q-breathers: Localization in Normal Mode Space, and the Fermi-Pasta-Ulam Problem

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mpipks

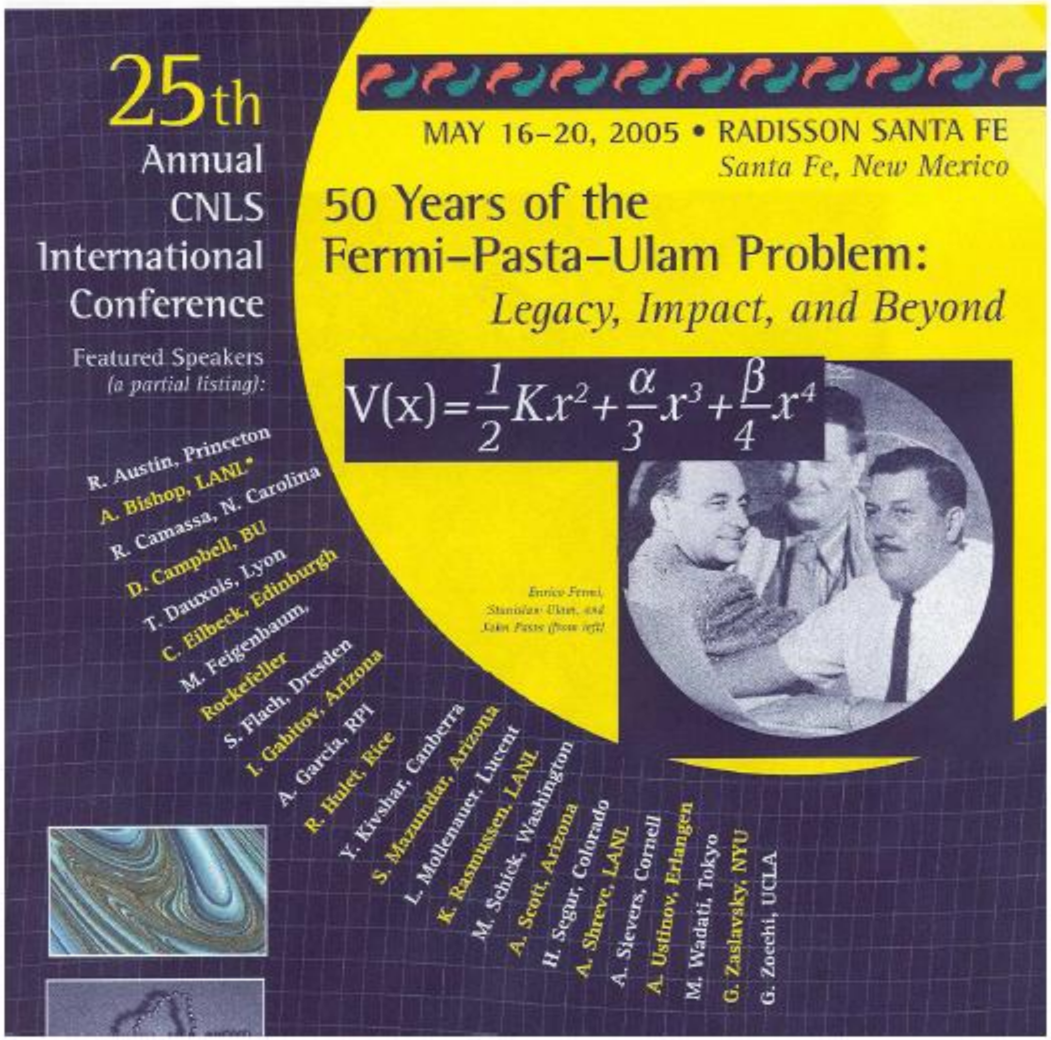
Road map:

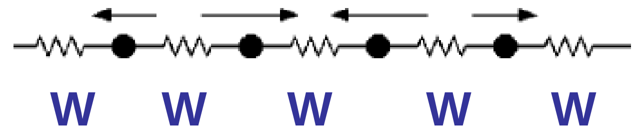
- paradox and problems
- KAM, FPU and Toda
- periodic orbits (q-breathers)
- scaling

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

PART ONE:

THE PARADOX AND THE PROBLEMS





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

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

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

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

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

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:

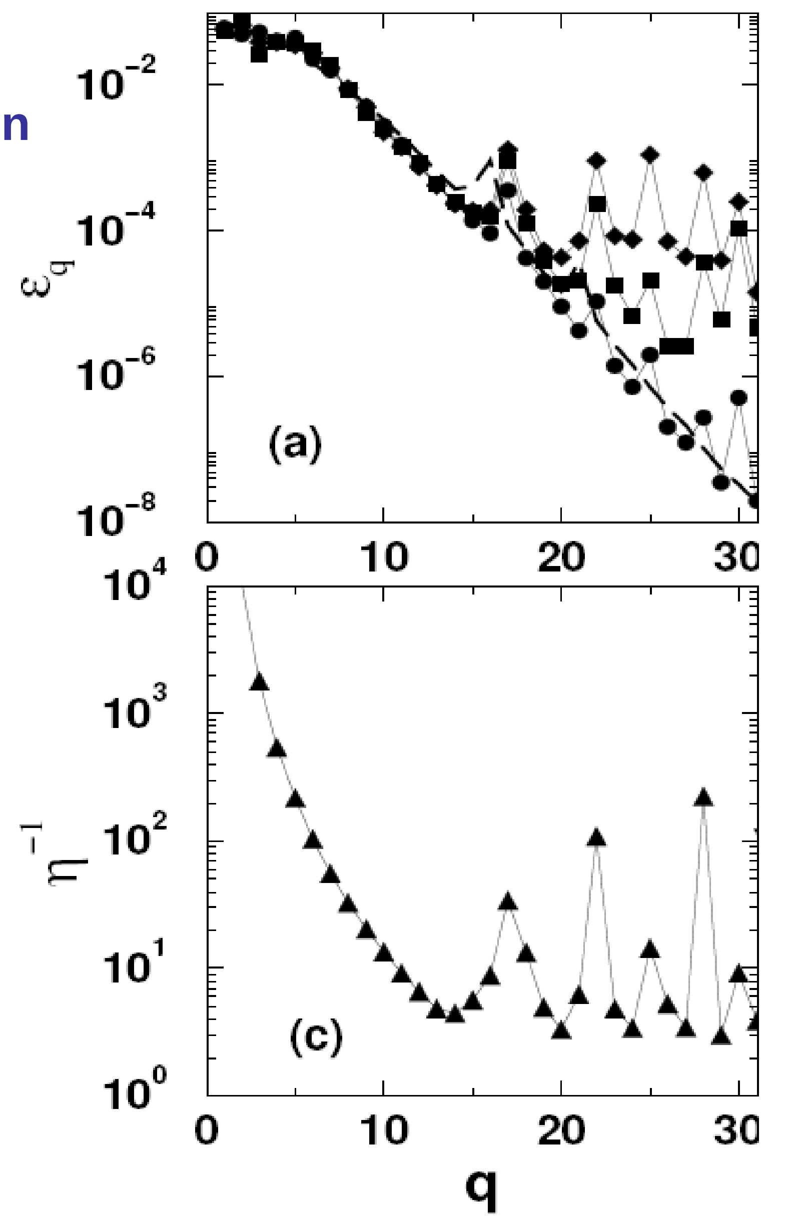
$$E_q = \frac{1}{2}(\dot{Q}_q^2 + \omega_q^2 Q_q^2)$$

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

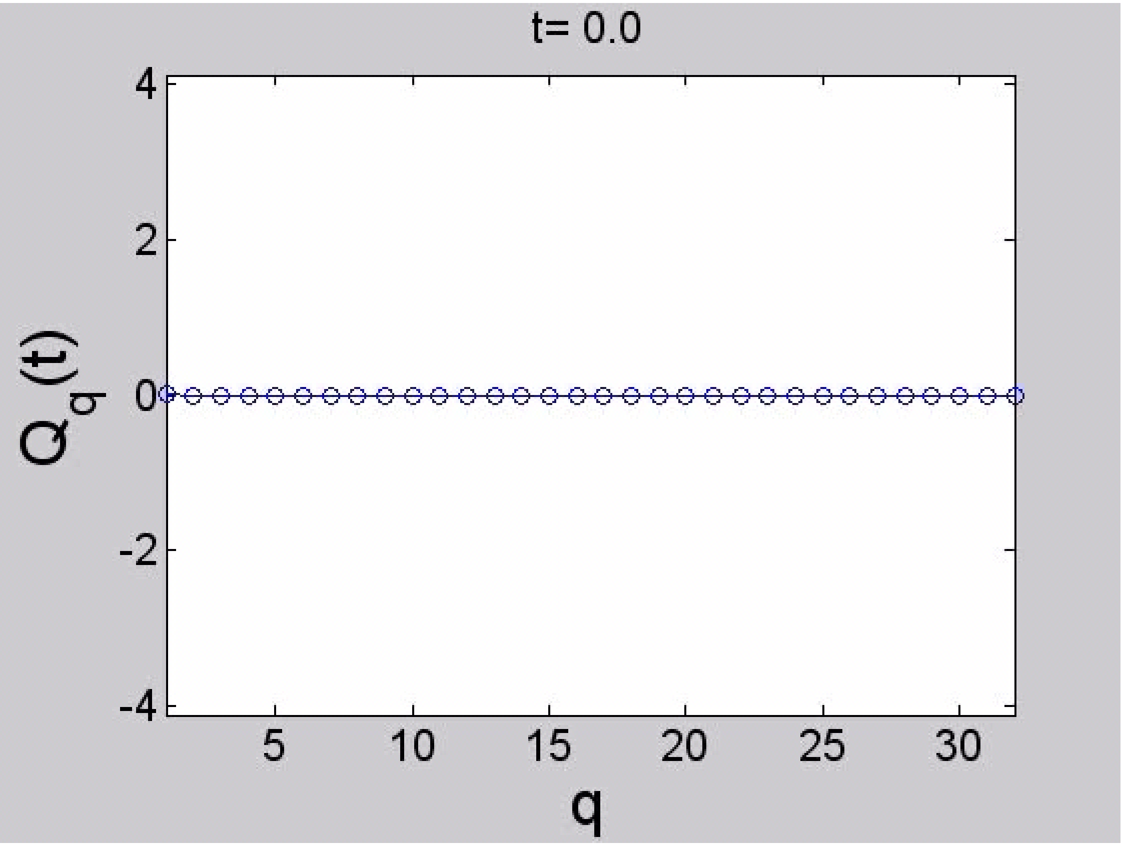
- excite $q = 1$ mode
- observe nonequipartion of mode energies
- no transition to thermal equilibrium
- energy is localized in a few modes for long time **FPU 1**
- recurrence of energy into initially excited mode **FPU 2**
- two thresholds in energy and N **FPU 3**
- two pathways of understanding:
  $\rightarrow$ 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

