FPU: problems, myths, q-breathers

S. Flach, MPIPKS Dresden

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Road map:

- paradox and problems
- myths
- periodic orbits (q-breathers)
- scaling

Together with: M. Ivanchenko, O. Kanakov, K. Mishagin, T. Penati, A. Ponno

What will I talk about?

- **networks of oscillators**
- **localization of excitations of energy takes place**
- **invariant structures: periodic orbits – one-dimensional manifolds in (in)finite dimensional phase spaces**
- **why networks: cut the interactions, excite one oscillator, get a periodic orbit which is localized**
- **turn on the interactions – periodic orbit generically survives**

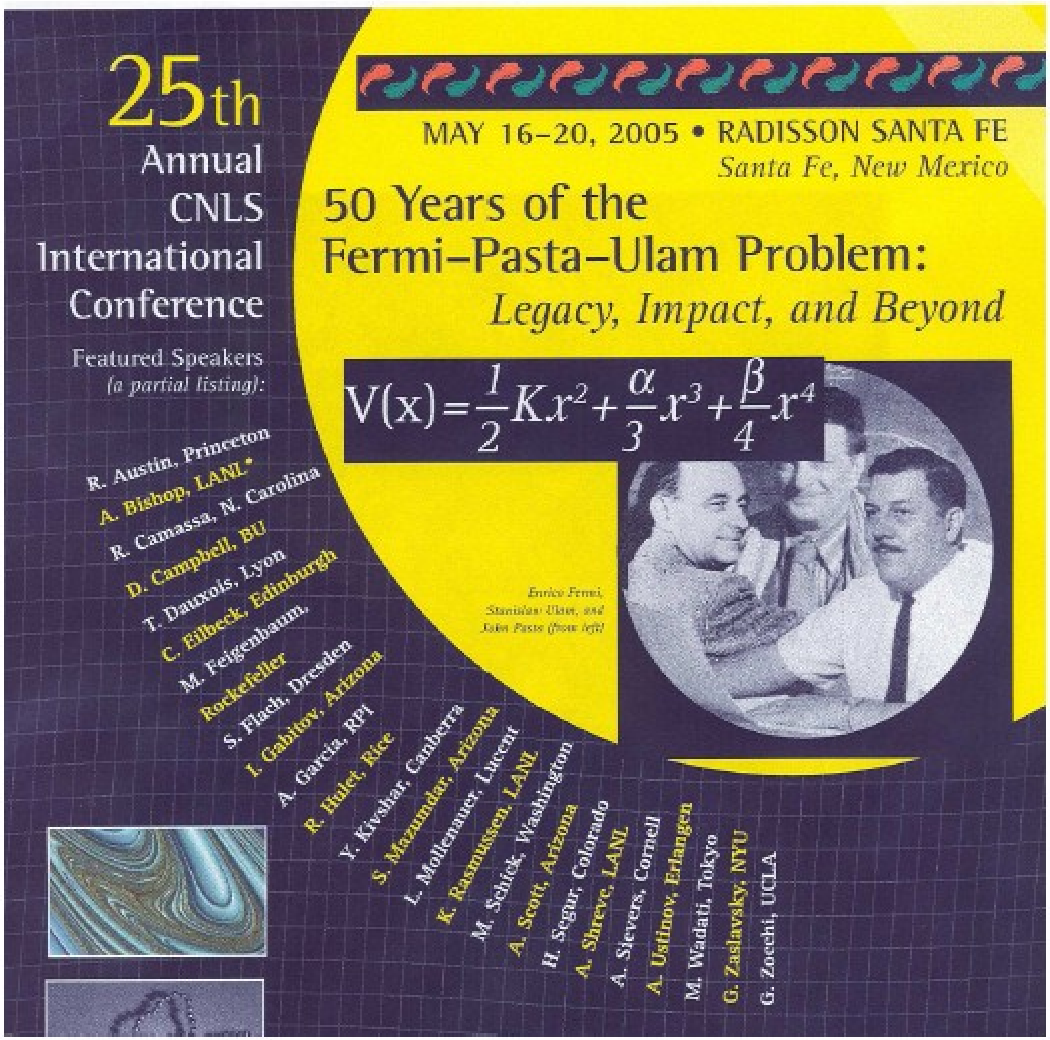
- ***think about normal modes of a linear problem – nonlinearity spans interaction network between normal modes***

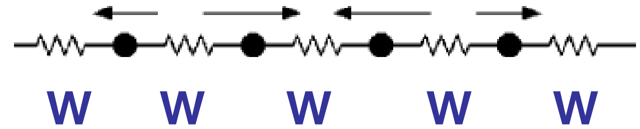
- ***q-breathers are time-periodic solutions localized in normal mode space***

- ***they delocalize when the dispersion becomes linear or flat, or when the energy and/or nonlinearity are large enough***

PART ONE:

THE PARADOX AND THE PROBLEMS





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

$$\ddot{x}_l = -W'(x_l - x_{l-1}) + W'(x_{l+1} - x_l)$$

The equations of motion are for a nonlinear finite atomic chain with fixed boundaries and nearest neighbour interaction

N **particles,** $x_0 = x_{N+1} = 0$:

$$x_n(t) = \sqrt{\frac{2}{N+1}} \sum_{q=1}^{N} Q_q(t) \sin\left(\frac{\pi q n}{N+1}\right) \,,\ \omega_q = 2\sin\left(\pi q / 2(N+1)\right)$$

α **model (** $\beta = 0\,,\ \alpha \neq 0$**):**

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\alpha \sum_{i,j=1}^{N} A_{q,i,j} Q_i Q_j}{\sqrt{2(N+1)}}$$

β **model (** $\beta \neq 0\,,\ \alpha = 0$**):**

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\beta \sum_{i,j,m=1}^{N} C_{q,i,j,m} Q_i Q_j Q_m}{2(N+1)}$$

The interaction between the modes is purely nonlinear, selective but long-ranged!

