

# Discrete Breathers: Localizing Energy Through Nonlinearity and Discreteness

S. Flach, MIPKS Dresden



## Road map:

- collecting evidence:
  - bifurcations and symmetry breaking
  - table and computational experiments
- discrete breathers: time-periodic and spatially localized
- proving their existence, and computing them
- small fluctuations: stability and scattering
- experimental observations

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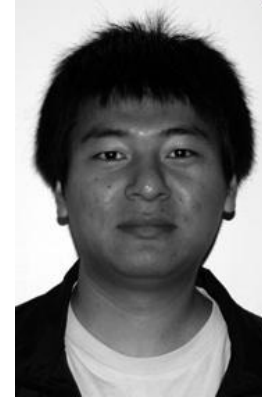
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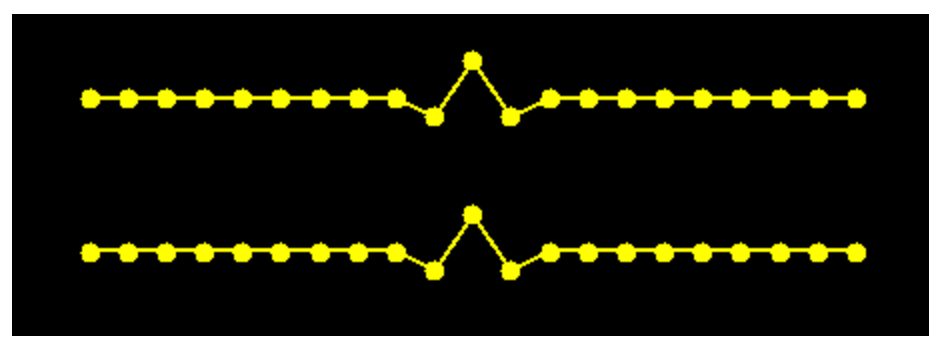
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## A few preliminaries

- 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

**PART ONE:**

**COLLECTING EVIDENCE**

one classical anharmonic oscillator:

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

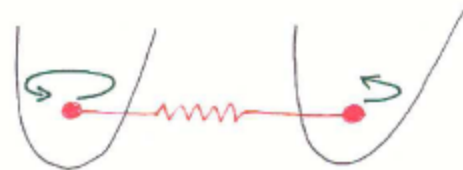
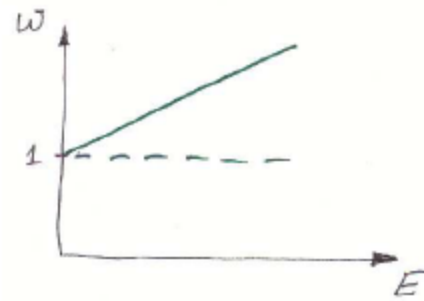
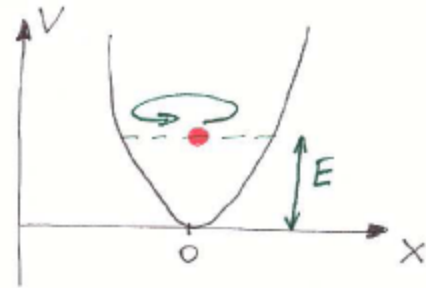
The frequency of oscillations is depending on the energy:

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

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:  
 $H(1, 2) = H(2, 1)$



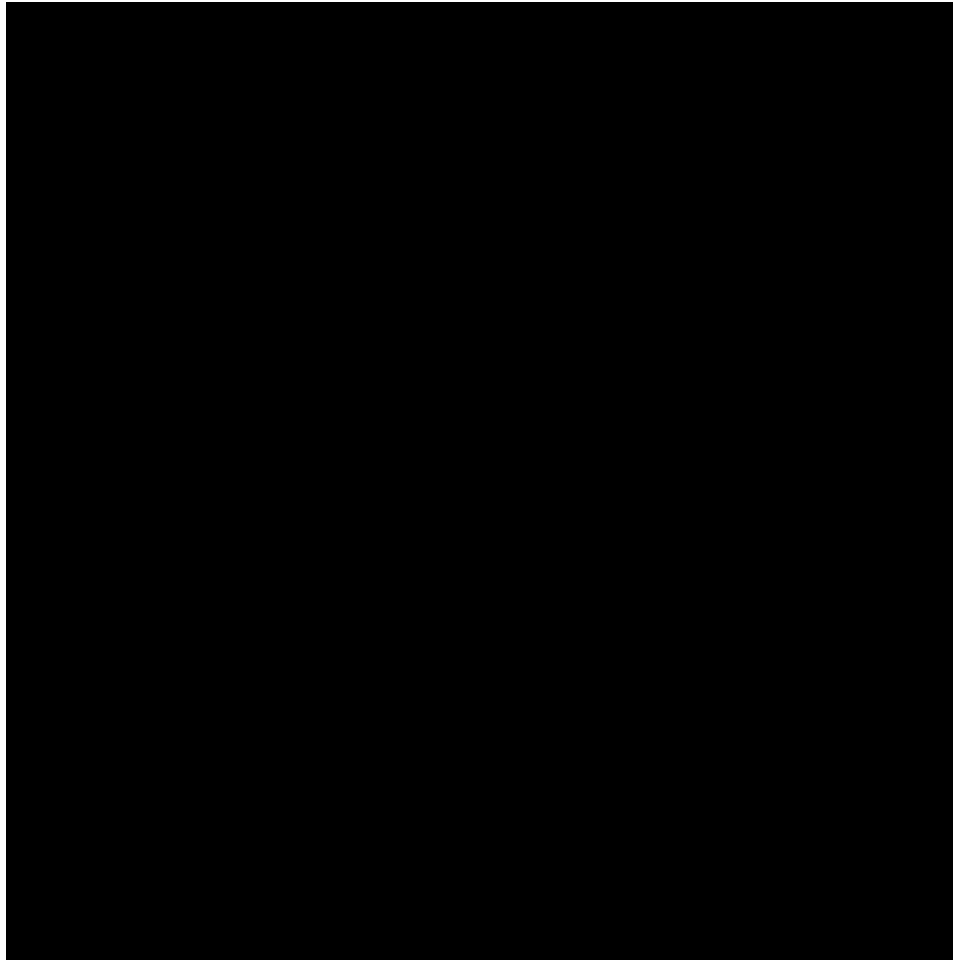
## **Table experiments with coupled magnetic pendula**

Two magnetic pendula, small amplitudes

**Gravitational potential:  $-\cos(x)$  , anharmonic!**

Two magnetic pendula, small amplitudes

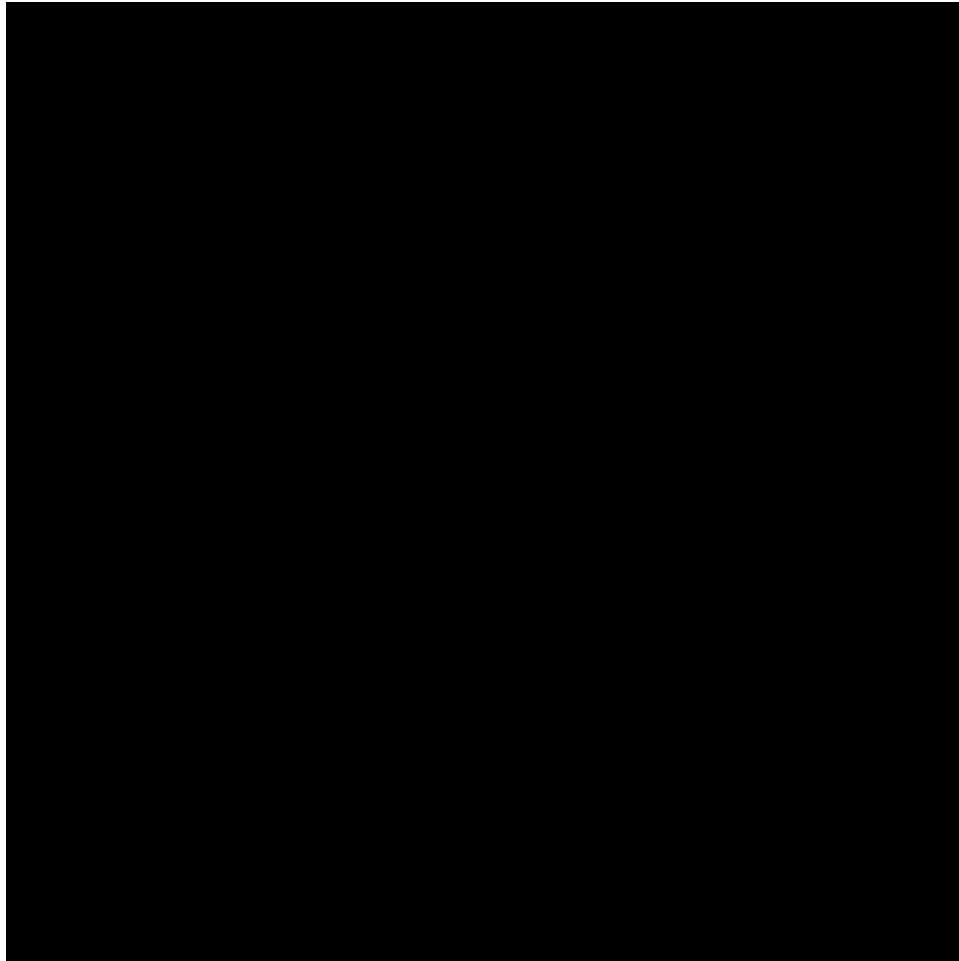
**Gravitational potential:  $-\cos(x)$  , anharmonic!**