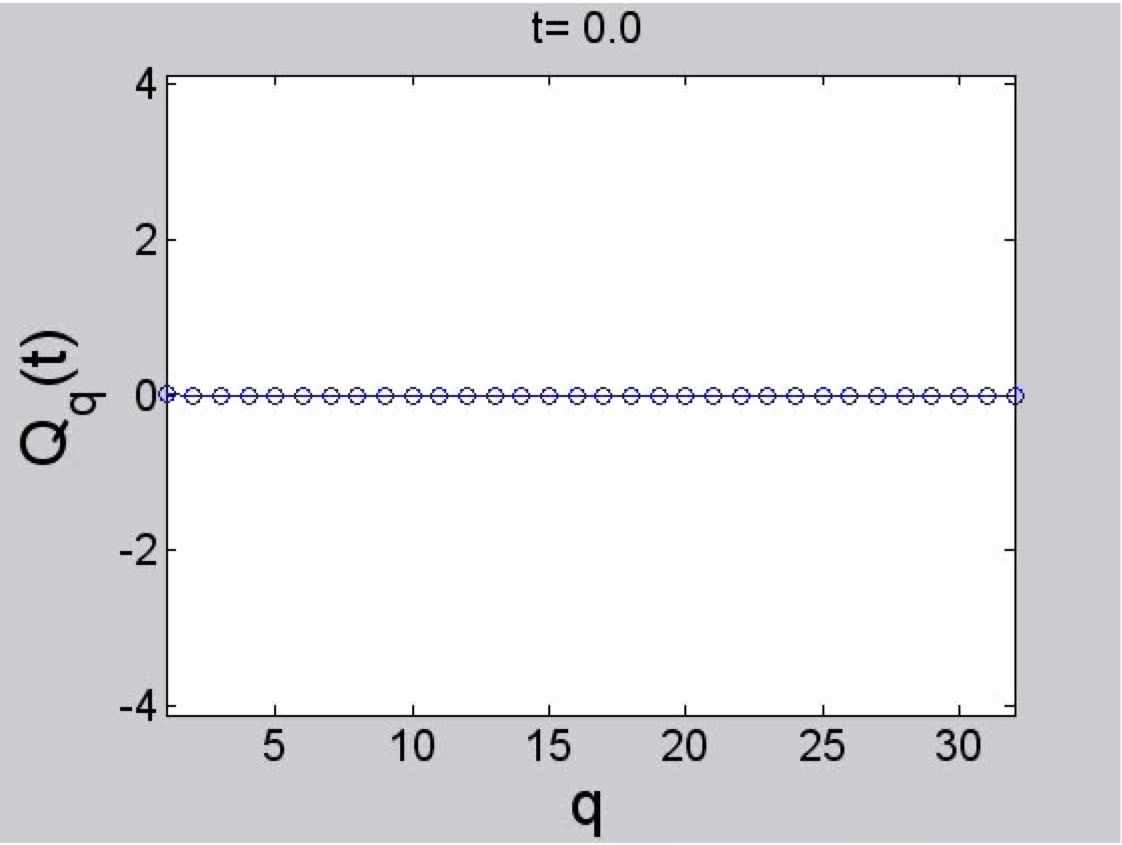
Movies: let us see what FPU observed



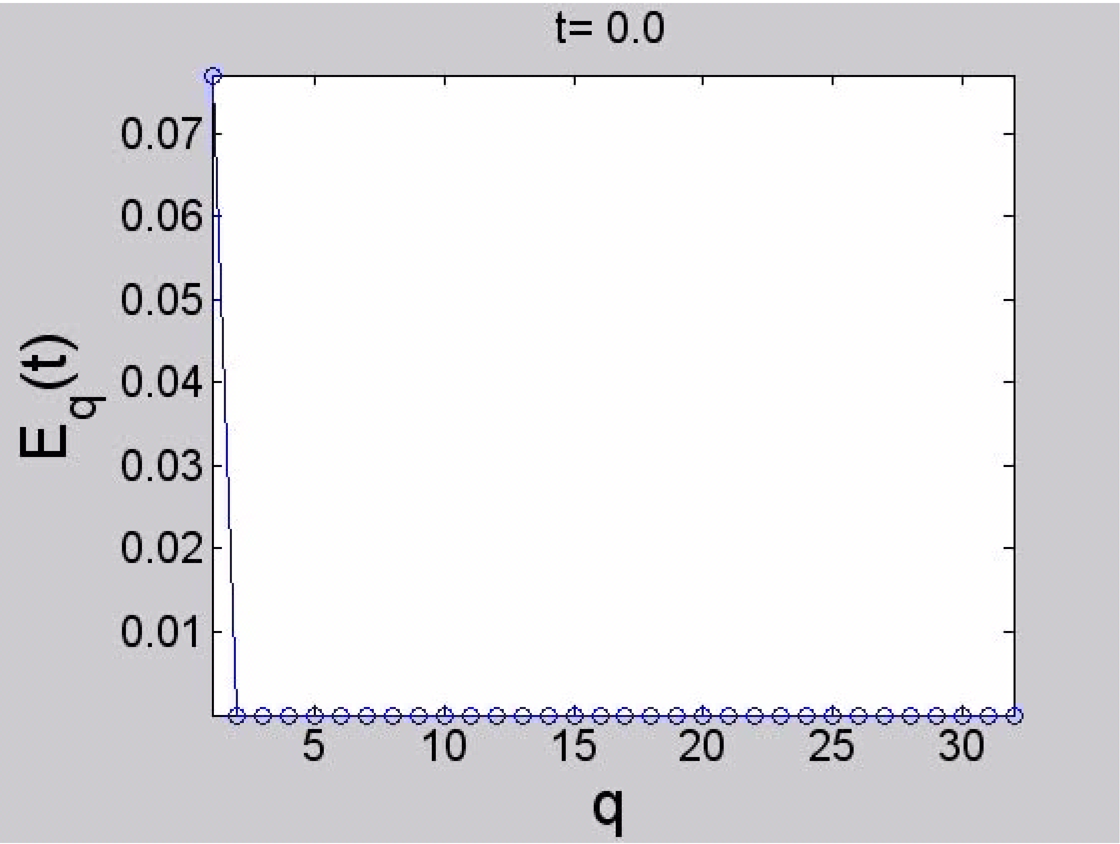
Evolution of normal mode coordinates



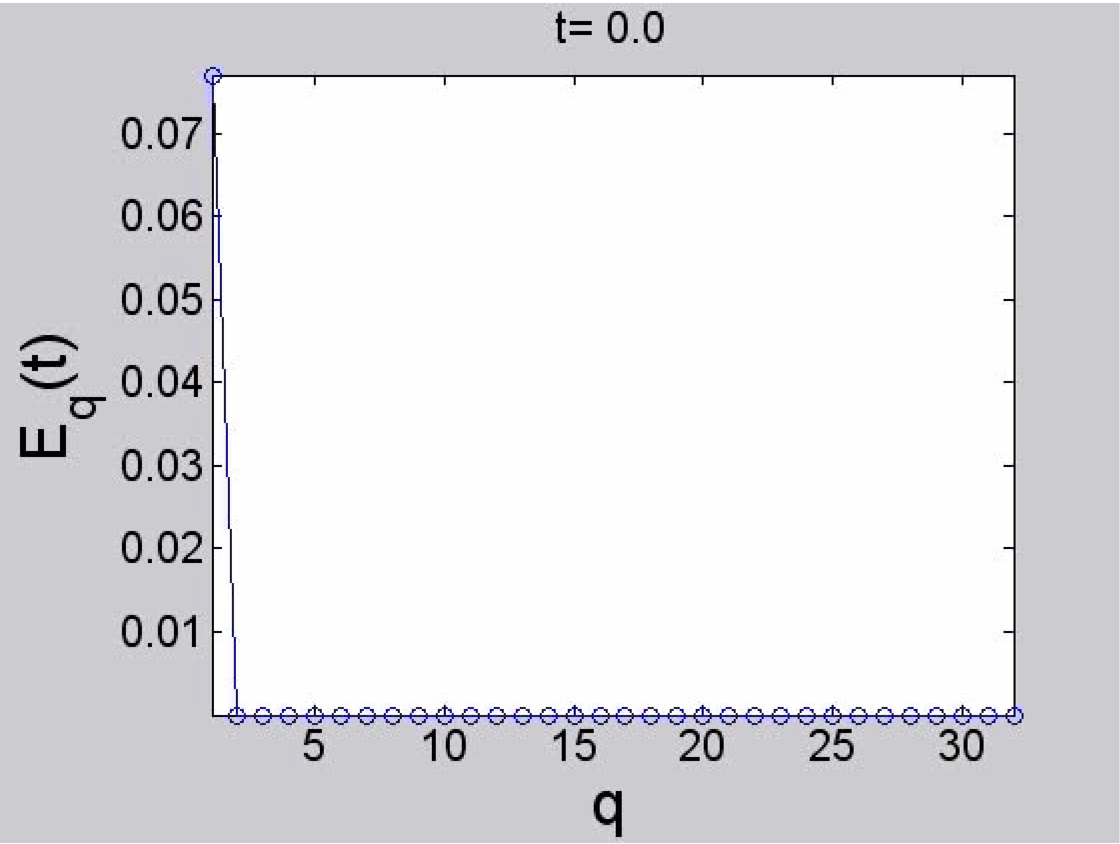
Evolution of normal mode coordinates



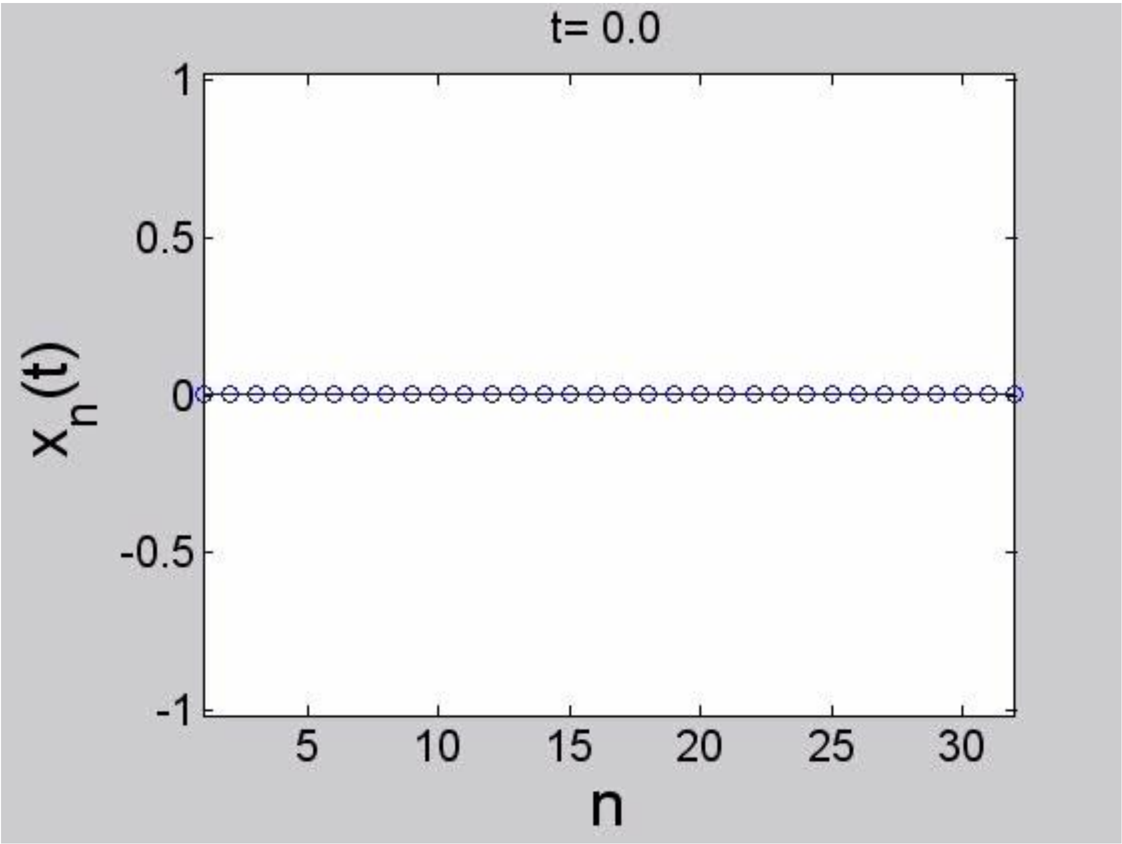
Evolution of normal mode energies



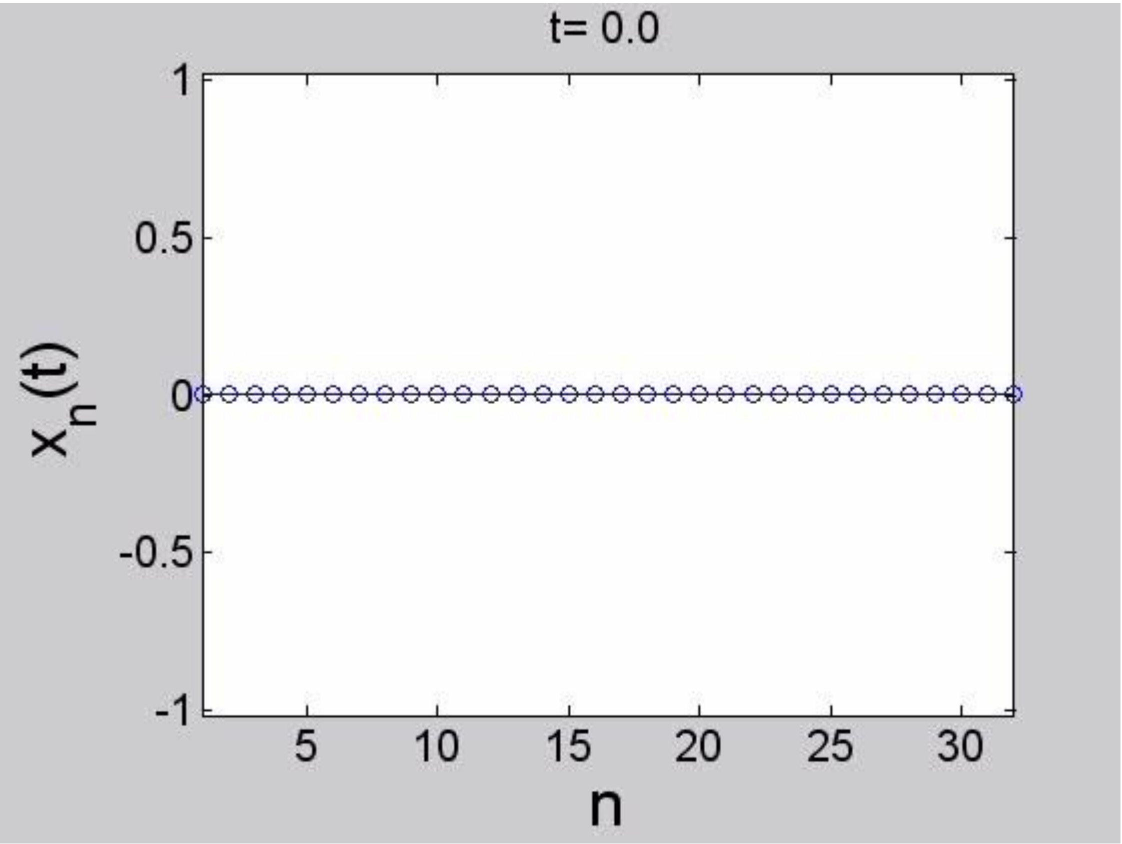
Evolution of normal mode energies



Evolution of real space displacements

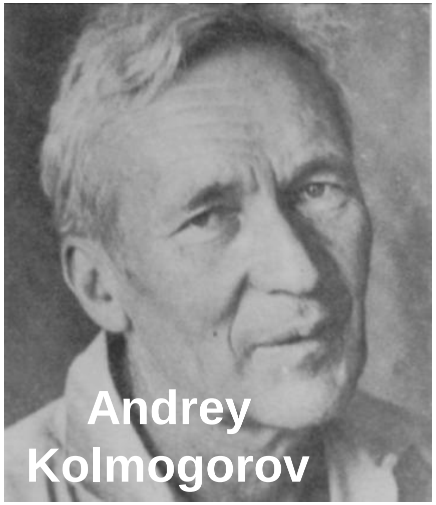


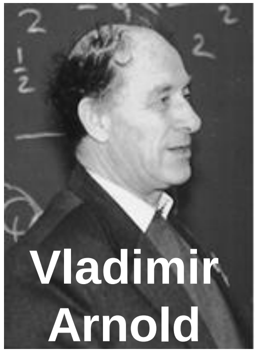
Evolution of real space displacements



