Enrico Fermi and the birth of modern nonlinear physics

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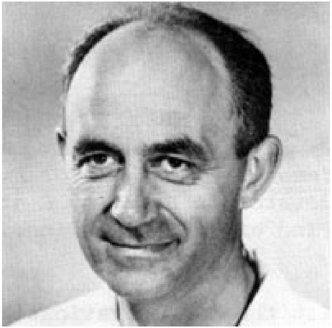
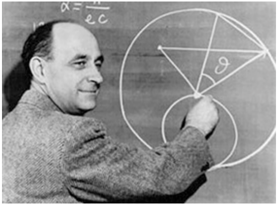
Enrico Fermi



- E. Fermi, Dimostrazione che in generale un sistema meccanico è quasi-ergodico. Nuovo Cimento (1923)
- E. Fermi, J. Pasta and S. Ulam, Studies of nonlinear problems. Los Alamos Report LA-1940, 978 (1955)

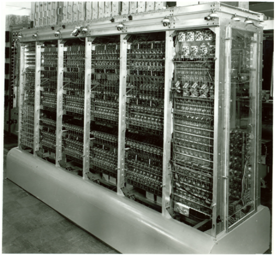
Fermi, Pasta, Ulam in Los Alamos



Enrico Fermi (1901-1954)

John Pasta (1909-1984)

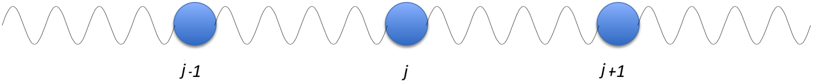
Stanislaw Ulam (1918-1984)



MANIAC I (1952-1957)

The weakly nonlinear 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

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

The result expected by Fermi

Equipartition of *linear* energy in momentum space (k-space)

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

then

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

with

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

The Los Alamos report

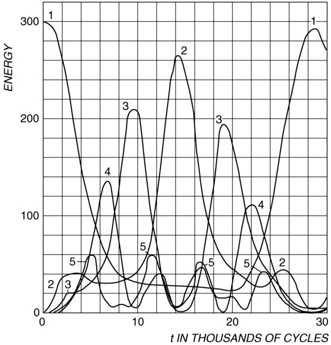
STUDIES OF NON LINEAR PROBLEMS

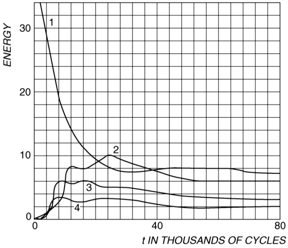
E. Fermi, J. Pasta, and S. Ulam

Document LA-1940 (May 1955).

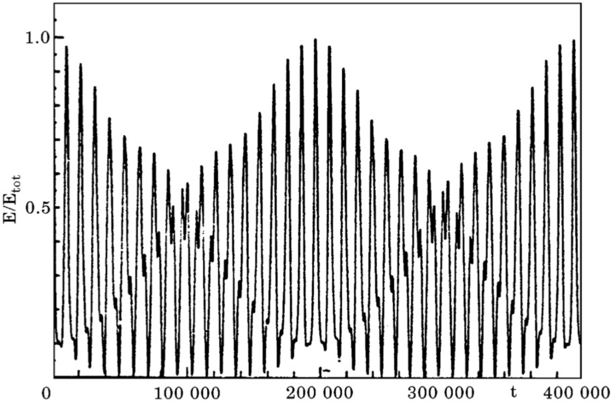
A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted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

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





The super-recurrence of Tuck and Menzel



Tuck, J. L., Menzel, M. T. (1972), Advances in Mathematics, 9(3), 399-407.

Following up on the “little discovery”

- “Experimental mathematics”
- Soliton theory
- Theory of integrable PDEs
- Hamiltonian Chaos

Ten years after FPU: solitons in physics

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

$$\eta_t + \eta\eta_x + \varepsilon^2\eta_{xxx} = 0$$

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

Numerical simulations of the KdV

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

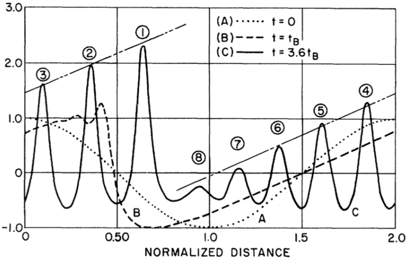


FIG. 1. The temporal development of the wave form $u(x)$.

