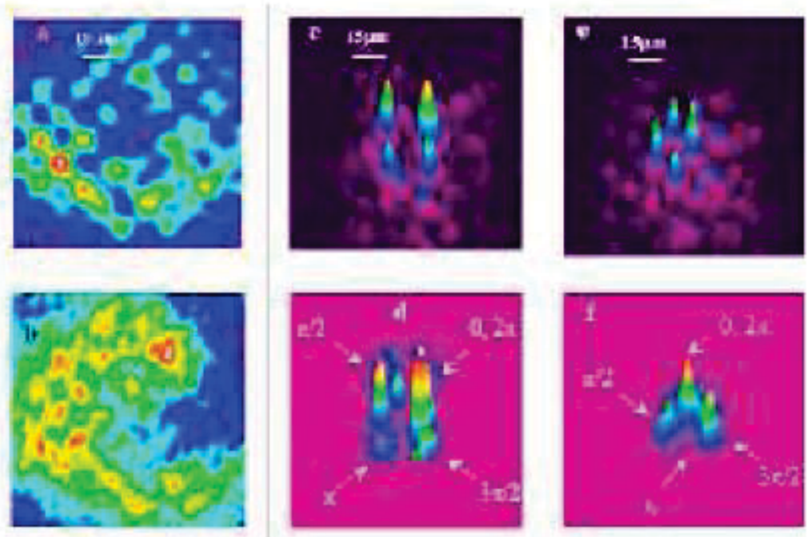
Breathers in optically induced nonlinear photonic 2d lattices based on SBN:75
Fleischer et al 2004





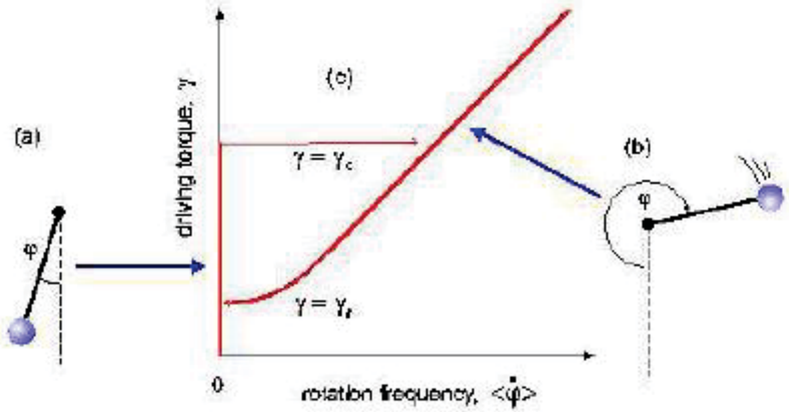
Vortex-ring breathers

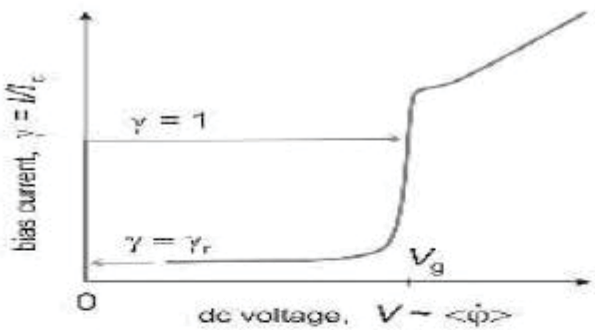


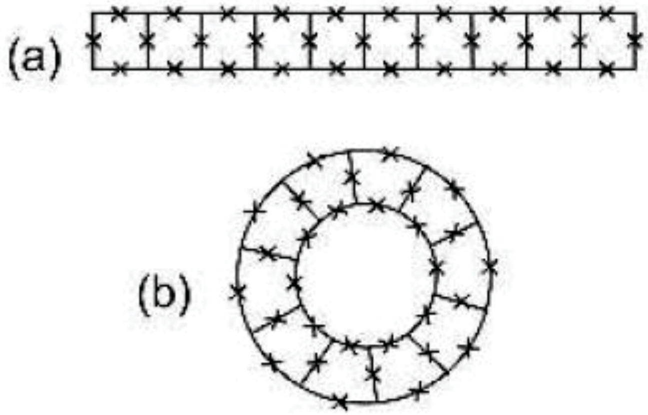


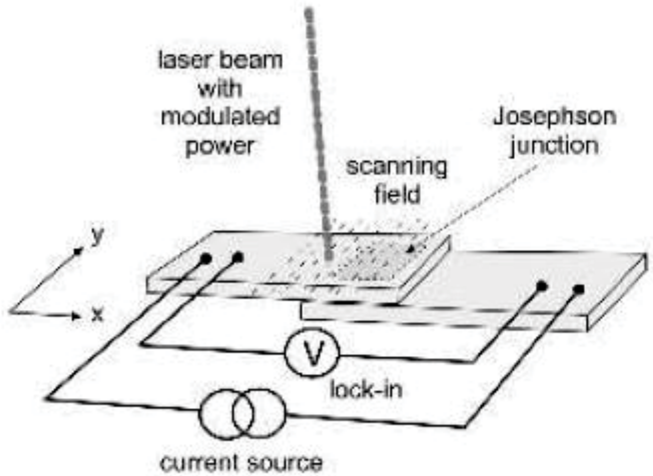
Josephson junction ladders
(Ustinov,Binder,Schuster)

