The Abdus Salam International Centre for Theoretical Physics

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Advanced Workshop on Energy Transport in Low-Dimensional Systems: Achievements and Mysteries

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Nonlinear Waves in Low-dimensional Systems - Part I

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

THE ENGINE
OF THE NEW
NEW ZEALAND

S. Flach

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Massey University
Auckland NZ

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

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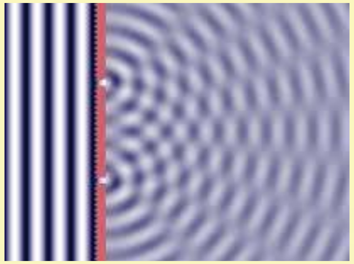
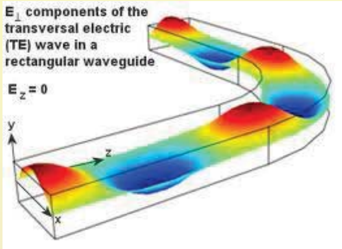
Waves

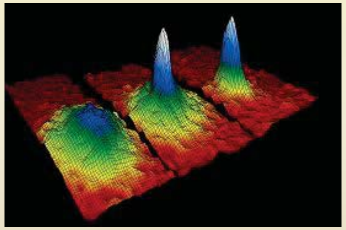
amplitude and phase in space and time

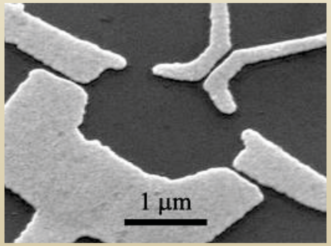


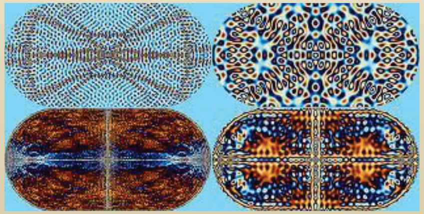
Linear waves: superposition, interference, phase coherence



e.g.
optical fibres
microwave cavities
atomic Bose-Einstein condensates
quantum billiards
quantum dots
superconducting networks
molecules, solids



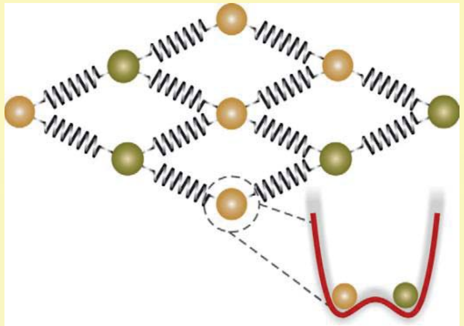


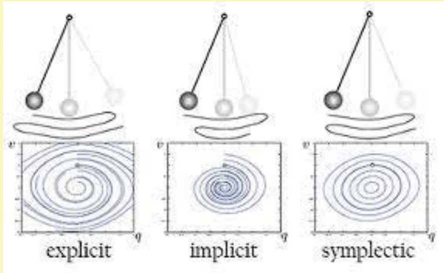


Why waves?

high intensities - qualitatively new properties:
nonlinear response
waves interact with each other
resonances
dynamical chaos
instability
rogue waves ... tsunami ...

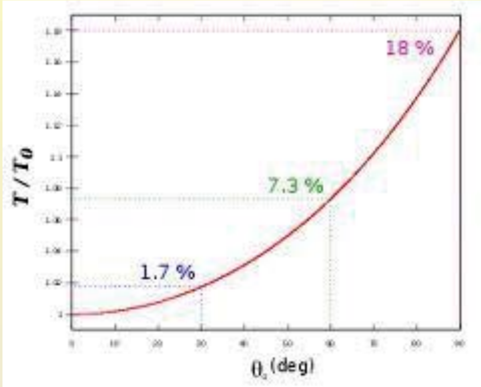
Lattice waves





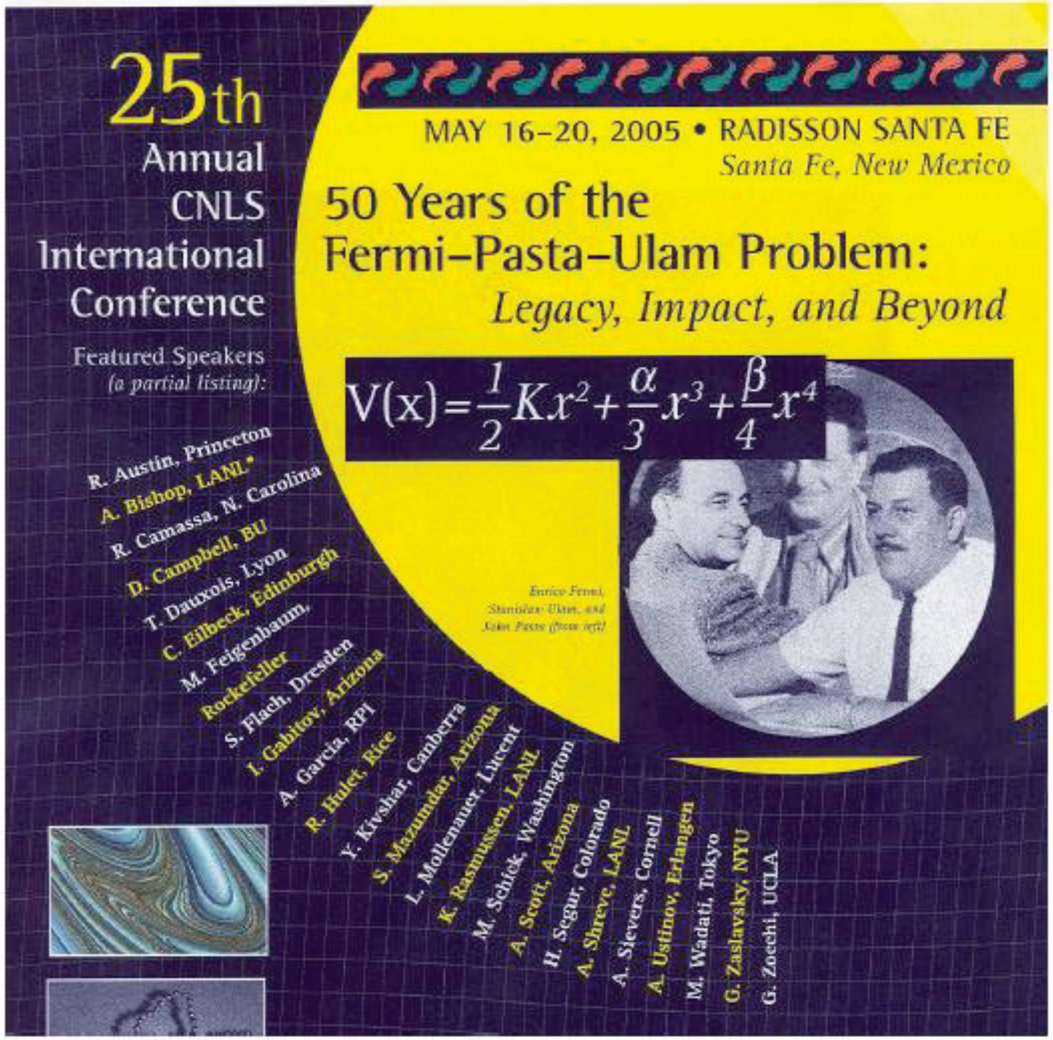
discretize space – introduce lattice
one oscillator per lattice point
oscillator state is defined by amplitude and phase
introduce interaction between oscillators

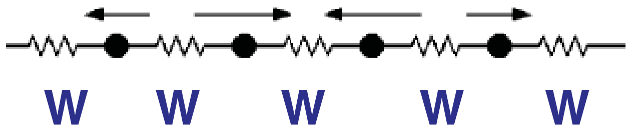
anharmonic potential = nonlinear wave equation
intensity increase changes frequency
in quantum world energy levels NOT equidistant



Typical excitations in condensed matter, optics, etc

FPU: the problem





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

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

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

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

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

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:

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

Longe range nonlinear interactions and localization?

Example: anharmonic oscillator

$$\ddot{x} = -x - \alpha x^2 - \beta x^3$$

$$x(t) = \sum_k A_k e^{ik\Omega t}$$

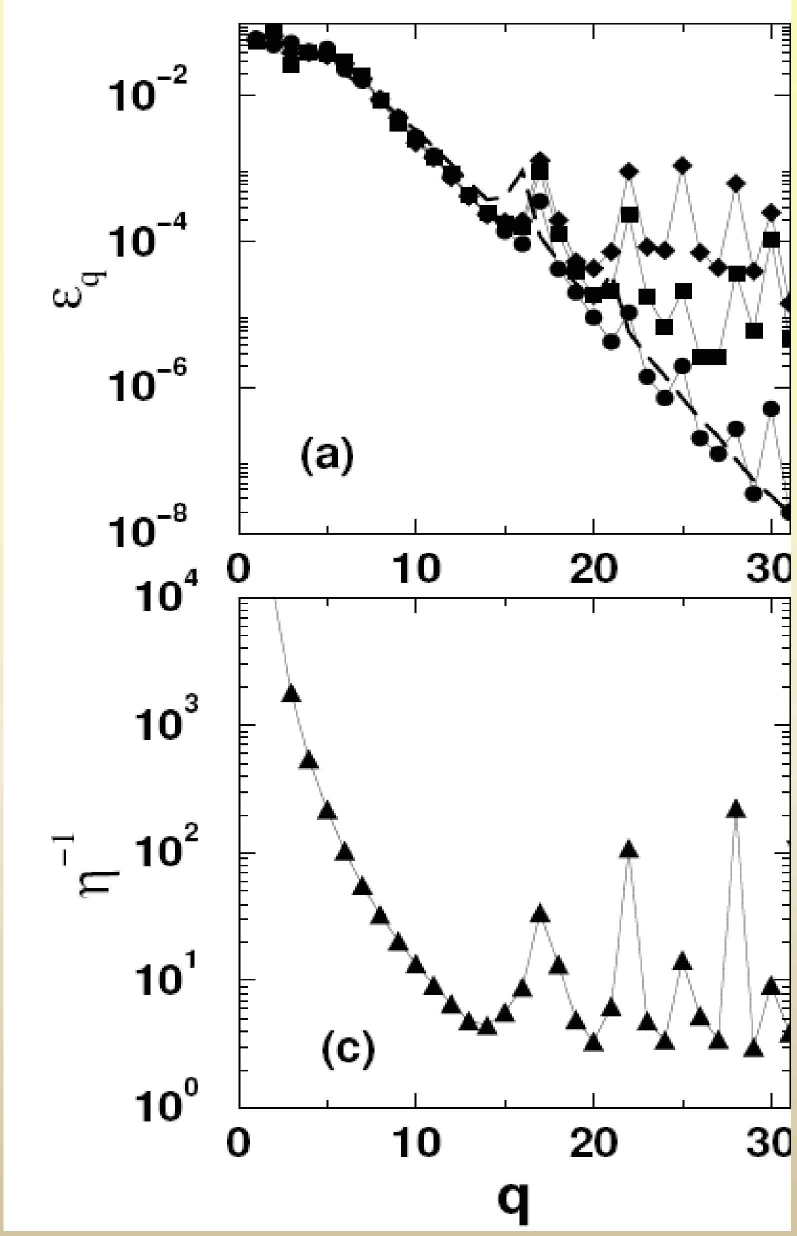
$$A_k = k^2\Omega^2 A_k - \alpha \sum_{k_1} A_{k_1} A_{k-k_1} - \beta \sum_{k_1,k_2} A_{k_1} A_{k_2} A_{k-k_1-k_2}$$

X(t) is an analytical periodic function and thus the Fourier series converges exponentially.
But would you guess that from the amplitude equations?

