The Abdus Salam International Centre for Theoretical Physics

2162-3

Advanced Workshop on Anderson Localization, Nonlinearity and Turbulence: a Cross-Fertilization

23 August - 3 September, 2010

INTRODUCTORY
Nonlinear Waves: The Fermi-Pasta-Ulam Problem of Equipartition and The Fate of Anderson Localization

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INTRODUCTORY

Nonlinear Waves:

The Fermi-Pasta-Ulam Problem of Equipartition and The Fate of Anderson Localization

S. Flach, MPIPKS Dresden

mpipks

Road map:

- introductory remarks

- the FPU paradox:
  KAM or CHAOS?

- Anderson localization + nonlinearity:
  LOCALIZATION or SPREADING?

PART ONE:

INTRODUCTORY REMARKS

Linear wave equations

$$d = 1 \quad \Delta = \frac{\partial^2}{\partial x^2} \; ; \; d = 2 \quad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \; ; \; \ldots$$

Linear Wave Equation : $\frac{\partial^2 u}{\partial t^2} = \Delta u$

Generalizations : $\frac{\partial^2 u}{\partial t^2} = (\Delta + V(x, y, \ldots)) \cdot u$

(Linear) Schrödinger equation : $i \dot{\Psi} = (-\Delta + V(x, y, \ldots)) \Psi$

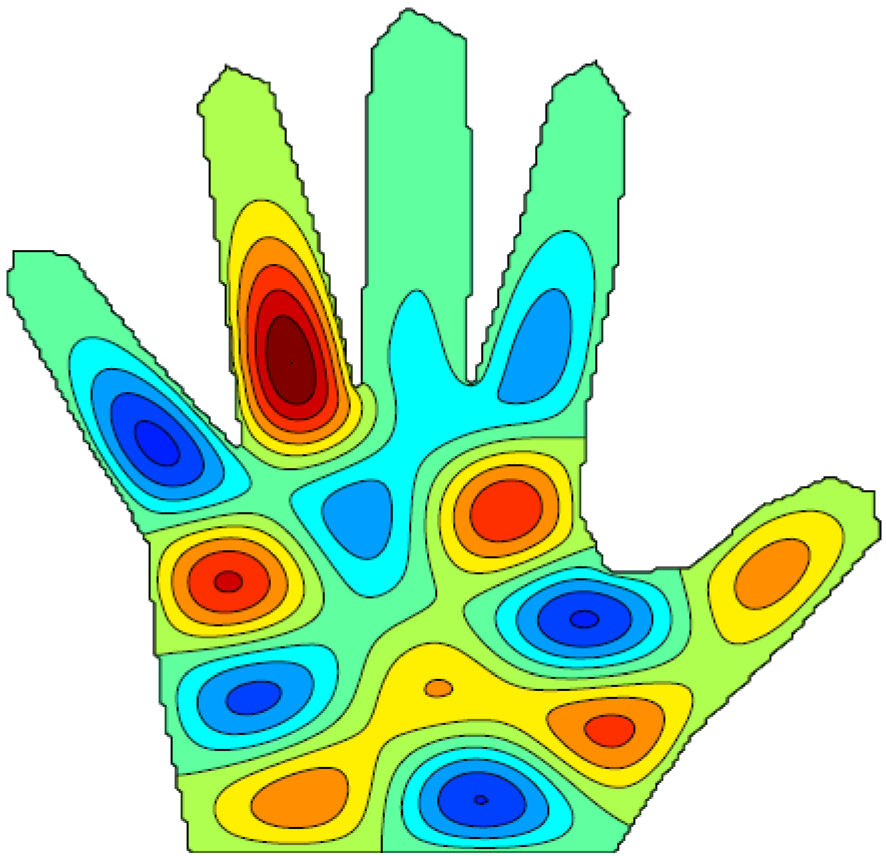
Define boundary values, solve eigenvalue problem

$$u(x,t) = A(x) \cdot e^{i\omega t} \qquad \Psi(x,t) = \varphi(x) \cdot e^{i\omega t}$$

$$-\lambda A = (\Delta + V) \cdot A \qquad -\lambda \varphi = (-\Delta + V) \varphi$$

$$\lambda \equiv \omega^2 \qquad \lambda \equiv \omega$$

An eigenfunction of a hand



Cleve Moler

Eigenvalues λ, Eigenfunctions A_λ, φ_λ

Superposition: the sum of two solutions is also a solution

Initial state: $\psi(x,0) = \sum\!\!\!\!\!\!\int c_\lambda \varphi_\lambda(x)$

$\Downarrow$

later time: $\psi(x,t) = \sum\!\!\!\!\!\!\int c_\lambda \varphi_\lambda(x) \cdot e^{i\lambda t}$

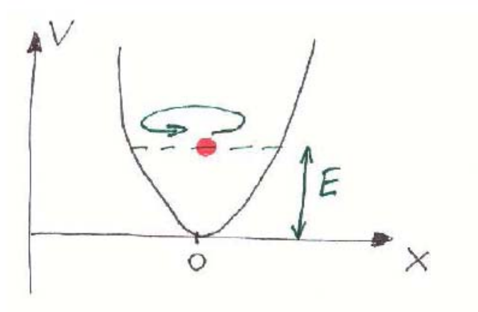
Discretizing space: $\Delta = \frac{\partial^2}{\partial x^2} \Rightarrow \Delta_d \cdot \varphi = \varphi_{n+1} + \varphi_{n-1} - 2\varphi_n$

still same properties

Integrability: angle $\theta_\lambda = \lambda t$, action $I_\lambda = \int |\varphi(x)|^2 dx$

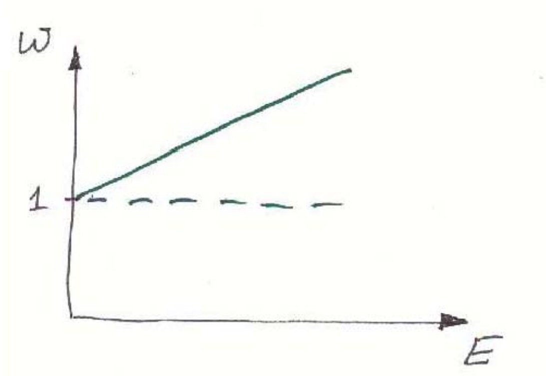
Hamiltonian $H = \sum\!\!\!\!\!\!\int \lambda I_\lambda$