**Linear regime, beating, no localization**

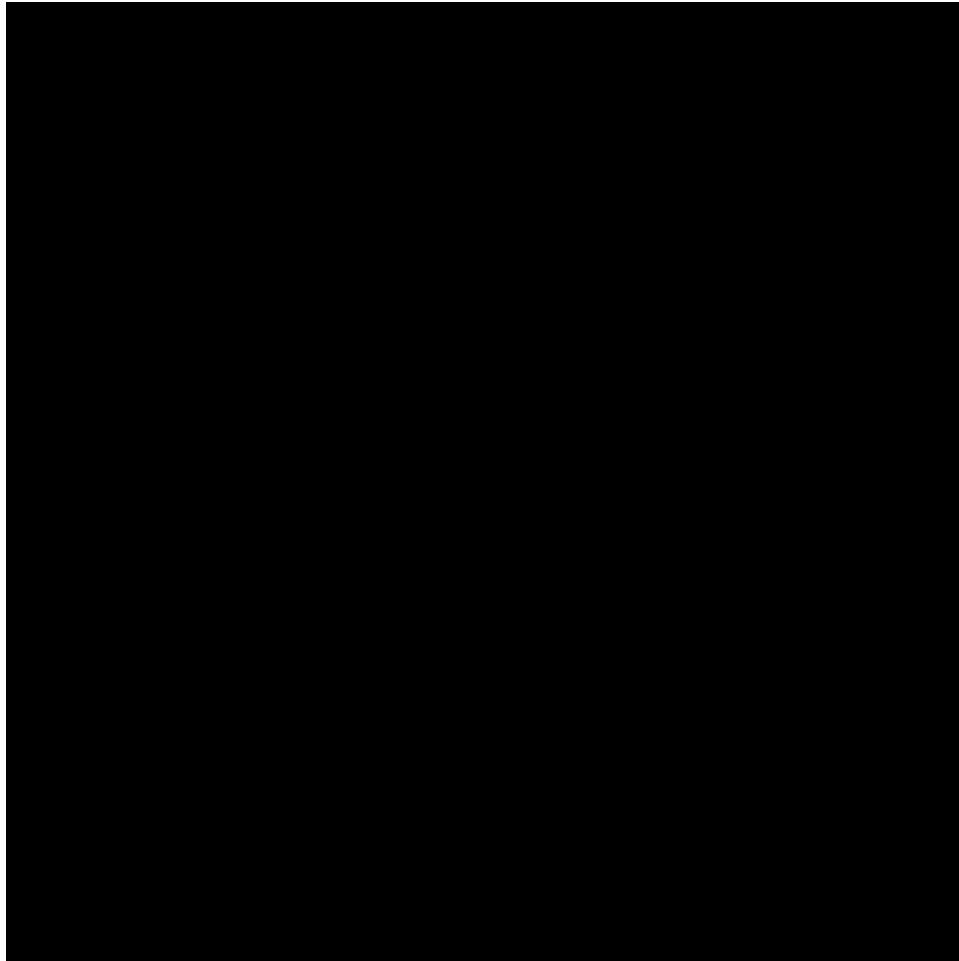


## Two magnetic pendula, large amplitudes



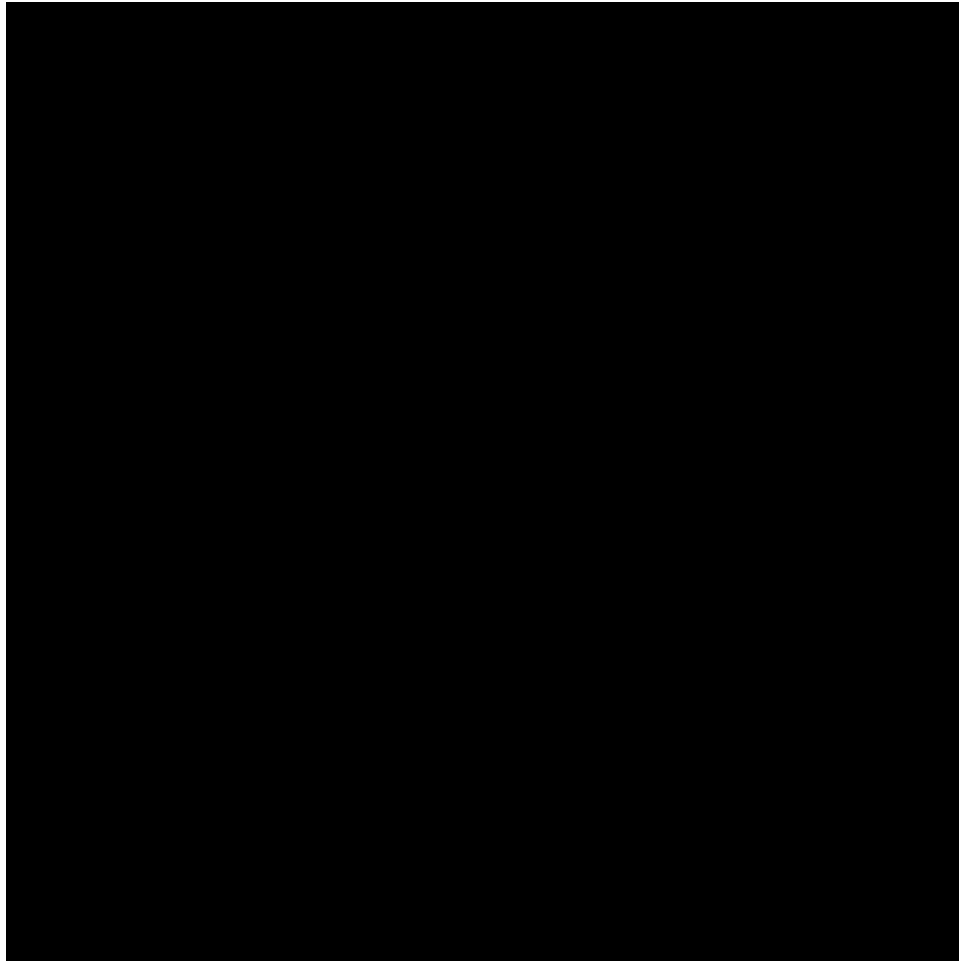
**Nonlinear regime, no beating, localization**

## Chain of magnetic pendula, small amplitudes



**Linear regime, wave spreading, delocalization**

## Chain of magnetic pendula, large amplitudes

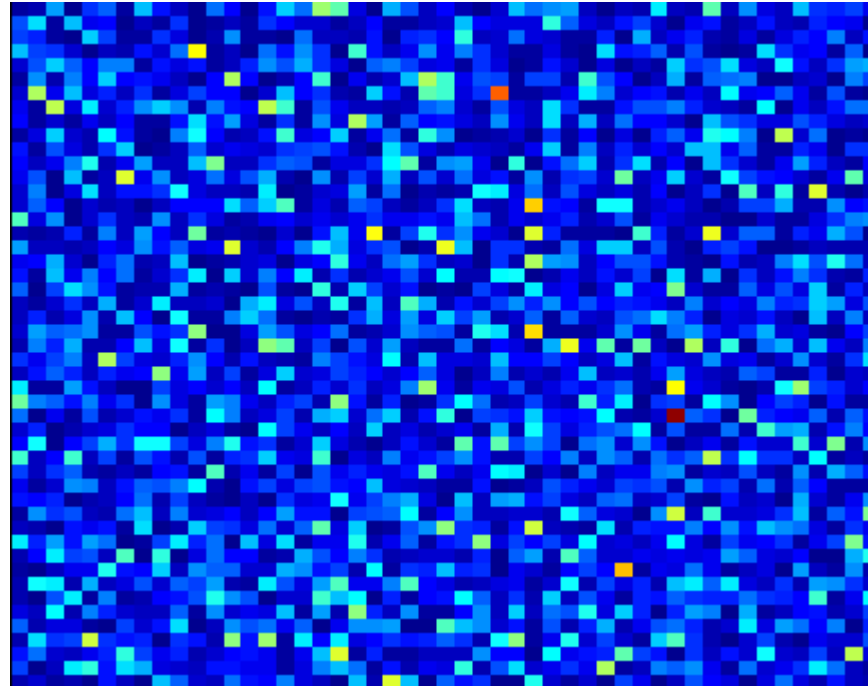


**Nonlinear regime, no wave spreading, localization**

## Cooling a two-dimensional lattice at the boundaries

- **a thermalized 2d lattice**
- **delocalized excitations are removed at the boundaries**
- **localized excitations will stay untouched**

# Cooling a two-dimensional lattice at the boundaries



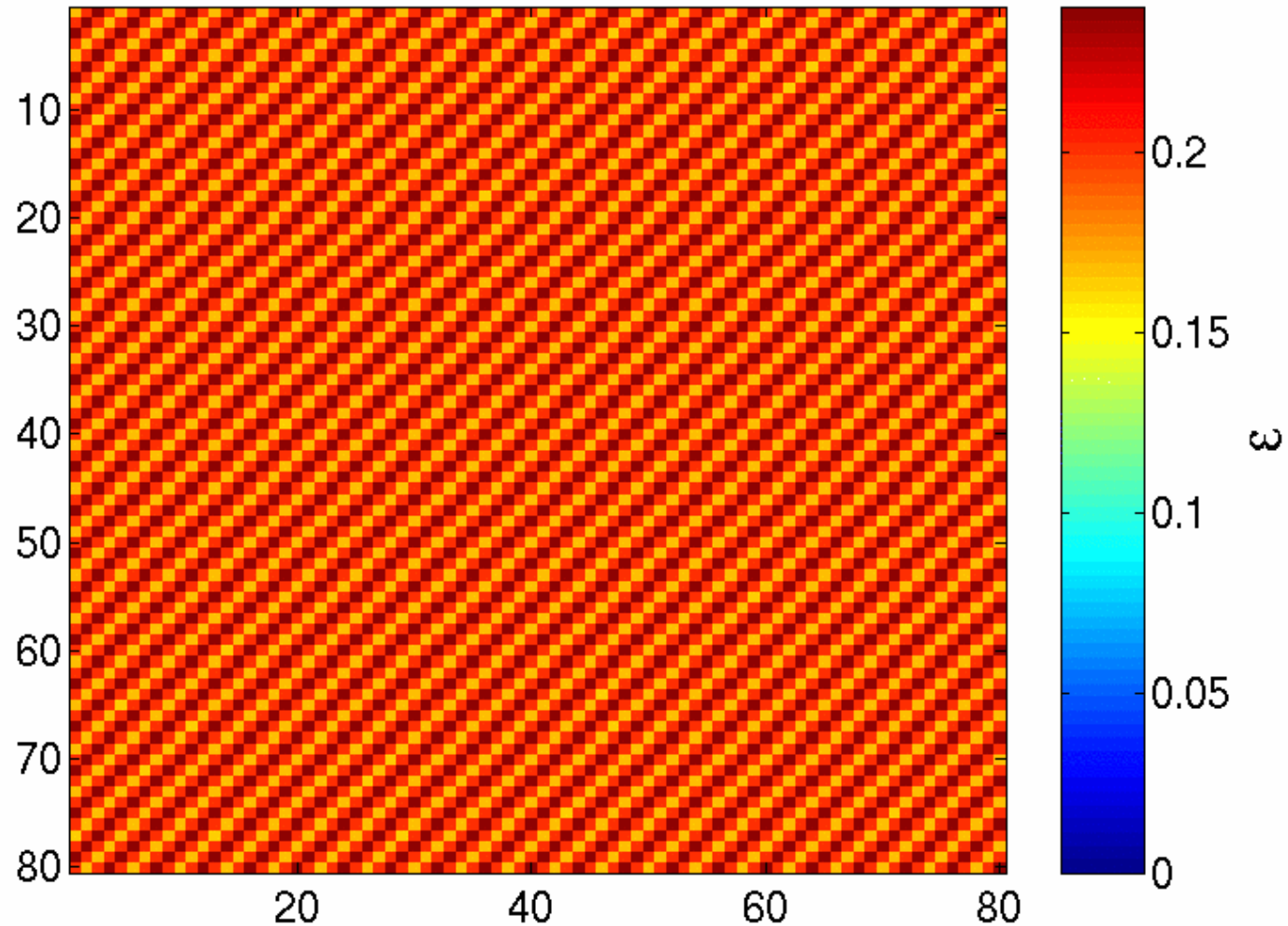
Originally designed by Bikaki et al (1999) to study slow energy relaxation of the remaining excitations