Severn river in England during high flood tides

Interaction of these solitons appeared to be elastic

Discovery of integrability of the KdV

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)

In 1972 Zakharov and Shabat proved integrability of the Nonlinear Schrödinger equation. After the discovery, many other equations were found to be integrable (Sine-Gordon, Davey-Stewartson, Kadomtsev-Petviashvili, Toda Lattice, etc.)

... but FPU is not integrable!!

FPU and Hamiltonian Chaos

- KAM theorem (1954)
  Given
  $$H(I,\theta,\varepsilon) = H_0(I) + \varepsilon H_1(I,\theta),$$
  under the assumption that H_0 is sufficiently regular and that
  $$\left|\frac{\partial \omega_i}{\partial I_j}\right| = \left|\frac{\partial^2 H_0}{\partial I_i \partial I_j}\right| \neq 0$$
  if $\varepsilon \ll 1$, then invariant tori (KAM tori) survive on the surface of constant energy
- Chirikov Criterium (Izraielev and Chirikov, 1966): stochasticity due to frequency overlap
  $$R = \frac{\Omega_k}{\omega_{k+1} - \omega_k} > 1 \tag{1}$$
  R is resonance overlap parameter, Ω_k is the nonlinear frequency correction (due to self interaction)

Existence of a critical energy ε_c for FPU

PHYSICAL REVIEW A VOLUME 31, NUMBER 2 FEBRUARY 1985

Equipartition threshold in nonlinear large Hamiltonian systems: The Fermi-Pasta-Ulam model

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Picture coming out:

- if $\varepsilon < \varepsilon_c$ the KAM tori are dominant and the system does not reach equipartition
- if $\varepsilon \geq \varepsilon_c$ the system reach equipartition according to statistical mechanics

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.

Recent numerical work

J Stat Phys (2013) 152:195–212
DOI 10.1007/s10955-013-0760-6

The Fermi-Pasta-Ulam Problem and Its Underlying Integrable Dynamics

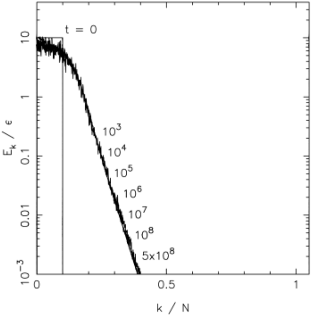
G. Benettin · H. Christodoulidi · A. Ponno

For small initial energy density two well separated time-scales are present:

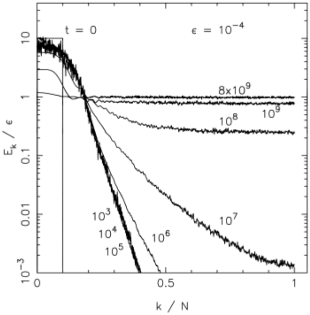
- metastable
- statistical equilibrium

Numerical simulations (Benettin et al. J Stat Phys 2013)

- The first time scale is the one in which FPU behaves essentially as an integrable system
- The second time scale is instead typical of a nonintegrable dynamics and statistical equilibrium is possible



Toda Lattice simulation



FPU simulation

The wave-wave interaction approach

Work in collaboration with L. Vozella, D. Proment and Y. L'vov

The large time behavior of the chain is ruled by exact resonant interactions

$$k_1 \pm k_2 \pm .... \pm k_m = 0$$
$$\omega(k_1) \pm \omega(k_2) \pm ... \pm \omega(k_m) = 0$$

Normal modes

Assuming periodic boundary conditions, we introduce the wave action variable

$$a_k = \frac{1}{\sqrt{2\omega_k}}(P_k - i\omega_k Q_k),$$

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

$$i\frac{da_1}{dt} = \omega_1 a_1 + \epsilon \sum_{k_2,k_3} V_{1,2,3}\Big(a_2 a_3 \delta_{1,2+3} + 2a_2^* a_3 \delta_{1,3-2} + a_2^* a_3^* \delta_{1,-2-3}\Big)$$

with the nonlinear parameter and matrix elements given by:

$$\epsilon = \alpha\sqrt{\sum \omega_k |a_k(t=0)|^2}, \quad V_{1,2,3} = -2sign(k_1 k_2 k_3)\sqrt{\omega_1 \omega_2 \omega_3}$$

The system is Hamiltonian with $H(a_k, a_k^*)$: $i da_k/dt = \partial H/\partial a_k^*$