The structure of the nonlinear coupling for the α-FPU model

$$\ddot{Q}_q + \omega_q^2 Q_q = -\frac{\alpha}{\sqrt{2(N+1)}} \sum_{l,m=1}^{N} \omega_q \omega_l \omega_m B_{q,l,m} Q_l Q_m$$

$$B_{q,l,m} = \sum_{\pm} \left(\delta_{q \pm l \pm m, 0} - \delta_{q \pm l \pm m, 2(N+1)} \right)$$

The harmonic energy of a normal mode with mode number q:

$$E_q = \frac{1}{2}(\dot{Q}_q^2 + \omega_q^2 Q_q^2)$$

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FPU-paradox Fermi, Pasta, Ulam, Tsingou(1955) :

- excite $q = 1$ mode
- observe nonequipartion of mode energies
- no transition to thermal equilibrium
- energy is localized in a few modes for long time **FPU 1**
- recurrence of energy into initially excited mode **FPU 2**
- two thresholds in energy and N **FPU 3**
- two pathways of understanding:
  $\longrightarrow$ stochasticity thresholds, nonlinear resonances, similarity to Landau's quasiparticle approach Israilev, Chirikov (1965)
  $\longrightarrow$ continuum limit, KdV, solitons Zabusky, Kruskal (1965)

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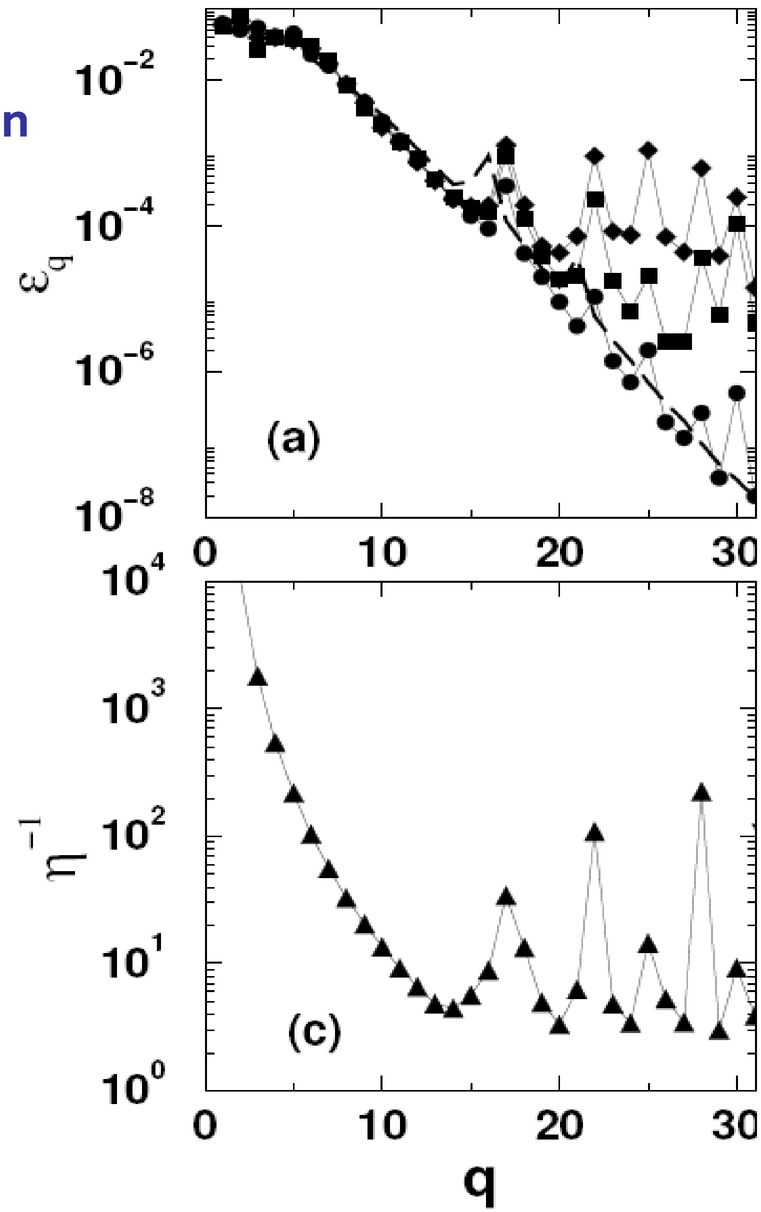
Galgani and Scotti (1972): exponential localization



Movies: let us see what FPU observed

Evolution of normal mode coordinates

Evolution of normal mode energies

Evolution of real space displacements

Joseph Ford, Physics Reports 213 (1992) 271:

- It was Freeman Dyson who provided the most penetrating comment ' Ford's explanation cannot be regarded as the complete answer'. Indeed, Dyson's comment applies equally well to all efforts at integrable approximation …

- … in regard to the FPU problem, KdV is highly ingenious and delightfully intuitive, but in the end nothing more than another integrable approximation …

true?

1. Solitons (Zabusky/Kruskal, KdV) explain the paradox
2. Estimate of Izrailev/Chirikov gives the correct value for the stochasticity threshold for long wavelength
3. Estimate of Izrailev/Chirikov predicts that the stochasticity threshold energy density tends to zero for large systems

recent results

- resonant layer of modes with strong interaction
- boundary of layer – scaling laws
- short time scales – formation of natural packet
- large time scales – destruction of packet, equipartition
- large energy densities – merging of time scales
- scaling with intensive quantities?

work by DeLuca, Lichtenberg, Liebermann, Shepelyansky, Giorgilli, Galgani, Benettin, Livi, Paleari, Bambusi, Ponno, Ruffo, Bountis and others

PART TWO:

q-BREATHERS

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q-breathers - the recipe

PRL 95 (2005) 064102, PRE 73 (2006) 036618

- start with $\alpha = \beta = 0$ and some finite size N
- consider periodic orbits $Q_{q \neq q_0} = \dot{Q}_{q \neq q_0} = 0$
- choose one with energy E_{q_0}
- gradually switch on nonlinearity (interaction) α, β and continue periodic orbit at the same chosen energy

You will obtain a q-breather:
a time-periodic solution localized in q-space

The observed FPU-paradox including the famous recurrence is a perturbed q-breather trajectory, recurrence is just beating

Existence proof: use nonresonance for finite N and Lyapunov orbit continuation!

Nonresonance condition (follows from Conway/Jones 1976):

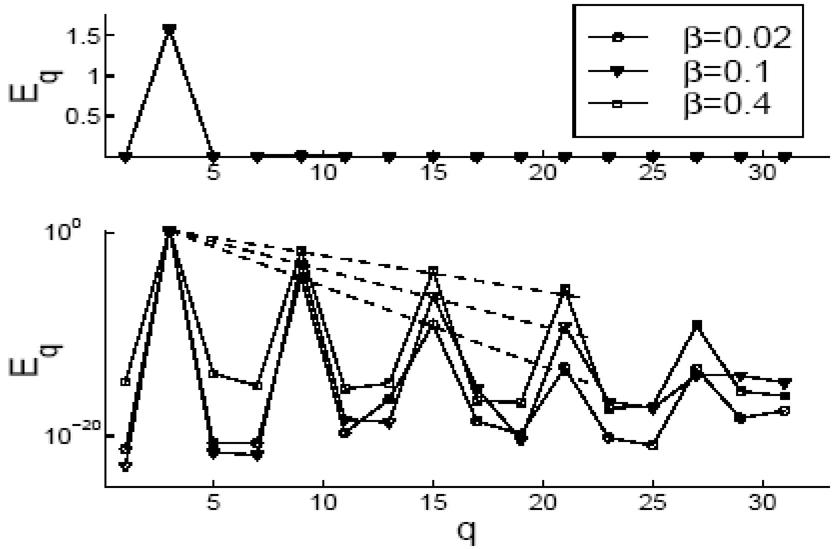
$$n\omega_{q_0} \neq \omega_{q \neq q_0}$$

And Lyapunov's Theorem for Non-Degenerate Weakly Coupled Anharmonic Oscillators

SO WE NEED A FINITE SYSTEM IN REAL SPACE!