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 oscillation frequency depends on energy:



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

Nonlinear wave equations

examples:

$$\frac{\partial^2 u}{\partial t^2} = (\Delta + V(x))u + u^3 + \dots$$

$$i\dot{\psi} = (-\Delta + V(x))\psi + |\psi|^2\psi + \dots$$

why? • field excites medium $\Rightarrow$ <u>non</u>linear response

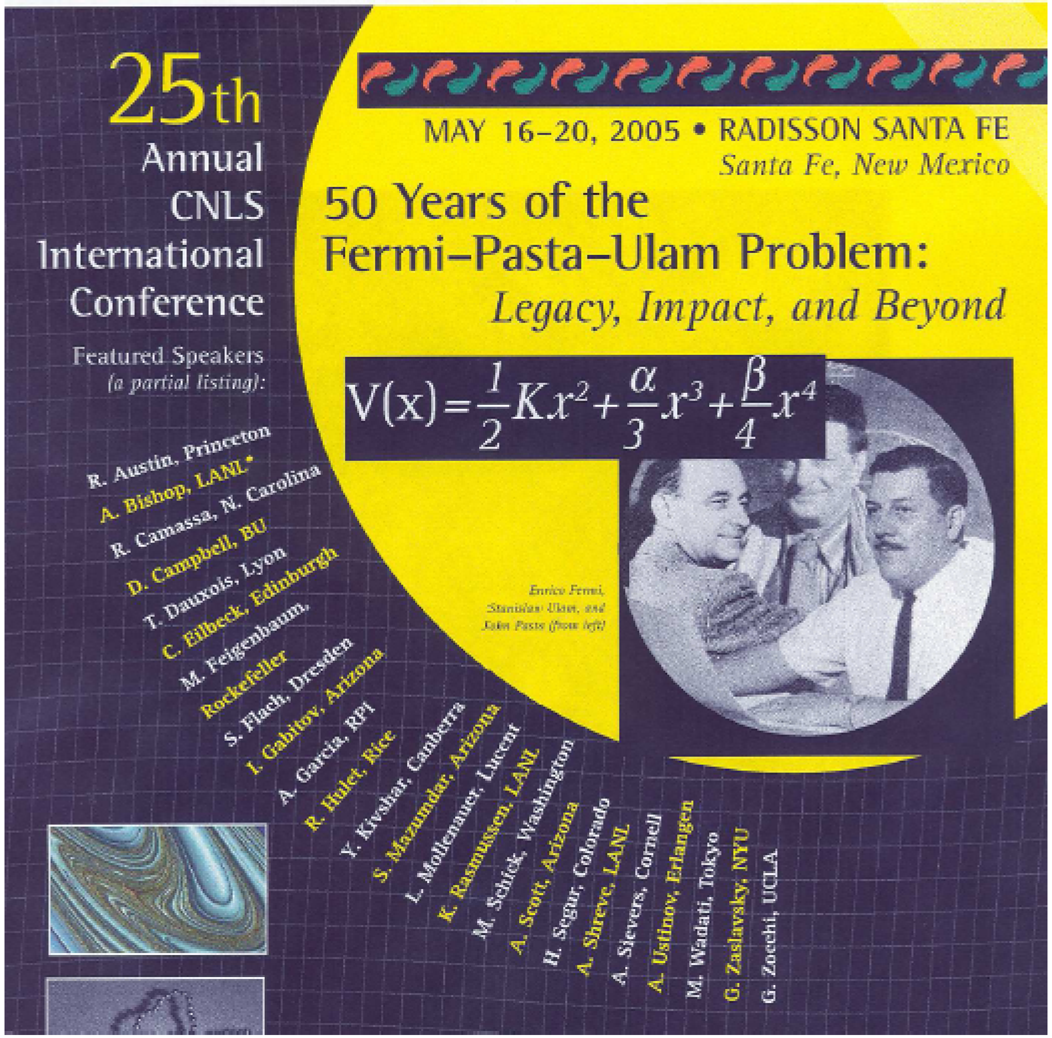
• many quantum particles
interact (scatter),
mean field approximation,
similar to effective medium $\Rightarrow$ nonlinear
response

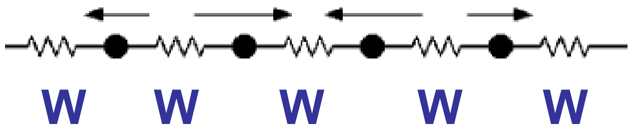
<u>Consequence?</u>

• loss of superposition
• loss of integrability (in general)
• deterministic chaos possible
• regular dynamics may survive (KAM)

PART TWO:

THE FPU PARADOX: KAM OR CHAOS?





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

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

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

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

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

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

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:

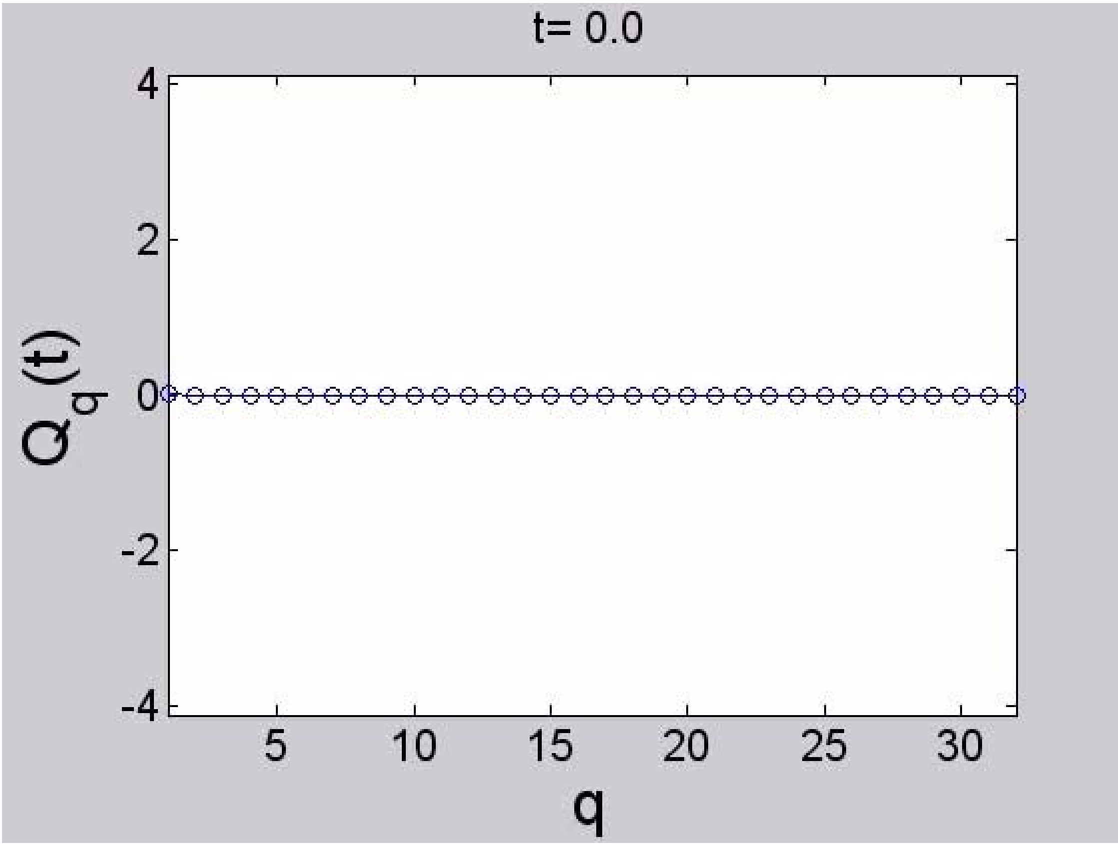
$$E_q = \frac{1}{2}(\dot{Q}_q^2 + \omega_q^2 Q_q^2)$$

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

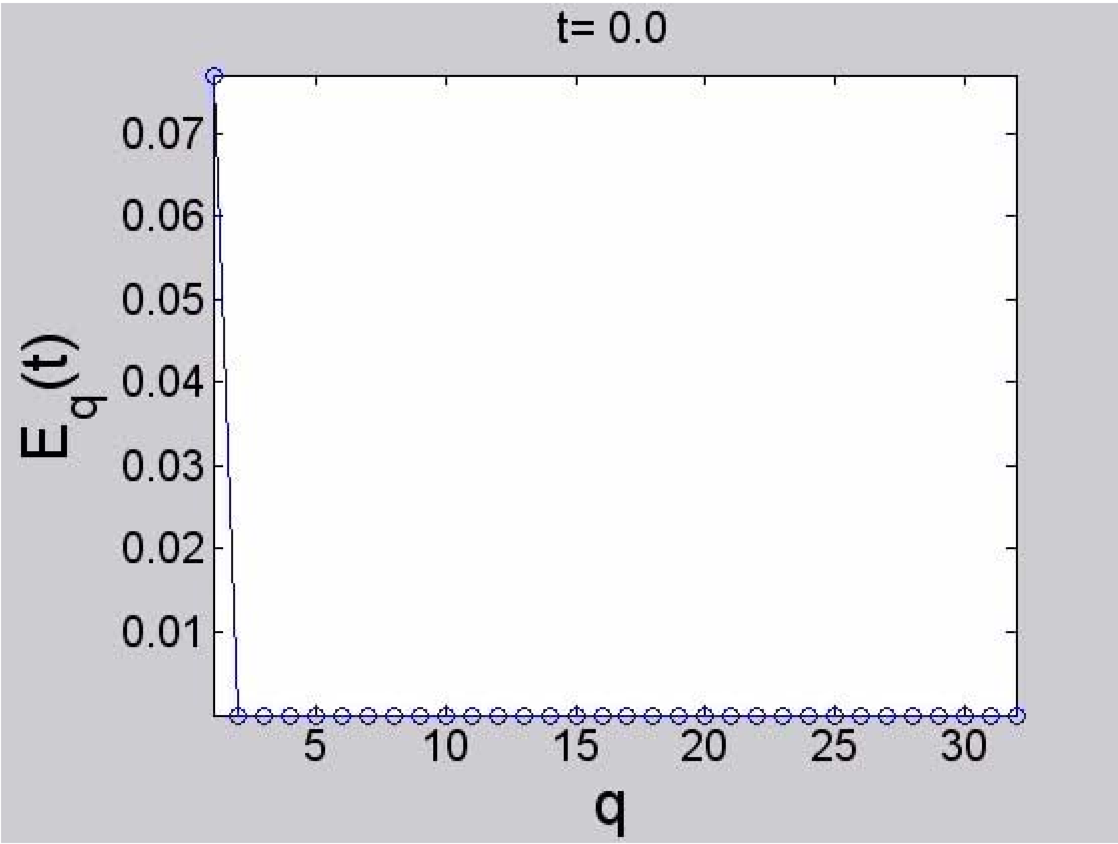
- excite $q = 1$ mode
- observe nonequipartion of mode energies
- no transition to thermal equilibrium
- energy is localized in a few modes for long time **FPU 1**
- recurrence of energy into initially excited mode **FPU 2**
- two thresholds in energy and N **FPU 3**
- two pathways of understanding: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