Exciting a plane wave in a two-dimensional lattice

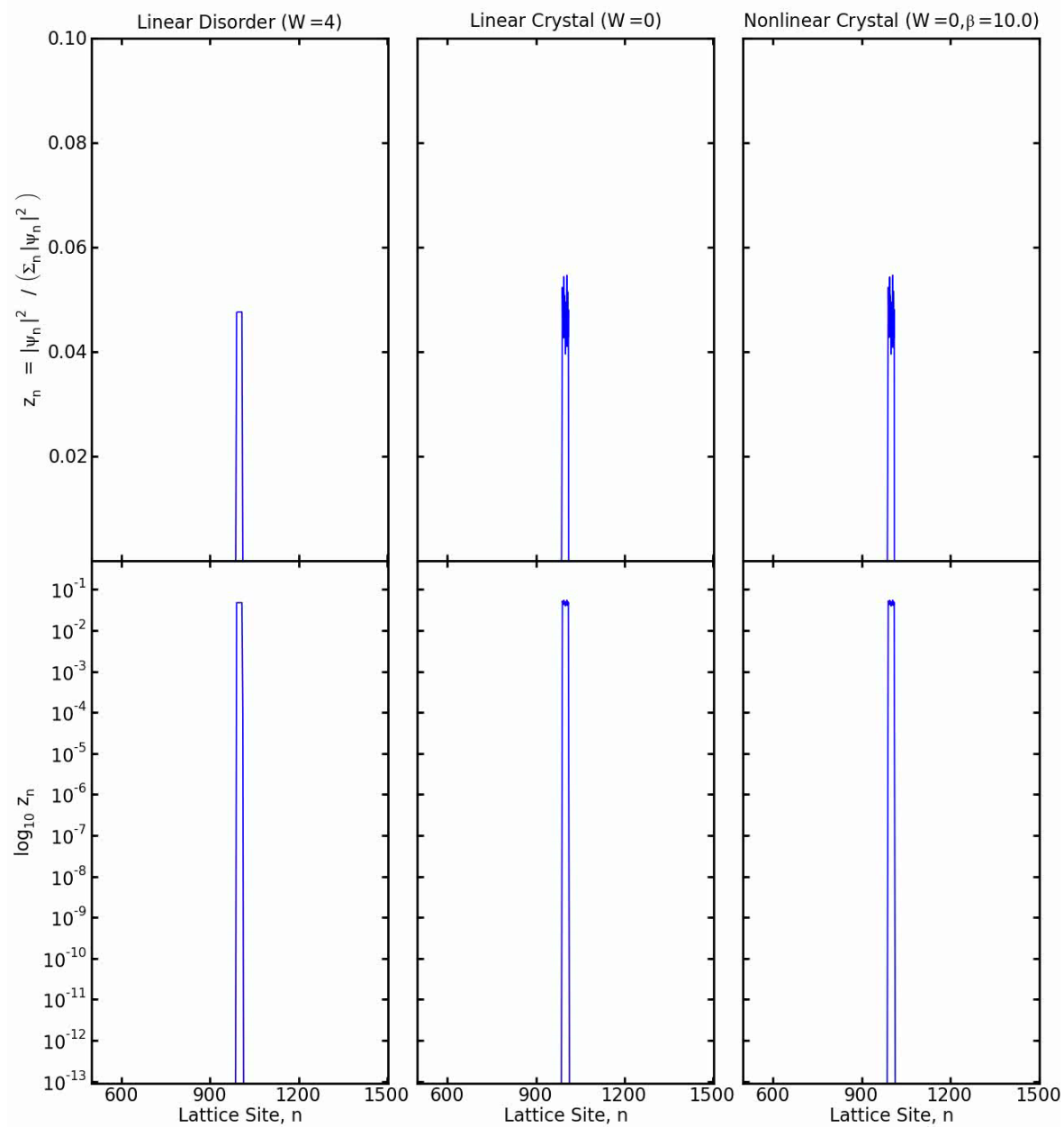
- **periodic boundary conditions**
- **plane wave is modulationally unstable**
- **what will it decay into?**

# Exciting a plane wave in a two-dimensional lattice

$\varepsilon=0.20$   $t=0$

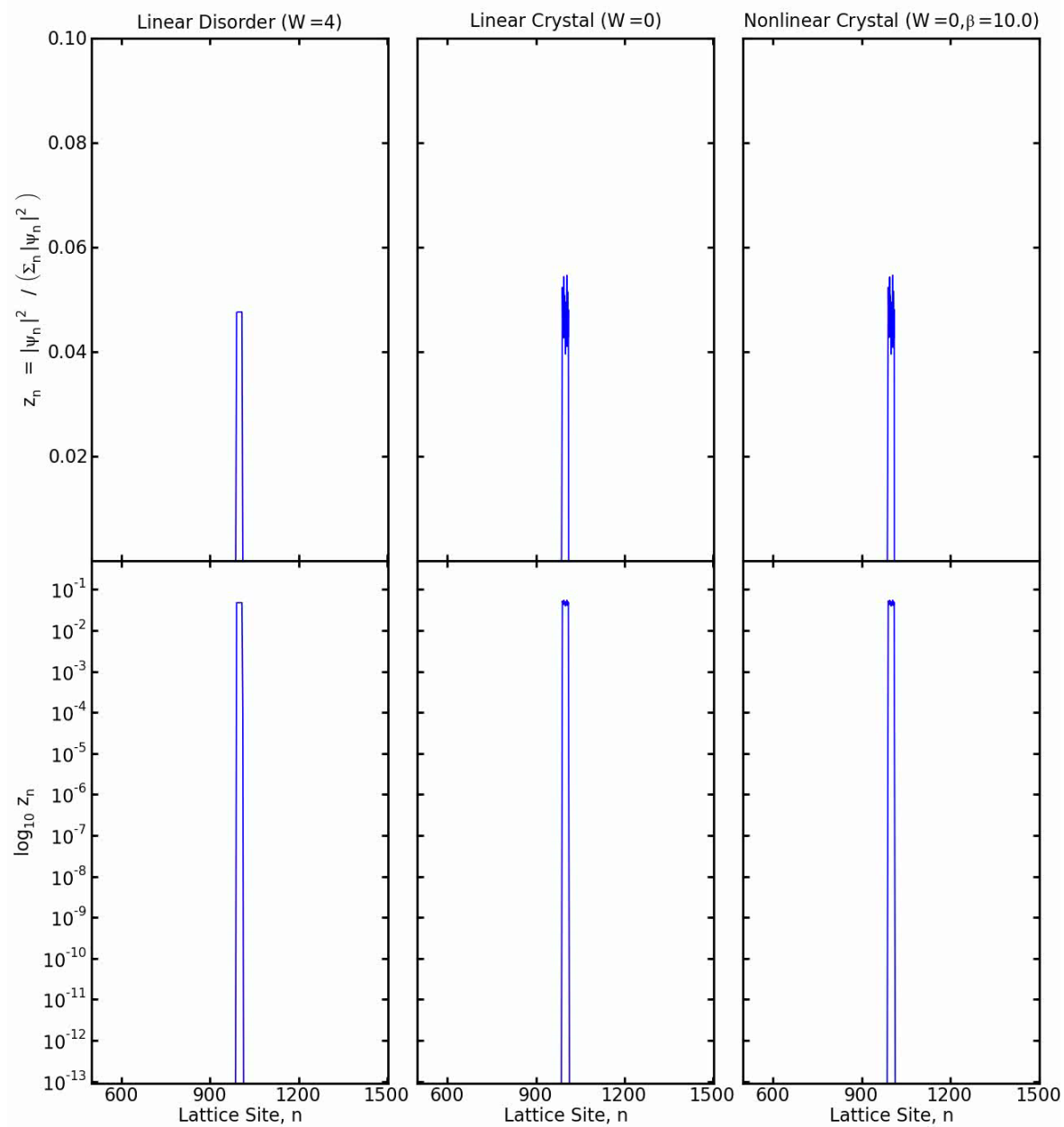


$\log_{10} t = -1.301$





$\log_{10} t = -1.301$



## **PART TWO:**

**DISCRETE BREATHERS –  
TIME-PERIODIC ORBITS  
LOCALIZED IN SPACE**

A few more definitions first, using a simple model class

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

$$V(0) = W(0) = V'(0) = W'(0) = 0$$

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

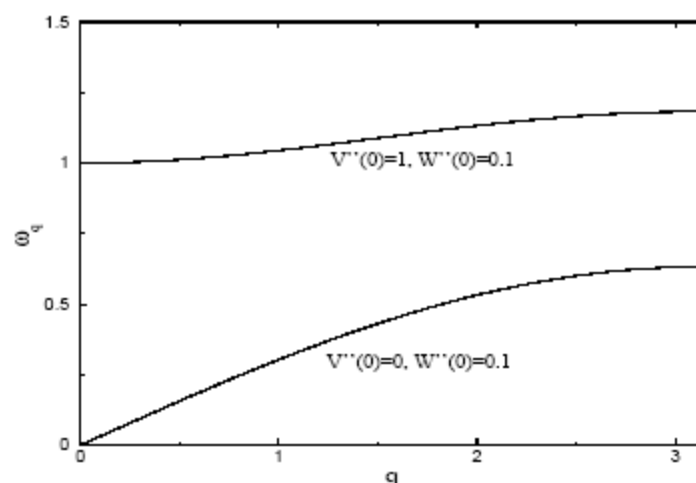
Equations of motion:

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

Small amplitude plane waves:

$$x_l(t) \sim e^{i(\omega_q t - ql)}, \quad \omega_q^2 = V''(0) + 4W''(0) \sin^2\left(\frac{q}{2}\right)$$

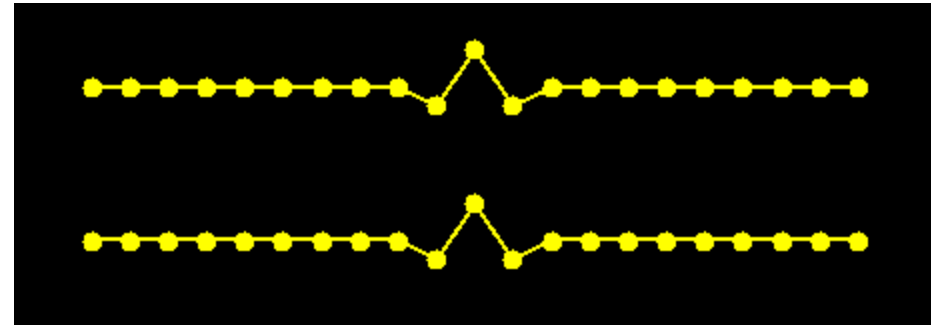
For  $N$  sites trajectories evolve in a  $2N$ -dimensional phase space!