Kolmogorov – Arnold – Moser (KAM) theory

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



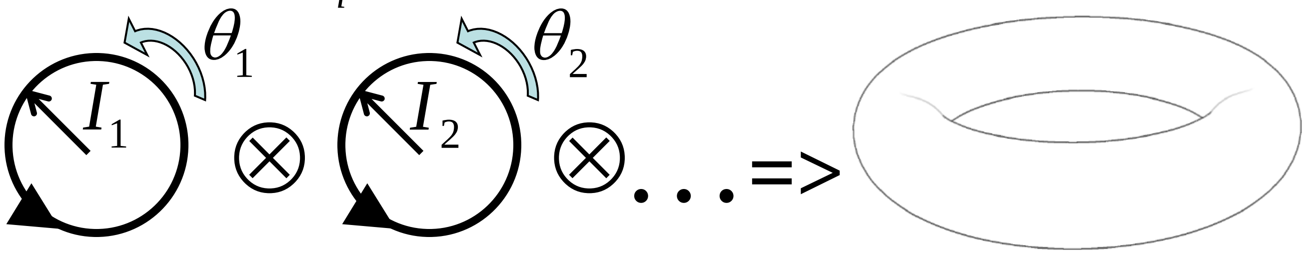


Integrable classical Hamiltonian $\hat{H}_0$, ***d>1*:**

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 $\partial I_i / \partial t = 0$



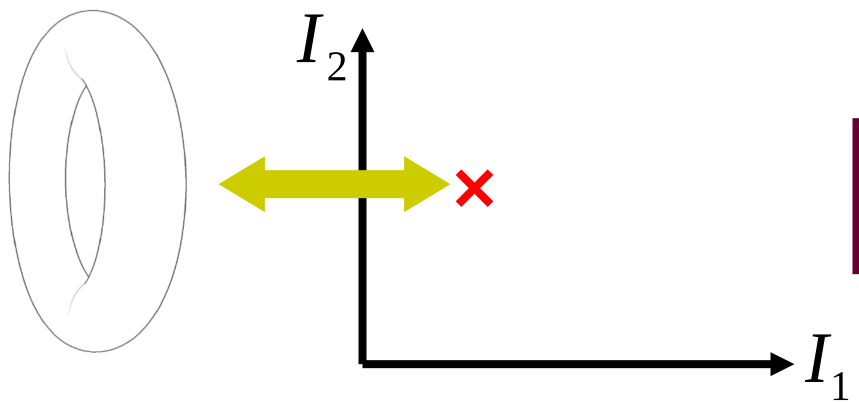
Q: Will an arbitrary weak perturbation $\hat{V}$ of the integrable Hamiltonian $\hat{H}_0$ destroy the tori and make the motion ergodic (when each point at the energy shell will be reached sooner or later) **?**