$$\ddot{\varphi} + \alpha\dot{\varphi} + \sin\varphi = \gamma$$



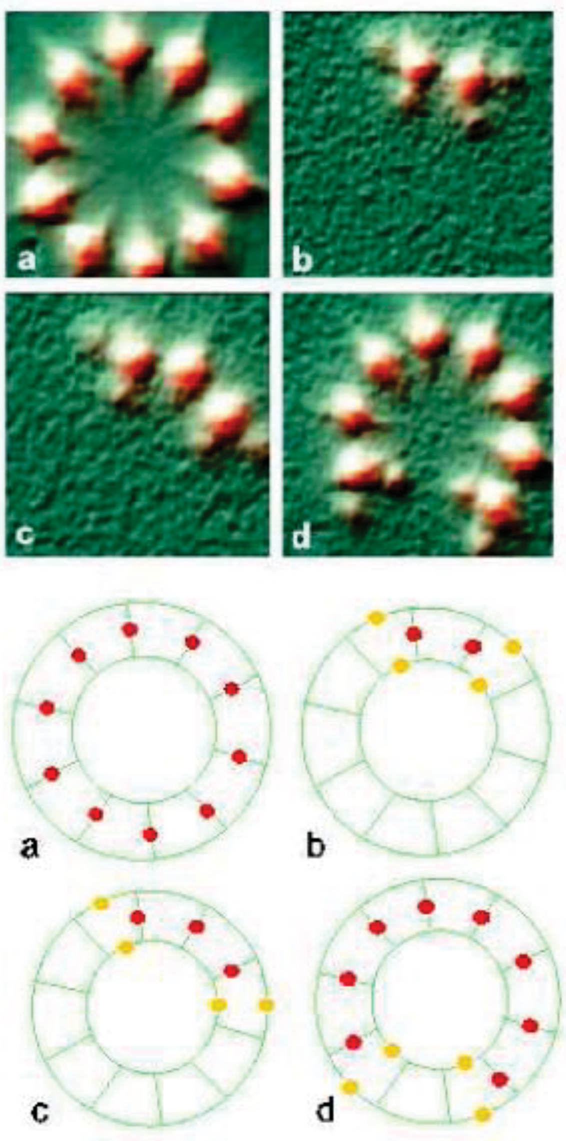






Josephson junction networks

Ustinov et al



The zoo of rotobreathers

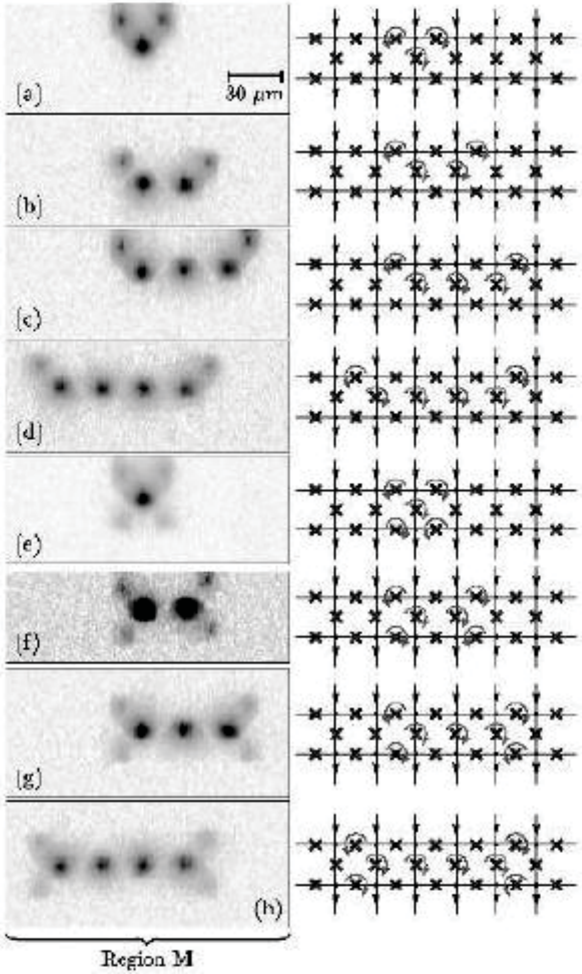
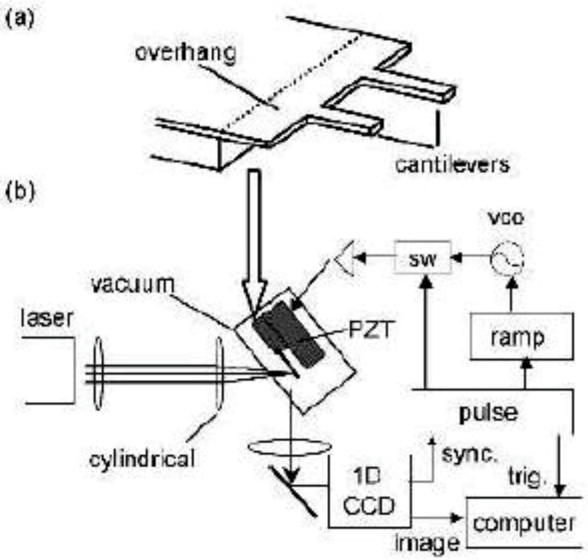