The β model case

Numerical solutions for $N = 32$, $q_0 = 3$, only odd modes are excited:



Asymptotic expansion of solution:

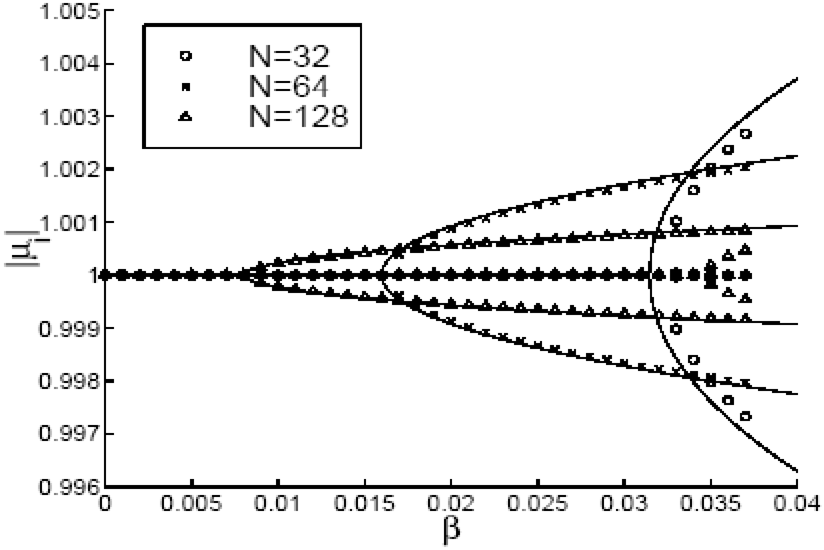
$$E_{(2n+1)q_0} = \lambda^{2n} E_{q_0} \ , \ \lambda = \frac{3\beta E_{q_0}(N+1)}{8\pi^2 q_0^2}$$

coincides with boundary estimate of natural packet by Shepelyansky!

QB solution localizes exponentially with exponent $\ln \lambda / q_0$

Cascade-like perturbation theory 3,3+3+3=9,9+3+3=15,15+3+3=21,etc

Numerical computation of Floquet eigenvalues



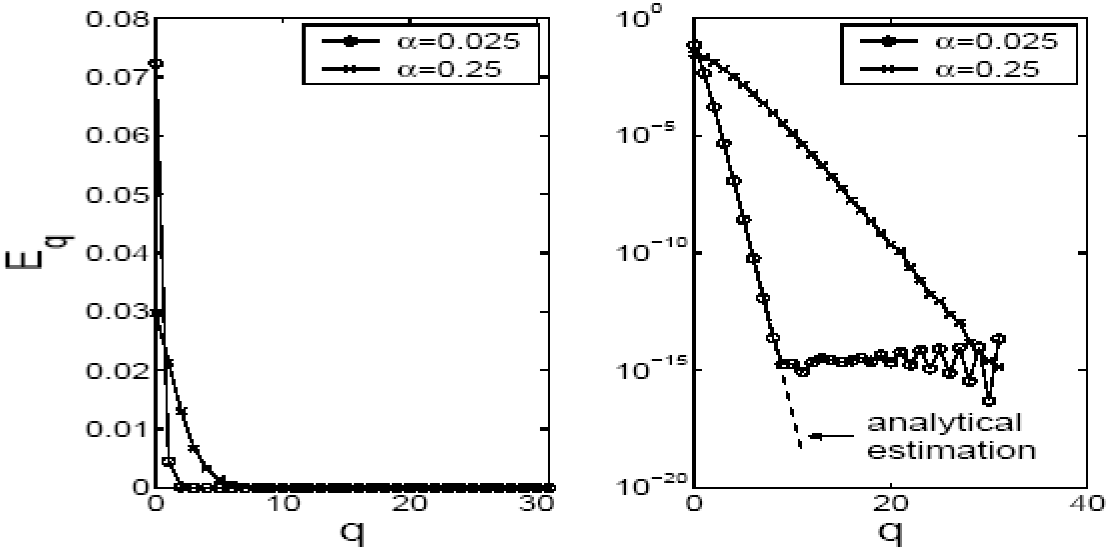
Secular perturbation theory:

$$|\mu_{j_1 j_2}| = 1 \pm \frac{\pi^3}{4(N+1)^2}\sqrt{R - 1 + O\left(\frac{1}{N^2}\right)}\ ,\ R = 6\beta E(N+1)/\pi^2$$

The QB solution turns unstable for $R = 1$.
This condition coincides with the transition to weak chaos according to DeLuca,Lichtenberg,Liebermann!

The α model case

Numerical solutions for $N = 32$, $q_0 = 1$, energy 0.077 of original FPU trajectory:

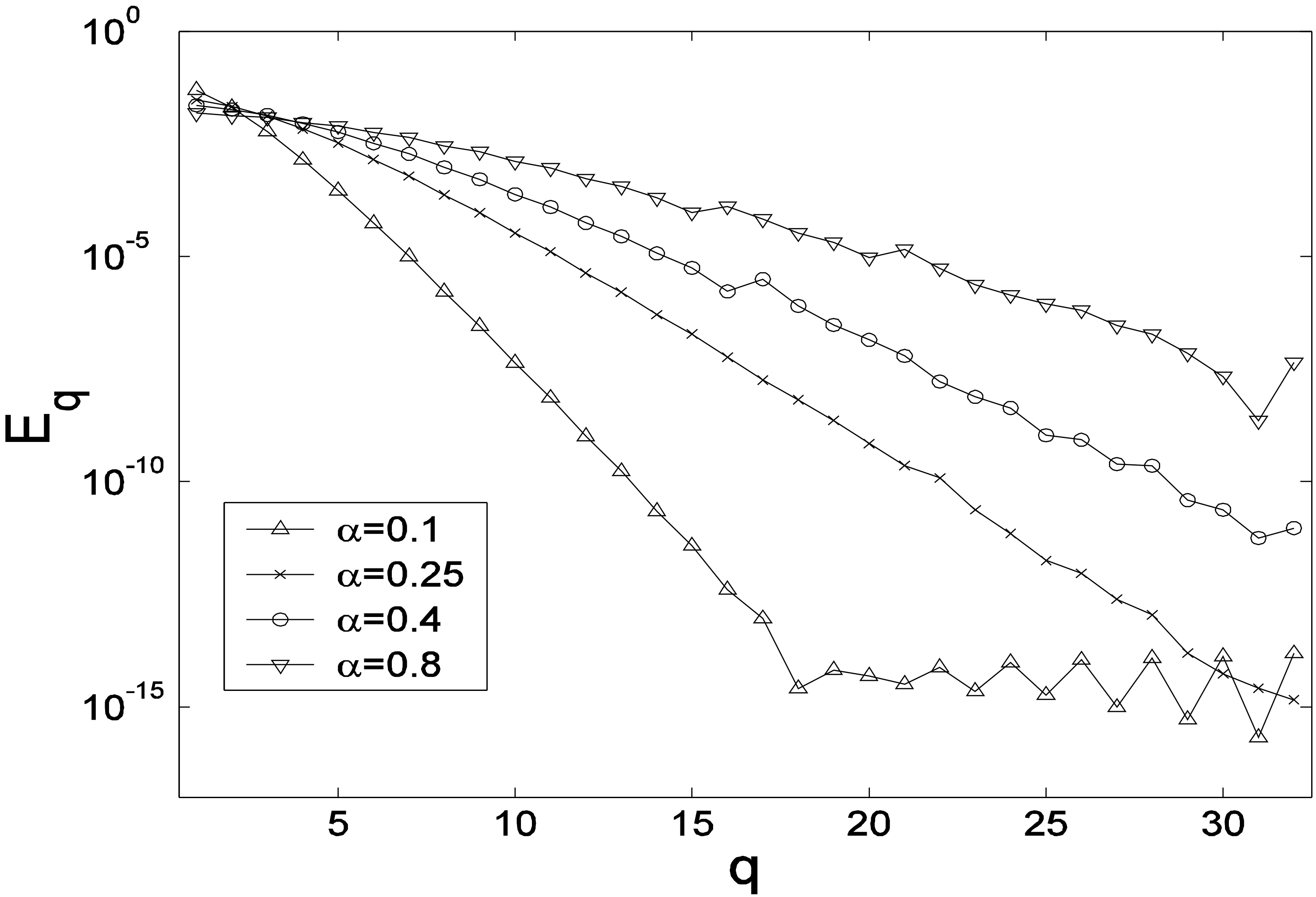


Asymptotic expansion of solution:

$$E_{nq_0} = \epsilon^{2n-2} n^2 E_{q_0} \ , \ \epsilon = \frac{\alpha \sqrt{E_{q_0}^{(0)}} (N+1)^{3/2}}{\pi^2 q_0^2}$$

coincides with boundary estimate of natural packet by Shepelyansky!

QB solution localizes exponentially with exponent $2 \ln \epsilon / q_0$



Evolution of normal mode energies

Evolution of normal mode coordinates

Evolution of real space displacements

PART THREE:

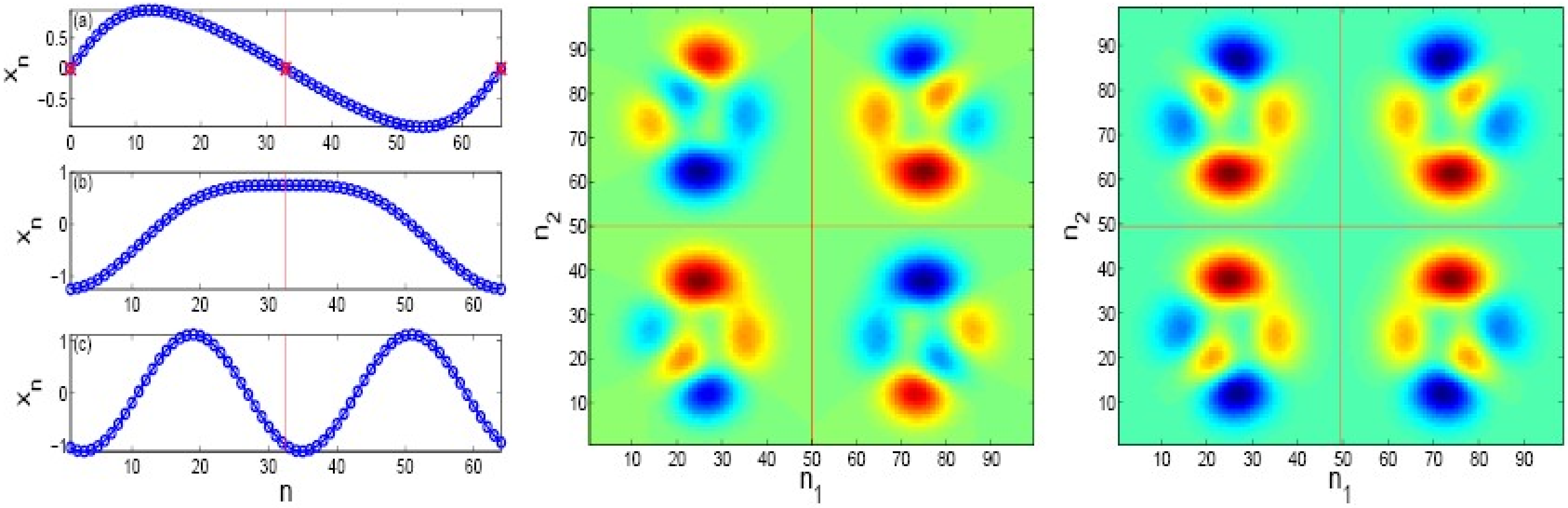
GOING BEYOND

Scaling of q-breathers to large system size

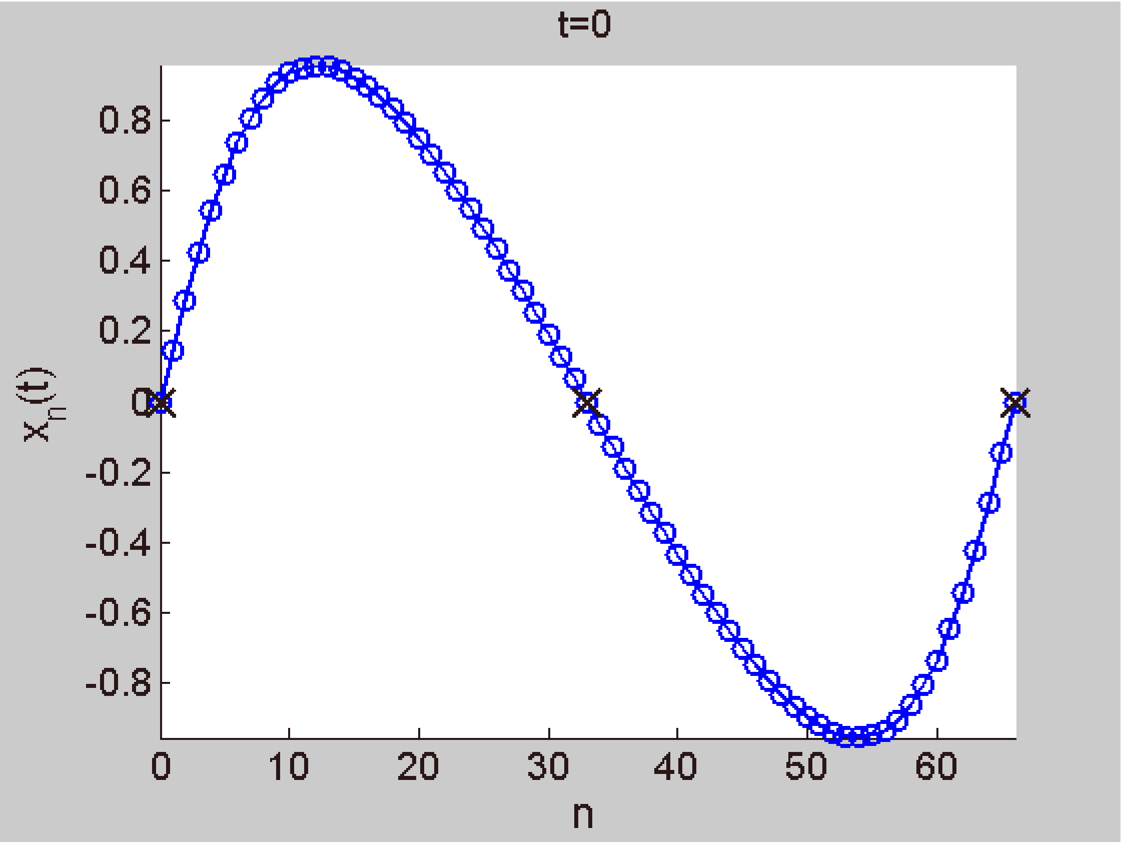
Establish existence of q-breather for given size N and any boundary condition, consider new size rN and scale!

PLA 365 (2007) 416

$$\tilde{Q}_{\tilde{q}}(t) = \begin{cases} \sqrt{r} Q_q(t) & \tilde{q} = rq \,, \\ 0 & \tilde{q} \neq rq \,, \end{cases} \quad q = \overline{1, N}$$



Thus scaled q-breathers exist for infinite size systems!



t=0
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
$x_n(t)$
0
10
20
30
40
50
60
n

Scaling of localization length of q-breathers

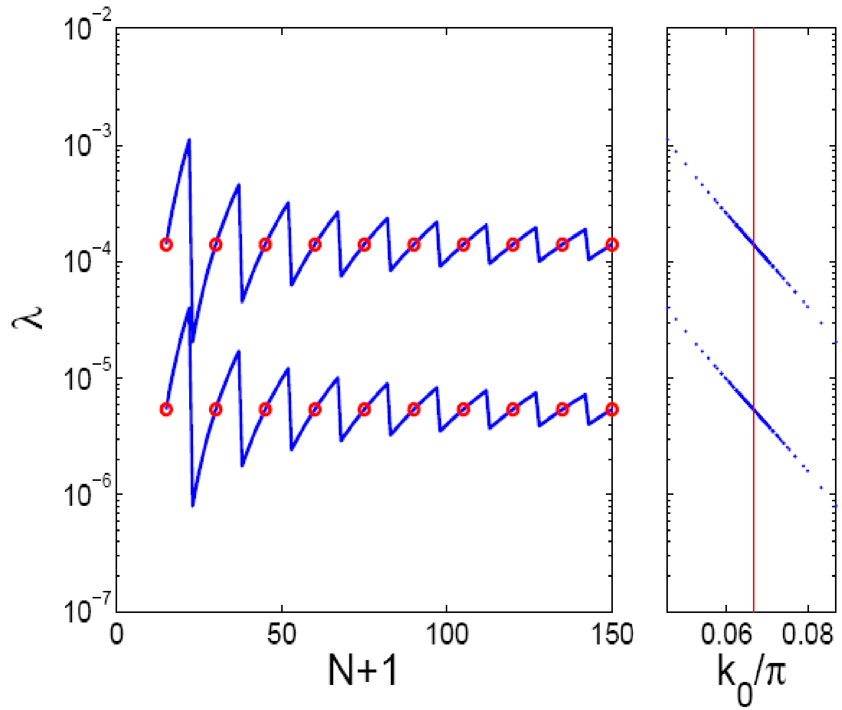
PLA 365 (2007) 416

$$\ln \varepsilon_k = \left(\frac{k}{k_0} - 1 \right) \ln \sqrt{\lambda} + \ln \varepsilon_{k_0} , \qquad \sqrt{\lambda} = \frac{3\beta}{2^{2+D}} \frac{\varepsilon_{k_0}}{k_0^2}$$