Movies: let us see what FPU observed

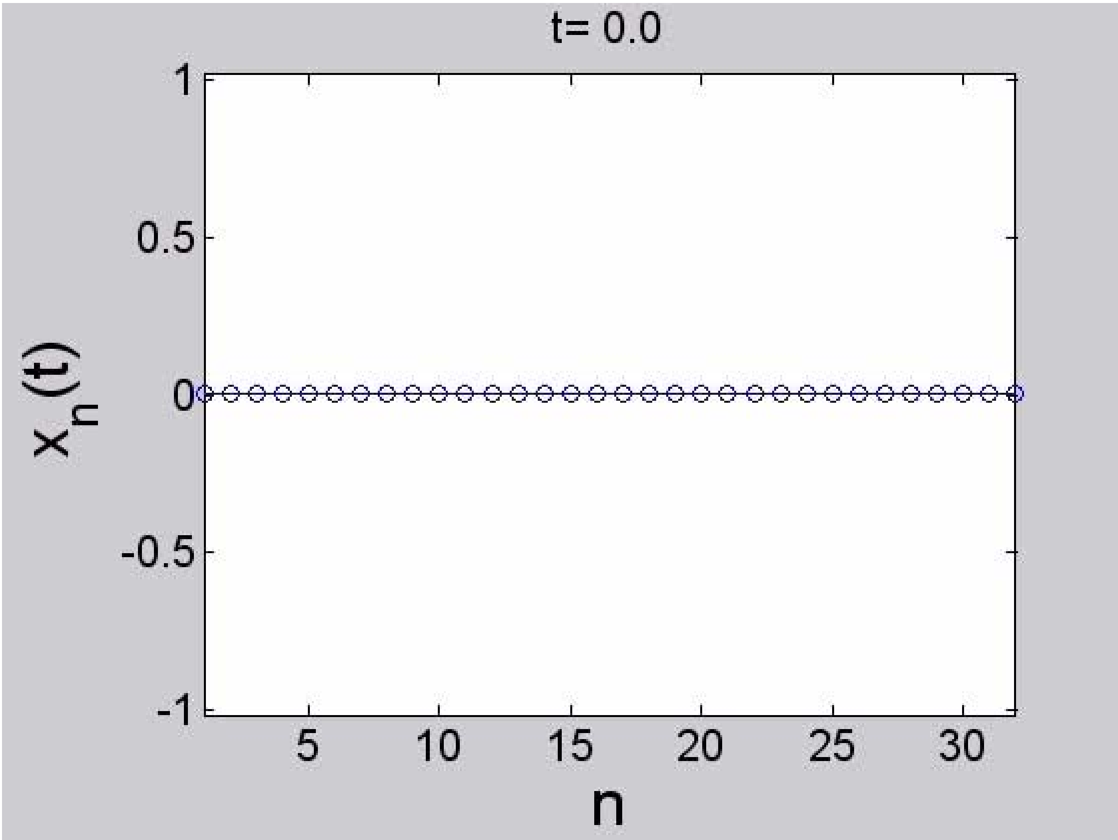
Evolution of normal mode coordinates



Evolution of normal mode energies

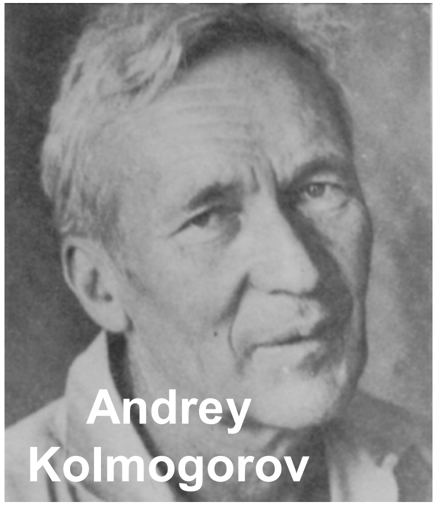


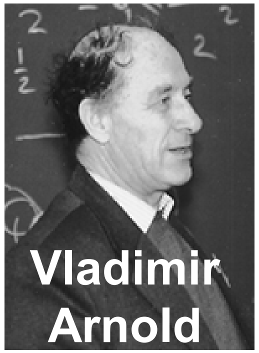
Evolution of real space displacements



Kolmogorov – Arnold – Moser (KAM) theory

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



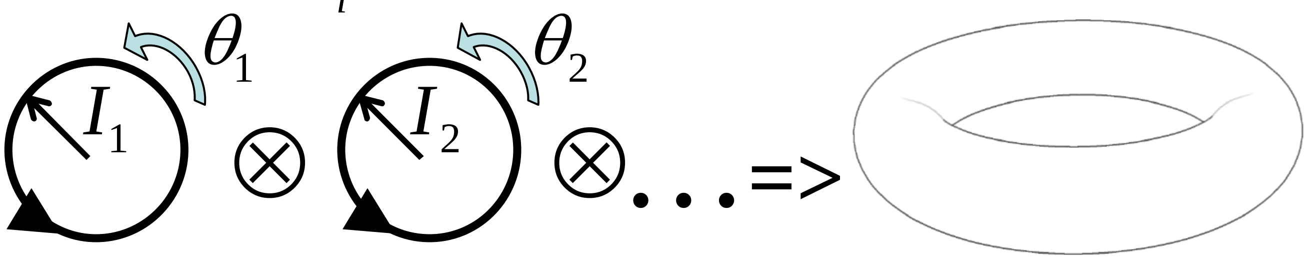


Integrable classical Hamiltonian $\hat{H}_0$, ***d>1***:

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

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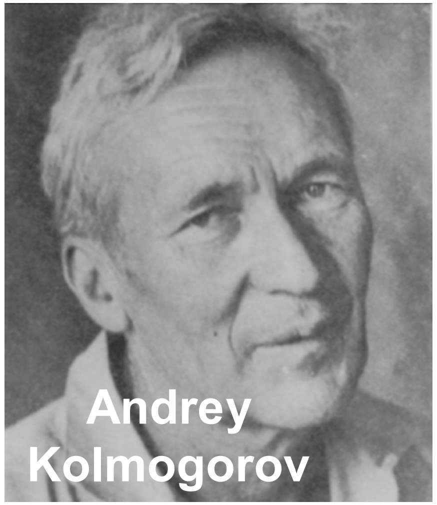
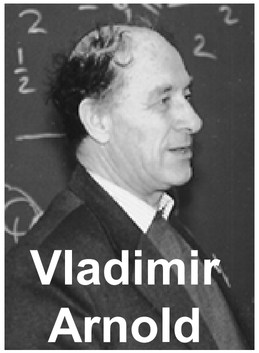
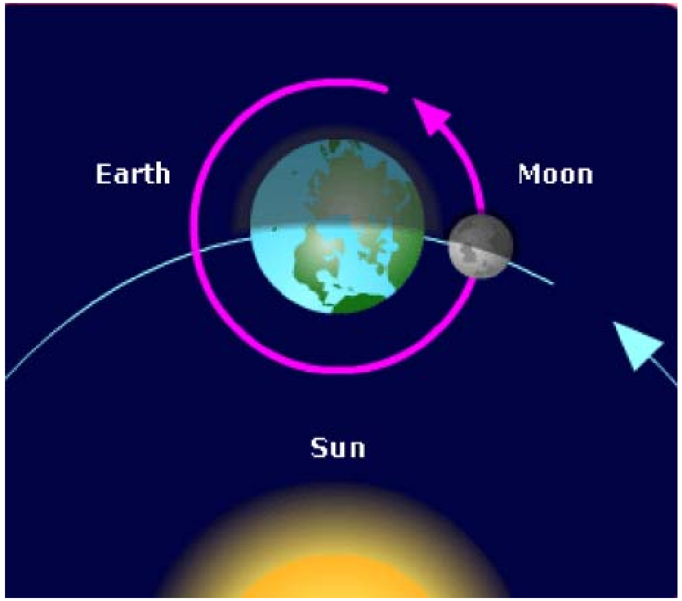
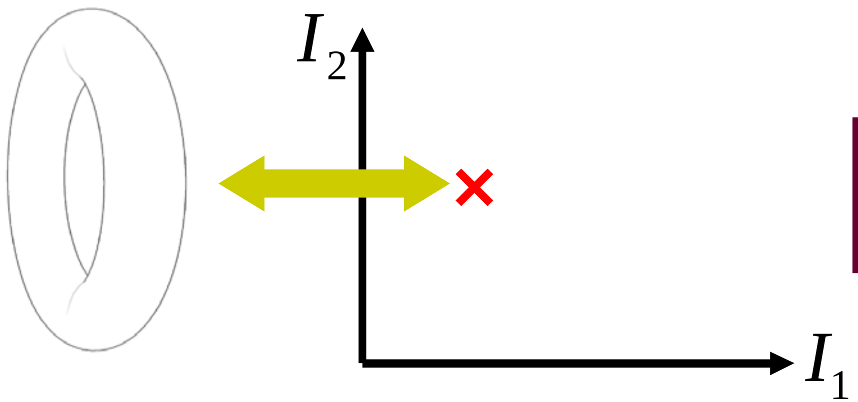




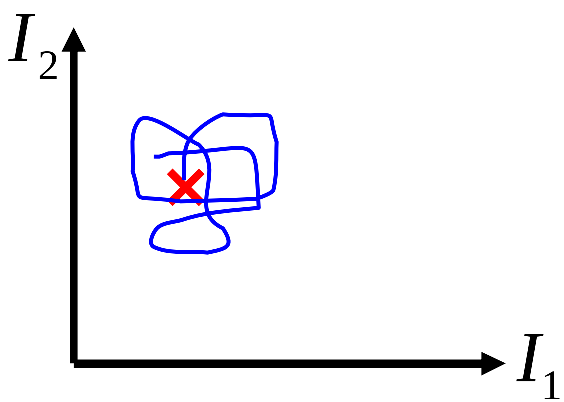


KAM theorem:

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 ?

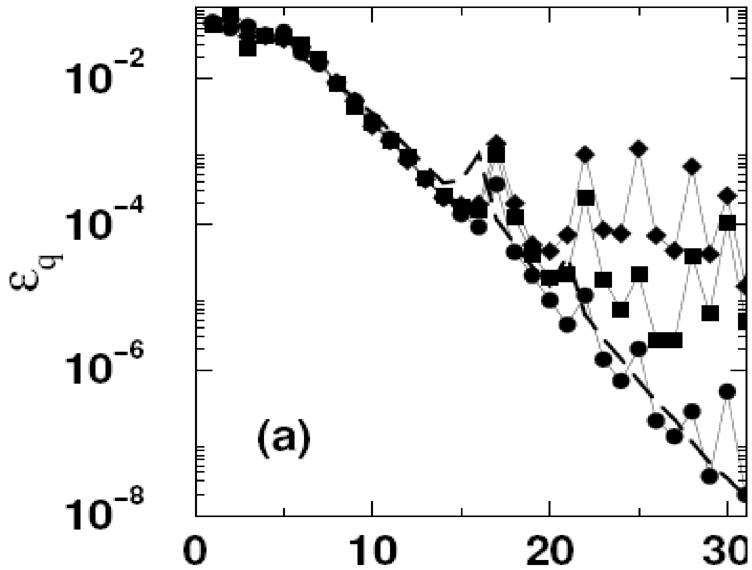
- KAM applies to finite systems
- Does it apply to waves in infinite systems?
- How are KAM thresholds scaling with number of degrees of freedom?
- Will nonlinear waves observe KAM regime?
- If they do – then localization remains
- If they do not – waves can delocalize

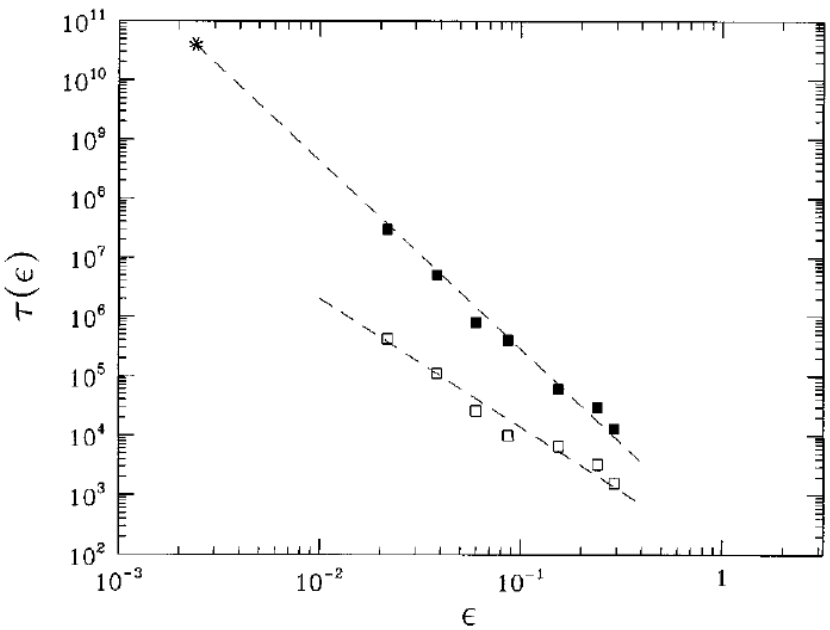
Galgani and Scotti (1972):
exponential localization after short transient

Galgani, Giorgilli, Benettin, Ponno, Penati, and many many others (… much later …):
slow delocalization in tails, equipartition
After potentially very long second time scale

Ivanchenko, Kanakov, Penati, SF (2005+):
exact periodic orbits (q-breathers) exp. localized in mode space (dashed line)

Casetti, Cerruti-Sola, Pettini, Cohen (1997):
scaling of second time scale





After 40 years of investigations: a set of NoAnswers on:

- obtaining two time scales in the thermalization process?