Group velocity  $v_g(q)$ :

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

- 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:

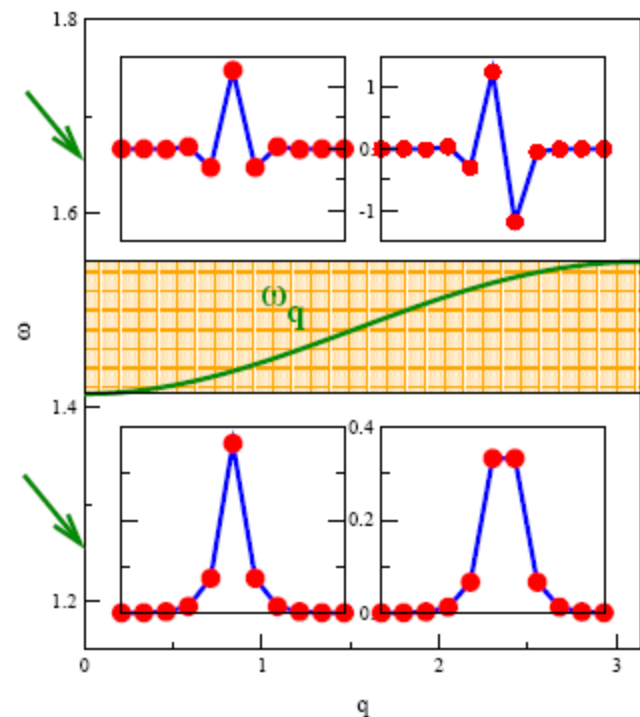
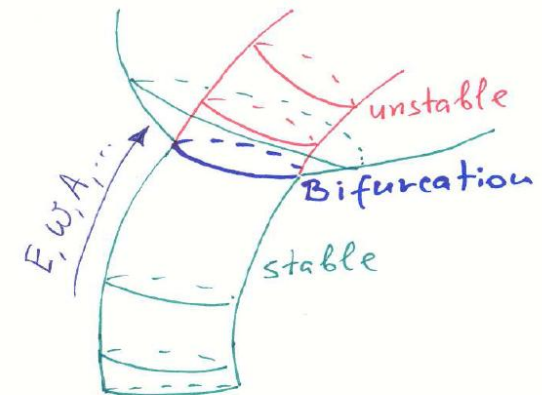
time-periodic, spatially localized solutions  
of the equations of motion with finite  
energy (action) with frequency  $\Omega_b$

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

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

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

Phase Space



## Necessary ingredients:

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

## Necessary condition for existence (Flach 1994):

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

Thus:

in general no localized excitations with quasiperiodic time dependence (Flach 1994)

Ansatz:  $x_l(t) = \sum_k A_{kl} e^{ik\omega_b t}$

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.

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

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  $F: SL_{T,1} \times \mathbb{R} \rightarrow SM_{T,0}$  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

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

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

## Localization in space?

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

$$A_{kl} \sim AG_{k\Omega_b}(l)$$

$$G_{k\Omega_b}(l) = \int \frac{\cos(ql)}{-(k\Omega_b)^2 + \omega_q^2} d^d q$$

$$r = \ln(|\lambda_k(\Omega_b)|)l \equiv \delta l$$

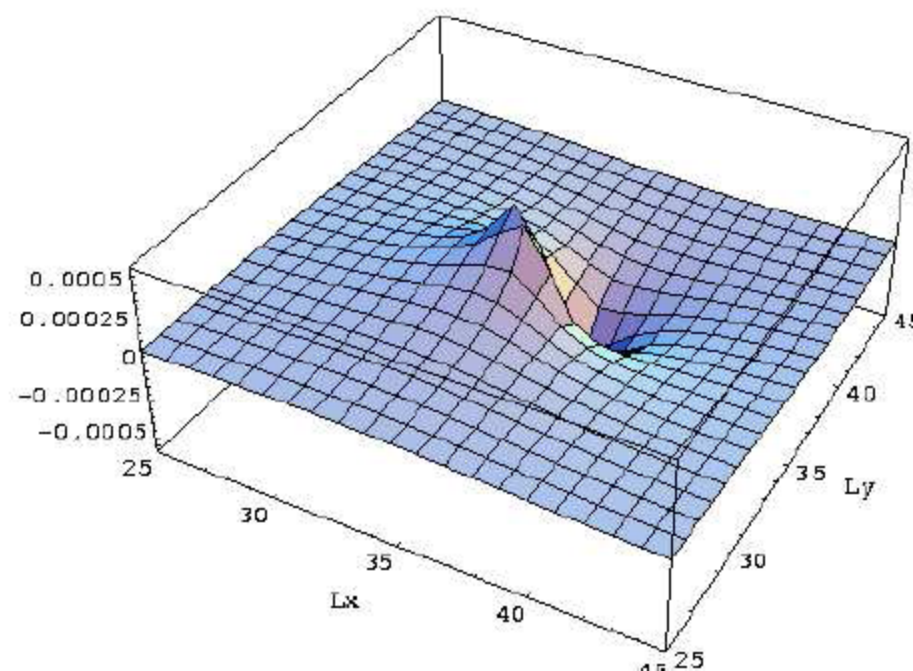
$$G(x) \sim e^{-x}, \quad d = 1$$

$$G(x) \sim \int \frac{e^{-x\sqrt{1+\xi^2}}}{\sqrt{1+\xi^2}} d\xi, \quad d = 2$$

$$G(x) \sim \frac{1}{x} e^{-x}, \quad d = 3$$

'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:

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

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

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

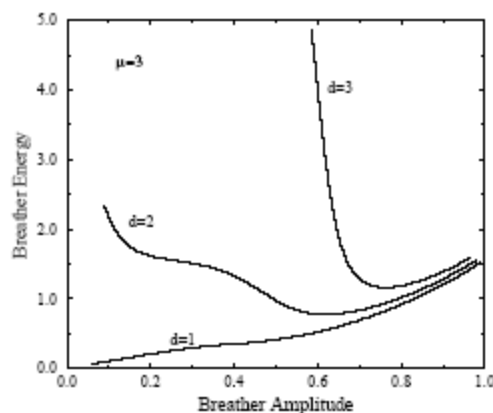


Fig.1 Flach,Kladko,MacKay

The breather zoo of localized:

vibrations

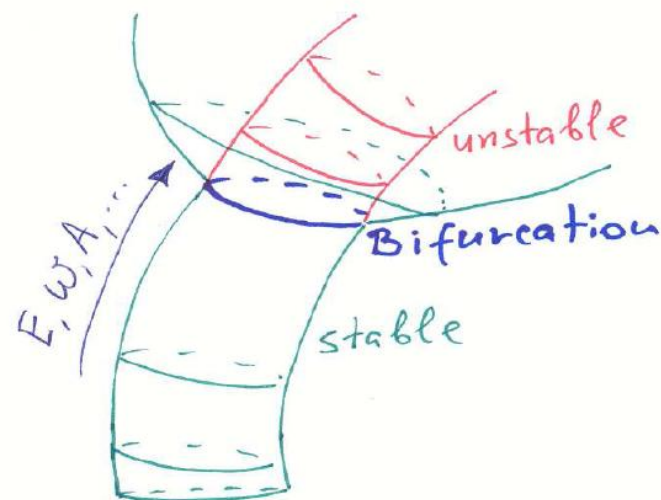
rotations

spin excitations

bound states with quasiparticles

...

Phase Space



# **PART THREE:**

## **SMALL FLUCTUATIONS – 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  $\epsilon_l(t)$ :

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

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

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

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

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  $\mathcal{U}(t)$

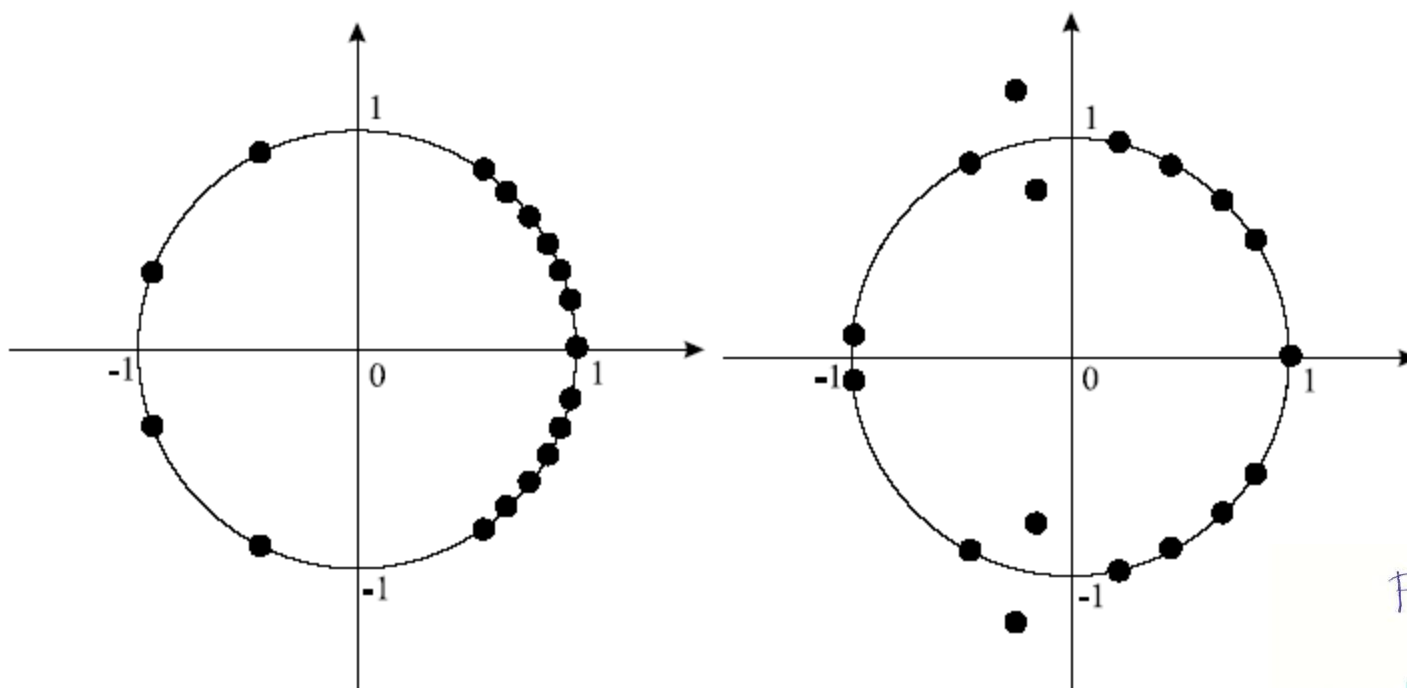
$$\begin{pmatrix} \pi(t) \\ \epsilon(t) \end{pmatrix} = \mathcal{U}(t) \begin{pmatrix} \pi(0) \\ \epsilon(0) \end{pmatrix}$$