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

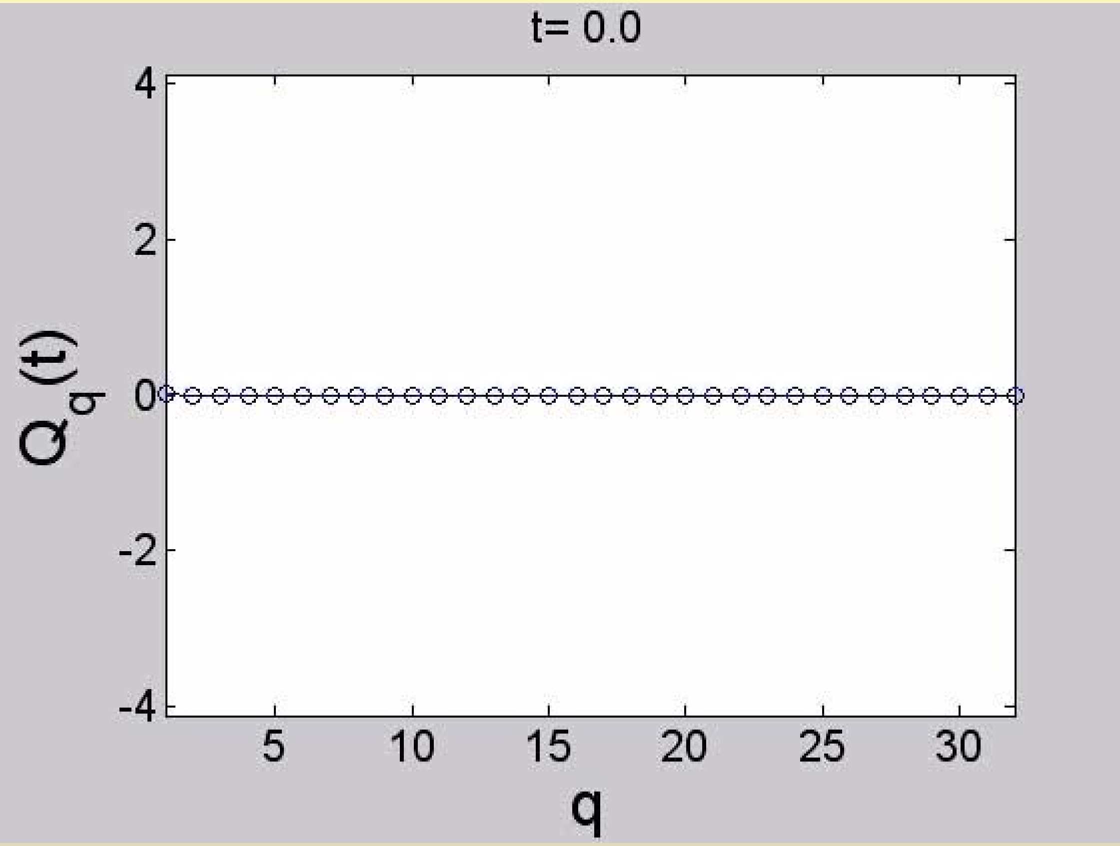
- excite $q = 1$ mode
- observe nonequipartion of mode energies
- no transition to thermal equilibrium
- energy is localized in a few modes for long time **FPU 1**
- recurrence of energy into initially excited mode **FPU 2**
- two thresholds in energy and N **FPU 3**
- two pathways of understanding: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