- relation to weakly nonintegrable systems and KAM theorem?

- why do we need spatially localized solitons to explain exponentially strong localization in normal mode space?
  (in fact there IS no reduction in the KdV approach, one needs roughly as many solitons, as normal modes are excited)

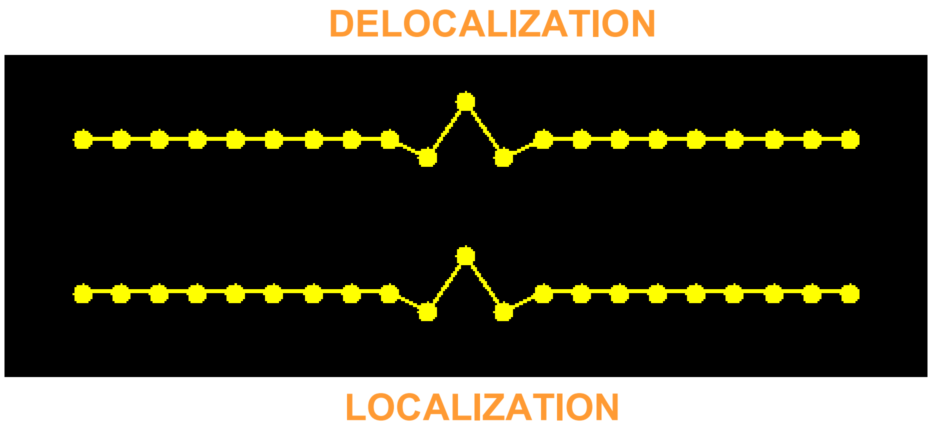
- are there exact invariant low-dimensional manifolds for the nonintegrable model which relate to the observations?

- are the Chirikov-Izrailev thresholds correct?

PART THREE:

ANDERSON LOCALIZATION
+
NONLINEARITY
=
(DE)LOCALIZATION ?

Defining the problem



- a disordered medium
- linear equations of motion: all eigenstates are Anderson localized
- add short range nonlinearity (interactions)
- follow the spreading of an initially localized wave packet

Will it delocalize?

Yes because of nonintegrability and ergodicity

No because of energy conservation –
spreading leads to small energy density,
nonlinearity can be neglected,
dynamics becomes integrable, and
Anderson localization is restored

Model : The discrete nonlinear Schrödinger Equation

$$\mathcal{H}_D = \sum_l \epsilon_l |\psi_l|^2 + \frac{\beta}{2}|\psi_l|^4 - (\psi_{l+1}\psi_l^* + \psi_{l+1}^*\psi_l)$$

ϵ_l uniformly from $\left[-\frac{W}{2}, \frac{W}{2}\right]$ $\qquad \dot{\psi}_l = \partial \mathcal{H}_D / \partial (i\psi_l^\star)$

$$i\dot{\psi}_l = \epsilon_l \psi_l + \beta|\psi_l|^2\psi_l - \psi_{l+1} - \psi_{l-1}$$

Conserved quantities: energy and norm $\quad S = \sum_l |\psi_l|^2$

Varying the norm is strictly equivalent to varying β

Equations model light propagation and cold atom dynamics
in structured media

$$i\dot{\psi}_l = \epsilon_l \psi_l + \beta |\psi_l|^2 \psi_l - \psi_{l+1} - \psi_{l-1}$$

The linear case: $\beta = 0 \qquad \psi_l = A_l \exp(-i\lambda t)$

Stationary states: $\lambda A_l = \epsilon_l A_l - A_{l-1} - A_{l+1}$

Normal mode (NM) eigenvectors: $A_{\nu,l} \; (\sum_l A_{\nu,l}^2 = 1)$

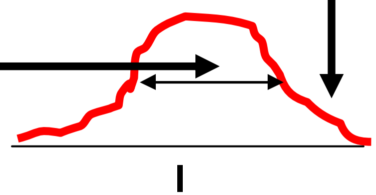
Eigenvalues: $\lambda_\nu \in \left[-2 - \frac{W}{2}, 2 + \frac{W}{2}\right]$

Width of EV spectrum: $\Delta_D = W + 4$

Asymptotic decay: $A_{\nu,l} \sim \mathrm{e}^{-l/\xi(\lambda_\nu)}$

Localization length: $\xi(\lambda_\nu) \leq \xi(0) \approx 100/W^2$

Localization volume of NM: V
V(W < 4) ≈ 3ξ V(W > 10) ≈ 1



Equations in normal mode space:

$$i\dot{\phi}_\nu = \lambda_\nu \phi_\nu + \beta \sum_{\nu_1,\nu_2,\nu_3} I_{\nu,\nu_1,\nu_2,\nu_3} \phi^*_{\nu_1} \phi_{\nu_2} \phi_{\nu_3}$$

$$I_{\nu,\nu_1,\nu_2,\nu_3} = \sum_l A_{\nu,l} A_{\nu_1,l} A_{\nu_2,l} A_{\nu_3,l}$$

NM ordering in real space: $X_\nu = \sum_l l A^2_{\nu,l}$

Characterization of wavepackets in normal mode space:

$z_\nu \equiv |\phi_\nu|^2 / \sum_\mu |\phi_\mu|^2 \qquad \bar{\nu} = \sum_\nu \nu z_\nu$

Second moment: $m_2 = \sum_\nu (\nu - \bar{\nu})^2 z_\nu$ → location of tails

Participation number: $P = 1/\sum_\nu z_\nu^2$ → number of strongly excited modes