Wave number: $k = \pi q/(N+1)$

Energy density: $\varepsilon = E/(N+1)$

$$\varepsilon_{k_0} = (1 - \lambda)\varepsilon$$

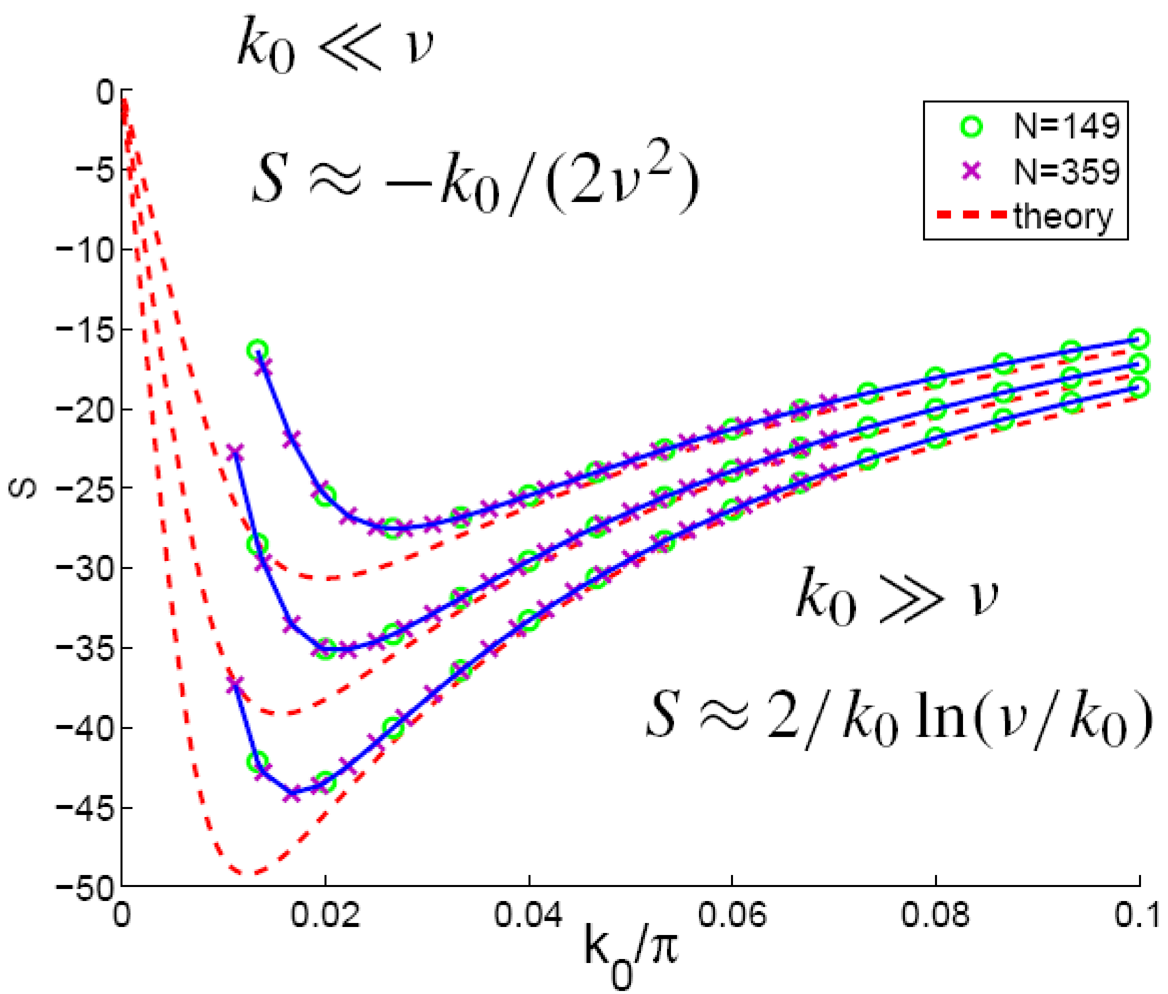


Slope S is the *negative inverse localization length* in k-space:

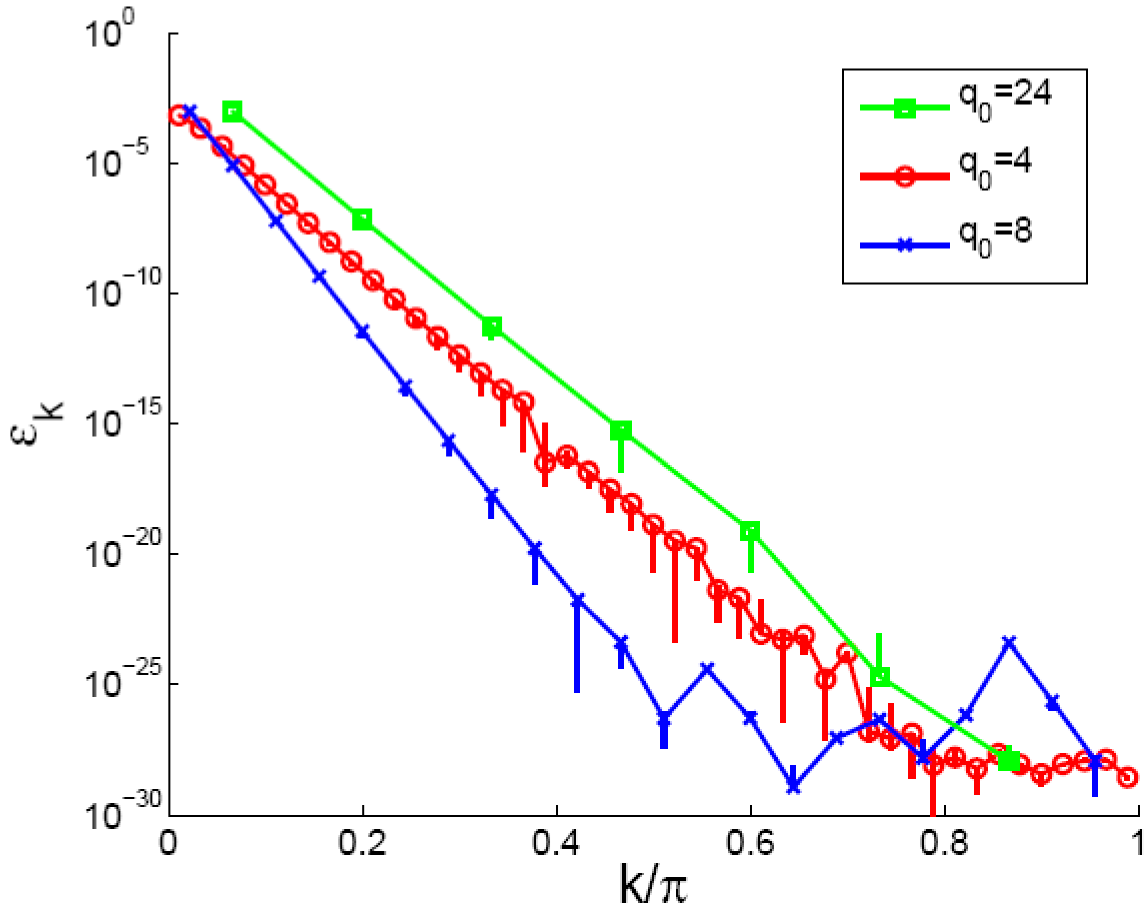
$$S = \frac{1}{k_0} \ln \sqrt{\lambda}\ , \ \sqrt{\lambda} = \frac{\sqrt{1 + 4\nu^4/k_0^4} - 1}{2\nu^2/k_0^2}\ , \ \nu^2 = \frac{3\beta}{8}\varepsilon$$