Galgani and Scotti (1972):
exponential localization

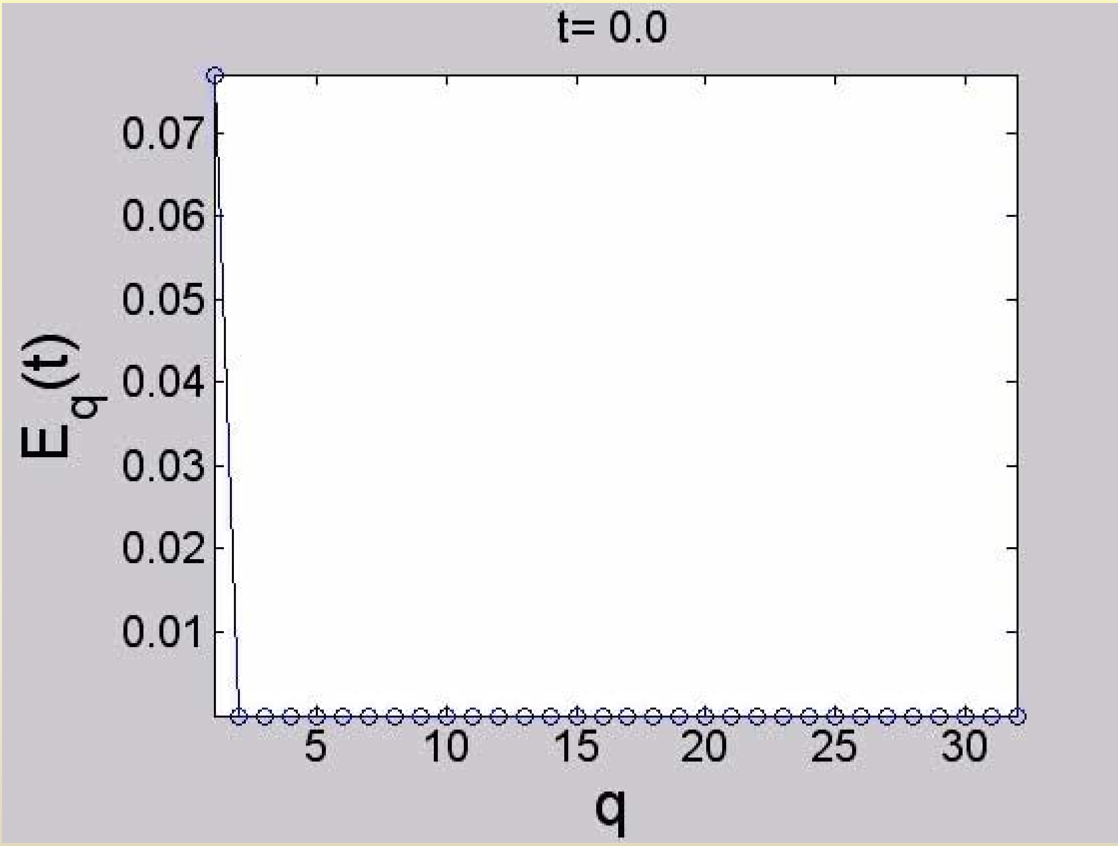


Movies: let us see what FPU observed

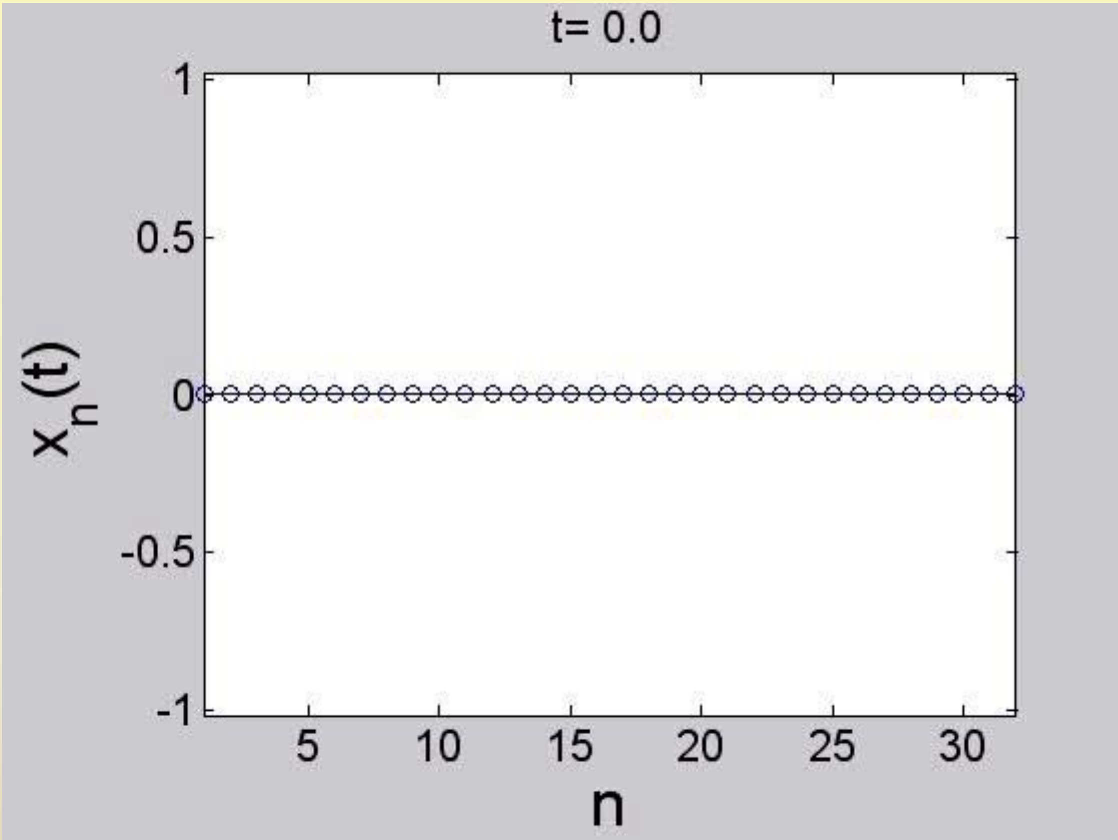
Evolution of normal mode coordinates



Evolution of normal mode energies

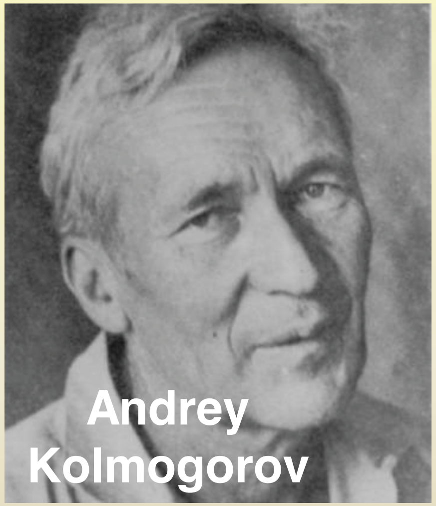


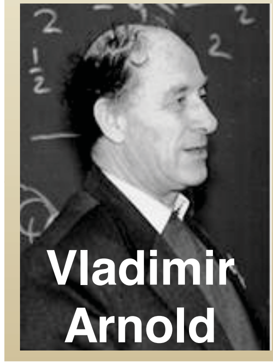
Evolution of real space displacements

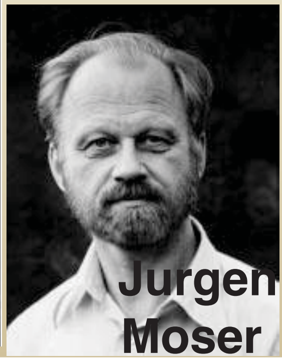


Kolmogorov – Arnold – Moser (KAM) theory

A.N. Kolmogorov,
Dokl. Akad. Nauk SSSR, 1954.
Proc. 1954 Int. Congress of Mathematics, North-Holland, 1957





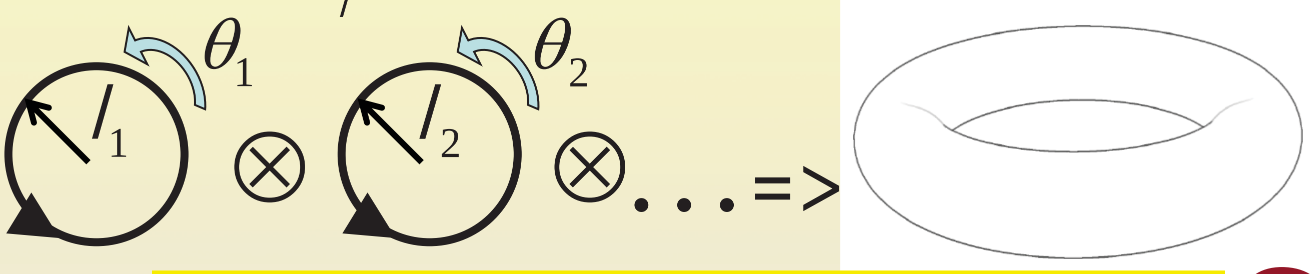


Integrable classical Hamiltonian $\hat{H}_0$, $d>1$:

Separation of variables: d sets of action-angle variables $I_1, \theta_1 = 2\pi\omega_1 t;.., I_2, \theta_2 = 2\pi\omega_2 t;..$

Quasiperiodic motion: set of the frequencies, $\omega_1, \omega_2, .., \omega_d$ which are in general incommensurate

Actions I_i are integrals of motion $\partial I_i / \partial t = 0$



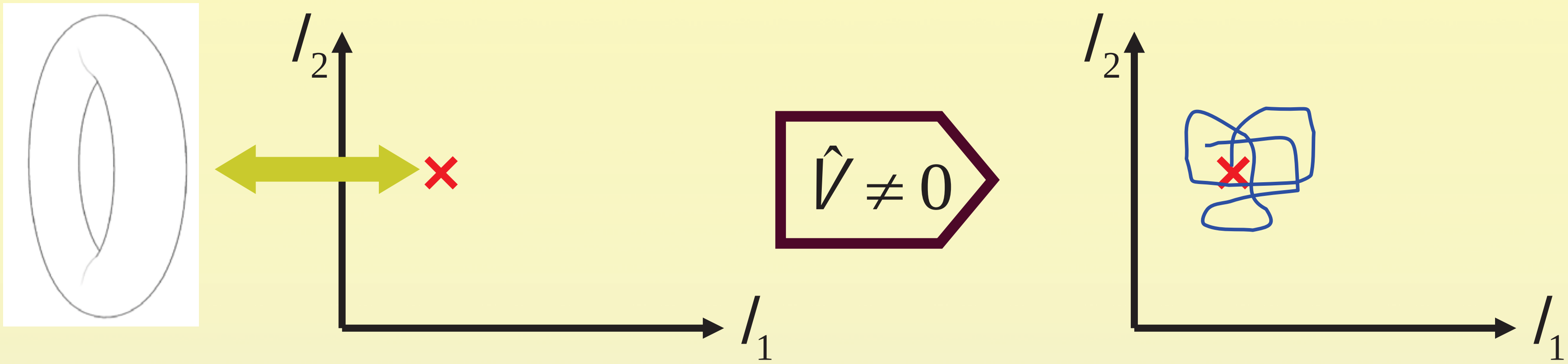
Q: Will an arbitrary weak perturbation $\hat{V}$ of the integrable Hamiltonian $\hat{H}_0$ destroy the tori and make the motion ergodic (when each point at the energy shell will be reached sooner or later) **?**

A: **Most of the tori survive weak and smooth enough perturbations**

KAM theorem

KAM theorem:

Most of the tori survive weak and smooth enough perturbations



Each point in the space of the **integrals of motion** corresponds to a torus and vice versa

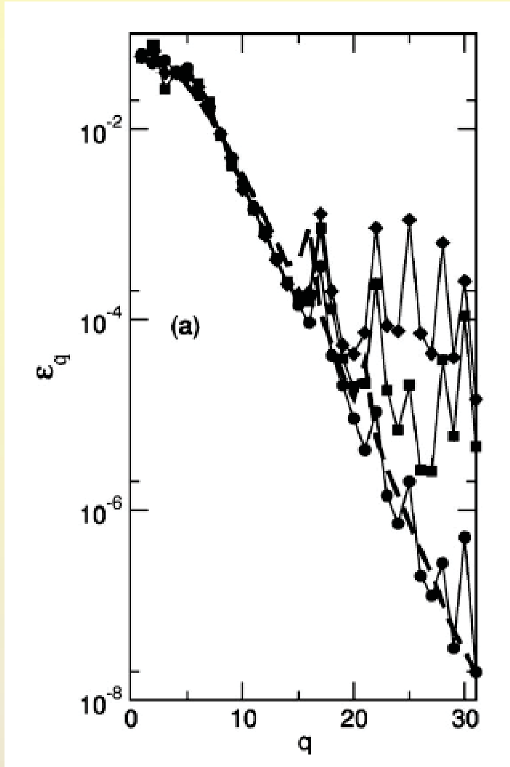
Finite motion.
Localization in the **space of the integrals of motion** ?

- KAM applies to finite systems
- Does it apply to waves in infinite systems?
- How are KAM thresholds scaling with number of degrees of freedom?
- Will nonlinear waves observe KAM regime?
- If they do – then localization remains
- If they do not – waves can delocalize

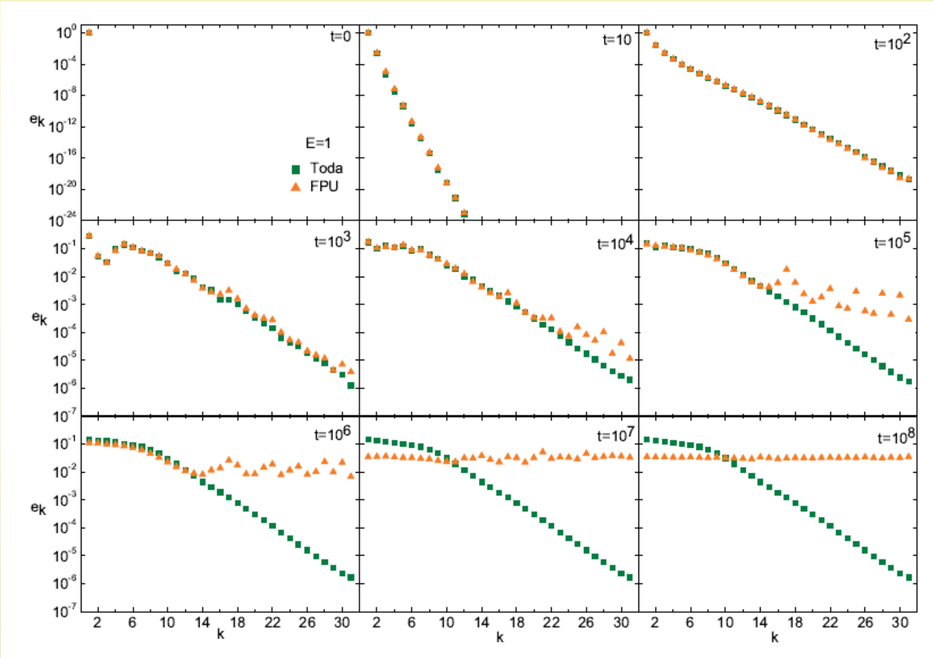
KAM?
Solitons (Zabusky,Kruskal 1965)?

two time scales
T1: formation of exponentially localized packet
T2: gradual destruction and equipartition

Galgani and Scotti (1972)



Ponno,Christodoulidi,Skokos,Flach (2011)



