An old problem from a new angle: FPU and anharmonic chains with wave turbulence

Revisiting the birth of modern nonlinear physics

Sergio Chibbaro

Sorbonne Université, Institut Jean Le Rond d'Alembert - Paris

sergio.chibbaro@sorbonne-universite.fr

in collaboration with
Miguel Bustamante (University College - Dublin)
Y. L'vov (Rensselaer Polytechnic Institute - New York)
Miguel Onorato and L. Pistone (Università di Torino - Torino)
D. Proment (University of East Anglia - Norwich)

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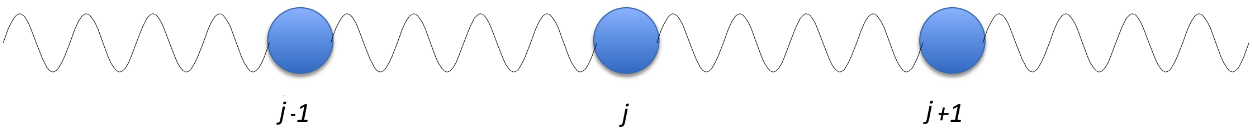
The weakly nonlinear one-dimensional chain model

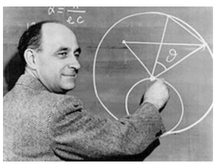
N equal masses connected by a weakly nonlinear spring



$$F \simeq -\kappa \Delta q + \alpha \Delta q^2 + \beta \Delta q^3 + \ldots$$

The system is Hamiltonian

$$H = \sum_{j=1}^{N} \left[\frac{1}{2m} p_j^2 + \frac{\kappa}{2} (q_j - q_{j+1})^2 \right] + \frac{\alpha}{3} \sum_{j=1}^{N} (q_j - q_{j+1})^3 + \frac{\beta}{4} \sum_{j=1}^{N} (q_j - q_{j+1})^4$$

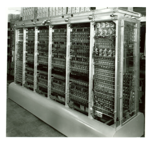


Enrico Fermi (1901-1954)

John Pasta (1909-1984)

Stanislaw Ulam (1918-1984)

Mary Tsingou-Menzel (1928-)



MANIAC I (1952-1957)

Premise

Ergodic problem and foundation of statistical mechanics

Poincaré Theorem (1895): the non existence of first integrals of motion (except for energy), in generic Hamiltonian systems

Fermi Theorem (1923): *In a generic Hamiltonian system with $N > 2$ degrees of freedom, no smooth surface can divide the phase space into two regions containing open invariant sets.*

Fermi argued that non-integrable Hamiltonian systems are generically ergodic, which would solve the ergodic problem.

Henri Poincaré
(1854-1912)

The result expected by Fermi and collaborators

Equipartition of *linear* energy in Fourier space for large times
Microcanonical ensemble values:

$$Q_k = \frac{1}{N}\sum_{j=0}^{N-1} q_j e^{-i\frac{2\pi kj}{N}}, \; P_k = \frac{1}{N}\sum_{j=0}^{N-1} p_j e^{-i\frac{2\pi kj}{N}},$$

then

$$E_k = |P_k|^2 + \omega_k^2 |Q_k|^2 = const$$

with

$$\omega_k = 2\left|\sin\left(\frac{\pi k}{N}\right)\right|$$

Remark: However for $\epsilon = 0$ normal modes are independent and the system is not ergodic. The statistical mechanics treatment can be well founded only in the non-integrable case.

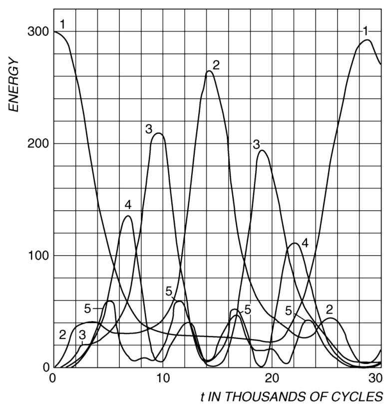
The Los Alamos report: an influential unpublished paper

STUDIES OF NON LINEAR PROBLEMS

E. Fermi, J. Pasta, and S. Ulam
Document LA-1940 (May 1955).

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer Maniac I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.



Among the first computer experiments and, perhaps, the first showing how simulations can be used as a powerful instrument able to provide new physical insights and ideas.