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

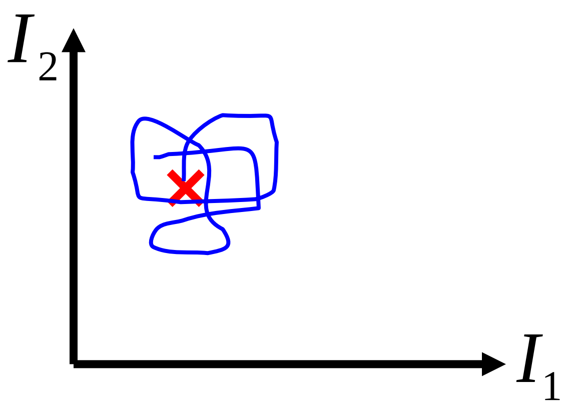
KAM theorem

KAM theorem:

Most of the tori survive weak and smooth enough perturbations



$$\hat{V} \neq 0$$



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** ?

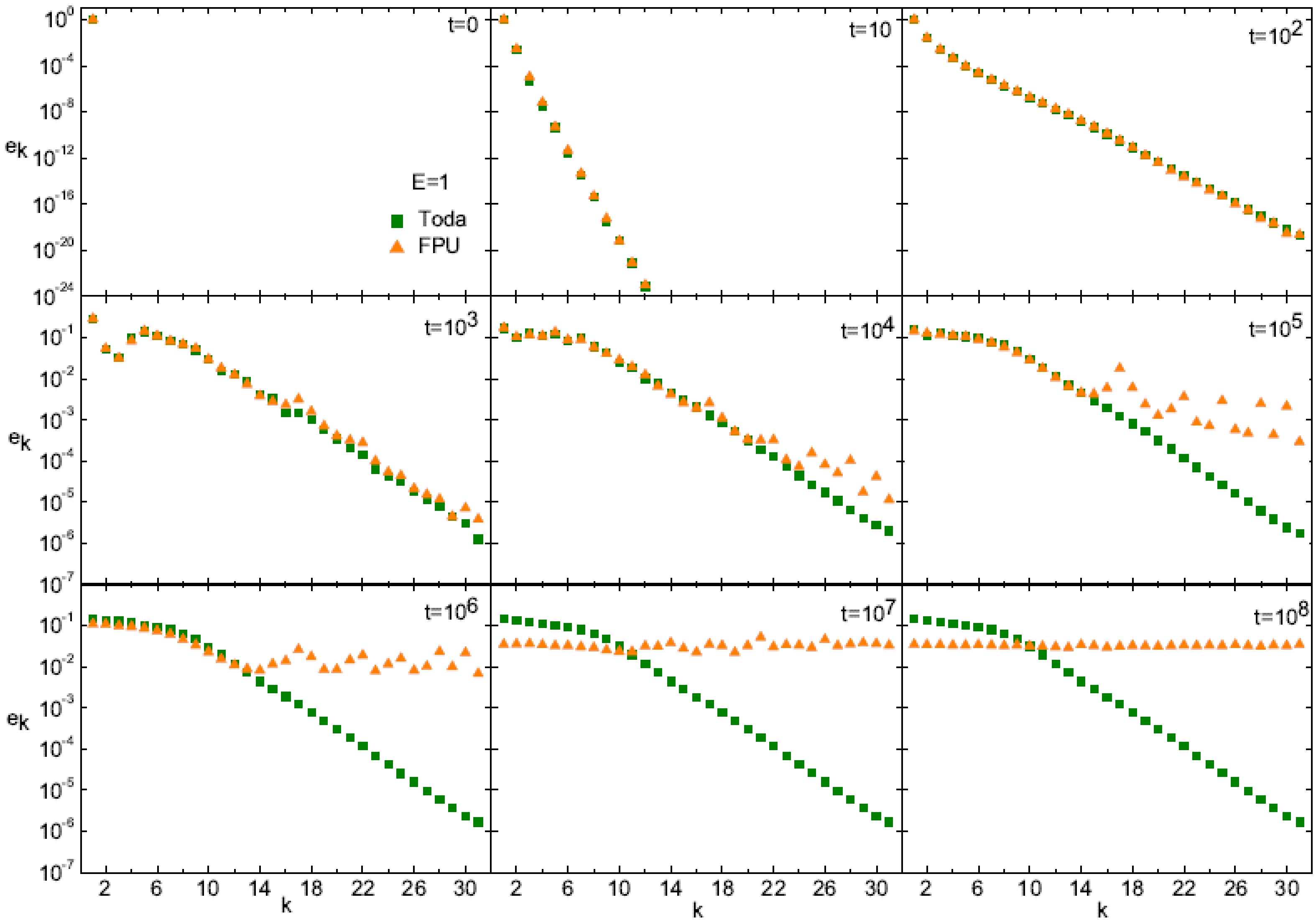
- KAM applies to finite systems
- Does it apply to waves in infinite systems?
- How are KAM thresholds scaling with number of degrees of freedom?
- Will nonlinear waves observe KAM regime?
- If they do – then localization remains
- If they do not – waves can delocalize