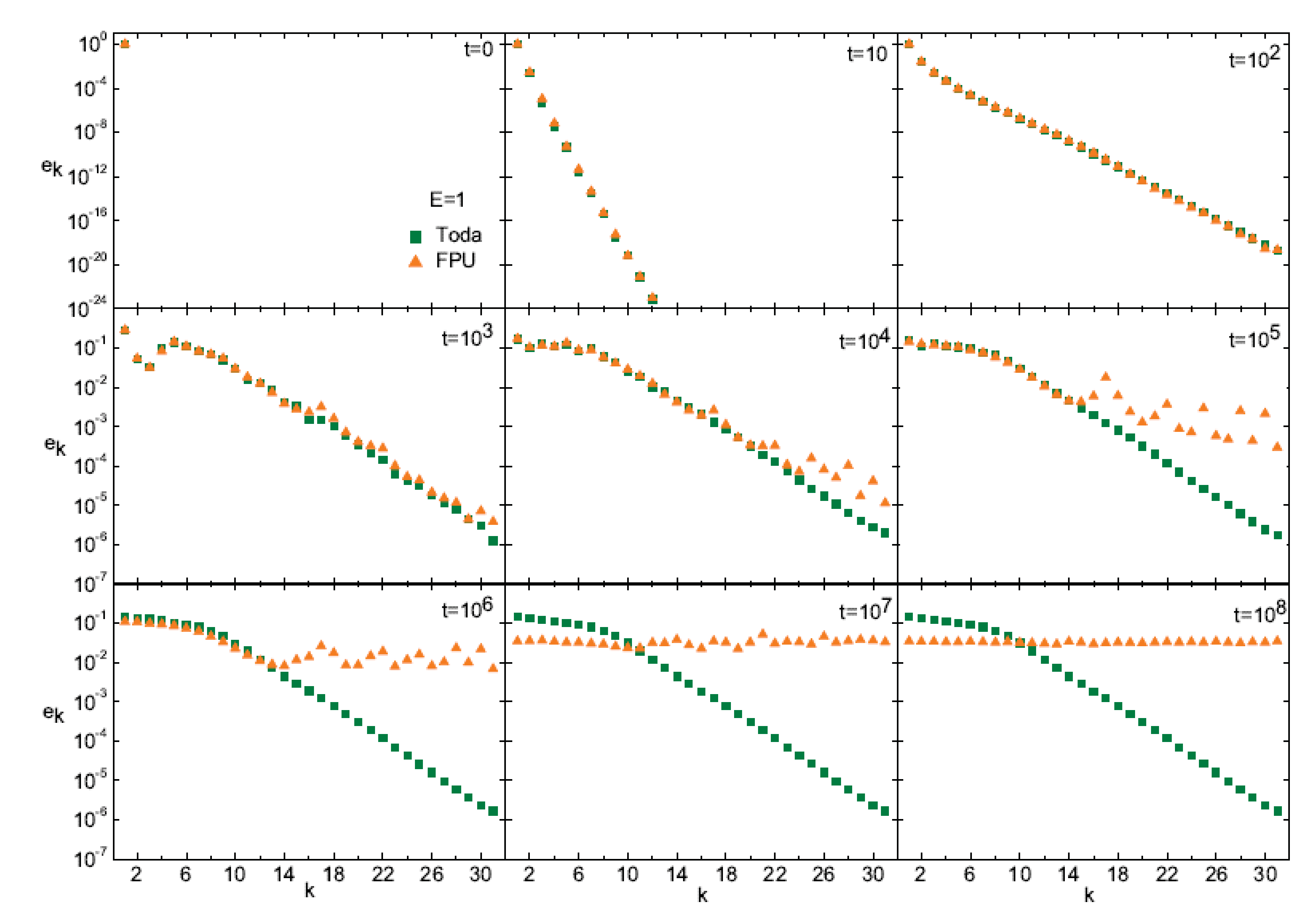
T1=10^2 ; T2=10^8

Comparing the integrable Toda to the nonintegrable FPU

$$H_T(q,p) = \sum_{n=0}^{N-1} \left[\frac{p_n^2}{2} + \frac{e^{2\alpha(q_{n+1}-q_n)} - 1}{4\alpha^2} \right]$$

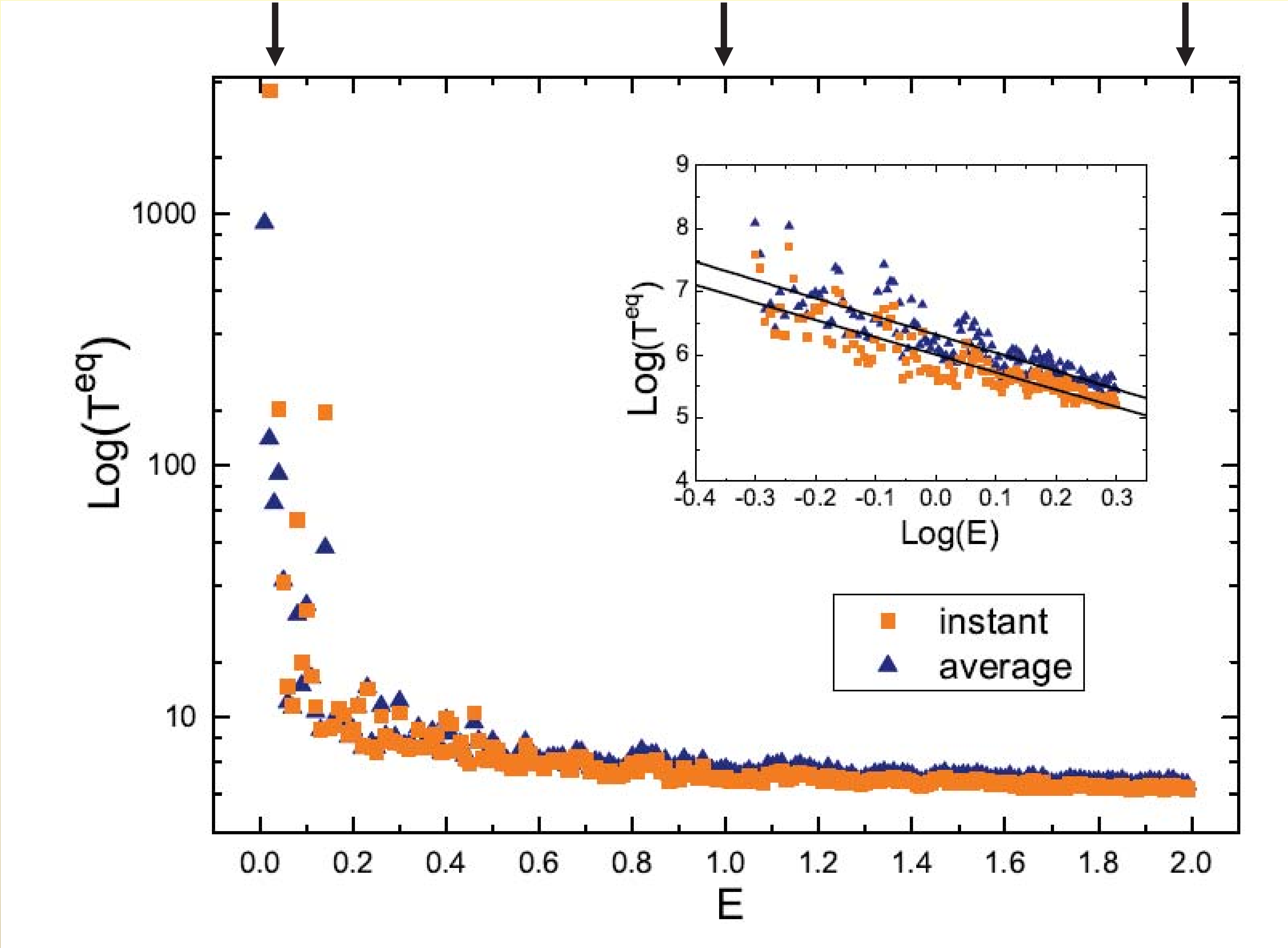
$$H_\alpha(q,p) = H_T(q,p) - \sum_{n=0}^{N-1} \sum_{r \geq 4} (2\alpha)^{r-2} \frac{(q_{n+1} - q_n)^r}{r!}$$

E. Christodoulidi, A. Ponno, Ch. Skokos, SF, Chaos 21, 043127 (2011)



T1=10^2 ; T2=10^8

T2 infinite? KAM? T2 >> T1 : weak chaos T2=T1 : strong chaos



q-breathers

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 by Flach et al (2006): 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!

A poor man's way to q-breathers

β-FPU, $q \ll N$

$$\ddot{Q}_{3q_0} = -\omega_{3q_0}^2 Q_{3q_0} - \frac{\beta}{N}\omega_{q_0}^4 Q_{q_0}^3$$

$$Q_{q_0} \sim A_{q_0} \cdot e^{i\omega_{q_0} t}$$

$$Q_{3q_0} \sim A_{3q_0} \cdot e^{3i\omega_{q_0} t}$$

identify the right resonance

$$A_{3q_0} \sim \frac{\beta\,\omega_{q_0}^4 \cdot A_{q_0}^3}{N(3\omega_{q_0} - \omega_{3q_0})(3\omega_{q_0} + \omega_{3q_0})}$$

Some relations:

$$3\omega_{q_0} + \omega_{3q_0} \sim \frac{q_0}{N} + O\left(\frac{q_0^3}{N^3}\right)$$

$$3\omega_{q_0} - \omega_{3q_0} \sim \frac{q_0^3}{N^3} + O\left(\frac{q_0^5}{N^5}\right)$$

$$E_q \sim \omega_q^2 A_q^2 \,, \quad E = \sum_q E_q$$

$$\varepsilon = E/N \,, \quad k = q/N$$

$$A_{3q_0} \sim \frac{\beta}{N} A_{q_0}^3$$

$$E_{3q_0} \sim \frac{\beta^2 N^2}{q_0^4} \cdot E_{q_0}^3$$

$$E_{3q_0} \sim \lambda^2 \cdot E_{q_0} \quad \ldots \quad E_{(2n+1)q_0} \sim \lambda^{2n} E_{q_0}$$

$$\Rightarrow \quad E_{q_0} = (1-\lambda^2) E$$

$$\boxed{\lambda \sim \frac{\beta N}{q_0^2} E_{q_0} = \frac{\beta\, \varepsilon_{k_0}}{k_0^2}}$$

exponential localization:

$$\varepsilon_k = \lambda^{k/k_0} \varepsilon_{k_0} = \varepsilon_{k_0} \cdot e^{-k \cdot \left[\frac{1}{k_0} \ln 1/\lambda\right]}$$

localization length: $\boxed{\xi_{loc} = -k_0 / \ln \lambda}$

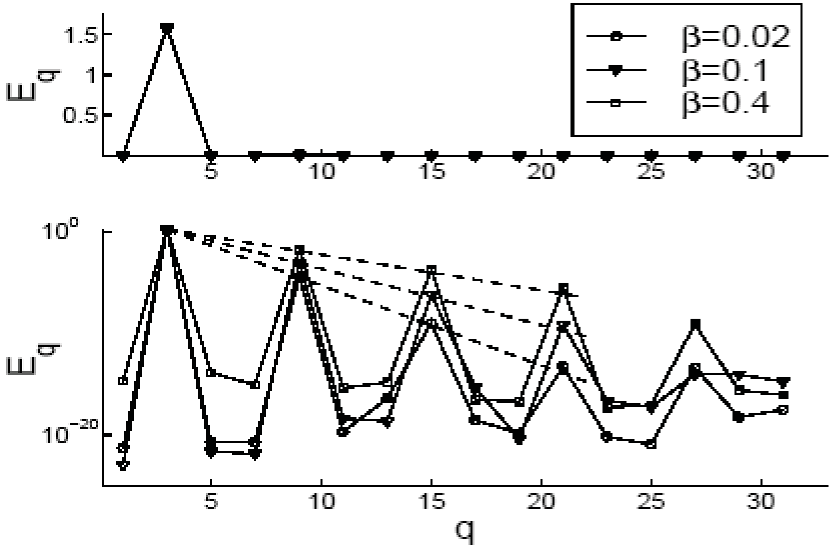
meaningful when $\boxed{\xi_{loc} < \pi}$

slope $S = -1/\xi_{loc}$

Flach, Ivanchenko, Kanakov PRL 95 (2005) 064102

The β model case

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



Asymptotic expansion of solution:

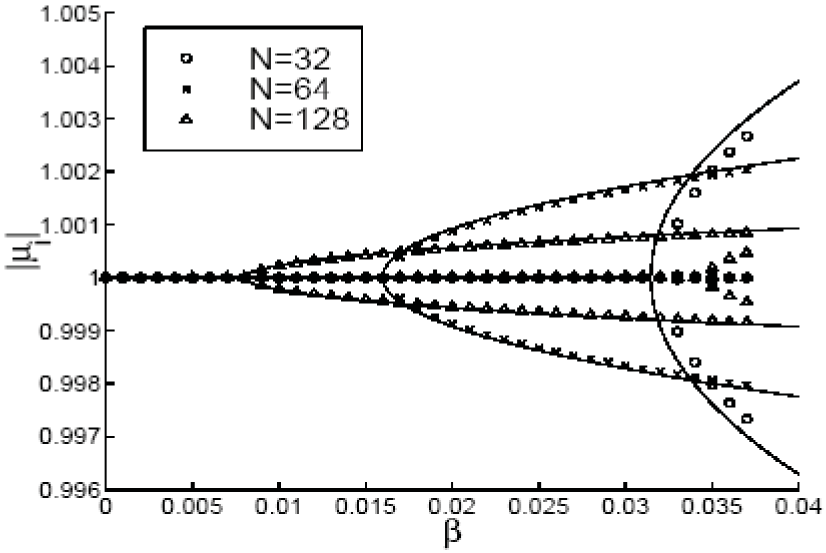
$$E_{(2n+1)q_0} = \lambda^{2n} E_{q_0} \ , \ \lambda = \frac{3\beta E_{q_0}(N+1)}{8\pi^2 q_0^2}$$

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:

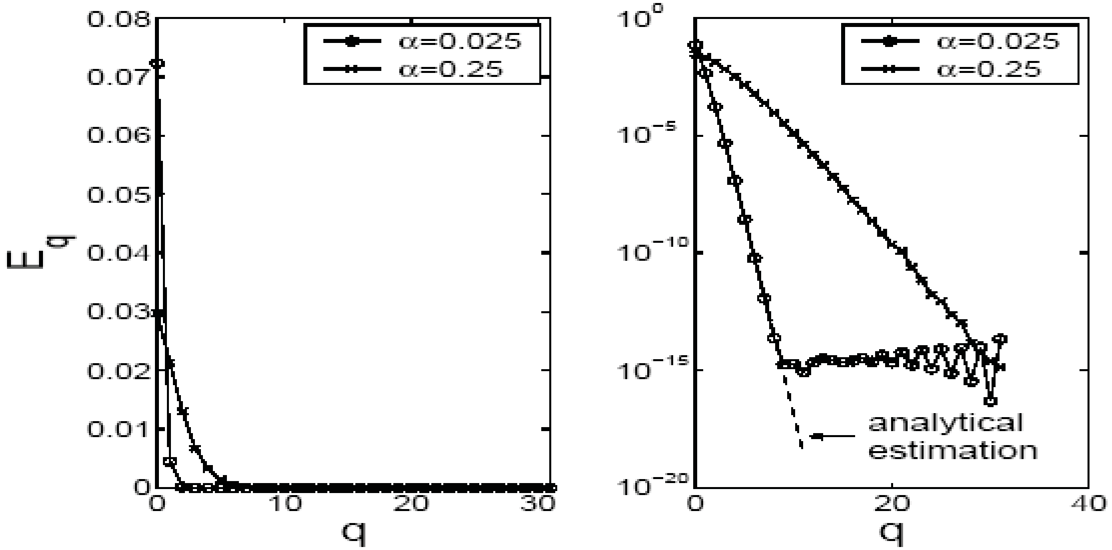
$$|\mu_{j_1 j_2}| = 1 \pm \frac{\pi^3}{4(N+1)^2}\sqrt{R - 1 + O\left(\frac{1}{N^2}\right)}\ ,\ R = 6\beta E(N+1)/\pi^2$$

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

Flach, Ivanchenko, Kanakov PRL 95 (2005) 064102

The α model case

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

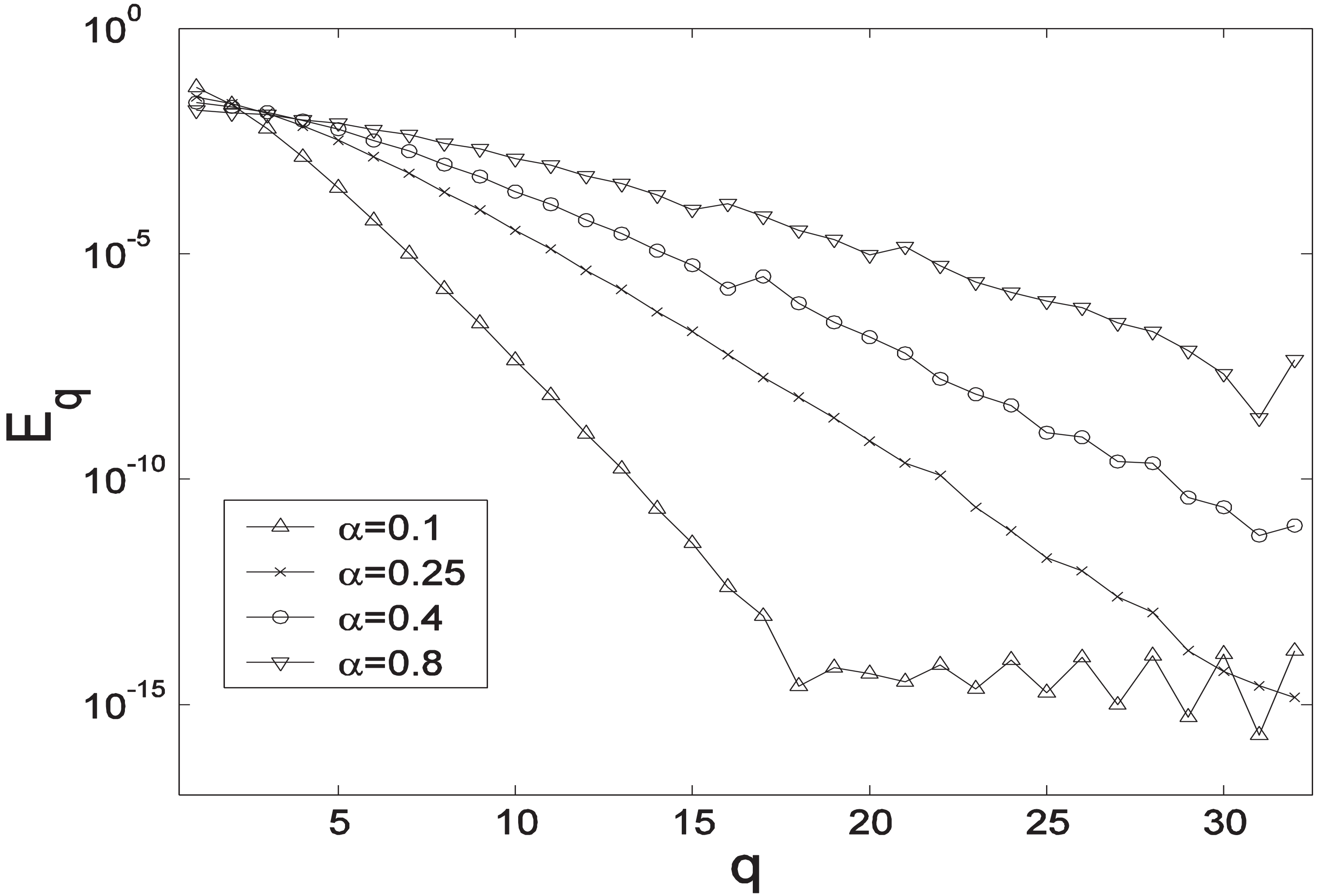


Asymptotic expansion of solution:

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

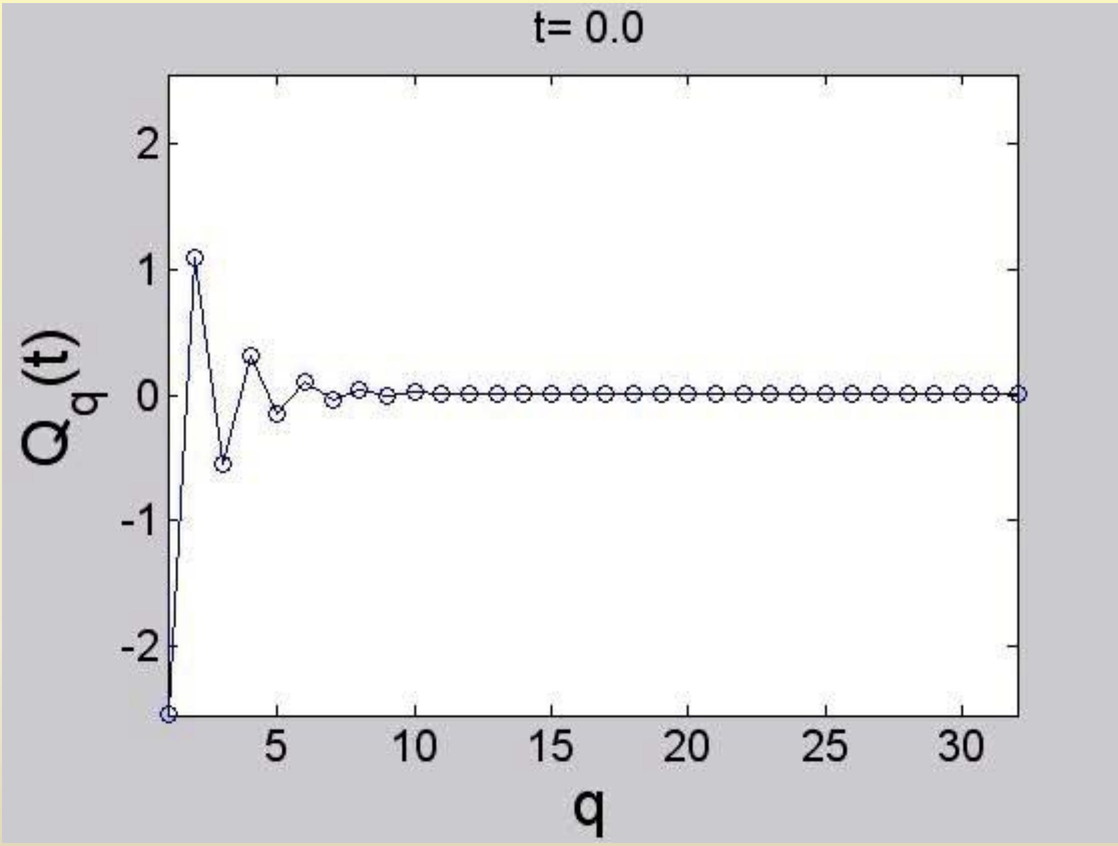
coincides with boundary estimate of natural packet by Shepelyansky!