First explanations: solitons and integrability in physics

In the limit of long waves (continuum limit) the α-FPU system reduces to the Korteweg-de Vries (KdV) equation:

$$\frac{\partial \eta}{\partial t} + \eta \frac{\partial \eta}{\partial x} + \frac{\partial^3 \eta}{\partial x^3} = 0$$

VOLUME 15, NUMBER 6 PHYSICAL REVIEW LETTERS 9 AUGUST 1965

INTERACTION OF "SOLITONS" IN A COLLISIONLESS PLASMA AND THE RECURRENCE OF INITIAL STATES

N. J. Zabusky
Bell Telephone Laboratories, Whippany, New Jersey
and
M. D. Kruskal

VOLUME 19, NUMBER 19 PHYSICAL REVIEW LETTERS 6 NOVEMBER 1967

METHOD FOR SOLVING THE KORTEWEG-deVRIES EQUATION*

Clifford S. Gardner, John M. Greene, Martin D. Kruskal, and Robert M. Miura
Plasma Physics Laboratory, Princeton University, Princeton, New Jersey
(Received 15 September 1967)

First explanations: solitons and integrability in physics

ZK showed, besides recurrence, the formation of train of solitons

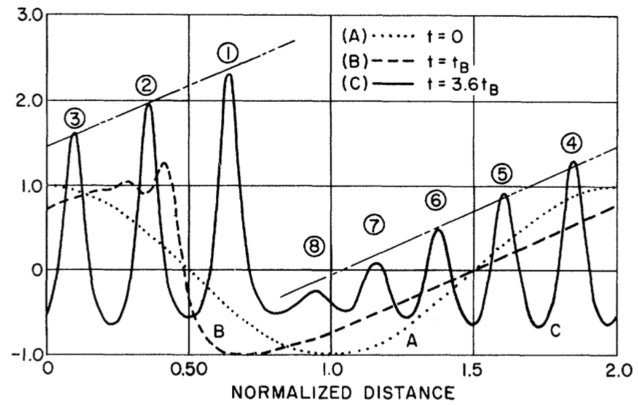


FIG. 1. The temporal development of the wave form $u(x)$.

Numerical simulation of the KdV equation*

First explanations: Hamiltonian Chaos

- KAM (1954) and Nekhoroshev (1977) theorems
$$H(I, \theta, \varepsilon) = H_0(I) + \varepsilon H_1(I, \theta),$$
if $\varepsilon \ll 1$, then invariant tori (KAM tori) survive on the surface of constant energy; Chaos can invade phase-space for large N
Physically: non- ergodic behaviors of non-integrable Hamiltonian systems are actually typical. Good properties are expected if $N \gg 1$.
The emerging picture for FPU system:
  - if $\varepsilon < \varepsilon_c$ the KAM tori are dominant and the system does not reach equipartition
  - if $\varepsilon \geq \varepsilon_c$ the system reaches equipartition according to statistical mechanics
- Chirikov Criterium (Izraielev and Chirikov, 1966): stochasticity due to frequency overlap
$$R = \frac{\Gamma_k}{\omega_{k+1} - \omega_k} > 1$$
R is resonance overlap parameter, Γ_k is the nonlinear frequency broadening

Physical Questions

(i) the regular behavior for small nonlinearities, and irregular for large ones, is peculiar of FPU Hamiltonian?

(ii) Does the system thermalize for arbitrary small nonlinearity for finite number of particles?

(iii) What are the characteristic times of the equipartition process as function of N and ϵ? What are the physical mechanisms ?

(iv) If there is a threshold, what is the dependence of ϵ_c on N (at fixed E)?

(v) for a given N, how small is the part of the phase space with regular behavior.

Among **Huge** literature:
Gallavotti ed. 2007 Lectures Notes in Physics Springer
Benettin & Ponno J. Stat. Phys. 2011

The models

- α-FPU

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) + \alpha \left[(q_{j+1} - q_j)^2 - (q_{j-1} - q_j)^2 \right]$$

- β-FPU

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) + \beta \left[(q_{j+1} - q_j)^3 - (q_{j-1} - q_j)^3 \right]$$

- Discrete Nonlinear Klein Gordon (DNKG)

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) - q_j - g q_j^3,$$

Hamiltonian formalism:

$$H_{\mathsf{lin}} = \sum_{j=0}^{N-1} \frac{1}{2} p_j^2 + \frac{1}{2}(q_j - q_{j+1})^2 + \frac{1}{2} m q_j^2,$$

$$H_{\mathsf{nlin}}^{(\alpha)} = \frac{\alpha}{3} \sum_{j=0}^{N-1} (q_j - q_{j+1})^3, \quad H_{\mathsf{nlin}}^{(\beta)} = \frac{\beta}{4} \sum_{j=0}^{N-1} (q_j - q_{j+1})^4, \quad H_{\mathsf{nlin}}^{(KG)} = \frac{\beta}{4} \sum_{j=0}^{N-1} q_j^4.$$

Normal modes

Assuming periodic boundary conditions, we introduce the wave action variable

$$a_k = \frac{1}{\sqrt{2\omega_k}}(\omega_k Q_k + iP_k),$$

with $P_k = \dot{Q}_k$ and $\omega_k = 2|\sin(\pi k/N)|$

Linear regime

$$\omega_k = \sqrt{m + 4\sin^2\left(\pi\frac{k}{N}\right)} \quad (m = 0 \text{ for the FPUT models}).$$