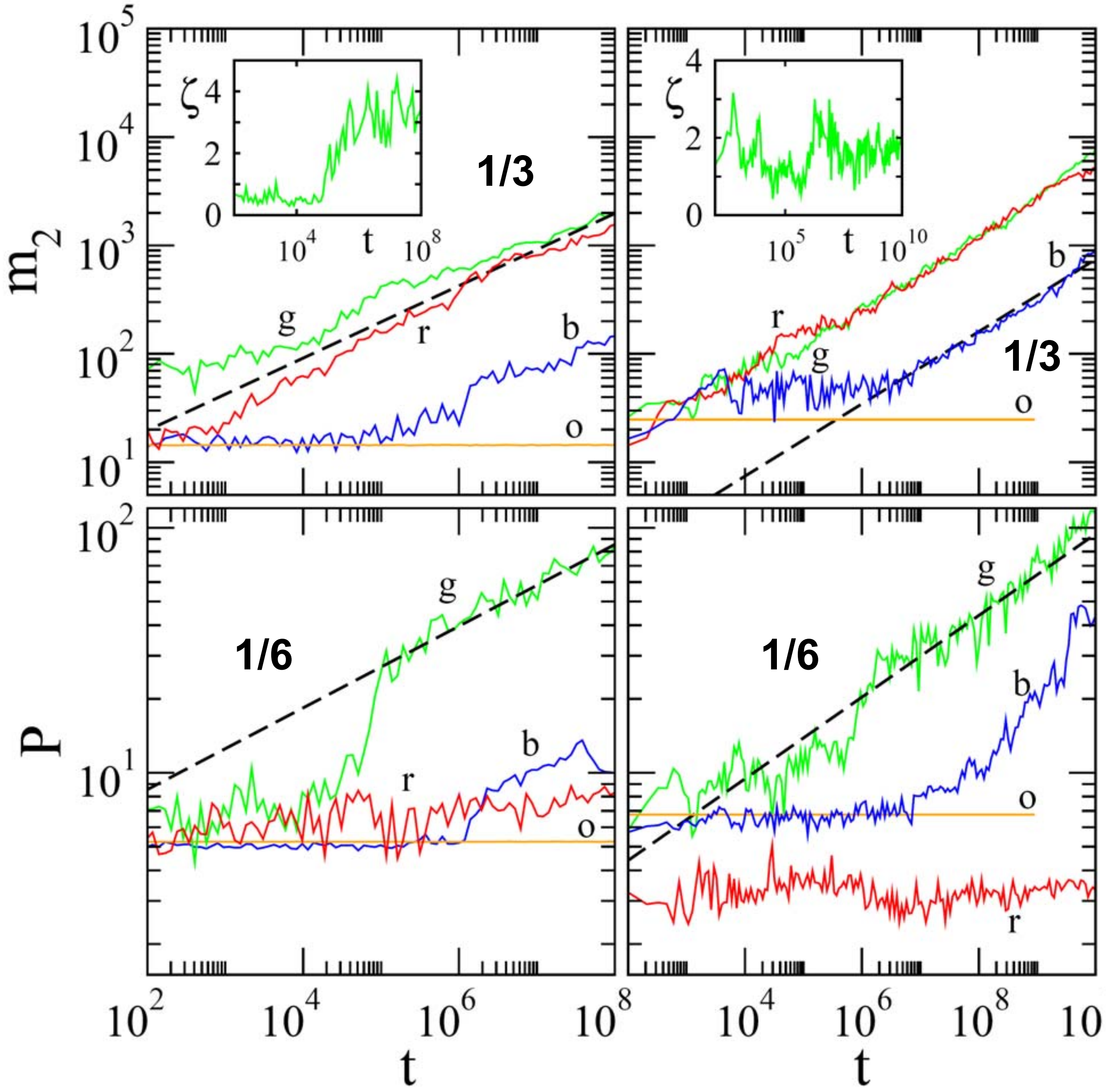
Compactness index: $\zeta = \dfrac{P^2}{m_2}$

→ K adjacent sites equally excited: $\zeta = 12$

→ K adjacent sites, every second empty or equipartition: $\zeta = 3$

Results for single site excitations $\psi_l = \delta_{l,l_0} \quad \epsilon_{l_0} = 0$

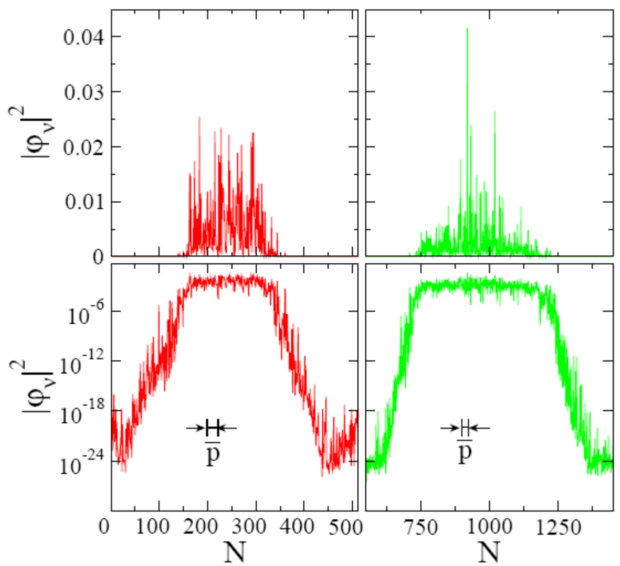
DNLS W=4, β= 0, 0.1, 1, 4.5 KG W=4, E= 0, 0.05, 0.4, 1.5



SF,Krimer,Skokos (2009)
Skokos,Krimer,Komineas,SF (2009)

Similar results by:
Molina (1998)
Shepelyansky,Pikovsky (2008)
Kopidakis,Komineas,SF,Aubry (2008)

Wavepacket spreads way beyond localization volume.
DNLS at $t = 10^8$



III A theorem for selftrapping

Kopidakis, Komineas, SF, Aubry (2008)

can not uniformly spread over the entire (infinite) lattice for the DNLS case. Indeed, with the notations

$$\mathcal{H}_D = \mathcal{H}_{NL} + \mathcal{H}_L \ , \tag{8}$$

$$\mathcal{H}_L = \sum_l \epsilon_l |\psi_l|^2 - (\psi_{l+1}\psi_l^* + c.c.) \ , \tag{9}$$

$$\mathcal{H}_{NL} = \sum_l \frac{\beta}{2} |\psi_l|^4 \equiv \frac{\beta}{2} P^{-1} \ , \tag{10}$$

where P is the participation number in real space, the single site excitation at time $t = 0$ yields

$$\mathcal{H}_L(t=0) = 0 \ , \ \mathcal{H}_{NL}(t=0) = \frac{\beta}{2} \ . \tag{11}$$