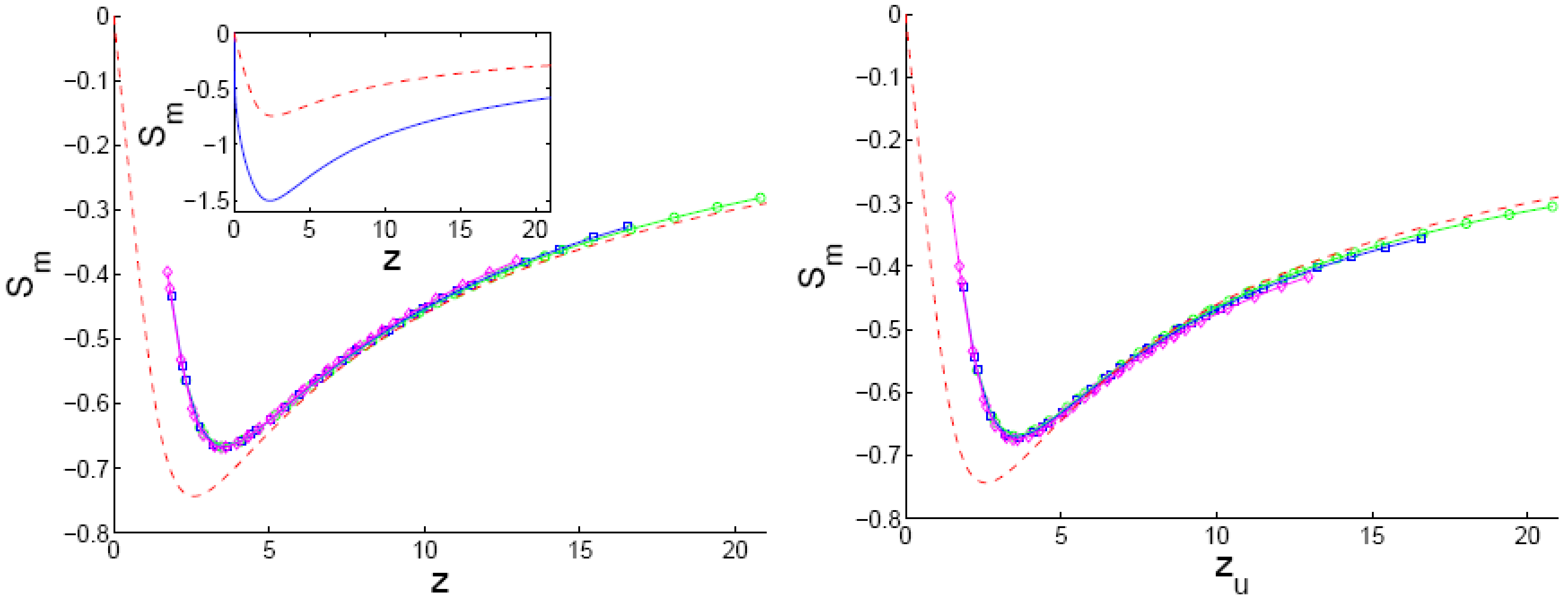
Master slope function: $S_m(z) = \nu S$

Rescaled wave number: $z = k_0/\nu$



$$\max(|S|) \approx 0.7432/\nu \ \text{at} \ k_{\min} \approx 2.577\nu$$

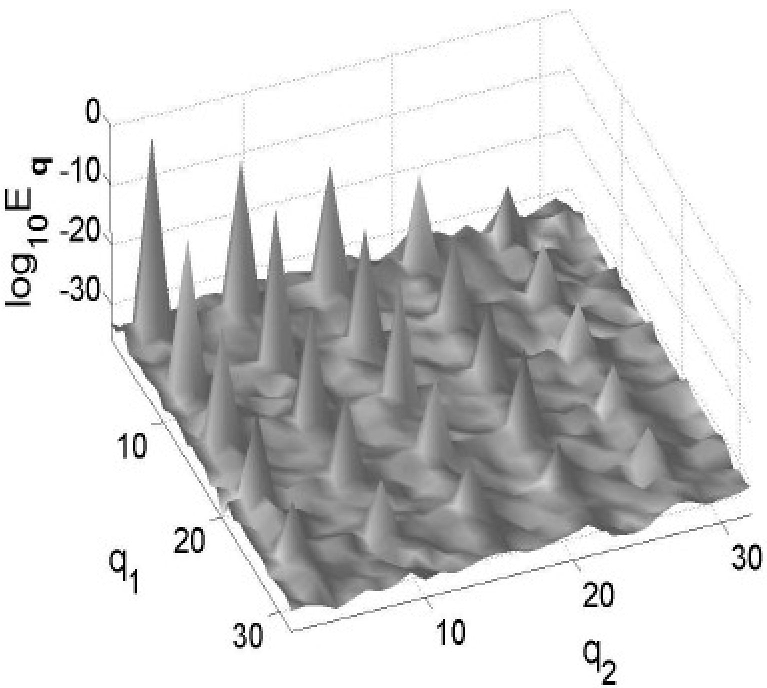

q0=24
q0=4
q0=8
εk
k/π
10^0
10^-5
10^-10
10^-15
10^-20
10^-25
10^-30
0
0.2
0.4
0.6
0.8
1

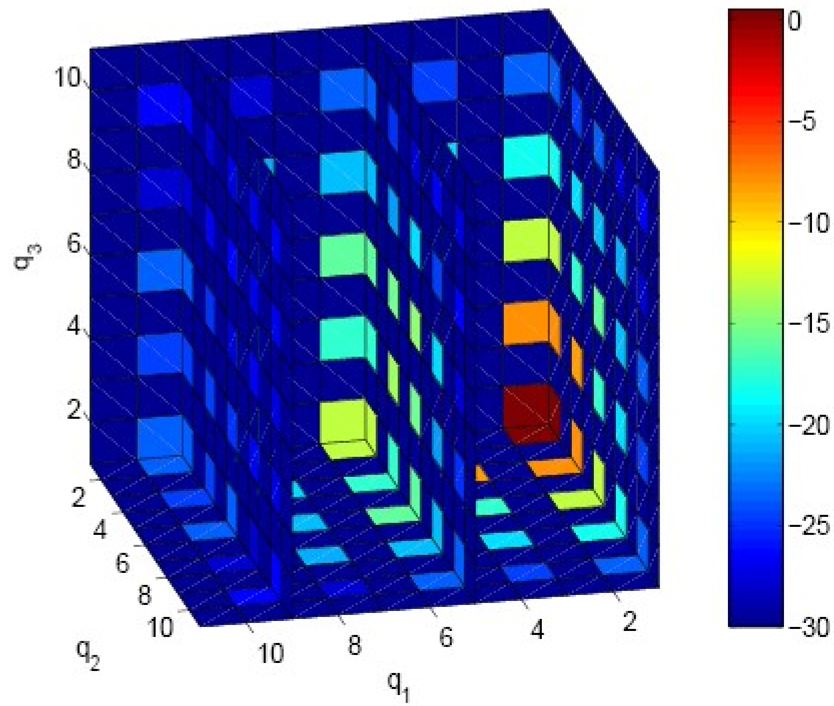


- Scaling works even in nonperturbative regime
- True also for upper band edge
- Similar results for α- FPU case
- In a certain region close to any band edge normal modes delocalize almost completely! Range depends only on ν!
- Position of minimum in S is identical to width of resonant layer!