Weakly nonlinear regime: perturbative approach

$$\beta \sim g \sim \alpha^2 \sim \epsilon$$

Normal form of Hamiltonian for all 4 models

$$\frac{H_{\mathsf{lin}}}{N} = \sum_{j=0}^{N-1} \omega_k \left| a_k \right|^2 ,$$

$$\frac{H_{\mathsf{nlin}}^{(\alpha)}}{N} = \alpha \sum_{k_1,k_2,k_3=0}^{N-1} A_{1,2,3} \left[\frac{1}{3} (a_1 a_2 a_3 + c.c.) \delta_{1+2+3}^{(N)} + (a_1^* a_2 a_3 + c.c.) \delta_{1-2-3}^{(N)} \right]$$

$$\frac{H_{\mathsf{nlin}}^{(\beta,\mathsf{KG})}}{N} = \beta \sum_{k_1,k_2,k_3,k_4=0}^{N-1} B_{1,2,3,4}^{(\beta,\mathsf{KG})} \left[\frac{1}{4} (a_1 a_2 a_3 a_4 + c.c.) \delta_{1+2+3+4}^{(N)} + \right.$$

$$\left. (a_1^* a_2 a_3 a_4 + c.c.) \delta_{1-2-3-4}^{(N)} + \frac{3}{2} a_1^* a_2^* a_3 a_4 \delta_{1+2-3-4}^{(N)} \right]$$

with

$$\delta_{1\pm2\pm3\pm4} = \delta(k_1 \pm k_2 \pm k_3 \pm k_4), \quad a_i = a(k_i, t), \qquad \mathbf{A}, \mathbf{B} = T(\mathbf{k})$$

Starting point for statistical theory!

Wave Turbulence in a nutshell

WT is the general statistical theory of weakly nonlinear dispersive waves.

- Look for an evolution equation for the correlator $\langle a(\kappa_i, t)a(\kappa_j, t)^* \rangle = n(\kappa_i, t)\delta(\kappa_i - \kappa_j)$
- BBGKY hierarchy: need of a closure
- Random-phase assumption and initial random apmlitudes
- Thermodynamic limit $N \to \infty$ $L \to \infty$
- **The main concept**: the existence of conservation laws associated to the wave scattering processes. Exact Resonances.

$$\begin{aligned} k_1 &= k_2 + k_3, \\ \omega_1 &= \omega_2 + \omega_3. \end{aligned}$$

Typical 3-waves scattering process (Ex. Capillary waves).

$$\frac{\partial n_1}{\partial t} = \int_{-\infty}^{+\infty} A_{123}^2 n_1 n_2 n_3 \left(\frac{1}{n_1} - \frac{1}{n_2} - \frac{1}{n_3} \right) \delta(\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3)\delta(\omega_1 - \omega_2 - \omega_3) \mathrm{d}\mathbf{k}_{23} \quad (1)$$

The Wave Kinetic Equation

Energy Conservation:

$$E = \int \omega(\kappa) n(\kappa, t) d\kappa, \qquad N = \int n(\kappa, t) d\kappa, \quad \text{scattering}$$

Existence of an H-theorem:

$$H = \int \ln(n(\kappa, t)) d\kappa, \quad \text{with} \quad \frac{dH}{dt} \leq 0$$

The Rayleigh-Jeans distribution

$$dH/dt = 0 \rightarrow n(k, t) = \frac{T}{\omega(\kappa) + \mu}$$

Thermalization time scale: nonlinear collision time

The thermodynamic limit in anharmonic chains

$$N \to \infty, \quad L \to \infty \quad \text{with} \quad \frac{L}{N} = \Delta x = const$$

Momentum space is continuous but space remains discrete.
Then the dispersion relations become:

$$\omega_k = \sqrt{m + 4\sin(k/2)^2}$$

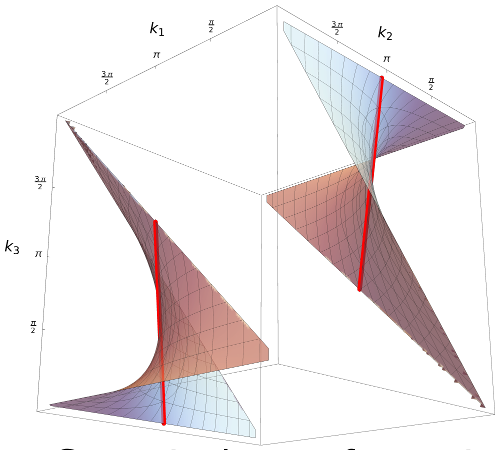
It is shown that 3-waves processes are not resonant

but the following 4-wave resonant interactions are satisfied in all chains:

$$k_1 + k_2 - k_3 - k_4 = 0$$
$$\omega_1 + \omega_2 - \omega_3 - \omega_4 = 0$$

Standard Wave Turbulence can be developed

The thermodynamic limit: Resonances



The continuous resonant manifold for resonances with $m = 0$, that is $\omega_1 + \omega_2 = \omega_1 + \omega_{1+2-3}$.