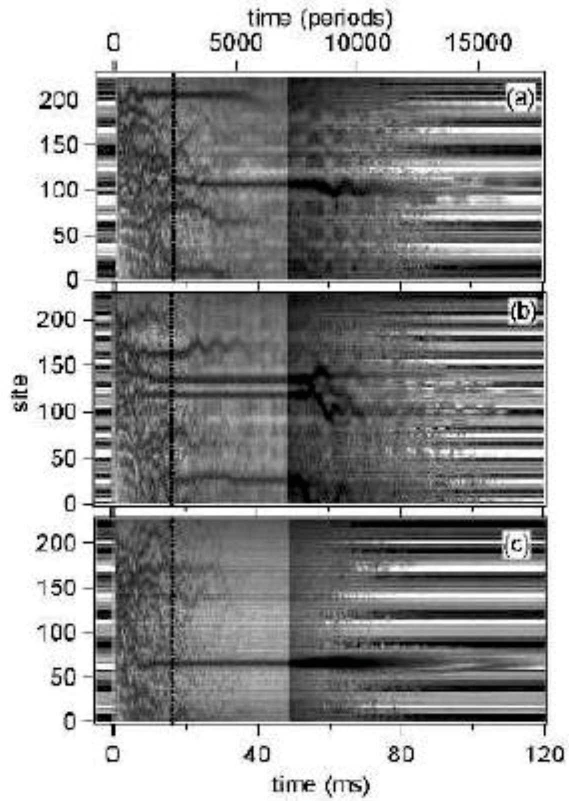
FIG. 2. Various localized states (discrete rotobreathers) measured by the low-temperature scanning laser microscope: (a)–(d) asymmetric rotobreathers; (e)–(h) symmetric rotobreathers. Region M is illustrated in Fig. 1(b).