Generalization to two- and three-dimensional lattices

PRL 97 (2006) 025505





K.G. Mishagin, S. Flach, O.I. Kanakov and M.V. Ivanchenko
arXiv:0801.1055v1

The Discrete Nonlinear Schrödinger Lattice

q-breathers are easily constructed as well!

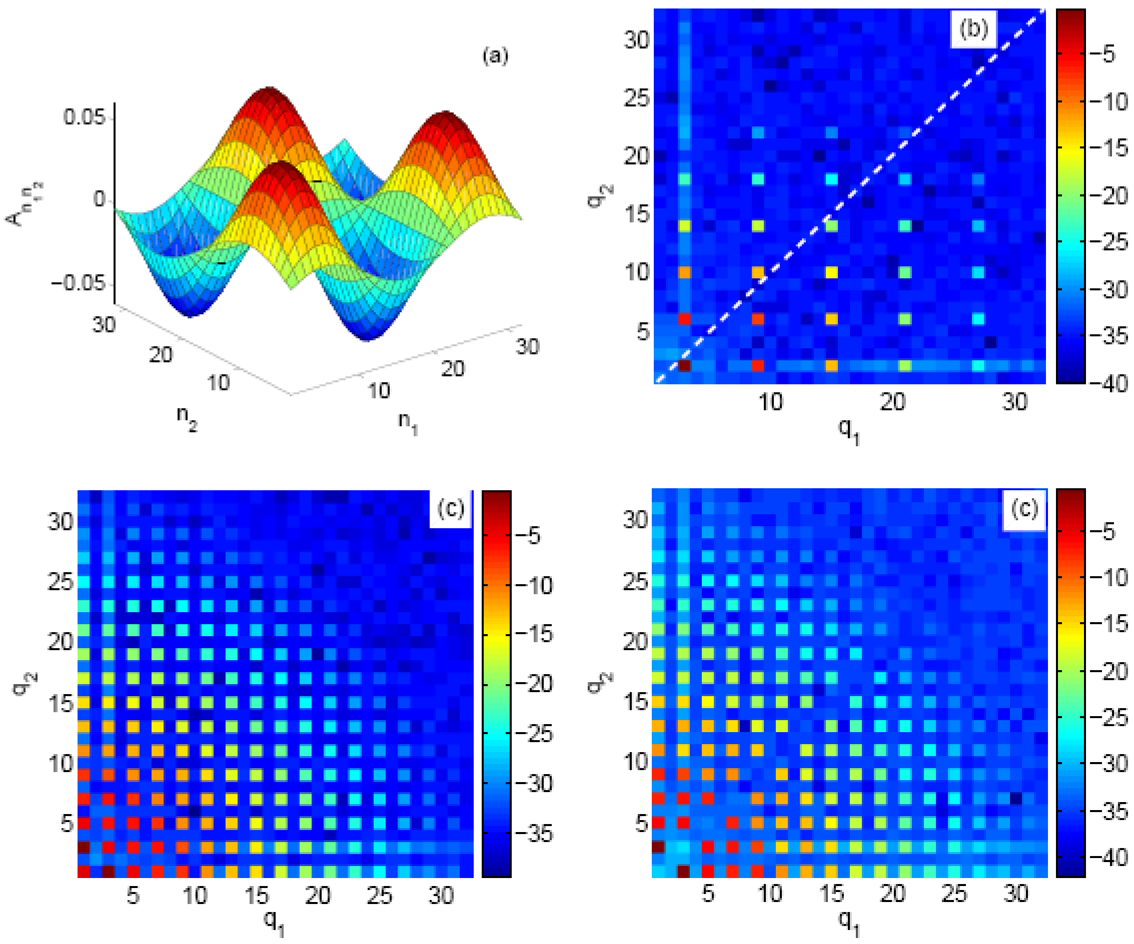
$$H = \sum_{\mathbf{n}} \Big(\sum_{\mathbf{m}\in \mathbf{D}(\mathbf{n})} \psi_{\mathbf{m}} \psi_{\mathbf{n}}^{*} + \frac{\mu}{2} |\psi_n|^4 \Big) \ , \ i\dot{\psi}_{\mathbf{n}} = \sum_{\mathbf{m}\in \mathbf{D}(\mathbf{n})} \psi_{\mathbf{m}} + \mu |\psi_{\mathbf{n}}|^2 \psi_{\mathbf{n}}$$

$$\psi_{\mathbf{n}}(t) = \left(\frac{2}{N+1} \right)^{d/2} \sum_{q_1,\ldots,q_d=1}^{N} Q_{\mathbf{q}}(t) \prod_{i=1}^{d} \sin \left(\frac{\pi q_i n_i}{N+1} \right)$$

$$i\dot{Q}_{\mathbf{q}} = -\omega_{\mathbf{q}} Q_{\mathbf{q}} - \frac{2^{d-2}\mu}{(N+1)^d} \sum_{\mathbf{p},\mathbf{r},\mathbf{s}} C_{\mathbf{q},\mathbf{p},\mathbf{r},\mathbf{s}} Q_{\mathbf{p}} Q_{\mathbf{r}}^{*} Q_{\mathbf{s}} \ , \ \omega_{\mathbf{q}} = -2 \sum_{i=1}^{d} cos \frac{\pi q_i}{N+1}$$

Solutions:

$$\psi_{\mathbf{n}} = \phi_{\mathbf{n}} \mathrm{e}^{i\Omega t} \ , \ Q_{\mathbf{q}} = A_{\mathbf{q}} \mathrm{e}^{i\Omega t}$$


(a)
(b)
(c)
(c)
$A_{n_1 n_2}$
n_1
n_2
q_1
q_2

Further reading:
- PRL 95 (2005) 064102
- PRE 73 (2006) 036618
- PRL 97 (2006) 025505
- PLA 365 (2007) 416
- Chaos 17 (2007) 023102
- New J Phys, in print; arXiv:0801.1055v1
- Physica D 237 (2008) 908
- AJP 76 (2008) 453

Summarizing the q-breather results

- Existence of q-breathers, their stability and localization in q-space explains nonequipartition (FPU-1)

- Localized perturbation of localized q-breathers - evolution on low-dimensional tori, rather short recurrence times (FPU-2)

- Stability thresholds of q-breathers - weak stochasticity thresholds; Localization thresholds of q-breathers - equipartion thresholds (FPU-3)

- q-breather concept can be applied to other nonlinear chains, higher dimensional nonlinear lattices, any nonlinear spatially extended dynamical system on a finite spatial domain (including continua)

- Quantization of q-breathers straightforward - quantum dressed phonons in finite systems