Canonical transformation to remove non resonant terms:

$$H^{(\alpha)} = \int_0^{2\pi} \omega_k \left|b_k\right|^2 \mathrm{d}k + \frac{\alpha^2}{2} \int_0^{2\pi} \bar{B}^{(\alpha)}_{1,2,3,4} b_1^* b_2^* b_3 b_4 \delta^{(2\pi)}_{1+2-3-4} \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4$$

$$H^{(\beta,KG)} = \int_0^{2\pi} \omega_k \left|b_k\right|^2 \mathrm{d}k + \frac{\beta}{2} \int_0^{2\pi} \bar{B}^{(\beta,KG)}_{1,2,3,4} b_1^* b_2^* b_3 b_4 \delta^{(2\pi)}_{1+2-3-4} \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4.$$

The thermodynamic limit: Time-scales

All three models are dynamically described by the Zakharov equation:

$$i\frac{\partial b_1}{\partial t} = \omega_1 b_1 + \int_0^{2\pi} W_{1,2,3,4} b_2^* b_3 b_4 \delta^{(2\pi)}_{1+2-3-4} \mathrm{d}k_2 \mathrm{d}k_3 \mathrm{d}k_4,$$

Coefficients $W_{1,2,3,4}$ depend on the particular system under consideration. The Kinetic equation reads:

$$\frac{\partial n_1}{\partial t} = \int_0^{2\pi} \mathrm{d}k_{2,3,4} W^2_{1,2,3,4} \delta^{(2\pi)}(k_1+k_2-k_3-k_4)\delta(\omega_1+\omega_2-\omega_3-\omega_4) n_1 n_2 n_3 n_4$$

The thermalization timescales T_{eq}:

$$T_{\text{eq}} \propto \alpha^{-4} \propto \epsilon_\alpha^{-2}$$

for the α-FPUT model and

$$T_{\text{eq}} \propto \beta^{-2} \propto \epsilon_{\beta,KG}^{-2}$$

for the DNKG and β-FPUT models. **Universal behaviour**.

Outside the Thermodynamic limit: small N régime

For N even, the above system has solutions for integer values of k:

- *Trivial solutions*: all wave numbers are equal or

$$k_1 = k_3,\ k_2 = k_4, \quad \text{or} \quad k_1 = k_4,\ k_2 = k_3$$

- *Nontrivial solutions*:

$$\{k_1, k_2; k_3, k_4\} = \left\{k_1, \frac{N}{2} - k_1; N - k_1, \frac{N}{2} + k_1\right\}$$

  with $k_1 = 1, 2, \ldots, \lfloor N/4 \rfloor$

However....

- Four-waves resonant interactions are isolated
- No efficient mixing (and thermalization) can be achieved via a four-wave resonant process (for weak nonlinearity)

Six-wave interactions

- check for exact resonances at higher order

$$i\frac{dc_1}{dt} = \omega_1 b_1 + \epsilon \sum_{k_2,k_3,k_4} T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2-3-4} +$$
$$+ \epsilon^2 \sum W_{1,2,3,4,5,6} c_2^* c_3^* c_4 c_5 c_6 \delta_{1+2+3-4-5-6}$$

Resonant conditions:

$$k_1 + k_2 + k_3 - k_4 - k_5 - k_6 = 0 \pmod N$$
$$\omega_1 + \omega_2 + \omega_3 - \omega_4 - \omega_5 - \omega_6 = 0$$

Non-isolated solutions exist for integer values of k with arbitrary N.

Removing non resonant interactions

Eliminate the non-resonant terms from the Hamiltonian using a near-identity (canonical) transformation from $\{ib, b^*\}$ to $\{ic, c^*\}$

$$\frac{H}{N} = \frac{H_{\text{integrable}}}{N} + \sum_{1,2,3,4,5,6} Z_{1,2,3,4,5,6} c_1 c_2 c_3 c_4^* c_5^* c_6^* \delta^{(N}_{1+2+3-4-5-6}, \tag{2}$$

where δ_N is the Kroneker modulo N.

$$\begin{aligned} \frac{H_{\text{integrable}}}{N} = & \sum_k \omega_k |b_k|^2 + \frac{1}{2}\sum_k W_{k,k,k,k} \left(|b_k|^2\right)^2 + \\ & \sum_{k_1 \neq k_2} W_{k_1,k_2,k_1,k_2} |b_{k_1}|^2 |b_{k_2}|^2 + \\ & + \sum_{k=1}^{\lfloor N/4 \rfloor} 2W_{k,\frac{N}{2}-k,-k,-\frac{N}{2}+k} \left(b_k^* b_{\frac{N}{2}-k}^* b_{-k} b_{-\frac{N}{2}+k} + c.c.\right), \end{aligned} \tag{3}$$

where $c.c.$ denotes complex conjugate.