Due to norm conservation $S = 1$ at all times, the harmonic energy part $\mathcal{H}_L$ is bounded from above and below [9]:

$$-2 - \frac{W}{2} \leq \mathcal{H}_L \leq 2 + \frac{W}{2} \,. \qquad (12)$$

Due to energy conservation, for all times the anharmonic energy part $\mathcal{H}_{NL}$ can therefore not become smaller than

$$\mathcal{H}_{NL}(t) \geq \frac{\beta}{2} - 2 - \frac{W}{2} \,. \qquad (13)$$

It follows with (10), that the participation number is bounded from above by a finite number, which diverges for $\beta = \Delta$:

$$P(t) \leq \frac{\beta}{\beta - \Delta} \text{ if } \beta \geq \Delta \,. \qquad (14)$$

Therefore no complete delocalization for some $\beta > \beta_c$ **= W+4 …**

Destruction of Anderson localization in the tails of a wave packet?

$$i\dot{\psi}_l = \epsilon_l \psi_l + \beta|\psi_l|^\sigma \psi_l - \psi_{l+1} - \psi_{l-1}$$

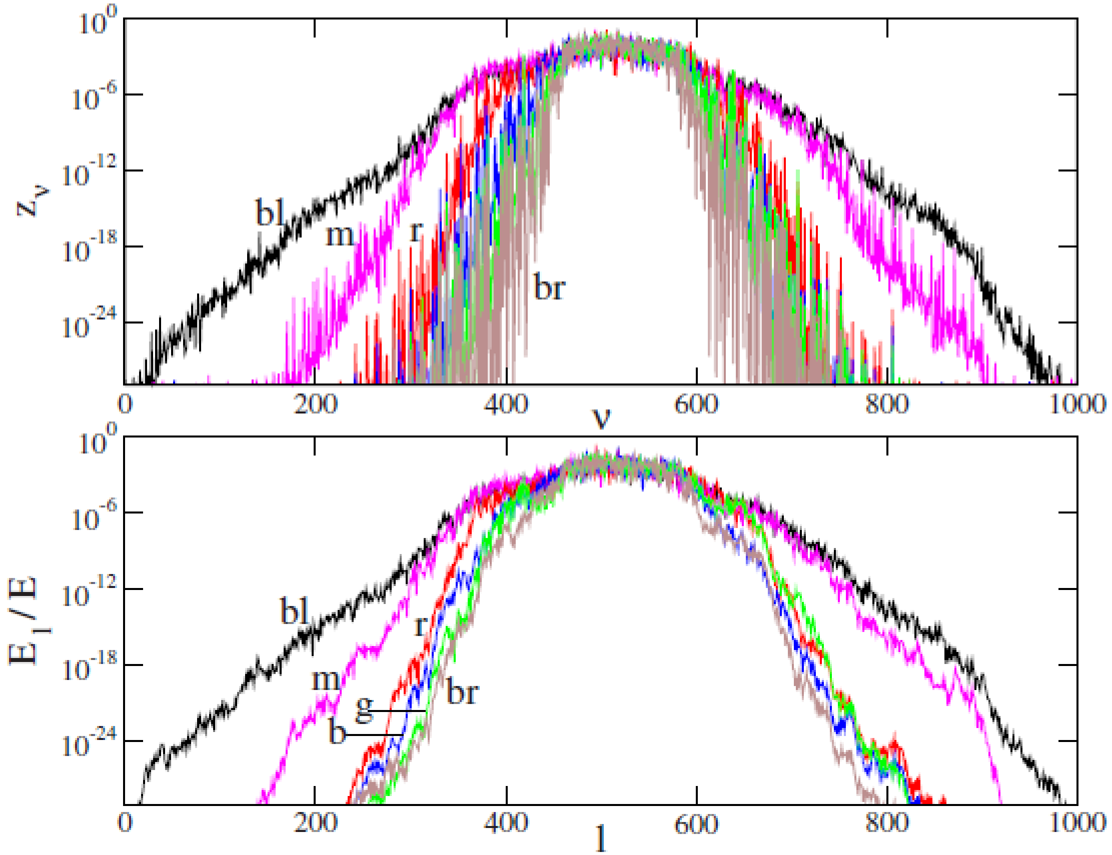


FIG. 7. (Color online) Normalized energy distributions in NM (upper plot) and real (lower plot) space for σ=0.05,0.2,0.8, 1.25,2.0,3.0 [(bl) black; (m) magenta; (r) red; (b) blue; (g) green;

Skokos,SF 2010

In a nutshell:

- strong nonlinearity: partial localization due selftrapping,
  but part of wavepacket may delocalize

- weak nonlinearity: Anderson localization on finite times: similar to FPU!
  After that – detrapping, and wavepacket delocalizes ?

- intermediate nonlinearity: wavepacket delocalizes without transients

- no signature of stop ?

- do results do depend on presence or absence of norm conservation ?

- is spreading is universal due to nonintegrability ?

$$\mathcal{H}_{int} = \sum_{\nu} \lambda_\nu J_\nu + \beta \sum_{\nu_1,\nu_2,\nu_3,\nu_4} I_{\nu_1,\nu_2,\nu_3,\nu_4} \sqrt{J_{\nu_1} J_{\nu_1} J_{\nu_1} J_{\nu_1}}$$

gives complete localization!

Open questions, problems, controversial opinions:

- is there a KAM regime at small but finite β, or not?
- will a spreading packet eventually enter a KAM regime, or not?
- is the spreading wave packet equilibrating inside, if yes, how?
- is the observed spreading Arnold diffusion, or not?
- will the spreading slow down into a kind of Arnold diffusion, or not?
- are the computational results affected by roundoff errors, or not?
- finite systems: how is the KAM threshold scaling with system size?
- characteristics of energy diffusion at finite norm/energy densities ?
- relation to turbulence? Lessons from there, or for it ?
- relation to quantum many body localization ?