It follows

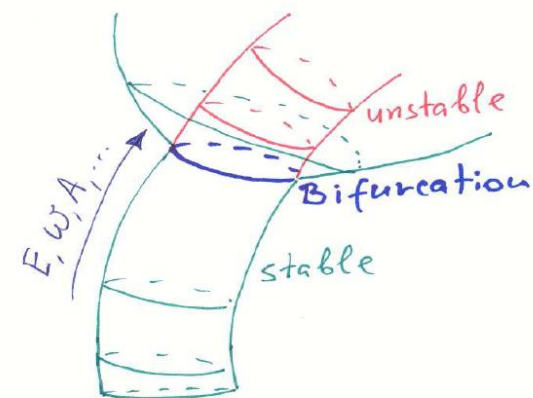
$$\rightarrow \mathcal{U}^T(t) \mathcal{J} \mathcal{U}(t) = \mathcal{J}$$

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

## Schematic view of the Floquet eigenvalues



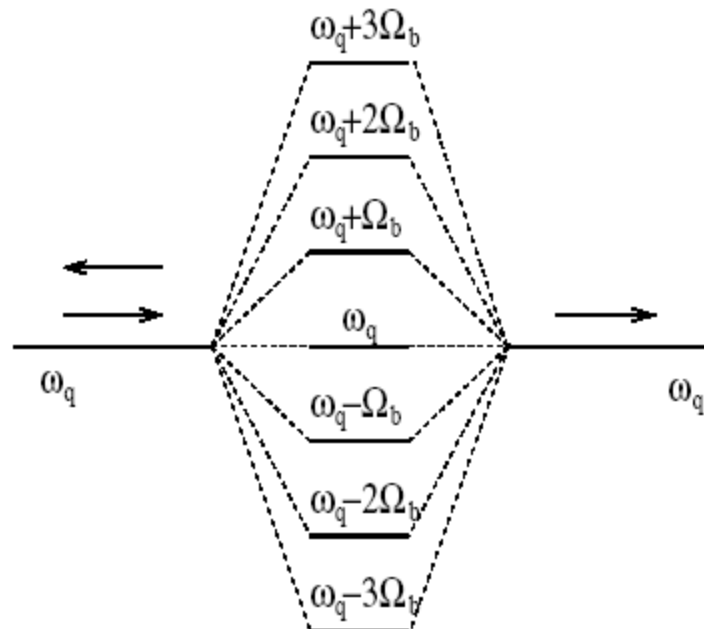
Phase Space



## Computing transmission up to machine precision

Scattering goes through the extended Floquet states:

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



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:

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

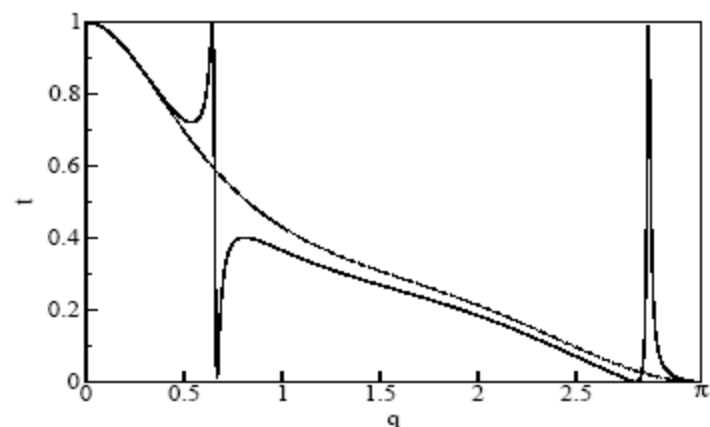
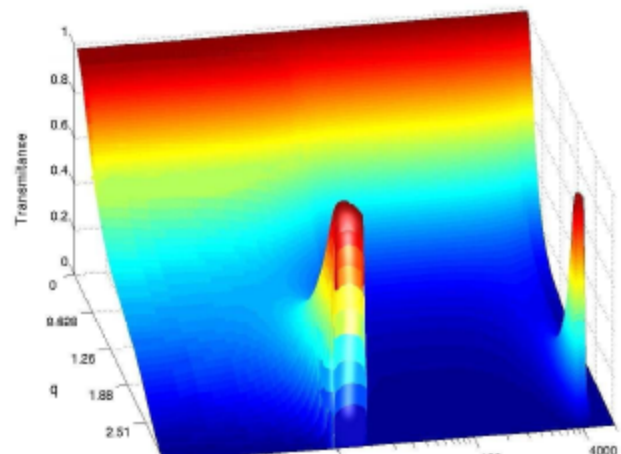
Fixing for the moment  $A, B$ , use standard Newton to find zeroes of  $G$ .

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:

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

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

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

Weak coupling:

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



**Linearize in small perturbations:**

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

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

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

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

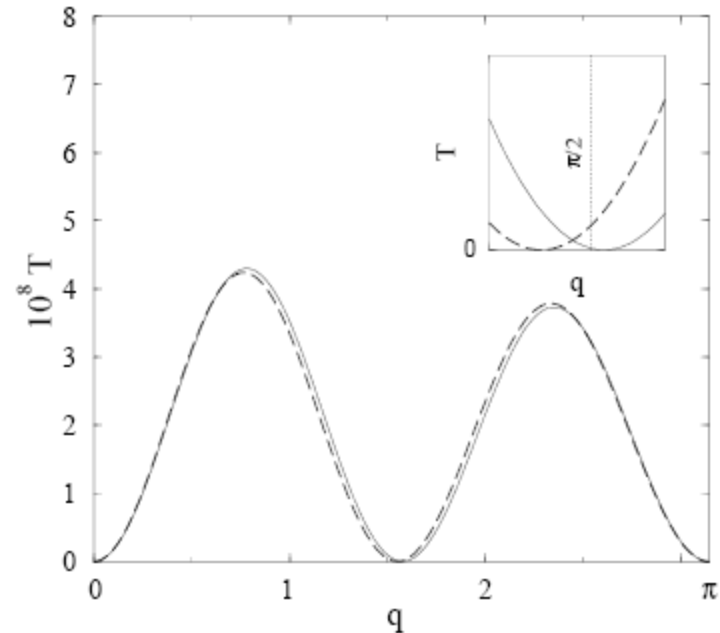
**Localized mode in closed channel!**

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).**

## 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)

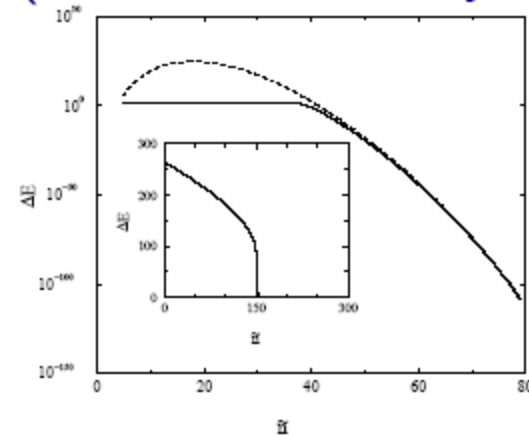


Fig.2 Aubry et al

## chaos assisted tunneling (Flach/Fleurov 1997-2001)

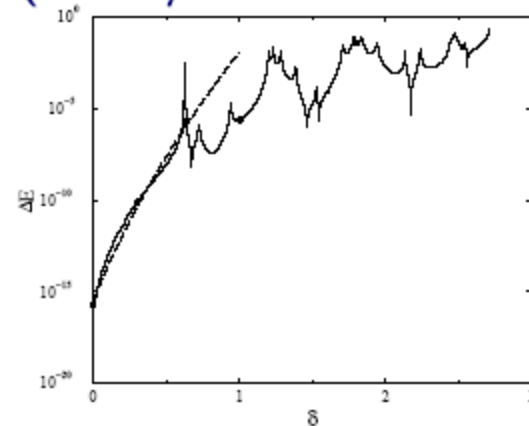


Fig.1 Flach et al

**PART FOUR:**

**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<sub>2</sub> crystal  
R. Bini et al J Chem Phys (1993)

# $N = 7$ : PtCl complexes

## B. I. Swanson et al PRL (1999)

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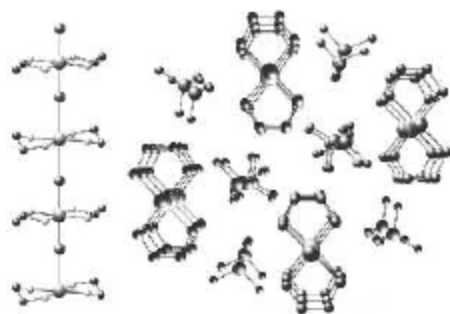
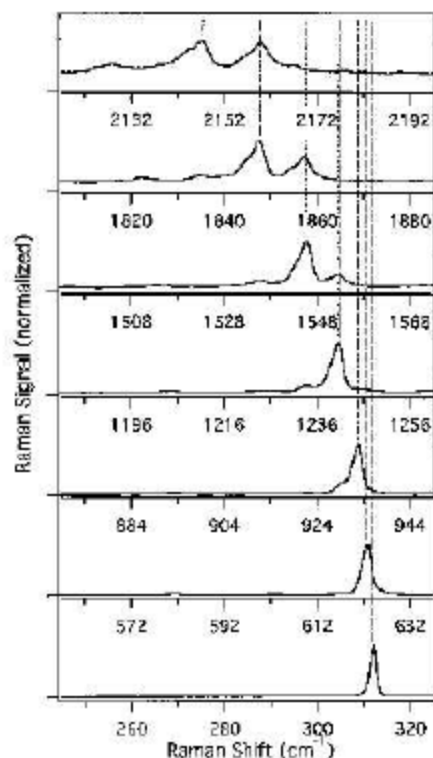