Estimation of the equipartition time scale for incoherent waves

Look for the evolution equation of $\langle c(k_i,t)c(k_j,t)^* \rangle = n(k_i,t)\delta_{i-j}$

$$\frac{\partial n_1}{\partial t} \sim \epsilon^2 \langle c_1^* c_2^* c_3^* c_4 c_5 c_6 \rangle$$
$$\frac{\partial \langle c_1^* c_2^* c_3^* c_4 c_5 c_6 \rangle}{\partial t} \sim \epsilon^2 \langle c_1^* c_2^* c_3^* c_4^* c_5 c_6 c_7 c_8 \rangle$$

therefore

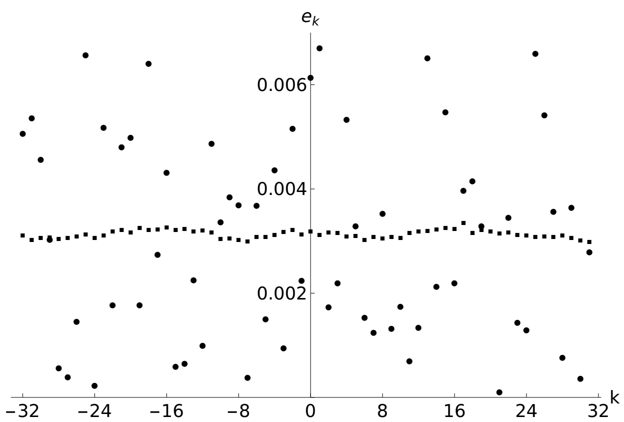
$$\frac{\partial n_1}{\partial t} \sim \epsilon^4 ....$$

and the time of equipartition scales as

$$\mathbf{t_{eq} \sim 1/\epsilon^4}$$

Numerical simulations

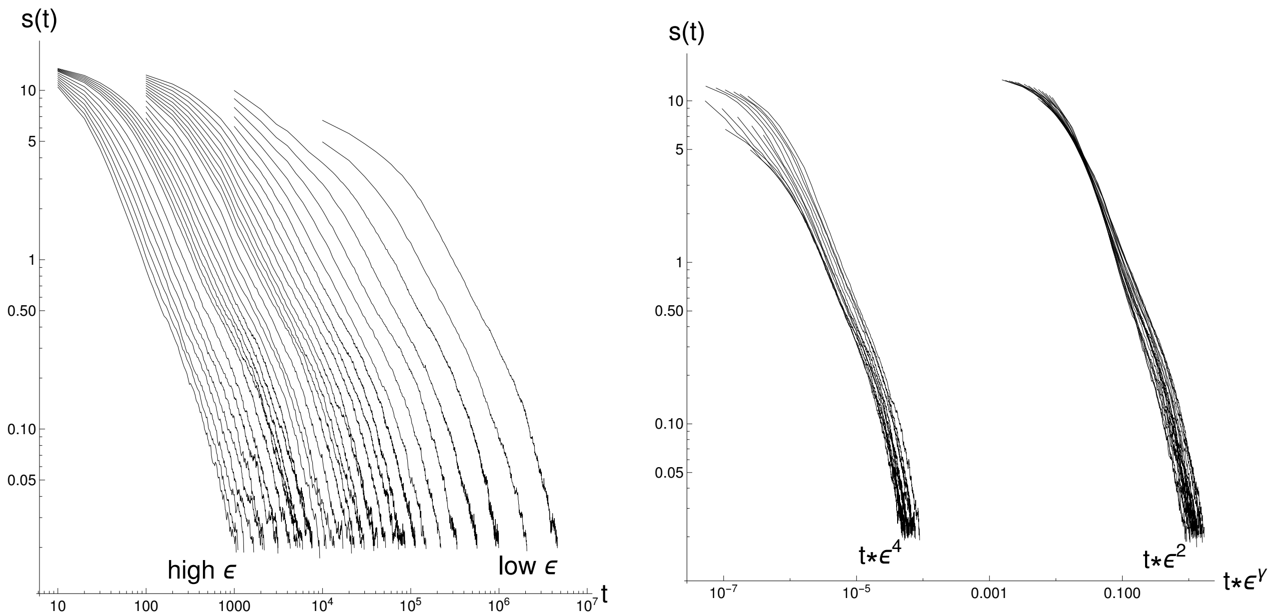
- Symplectic integrator (H. Yoshida, 1990 Phys. Lett. A)
- Numerical simulations with different values of N
- Generic Initial conditions
- ϵ is then selected
- 4096 realisations are made, each with a different set of ϕ_k