Breathers in driven micromechanical cantilever arrays
Sato et al 2003

Si_3N_4 **cantilevers**
l/w/p: 50/15/40 μm
PZT drive at 150kHz

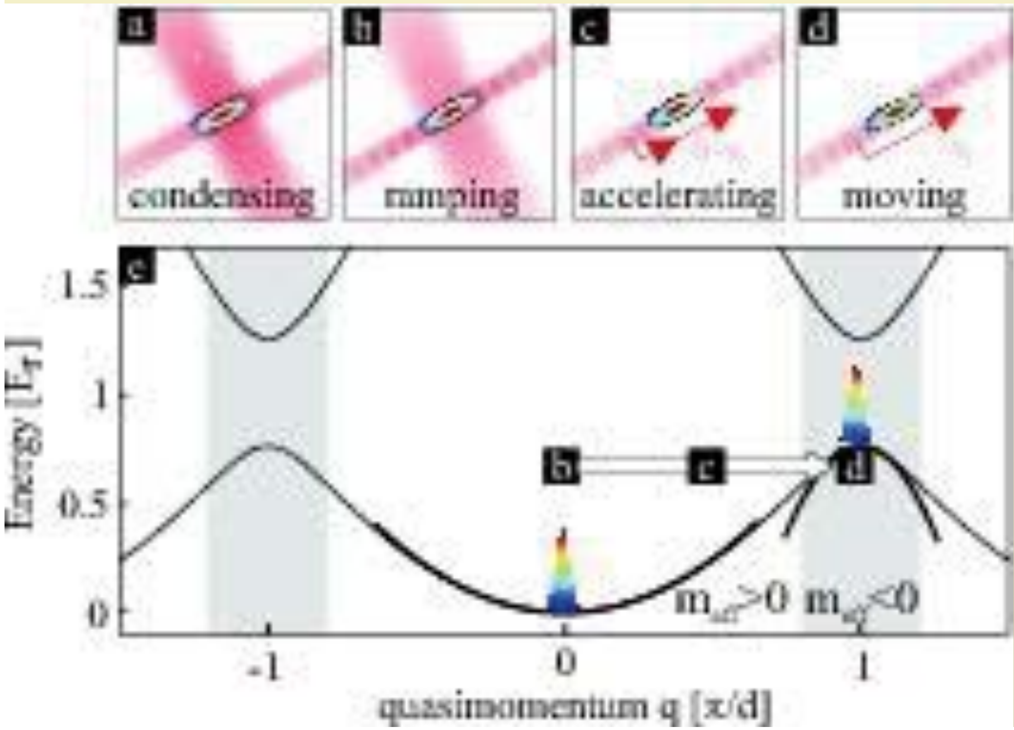


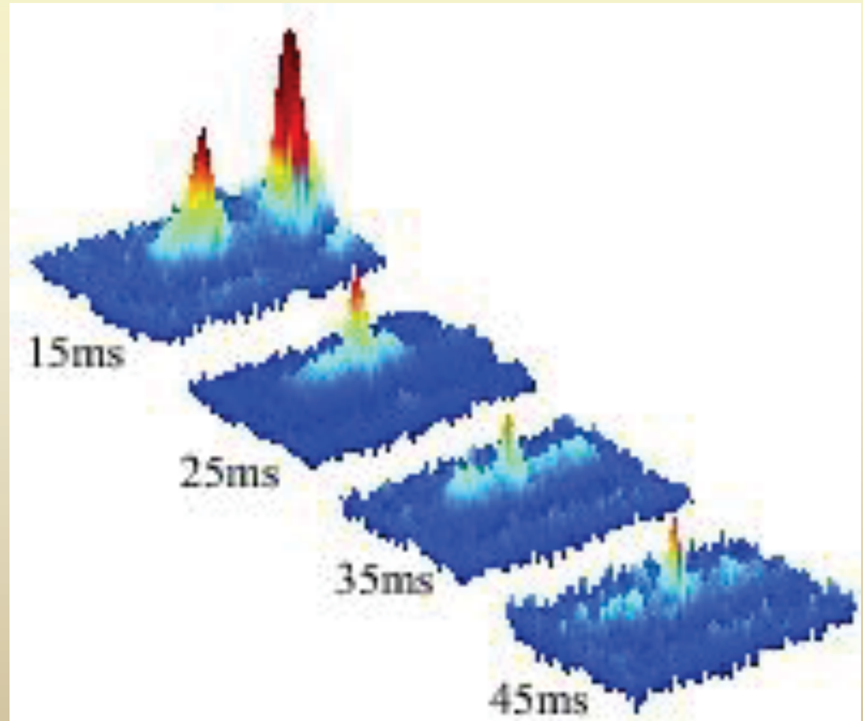
Detector:
He-Ne laser and CCD camera



BEC in an optical lattice (group of Oberthaler, 2004)

Prepare the BEC in the q=0 state, change quasimomentum by ramping, accelerating and moving.
Atoms interact repulsively, yet form a localized gap soliton state, which is stable. The atoms can not delocalize because the kinetic energy (of the first band) has a finite upper bound





Theory applied to:

- **interacting Josephson junction networks (classical regime)**
  DB existence, e/m wave scattering, quasiperiodic DBs, magnetic field influence
- **capacitively coupled Josephson junctions (quantum regime)**
  quantum breathers, tunneling, correlations, coherence, entanglement
- **electron-phonon interactions in crystals**
  interaction mediated many-phonon bound states
- **lattice spin excitations**
  FMs with easy plane and easy axis anisotropy
- **driven micromechanical cantilever arrays**
  modeling, routes to excite discrete breathers, response to AC fields
- **spatially modulated nonlinear optical waveguides**
  resonant scattering of probe light beams by spatial solitons, surface solitons
- **cold atoms in optical lattices**
  resonant matter wave scattering by BEC lattice solitons

SUMMARY OF LECTURE II

- nonlinearity and discreteness localize energy
- invariant manifolds – periodic orbits
- localization in real space, despite of translational inv.
- quantization yields slow tunneling of energy lumps
- breathers are robust with respect to perturbations
- breathers slow down relaxation, scatter waves
- breathers are observed in a wide variety of physical systems

Want to know more?

- http://www.pks.mpg.de/~flach
- Physics Reports 295 (1998) 181
- Physics Today 57(1) (2004) 43
- Physics Reports 467 (1-3) (2008) 1
- Rev. Mod. Phys. 82 (2010) 2257