Comparing the integrable Toda to the nonintegrable FPU

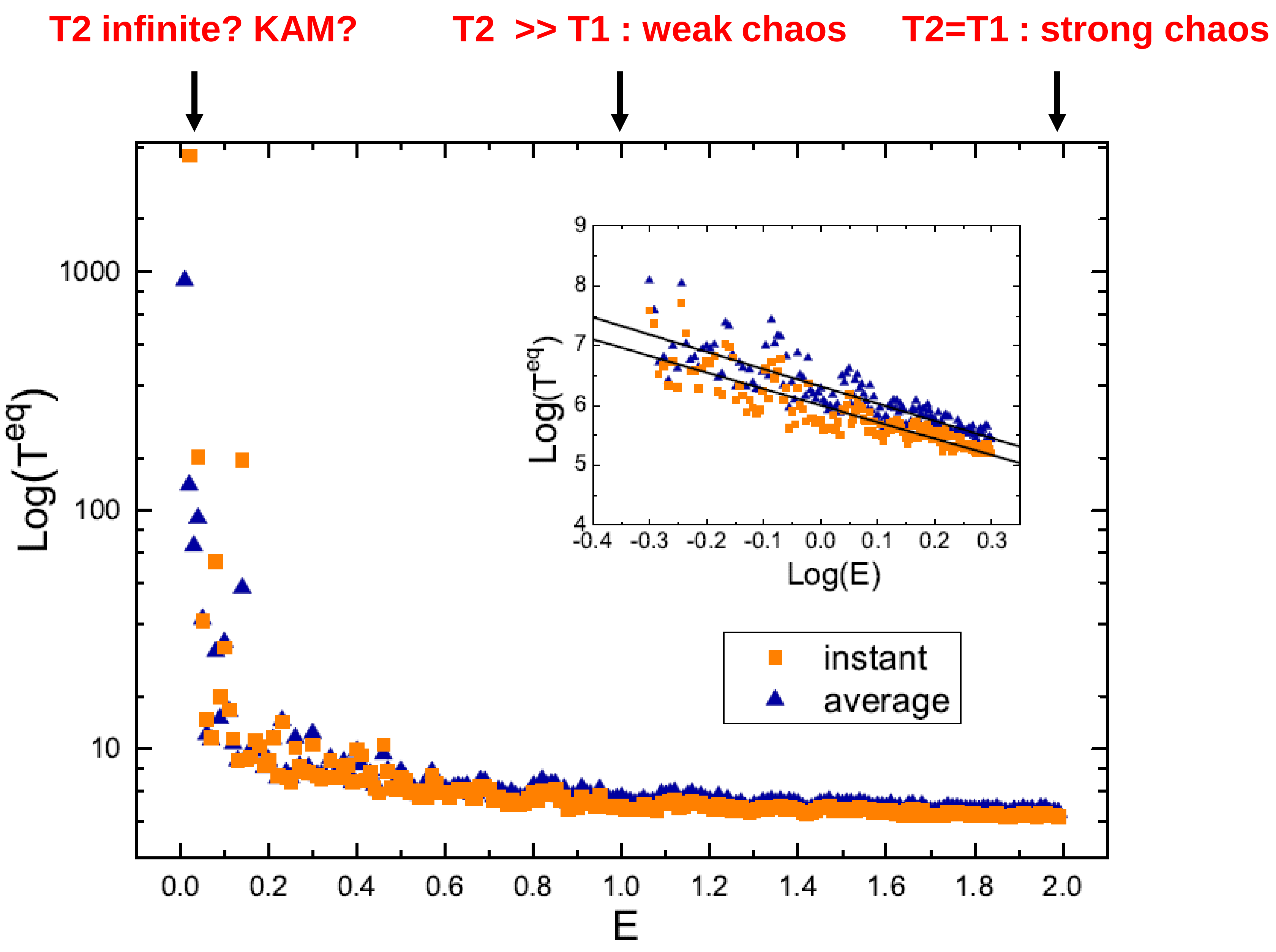
$$H_T(q,p) = \sum_{n=0}^{N-1} \left[\frac{p_n^2}{2} + \frac{e^{2\alpha(q_{n+1}-q_n)} - 1}{4\alpha^2} \right]$$

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

E. Christodoulidi, A. Ponno, Ch. Skokos, SF, in preparation



T1=10^2 ; T2=10^8


T2 infinite? KAM?
T2 >> T1 : weak chaos
T2=T1 : strong chaos
Log(T^eq)
1000
100
10
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
E
Log(T^eq)
9
8
7
6
5
4
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
Log(E)
instant
average

PART TWO:

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):

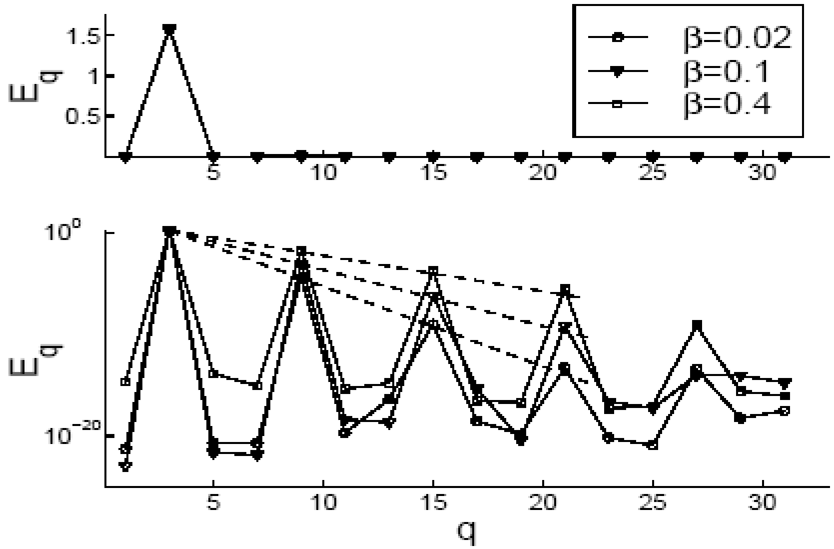
$$n\omega_{q_0} \neq \omega_{q \neq q_0}$$

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

SO WE NEED A FINITE SYSTEM IN REAL SPACE!

The β model case

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



Asymptotic expansion of solution:

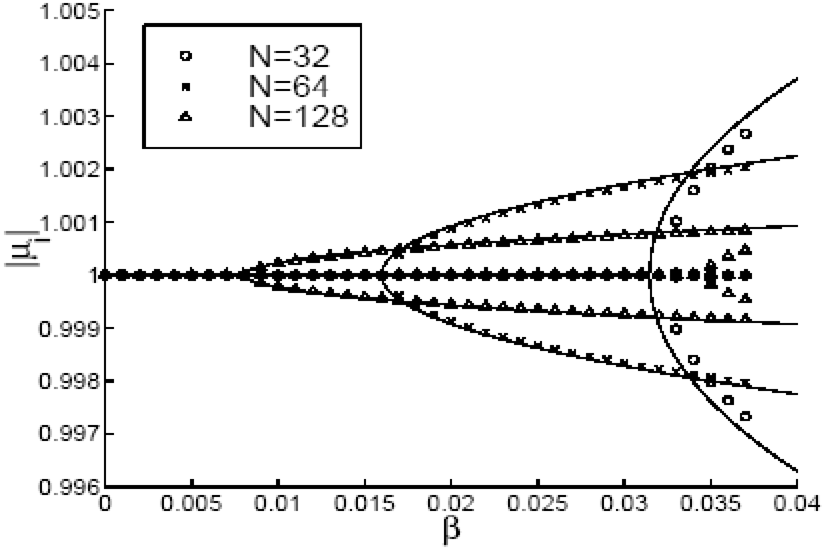
$$E_{(2n+1)q_0} = \lambda^{2n} E_{q_0} \; , \; \lambda = \frac{3\beta E_{q_0}(N+1)}{8\pi^2 q_0^2}$$

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:

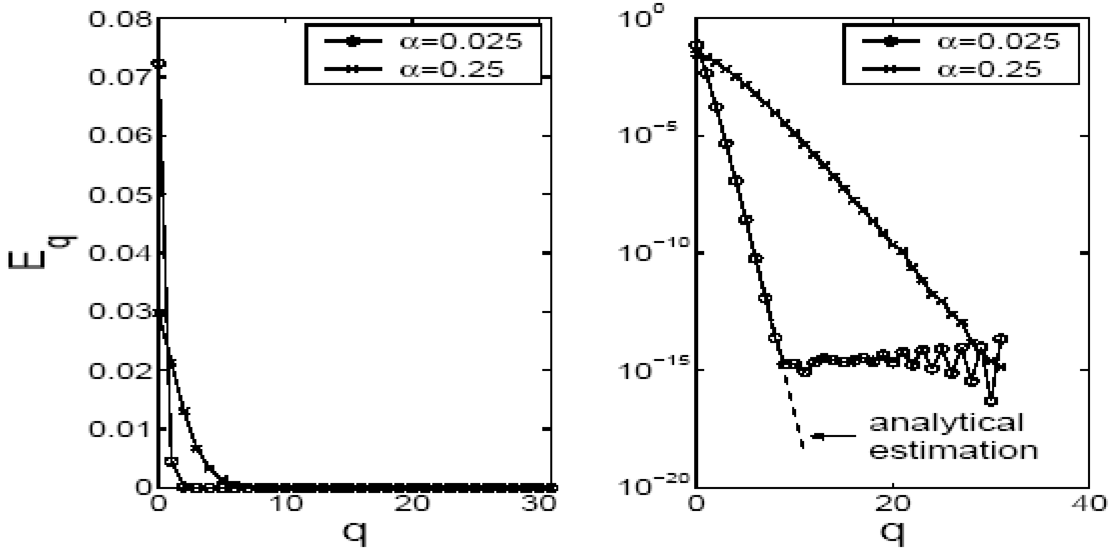
$$|\mu_{j_1 j_2}| = 1 \pm \frac{\pi^3}{4(N+1)^2}\sqrt{R - 1 + O\left(\frac{1}{N^2}\right)}\ ,\ R = 6\beta E(N+1)/\pi^2$$

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:

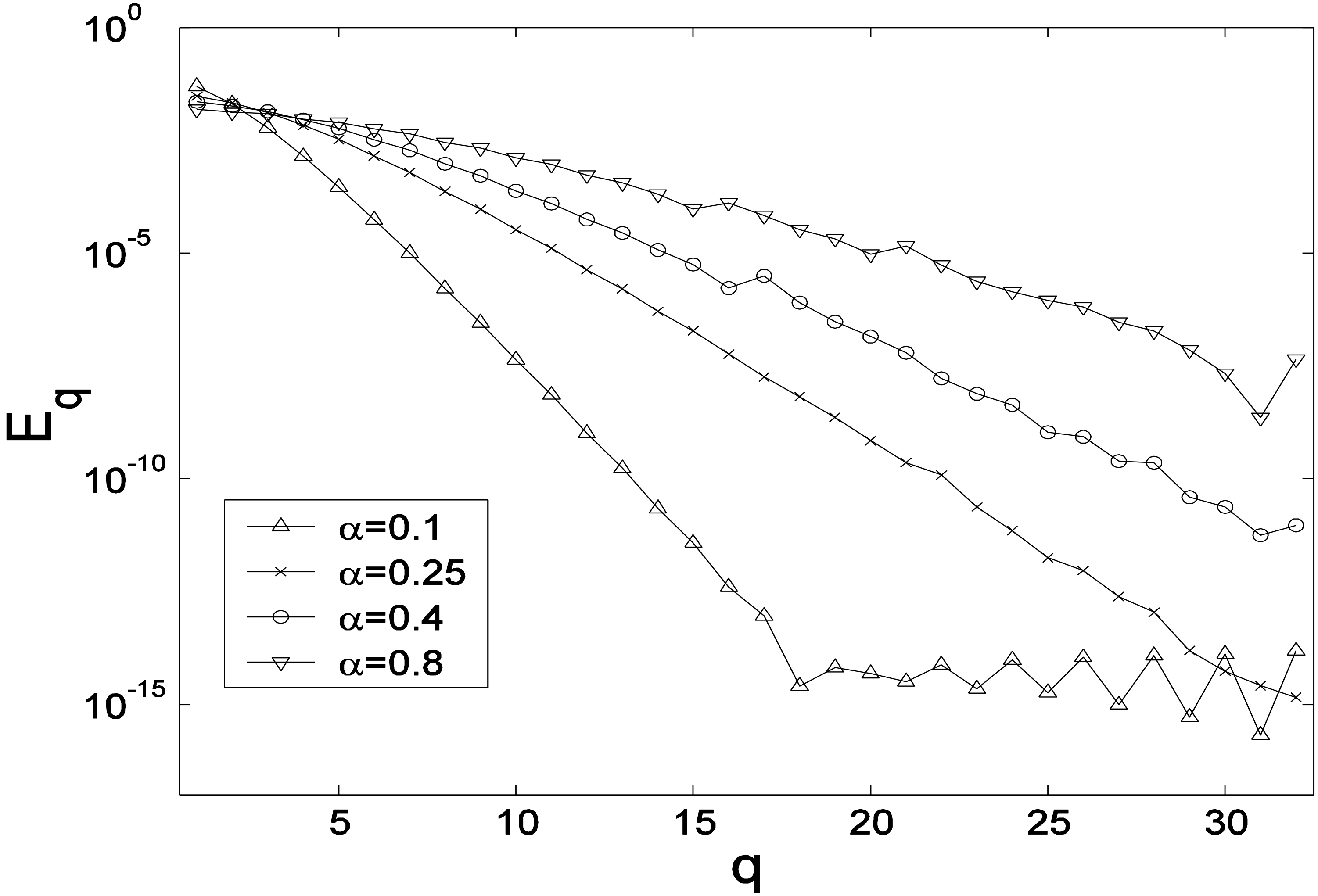


Asymptotic expansion of solution:

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

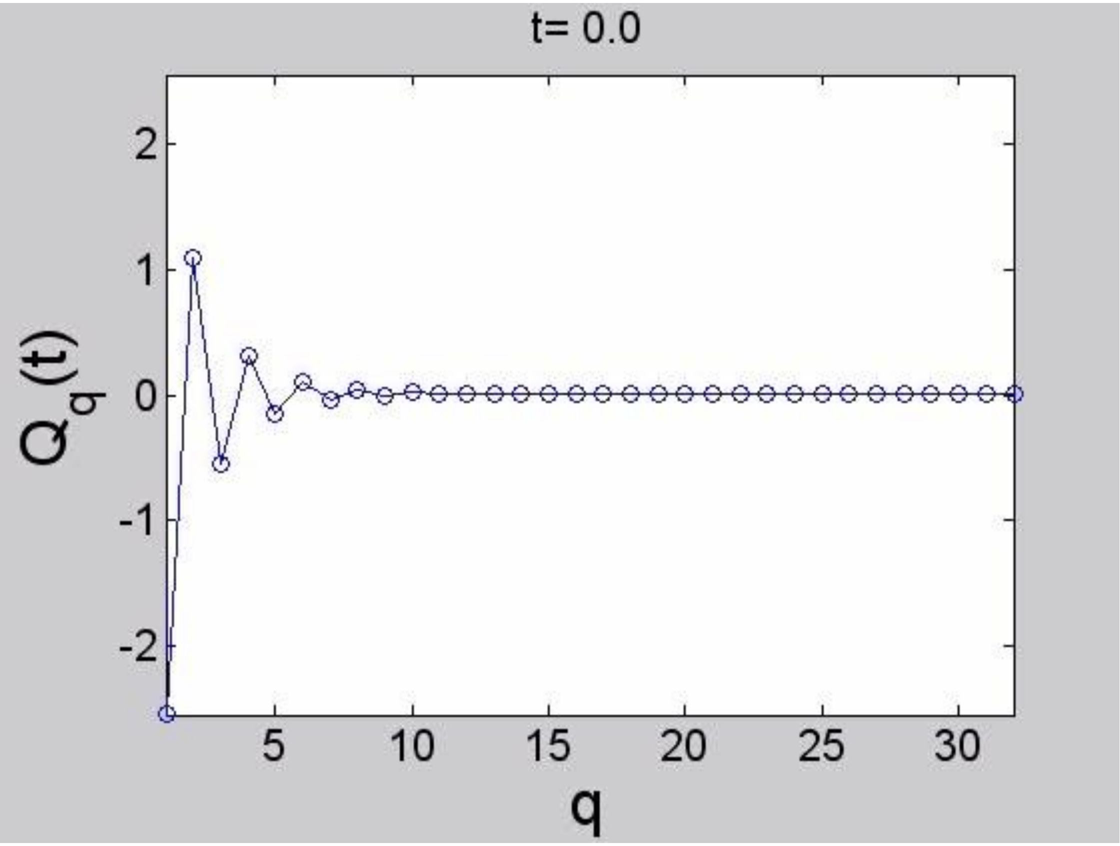
coincides with boundary estimate of natural packet by Shepelyansky!