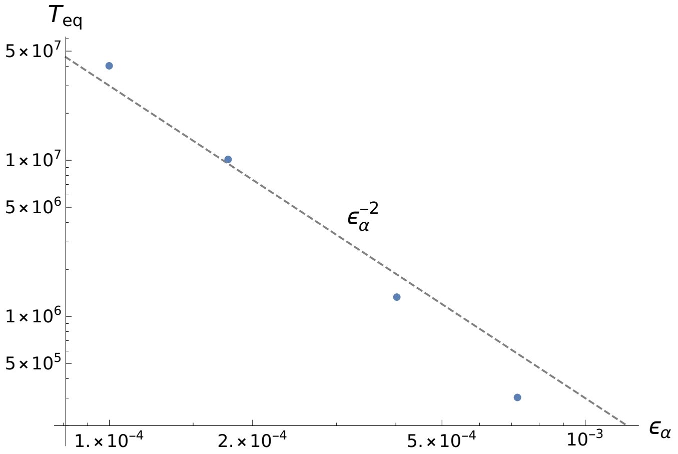
The initial distribution of e_k for the DNKG model with $m = 1$, $N = 64$ (circles), with $E = 0.2$ and $\mathcal{N} \simeq 0.129$. The thermalized final state is shown with the squares, and it approximately corresponds to a Rayleigh-Jeans distribution with $\mu = 0$.

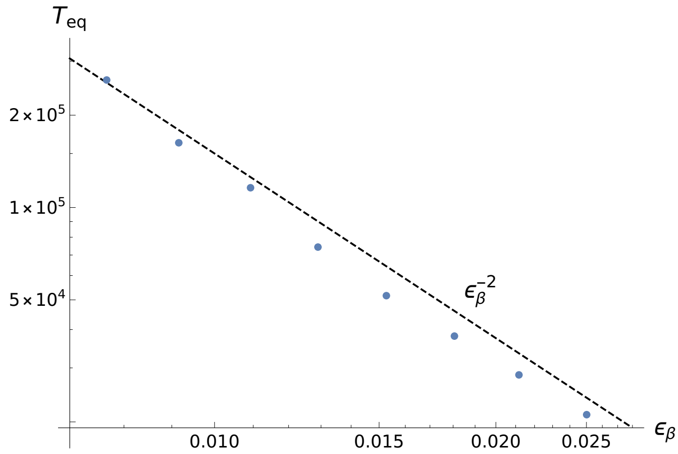
The Entropy: the example of DNKG

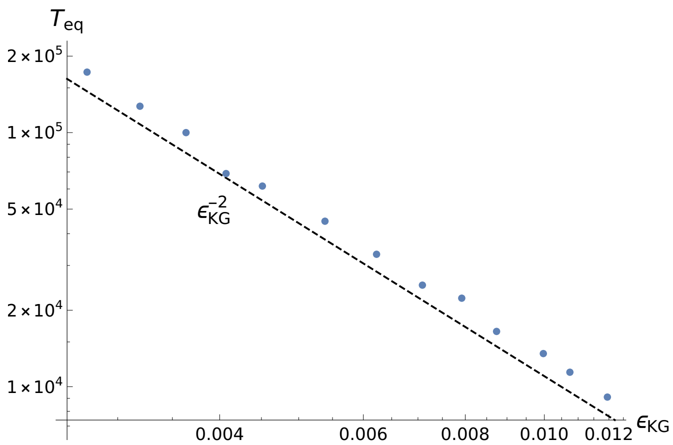
$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{E_{tot}} \omega_k \langle |a_k|^2 \rangle, \quad E_{tot} = \sum_k \omega_k \langle |a_k|^2 \rangle$$