FIG. 1. Structure of  $\{[\text{Pt}(\text{en})_2][\text{Pt}(\text{en})_2\text{Cl}_2](\text{ClO}_4)_4\}$  (en = ethylenediamine; H atoms are omitted) [11]. One PtCl chain is shown on the left. Each Pt atom is coordinated by two ethylenediamine units in a near square planar geometry, while  $\text{Cl}^-$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

letters to nature

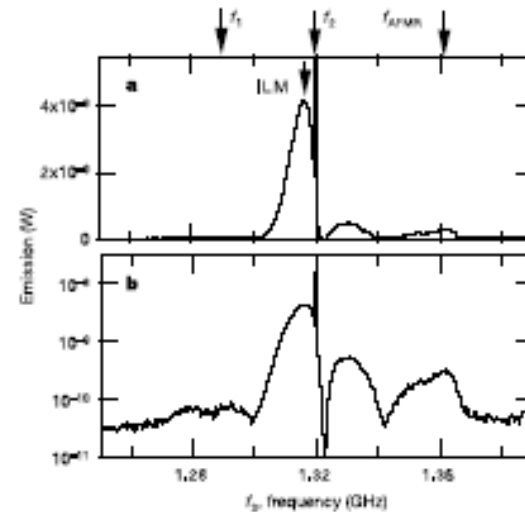
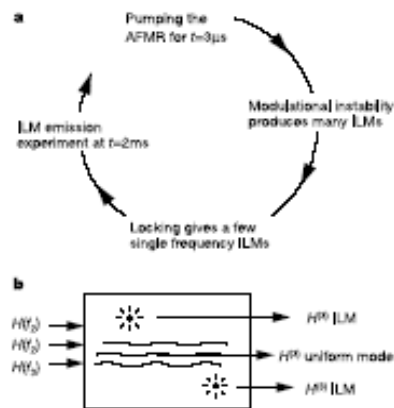
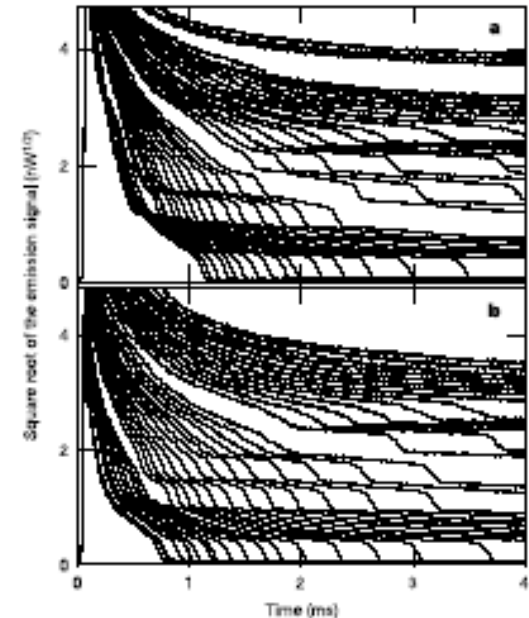


Figure 2 Snapshot of the mixing spectrum versus the probe oscillator frequency. **a**, Mixing data taken at 2 ms after the 3- $\mu\text{s}$ -long, 52 W pulse at  $f_1 = 1.29$  GHz. Here  $f_2 = 1.32$  GHz at a c.w. power of 240 mW. The weak ( $\sim 1$  mW) probe oscillator of variable frequency  $f_3$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



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

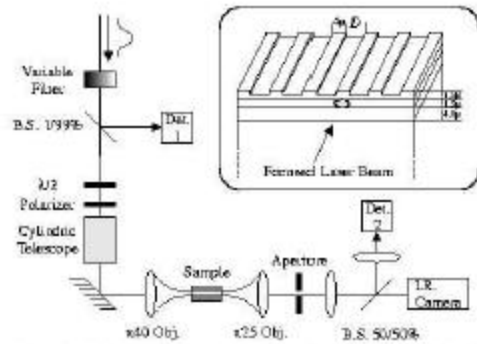
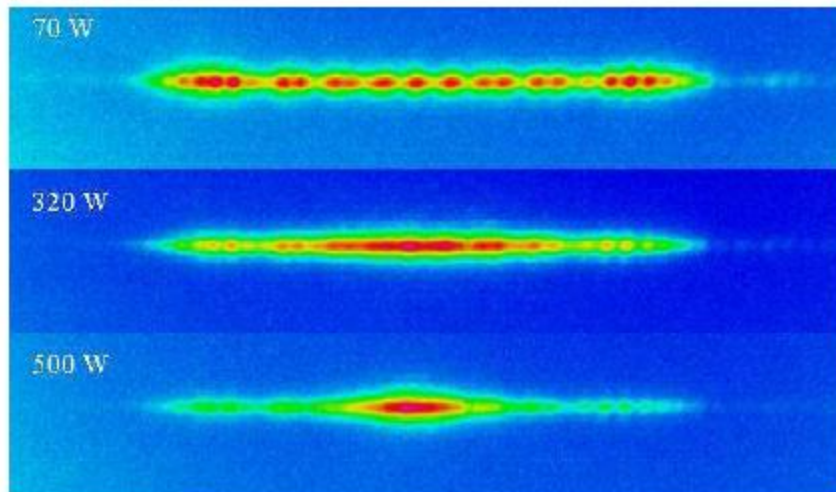


FIG. 2. The experimental setup. Inset: Schematic drawing of the sample. The sample consists of a  $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$  core layer and  $\text{Al}_{0.24}\text{Ga}_{0.76}\text{As}$  cladding layers grown on top of a GaAs substrate. A few samples were tested with different separations  $D$  between the waveguides.



## Nonlinear silica waveguides Cheskis et al 2003

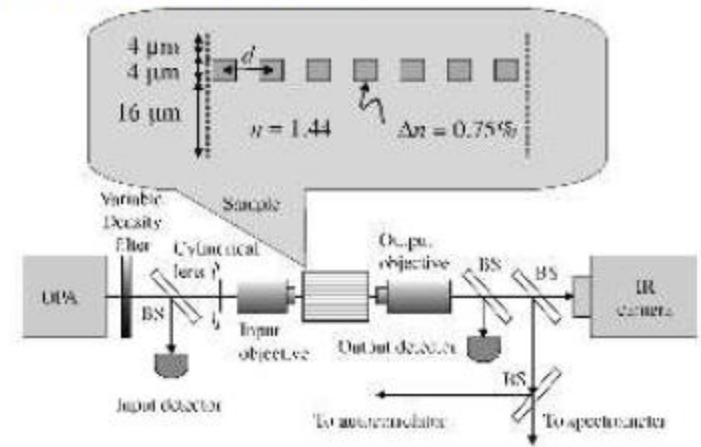


FIG. 1. Experimental setup and sample cross section.

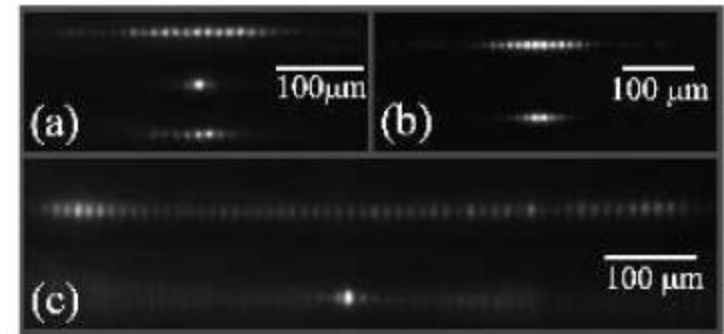
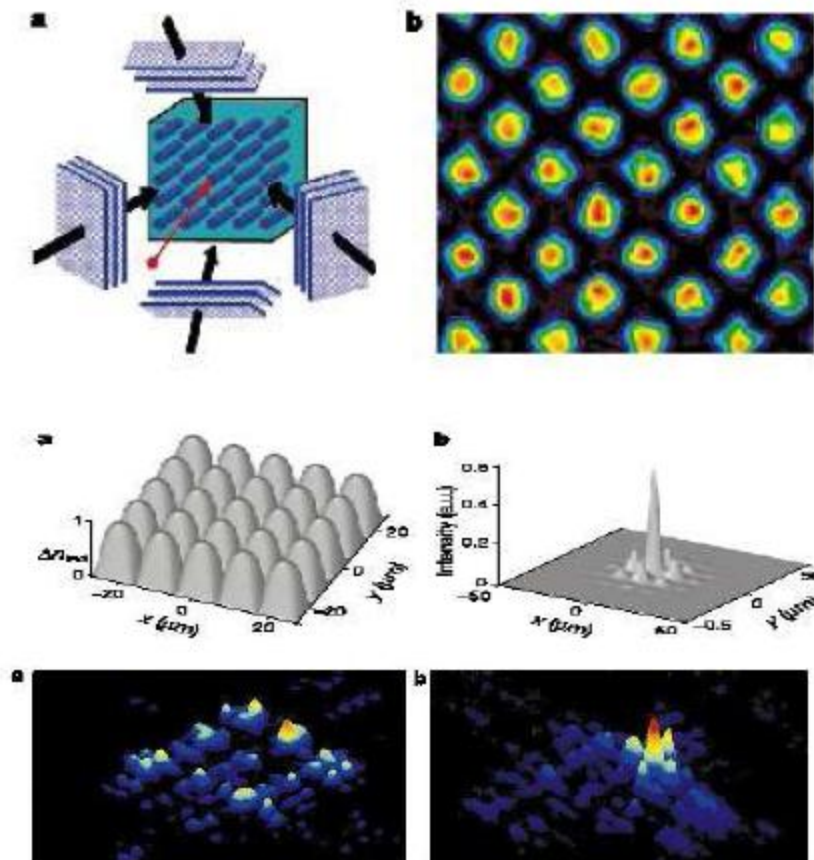