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

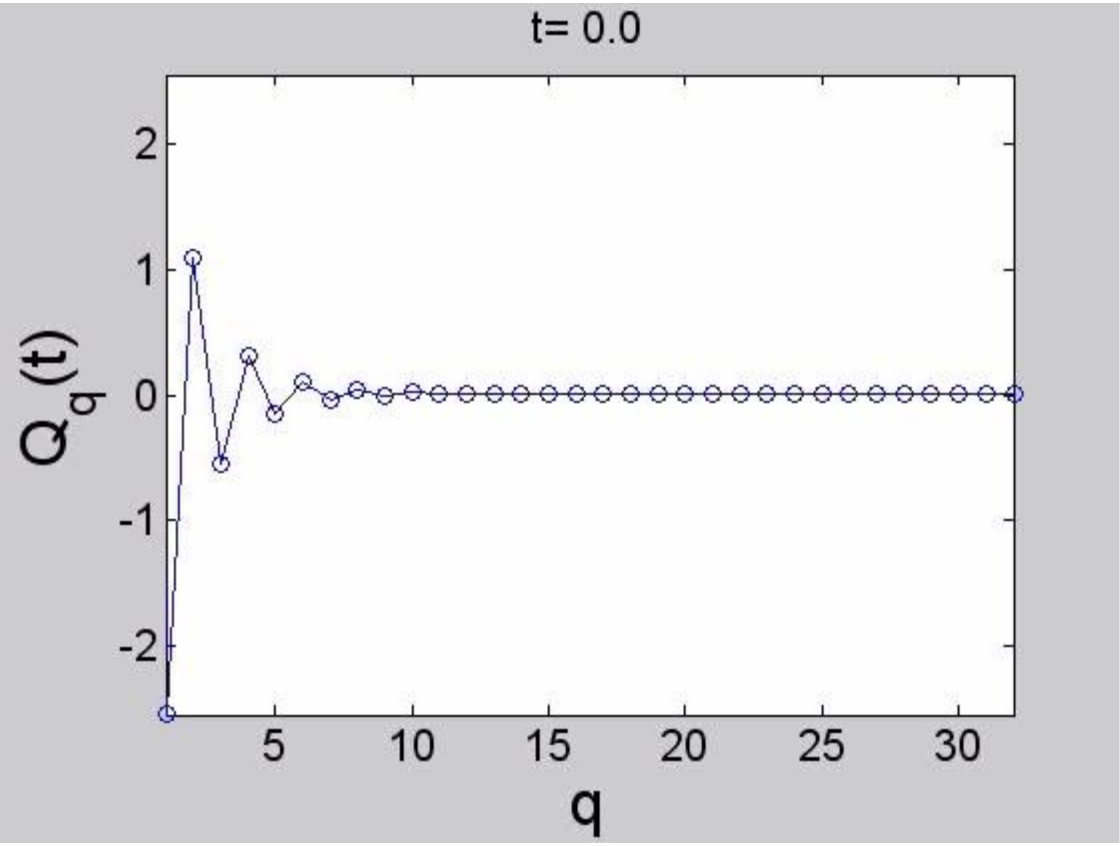


10^0
10^{-5}
10^{-10}
10^{-15}
E_q
5
10
15
20
25
30
q
α=0.1
α=0.25
α=0.4
α=0.8

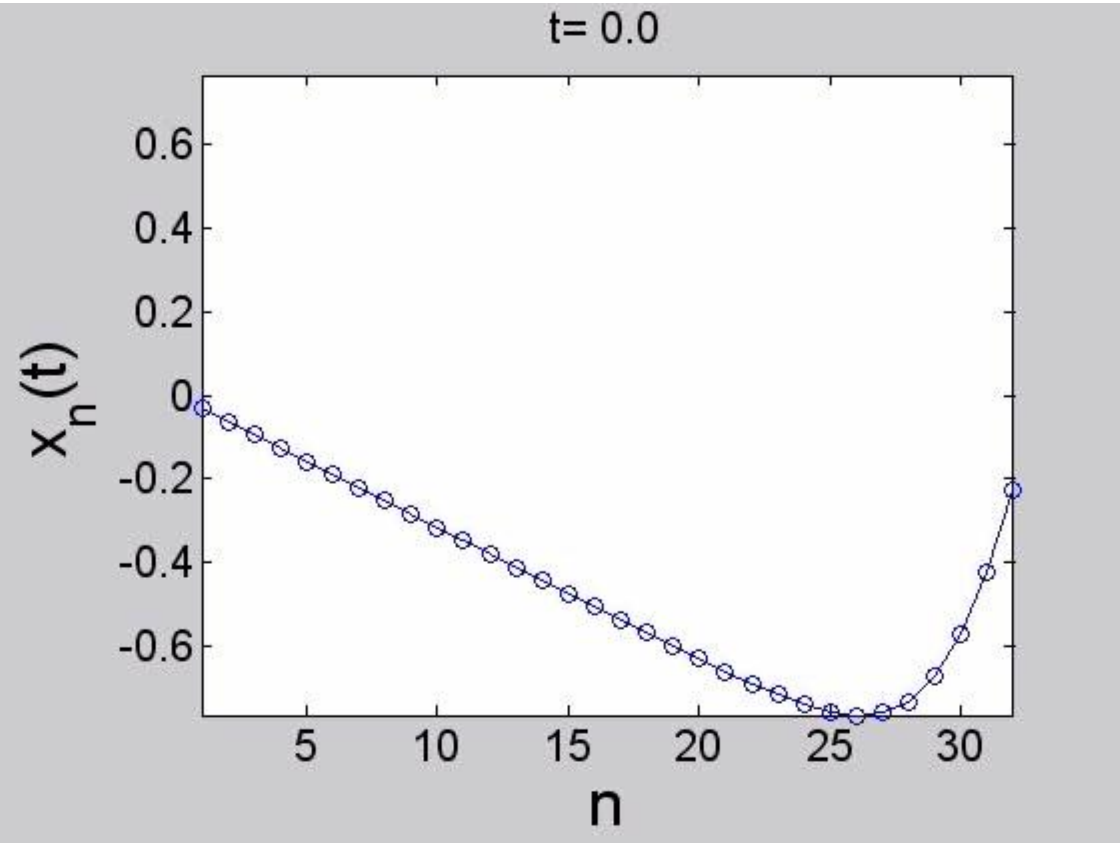
QB: Evolution of normal mode coordinates



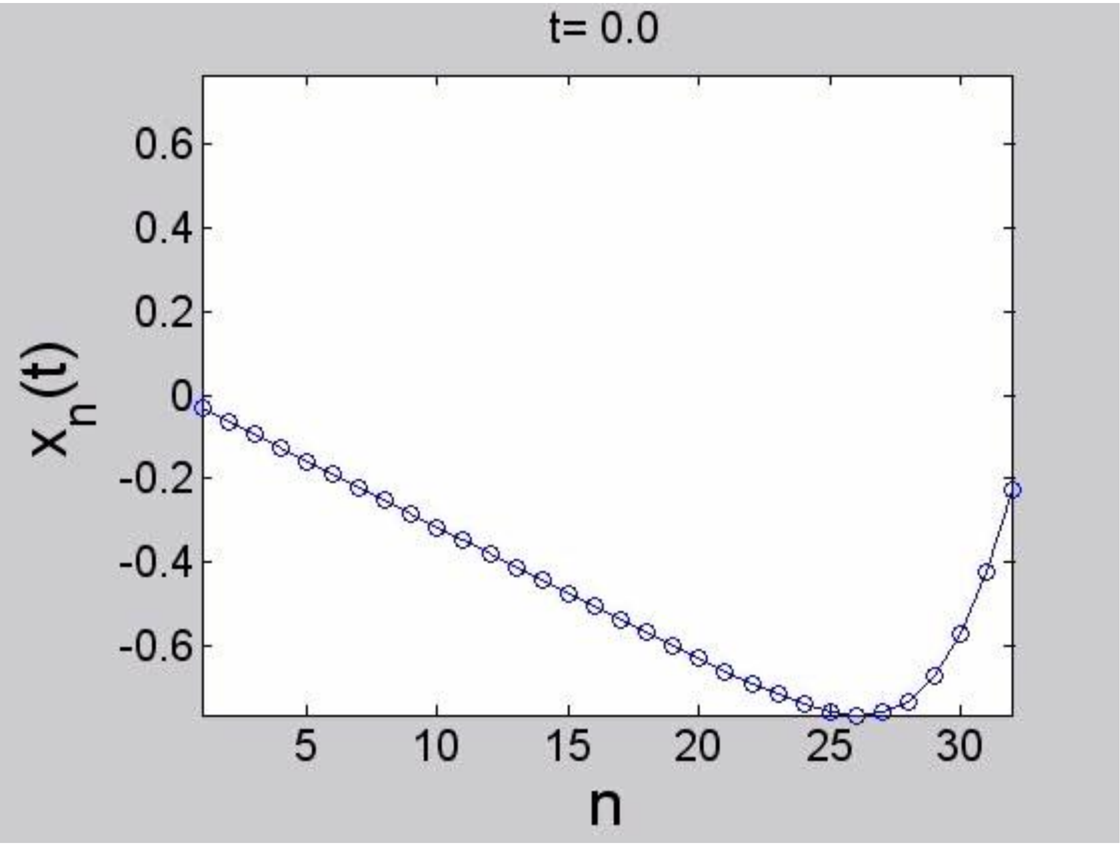
QB: Evolution of normal mode coordinates



QB: Evolution of real space displacements



QB: Evolution of real space displacements



PART THREE:

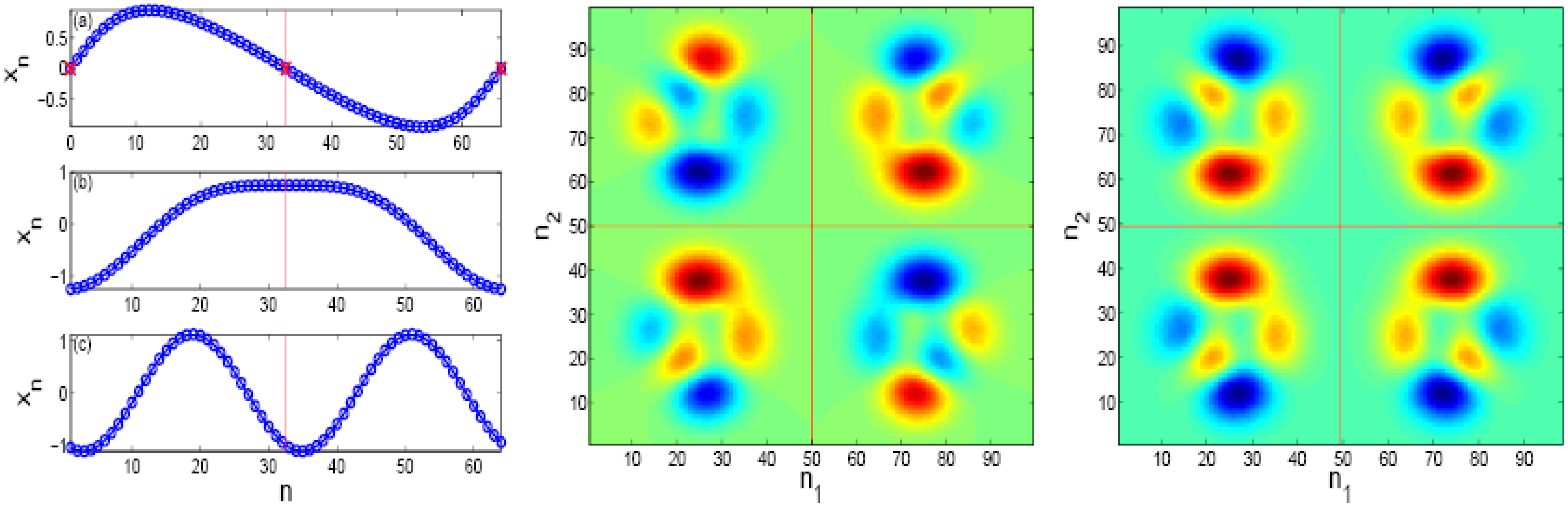
GOING BEYOND

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

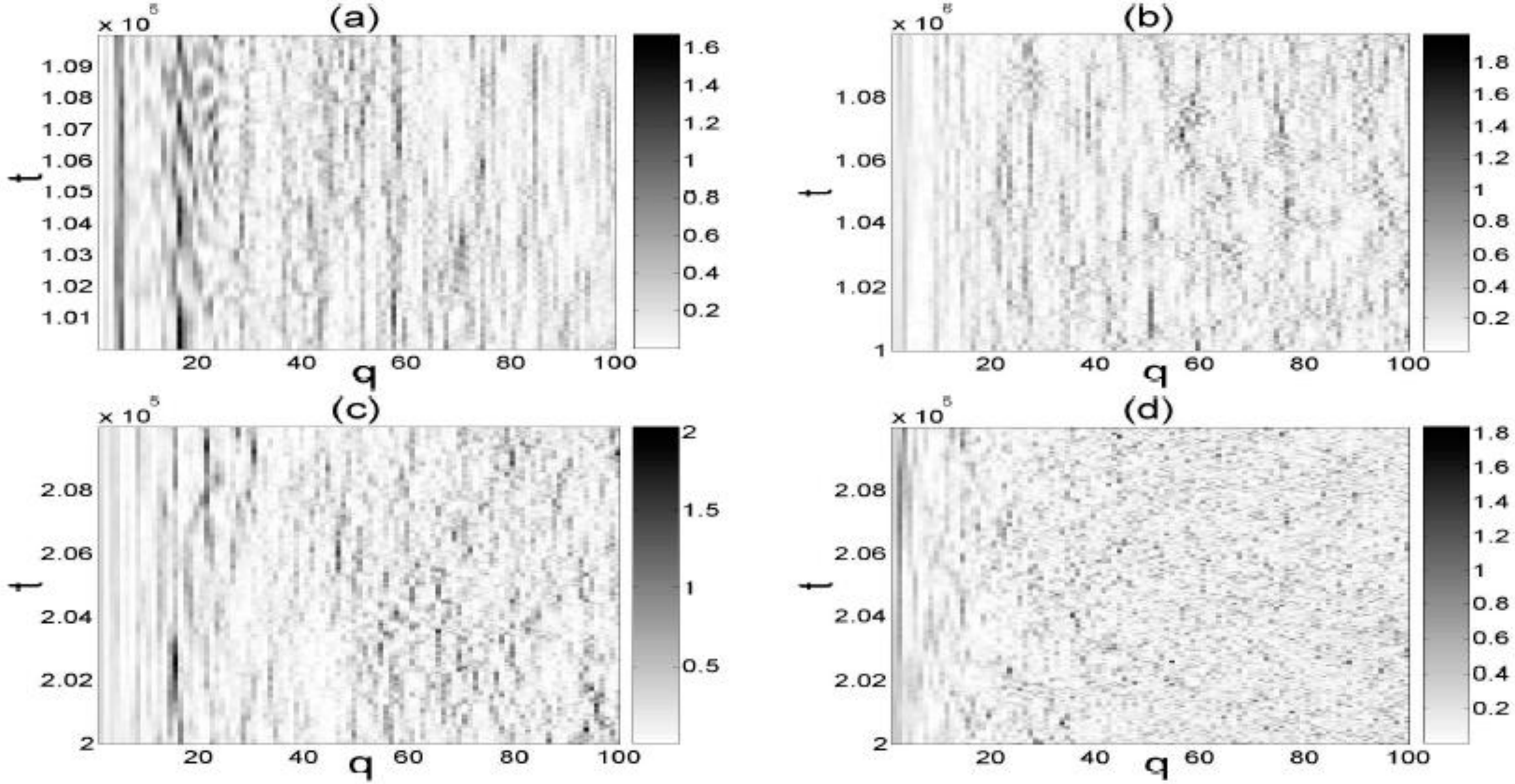
$$\tilde{Q}_{\tilde{q}}(t) = \begin{cases} \sqrt{r} Q_q(t) & \tilde{q} = rq \ , \\ 0 & \tilde{q} \neq rq \ , \end{cases} \quad q = \overline{1, N}$$



Thus scaled q-breathers exist for infinite size systems!

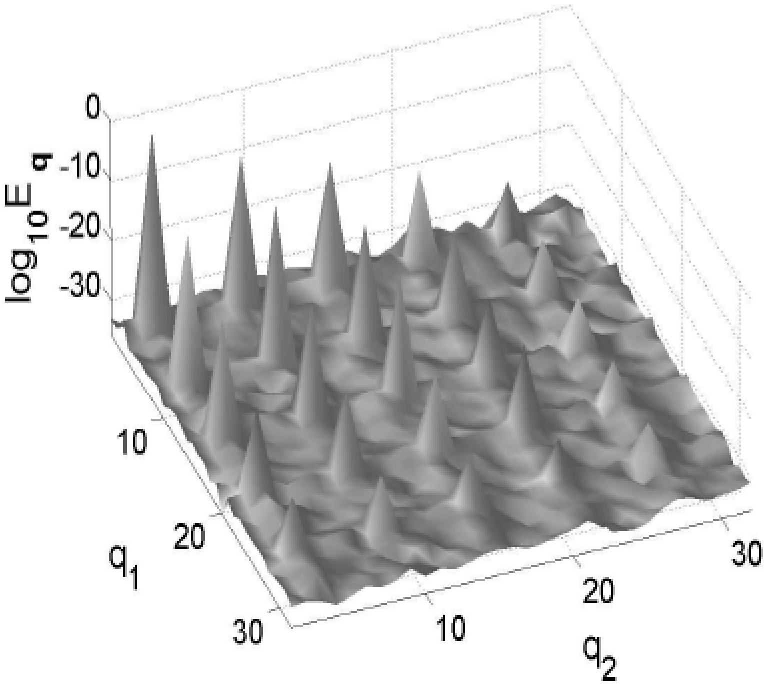
Dynamics in 'thermal' equilibrium

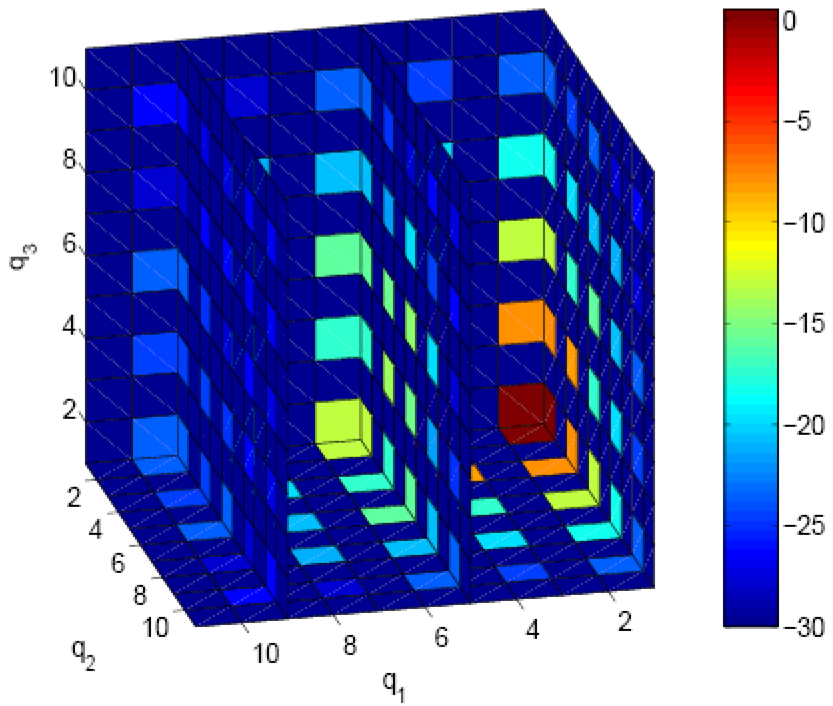
Space-time plots of modes energies E_q evolving from the random initial conditions for $N = 100, E/N = 0.2$ and (a) $\beta = 0.05$, (b) $\beta = 0.05$, (c) $\beta = 0.1$, (d) $\beta = 0.4$.



Generalization to two- and three-dimensional lattices

PRL 97 (2006) 025505





Further reading:

- PRL 95 (2005) 064102
- PRE 73 (2006) 036618
- PRL 97 (2006) 025505
- PLA 365 (2007) 416
- Chaos 17 (2007) 023102

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

Take Home Messages

- nonlinear dynamical systems – nonintegrability, chaos
- quasiperiodic motion destroyed, BUT:
- periodic orbits are generic low-d invariant manifolds
- spatial lattices: POs localize in real space – discrete breathers
- normal modes: POs localize in mode space – q-breathers
- breathers are essential periodic orbits which describe the evolution of relevant mode-mode interactions, correlations in and relaxations of complex systems