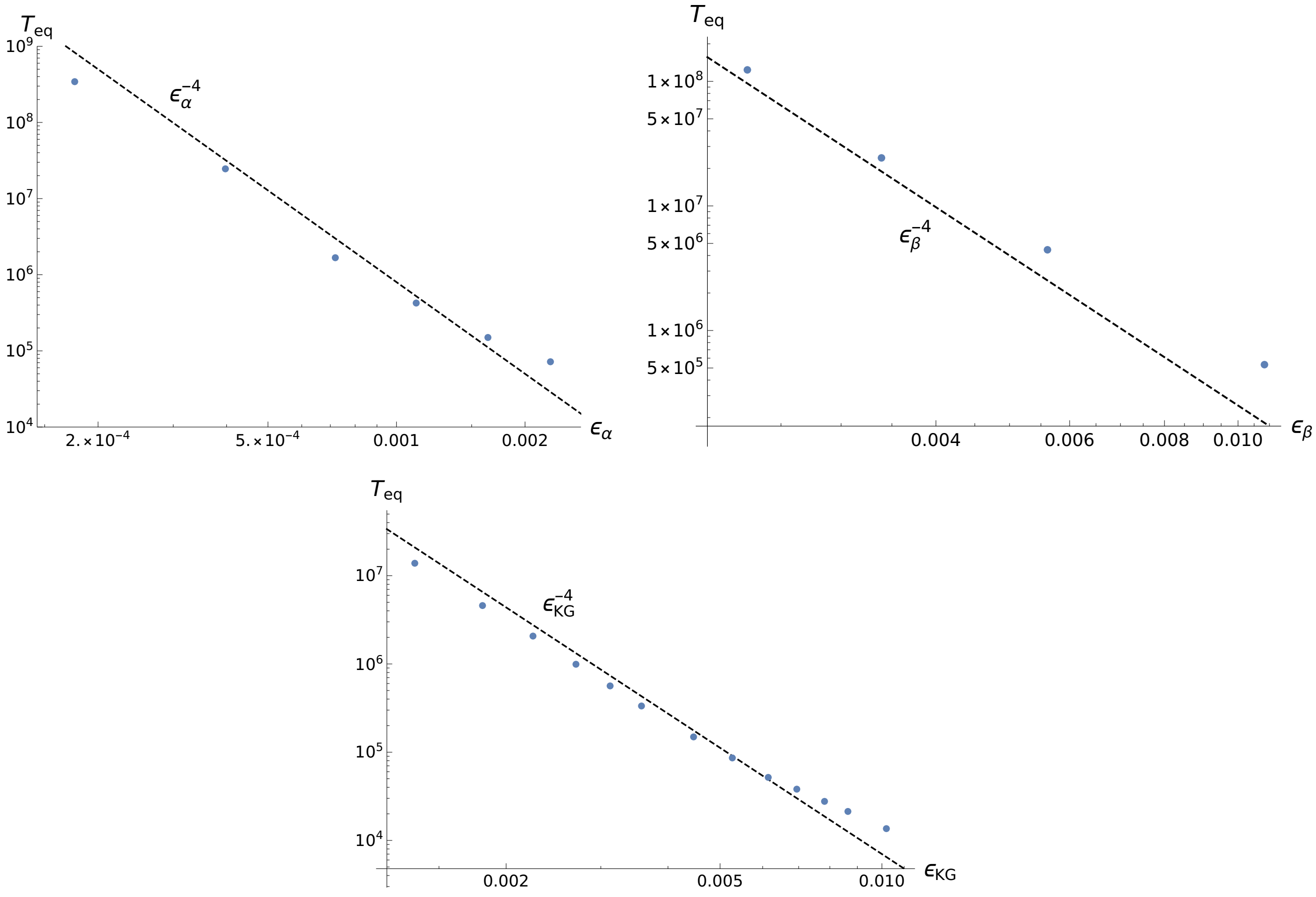
Scaling in time: Thermodynamic limit







Scaling in time: small N



DNKG simulations: frequency broadening

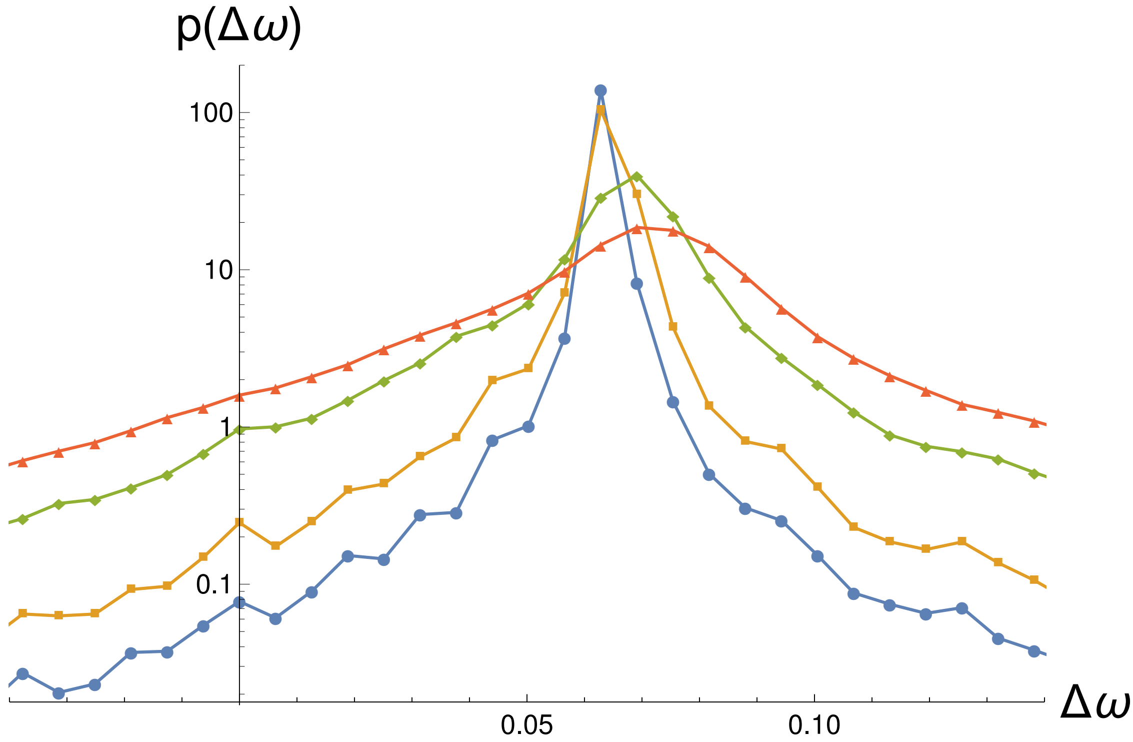


Figure: The dispersion of the frequency mismatch $\Delta\omega$, renormalized as a probability, for a $2 \to 2$ resonance with $N = 32$ and $k = \{1, -15, -11, -3\}$, with $\epsilon \simeq$ 0.0026 (●), 0.0052 (■), 0.0144 (◆), 0.023 (▲).