FIG. 2. Images of the sample's output facet under different excitation conditions. (a) Broad input beam (equal dispersion and diffraction lengths): top to bottom, 0.09, 0.45, and 0.74 MW. (b) The unstable mode is excited with the broad input beam: top, low power; bottom, high power. (c) Single waveguide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

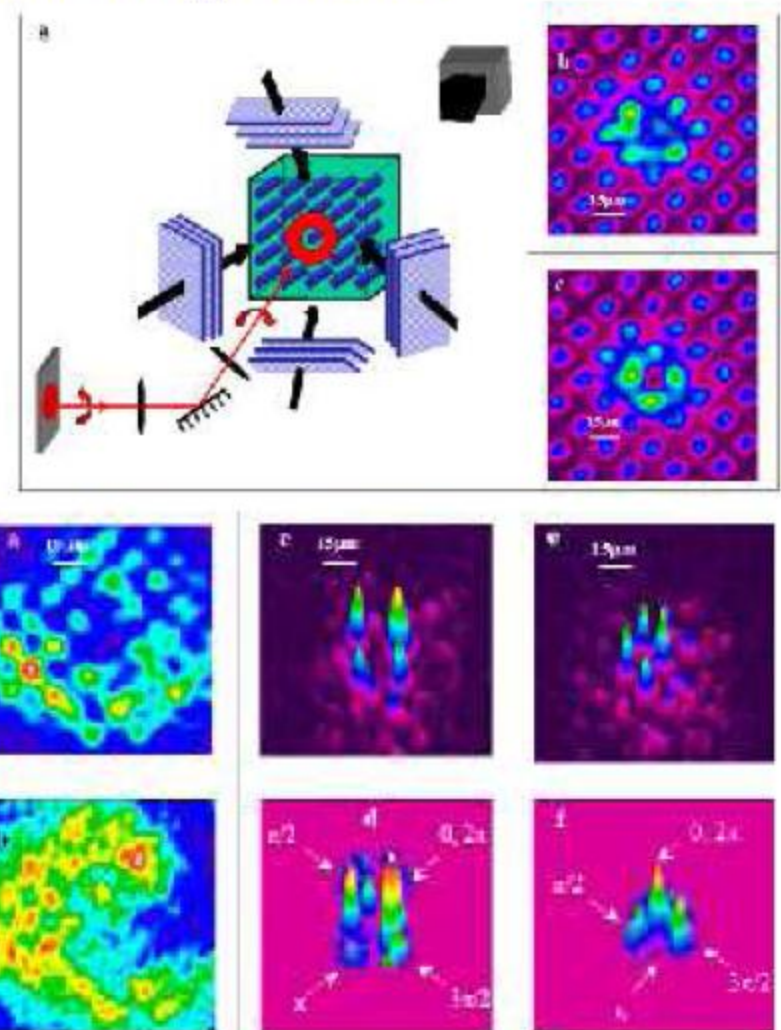


# Breathers in optically induced nonlinear photonic 2d lattices based on SBN:75

Fleischer et al 2004

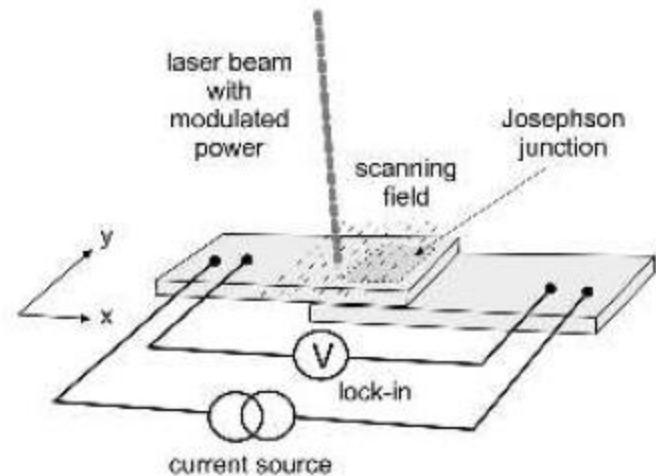
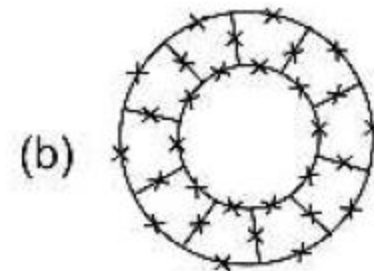
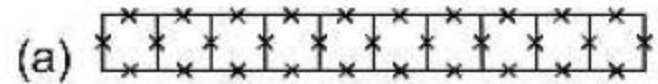
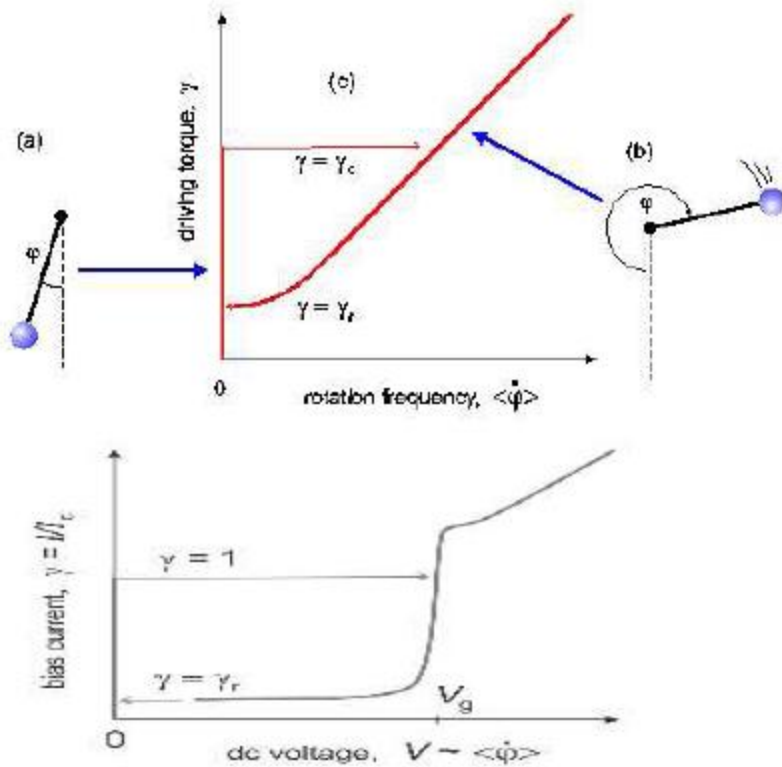


# Vortex-ring breathers



## Josephson junction ladders (Ustinov, Binder, Schuster)

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



# Josephson junction networks

Ustinov et al

## The zoo of rotobreathers

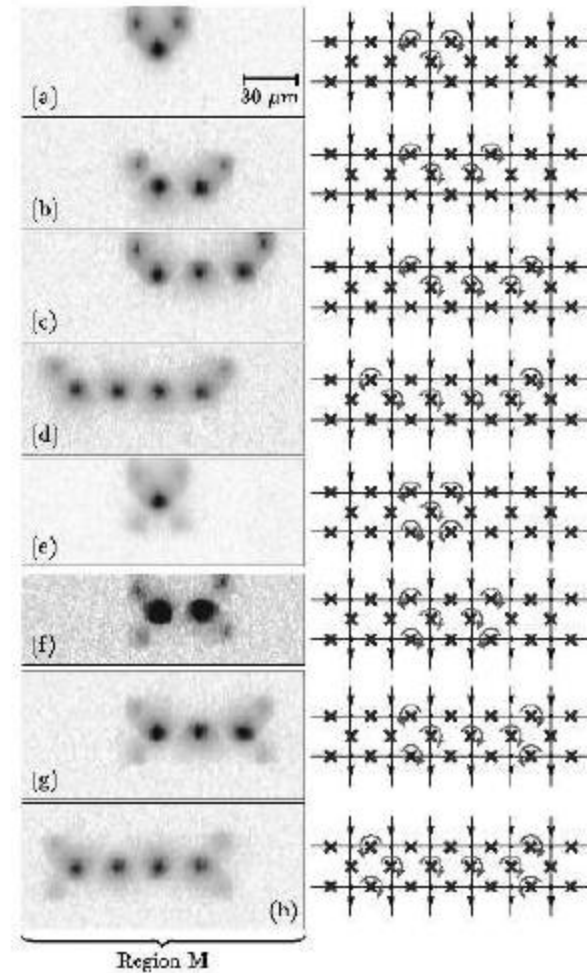
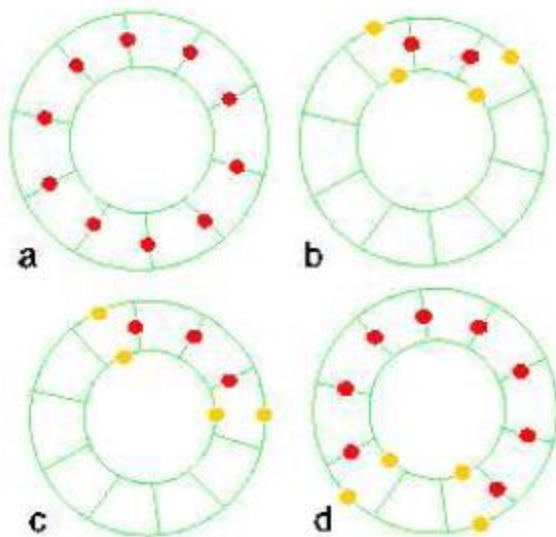
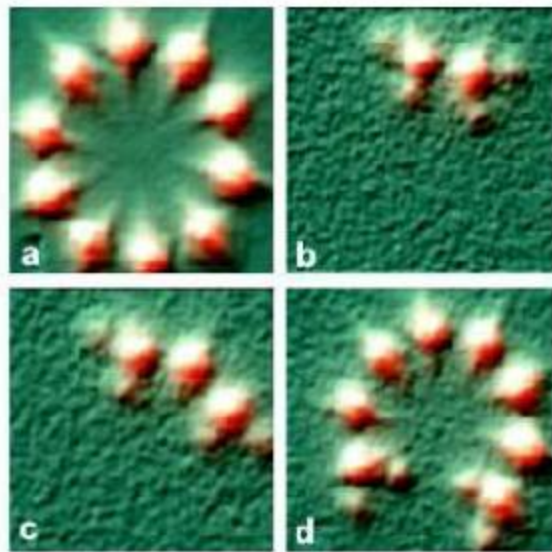


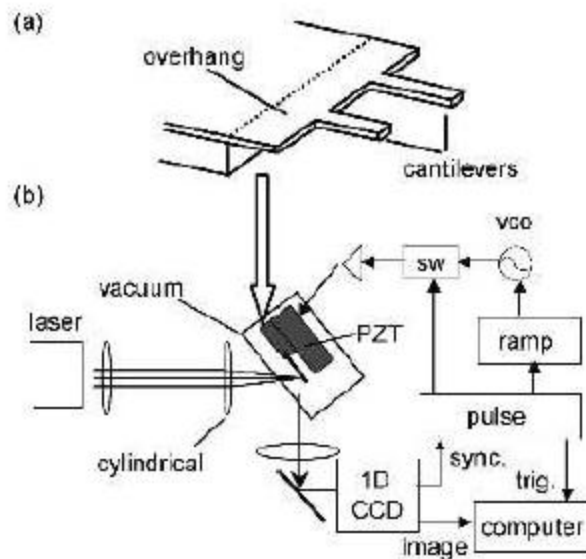
FIG. 2. Various localized states (discrete rotobreathers) measured by the low-temperature scanning laser microscope: (a)–(d) asymmetric rotobreathers; (e)–(h) symmetric rotobreathers. Region *M* is illustrated in Fig. 1(b).