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

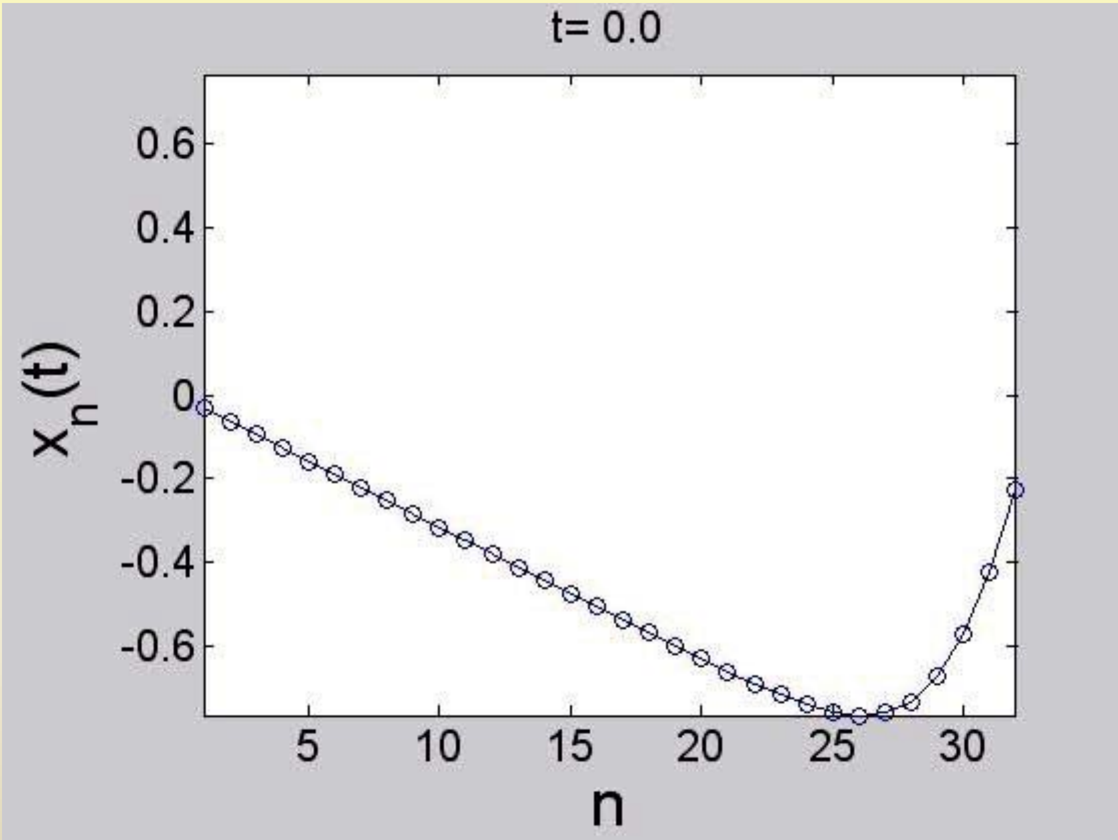


10^{0}
10^{-5}
10^{-10}
10^{-15}
E_q
5
10
15
20
25
30
q
α=0.1
α=0.25
α=0.4
α=0.8

QB: Evolution of normal mode coordinates



QB: Evolution of real space displacements



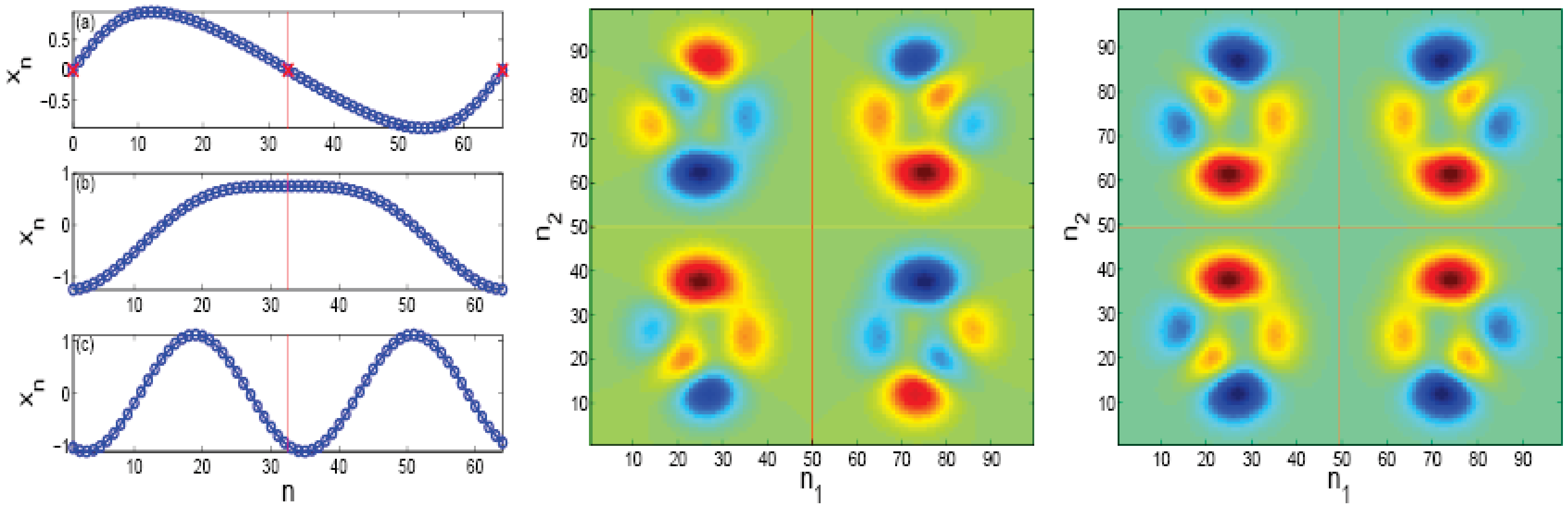
going beyond

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!

Scaling of localization length of q-breathers

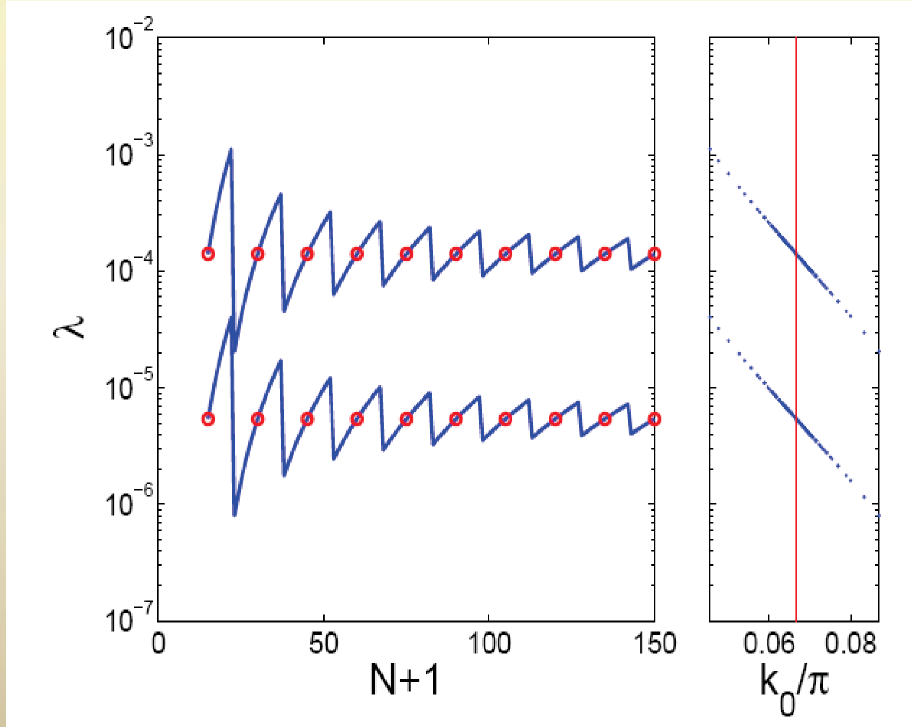
PLA 365 (2007) 416

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

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:

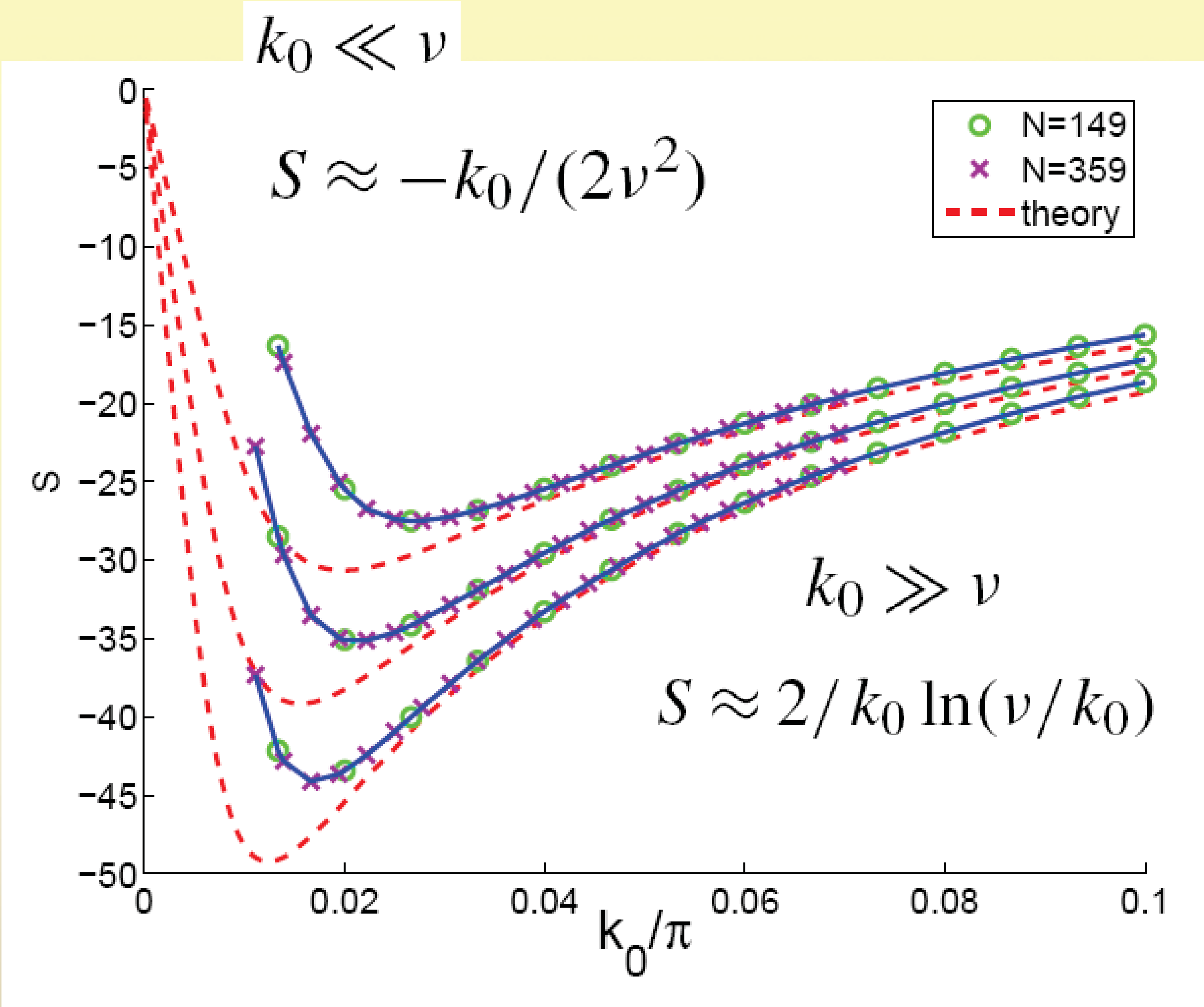
$$S = \frac{1}{k_0} \ln \sqrt{\lambda}\,, \quad \sqrt{\lambda} = \frac{\sqrt{1 + 4\nu^4/k_0^4} - 1}{2\nu^2/k_0^2}\,, \quad \nu^2 = \frac{3\beta}{8}\varepsilon$$

Master slope function:

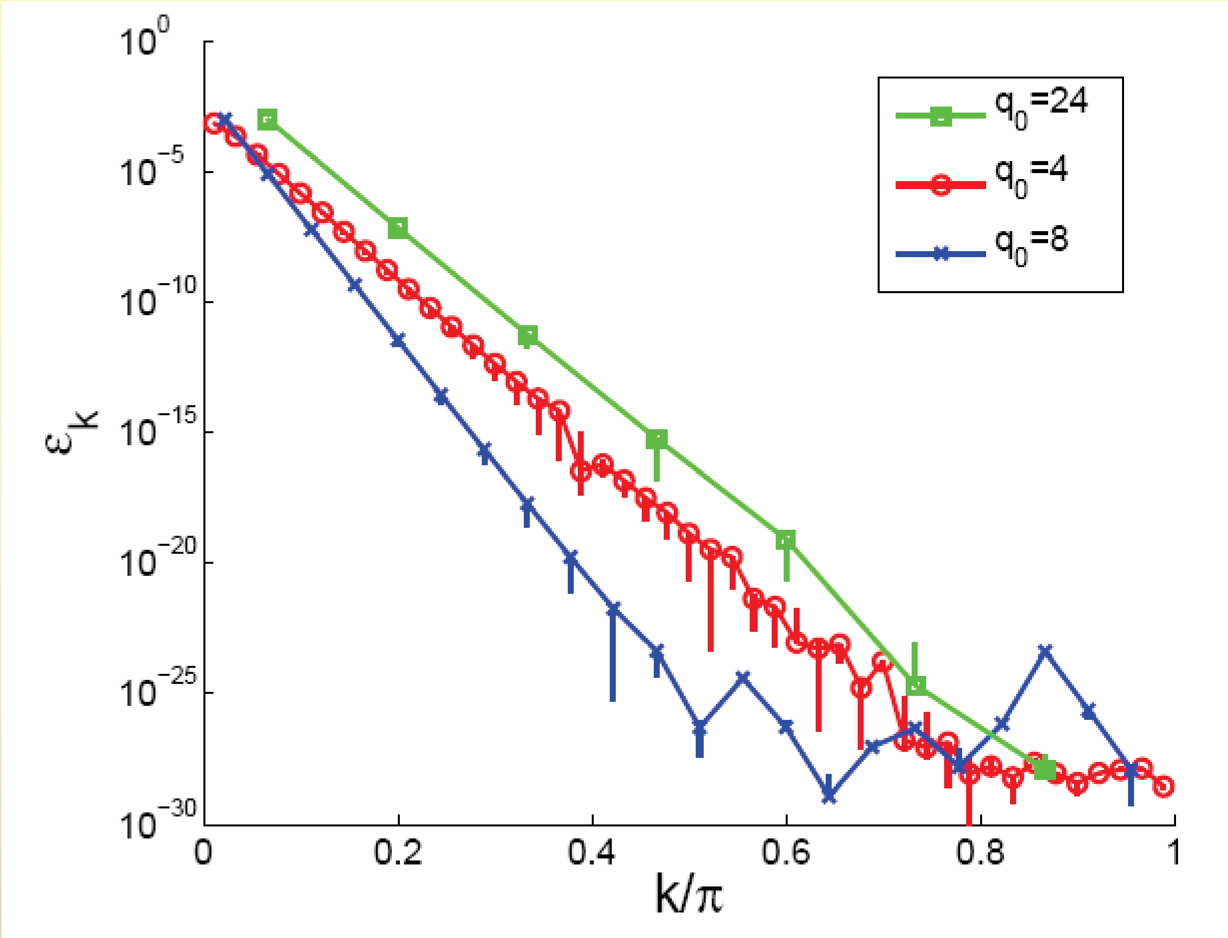
$$S_m(z) = \nu S$$

Rescaled wavenumber:

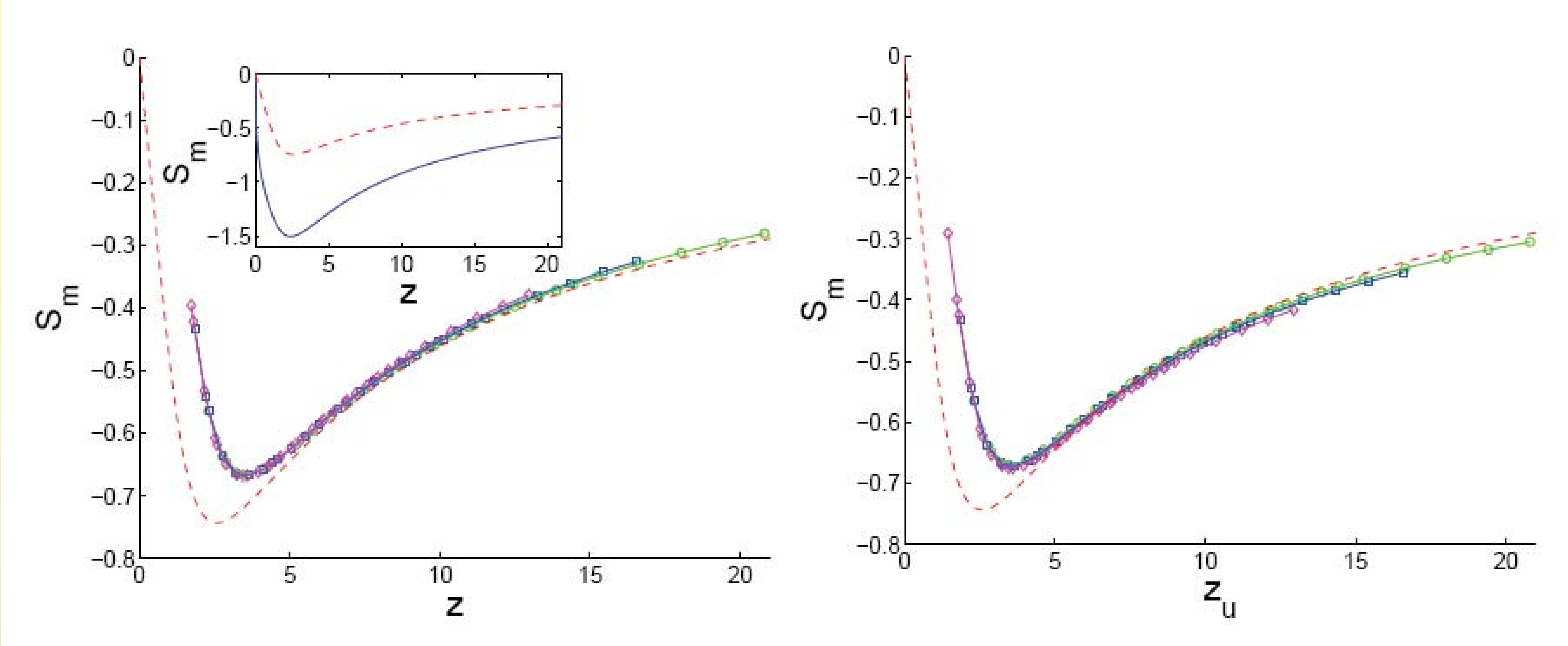
$$z = k_0/\nu$$



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



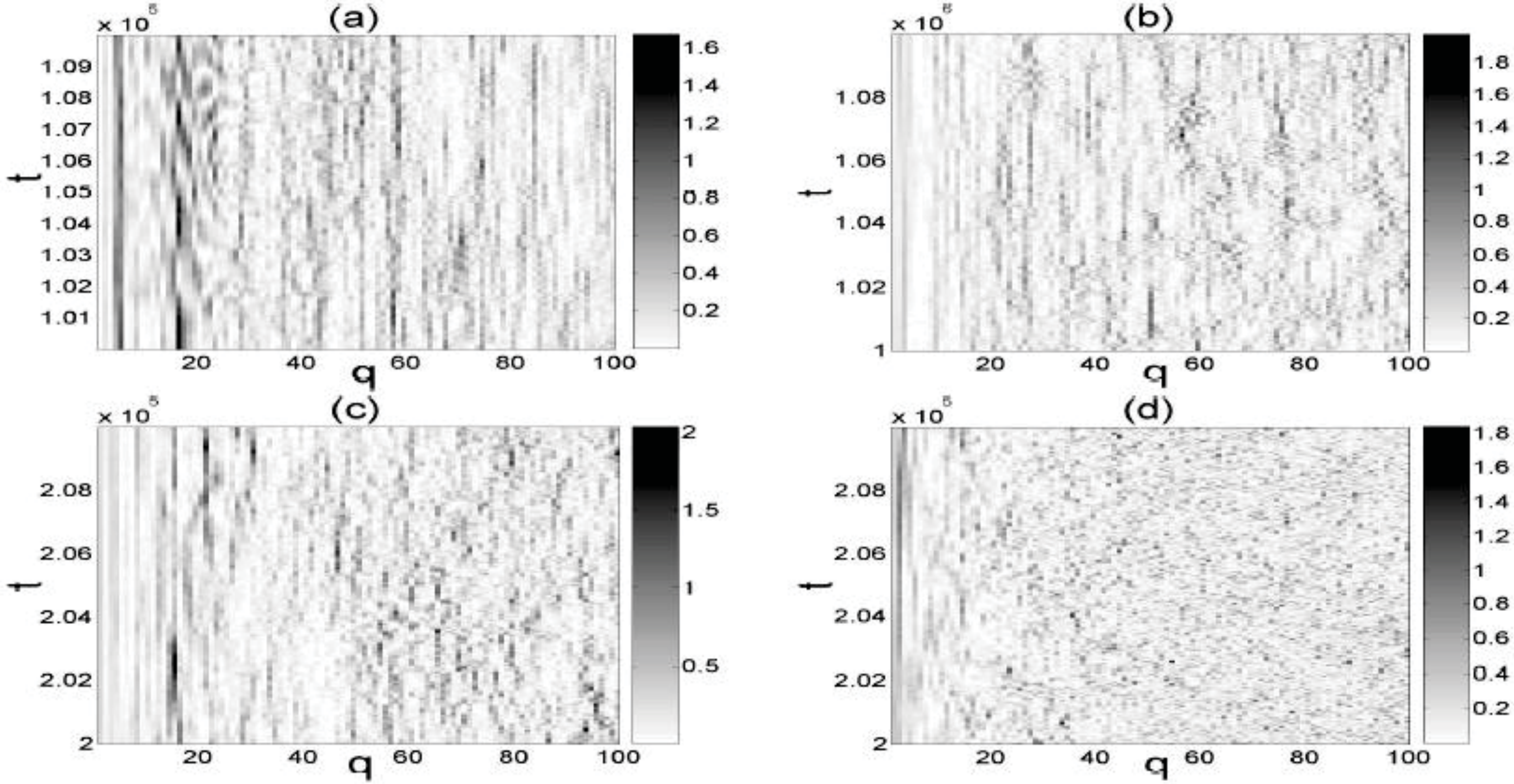
q_0=24
q_0=4
q_0=8
10^0
10^{-5}
10^{-10}
10^{-15}
10^{-20}
10^{-25}
10^{-30}
ε_k
0
0.2
0.4
0.6
0.8
1
k/π



- 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!

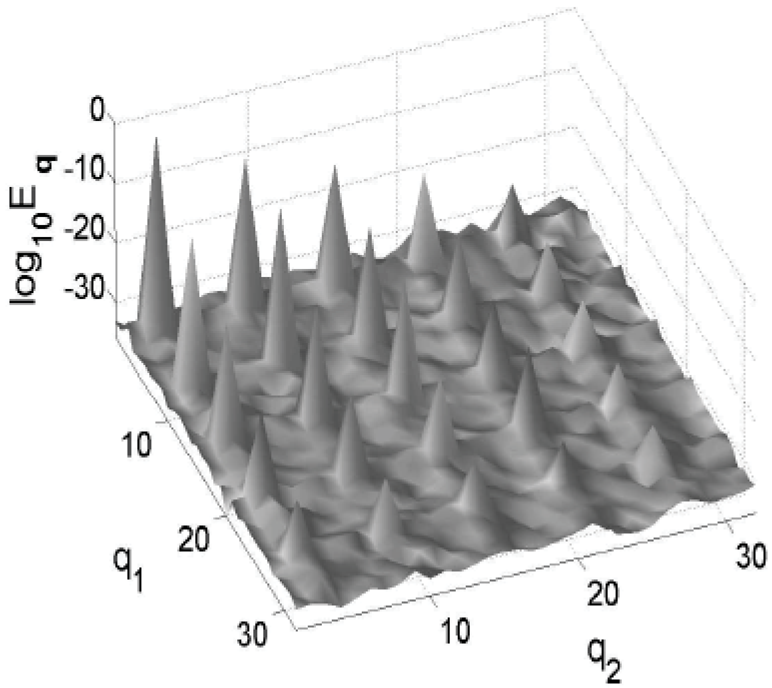
Dynamics in 'thermal' equilibrium

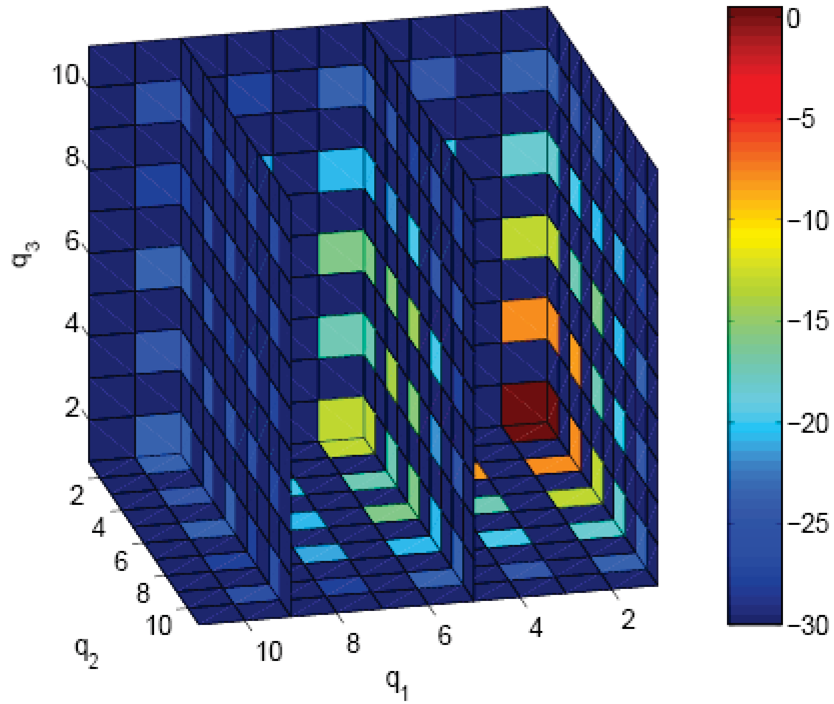
Space-time plots of modes energies E_q evolving from the random initial conditions for $N = 100, E/N = 0.2$ and (a) $\beta = 0.05$, (b) $\beta = 0.05$, (c) $\beta = 0.1$, (d) $\beta = 0.4$.



Generalization to two- and three-dimensional lattices

PRL 97 (2006) 025505





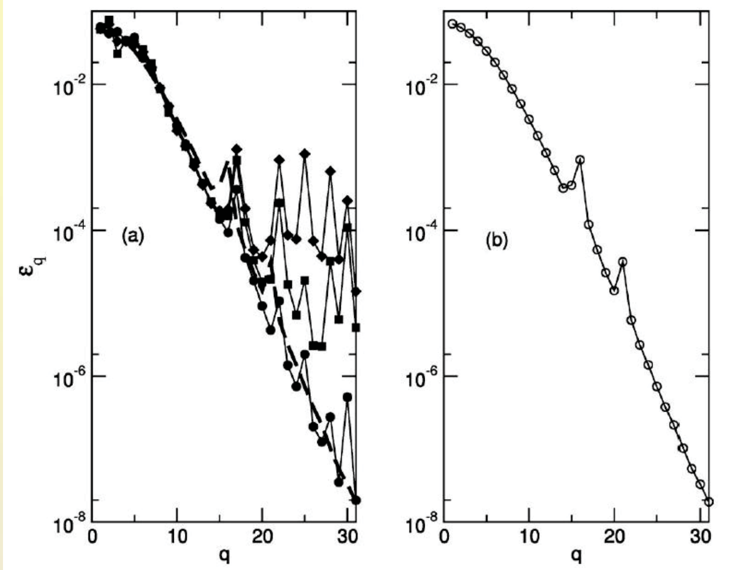
Summarizing the q-breather results

- 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

PRL 95, 064102 (2005) PHYSICAL REVIEW LETTERS

q-Breathers and the Fermi-Pasta-Ulam Problem

S. Flach,[1] M. V. Ivanchenko,[2] and O. I. Kanakov[2]



Solving FPU up to T1:

exact solutions – periodic orbits
existence proof for q-breathers
continuation of normal modes at linear limit
exponentially localized in mode space
dynamically stable
theory gives all characteristics

FPU trajectory is a perturbed q-breather,
recurrence is beating

Perspectives:

Theory for T2?
Theory for equipartition?
Where is KAM regime?

Further reading:
• PRL 95 (2005) 064102
• PRE 73 (2006) 036618
• PRL 97 (2006) 025505
• PLA 365 (2007) 416
• Chaos 17 (2007) 023102
• PRB 75 (2007) 214303
• New J Phys 10 (2008) 073034

Take Home Messages Lecture I

• nonlinear dynamical systems – nonintegrability, chaos

• quasiperiodic motion destroyed, BUT:

• periodic orbits are generic low-d invariant manifolds

• normal modes: POs localize in mode space – q-breathers

• q-breathers are essential periodic orbits which describe the evolution of relevant mode-mode interactions, correlations in and relaxations of complex systems

Further reading:
• Am J Phys 76 (2008) 453
• Physica D 237 (2008) 908
• Physica D 238 (2009) 581
• Chaos 21 (2011) 043127