DNKG equation: the Large Box Limit

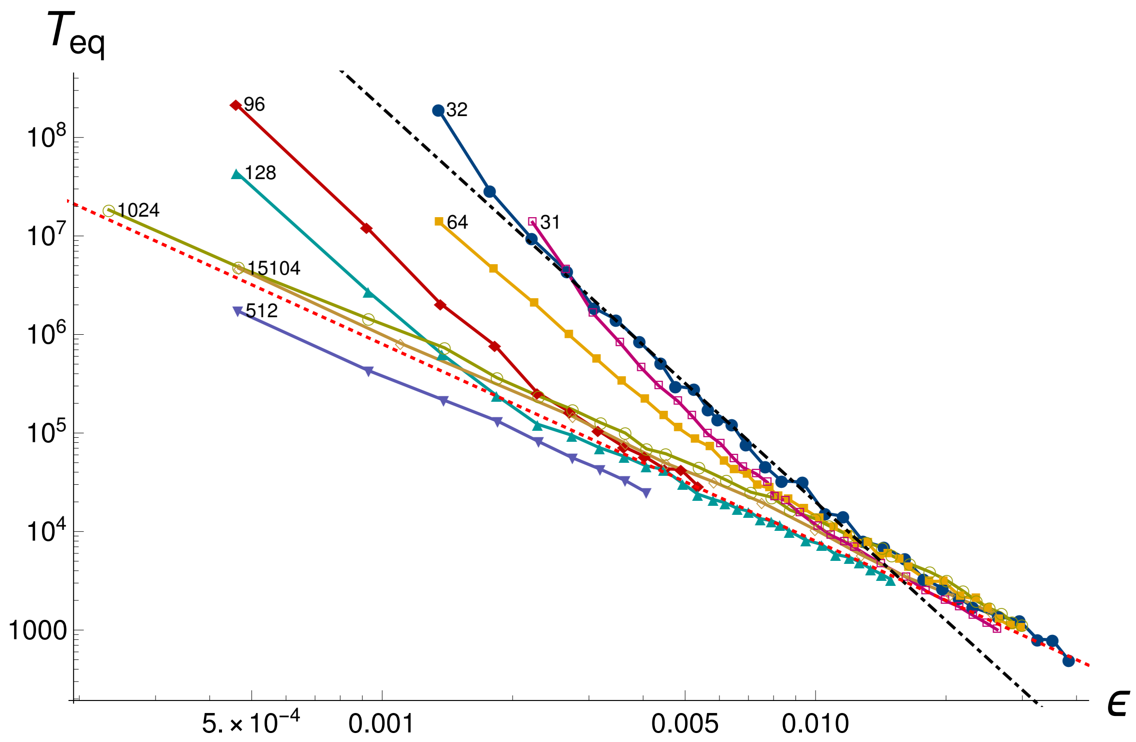


Figure: The scaling of T_{eq} on ϵ for multiple values of N, with $m = 1$ and $E = 0.1N/32$. Scaling laws ϵ^{-2} and ϵ^{-4} in red dotted and black dash-dotted lines for reference.

Conclusions and Perspectives

- The FPU/DNKG systems thermalize for arbitrary small nonlinearity
  Fermi intuition was right...

- The thermalization time scale is $1/\epsilon^2$ in the thermodynamic limit

- The thermalization time scale is $1/\epsilon^4$ in the weakly nonlinear regime for a finite number of particles

- After a (possibly long) transient, WT provides the universal mechanisms underlying anharmonic chains dynamics

$\rightarrow$ Possible specific bizarre cases in small systems ?

$\rightarrow$ What does it happen when some noise is added ? *Localisation* ?

$\rightarrow$ Is it possible to develop a *discrete* kinetic equation ?

E. Fermi with E. Amaldi in Varenna, 1954

The End

Literature and reviews

Some reviews:

- Ford, J. "The Fermi-Pasta-Ulam problem: paradox turns discovery." Physics Reports 213.5 (1992): 271-310.
- Berman, G. P., and F. M. Izrailev. "The Fermi-Pasta-Ulam problem: fifty years of progress." Chaos (Woodbury, NY) 15.1 (2005): 15104
- Carati, A., L. Galgani, and A. Giorgilli. "The Fermi-Pasta-Ulam problem as a challenge for the foundations of physics." Chaos: An Interdisciplinary Journal of Nonlinear Science 15.1 (2005): 015105-015105.
- Weissert, Thomas P. "The genesis of simulation in dynamics: pursuing the Fermi-Pasta-Ulam problem." Springer-Verlag New York, Inc., 1999.
- Gallavotti, G., ed. "The Fermi-Pasta-Ulam problem: a status report." Vol. 728. Springer, 2008.