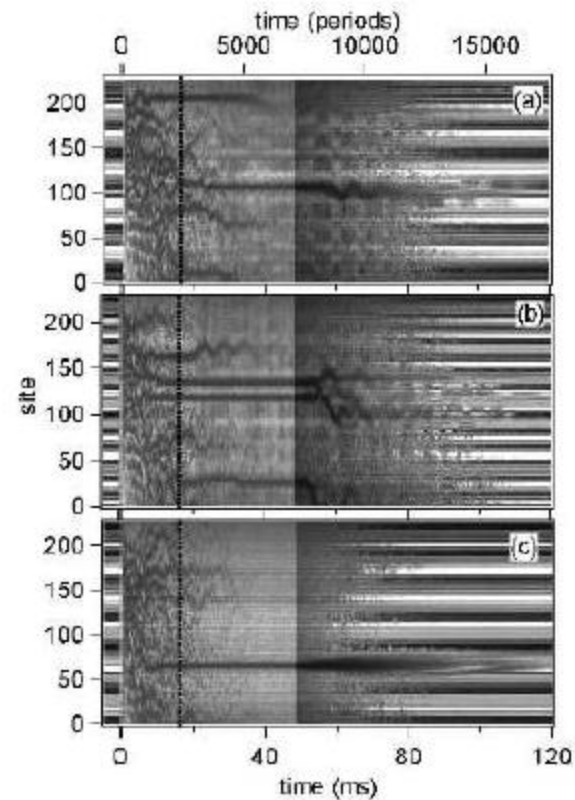
# Breathers in driven micromechanical cantilever arrays

Sato et al 2003

$\text{Si}_3\text{N}_4$  cantilevers  
 l/w/p: 50/15/40  $\mu\text{m}$   
 PZT drive at 150kHz

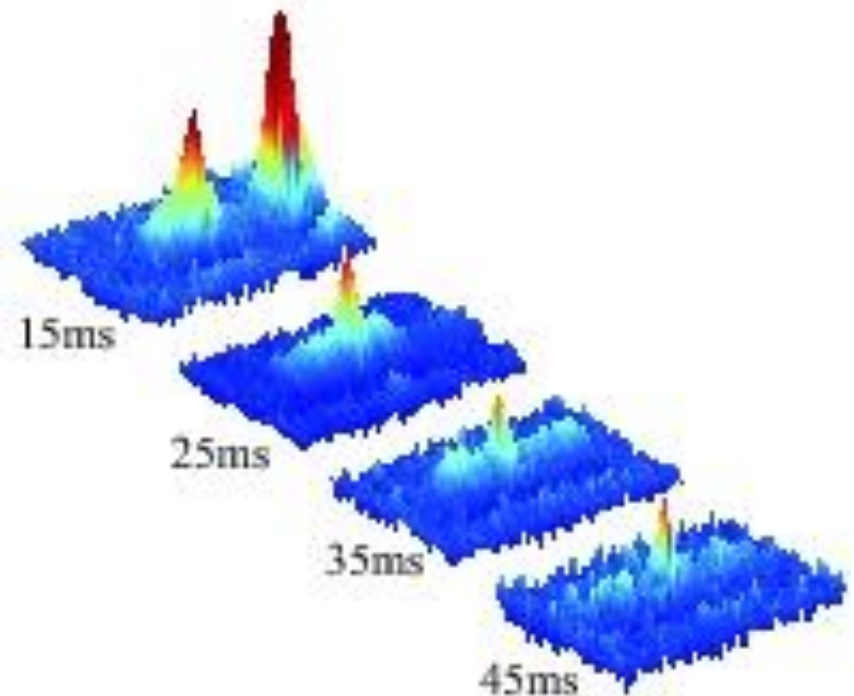
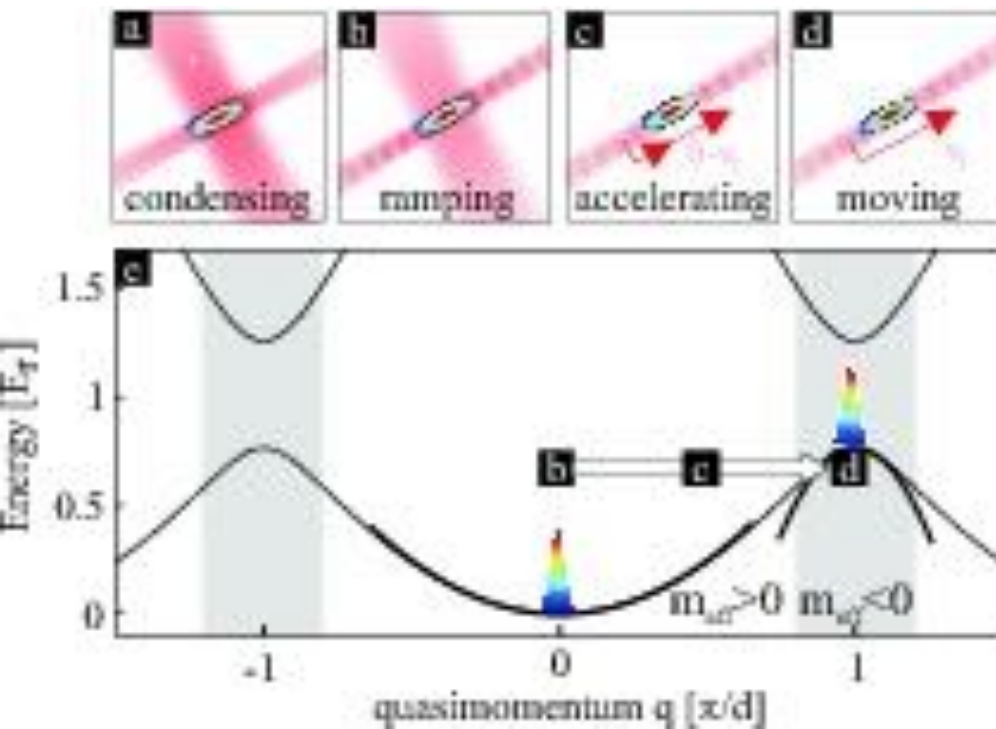


Detector:  
 He-Ne laser and CCD camera



## 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

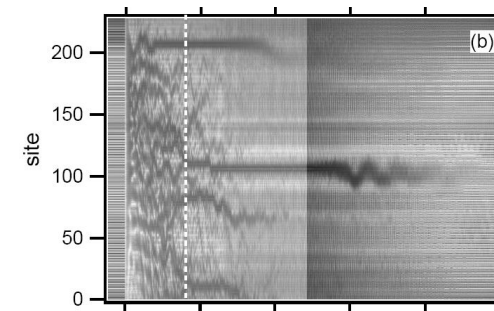
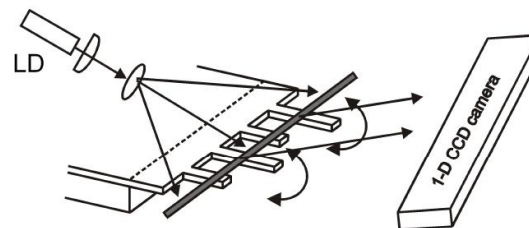
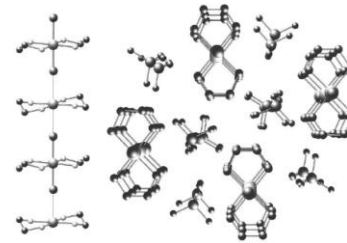
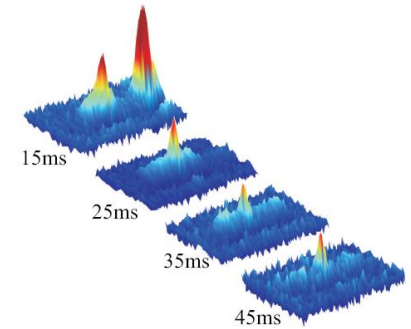
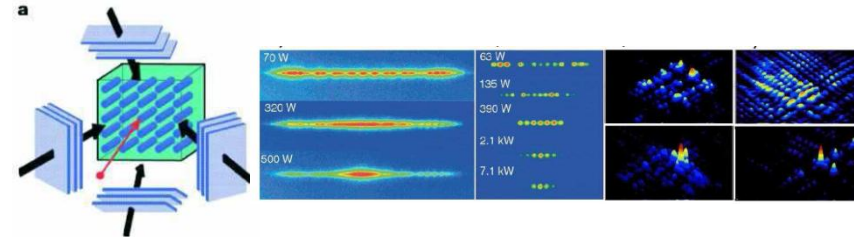
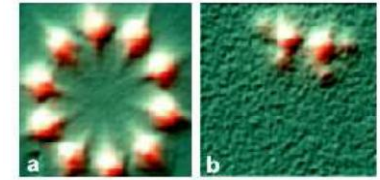


# Theory applied to:

- **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

# Experimentally observed and studied in:

- Josephson junction networks
- Coupled nonlinear optical waveguides
- BEC in optical lattices
- Driven micromechanical cantilever arrays
- Antiferromagnetic layered structures ( $(\text{C}_2\text{H}_5\text{NH}_3)_2\text{CuCl}_4$ )
- Poly- $\gamma$ -benzyl-L-glutamate (PBLG)
- H on Si(111), CO on Ru(001)
- PtCl based crystals,  $\alpha$ -Uranium



# SUMMARY

- 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