The interaction reppresentation

Introduce the following rotation

$$a'_k(t) = a_k(t)e^{i\omega_k t},$$

then

$$i\frac{da'_1}{dt} = \epsilon \sum_{k_2,k_3} V_{1,2,3}\left(a'_2 a'_3 e^{i\Delta\Omega^{(1)}t}\delta_{1,2+3} + 2a'^*_2 a'_3 e^{i\Delta\Omega^{(2)}t}\delta_{1,3-2} + \right.$$

$$\left. + a'^*_2 a'^*_3 e^{i\Delta\Omega^{(3)}t}\delta_{1,-2-3}\right)$$

$$\Delta\Omega^{(1)} = \omega_1 - \omega_2 - \omega_3$$
$$\Delta\Omega^{(2)} = \omega_1 + \omega_2 - \omega_3$$
$$\Delta\Omega^{(3)} = \omega_1 + \omega_2 + \omega_3$$

Non existence of exact triads interactions for α-FPU

Exact three-wave resonant interactions

$$k_1 \pm k_2 \pm k_3 = 0$$
$$\omega_1 \pm \omega_2 \pm \omega_3 = 0$$

Given

$$\omega_k = 2|\sin(\pi k/N)|$$

it is trivial to show that three-wave resonant interactions are forbidden

The canonical transformation

$$H = \sum_{k_1} \omega_1 |a_1|^2 + \epsilon \sum_{k_1,k_2,k_3} V_{1,2,3} \Big[(a_1^* a_2 a_3 + a_1 a_2^* a_3^*) \delta_{1,2+3} +$$

$$+ \frac{1}{3} (a_1^* a_2^* a_3^* + a_1 a_2 a_3) \delta_{1,-2-3} \Big]$$

Eliminate the cubic nonlinearity from the Hamiltonian using a canonical transformation from $\{ia, a^*\}$ to $\{ib, b^*\}$

$$a_1 = b_1 + \epsilon \sum_{k_2,k_3} (A^{(1)}_{1,2,3} b_2 b_3 \delta_{1,2+3} + A^{(2)}_{1,2,3} b_2^* b_3 \delta_{1,3-2} +$$

$$+ A^{(3)}_{1,2,3} b_2^* b_3^* \delta_{1,-2-3}) + O(\epsilon^2)$$

with $A^{(1,2,3)}_{1,2,3} = V_{1,2,3}/(\omega_1 \pm \omega_2 \pm \omega_3)$.

The reduced system

The reduced Hamiltonian

$$\tilde{H} = \sum_{k_1} \omega_1 |b_1|^2 + \frac{1}{2}\epsilon^2 \sum_{k_1,k_2,k_3,k_4} T_{1,2,3,4} b_1^* b_2^* b_3 b_4 \delta_{1+2,3+4} + O(\epsilon^3)$$

The equation of motion

$$i\frac{db_1}{dt} = \omega_1 b_1 + \epsilon^2 \sum_{k_2,k_3,k_4} T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2,3+4} + O(\epsilon^3),$$

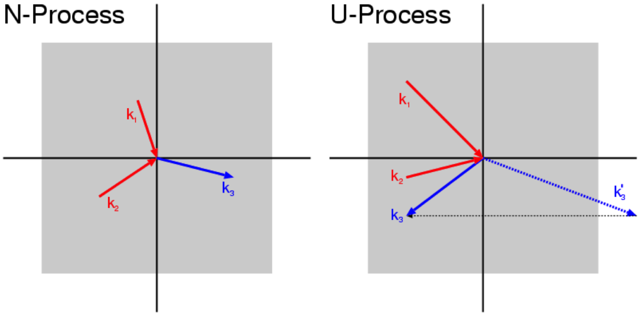
i.e. a four-wave interaction system

Four-wave resonant interactions in the α-FPU

Do 4-wave resonant interactions exist in the α-FPU system?

$$\begin{aligned} k_1 + k_2 &= k_3 + k_4 \\ \omega_1 + \omega_2 &= \omega_3 + \omega_4 \end{aligned} \tag{2}$$

Umklapp (flip-over) scattering



Normal process (N-process) and Umklapp process (U-process).
Example of an Umklapp scattering with $N = 32$ ($k_{max} = 16$),
$k_1 = 2$, $k_2 = 14$, $k_3 = -14$, $k_4 = 30$ $\rightarrow$ outside the Brillouin zone,
therefore the wave-number is flip-over $k_4' = k_4 - N = -2$

Four-wave resonant interactions in the α-FPU

$$k_1 + k_2 - k_3 - k_4 \overset{N}{=} 0,$$
$$\omega_1 + \omega_2 - \omega_3 - \omega_4 = 0$$

It is possible to show that 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*

$$\{k_1, k_2, -k_1, -k_2\}$$

with $k_1 + k_2 = mN/2$ and $m = 0, \pm 1, \pm 2, \ldots$

Four-wave resonant interactions in the α-FPU

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

The reduced Hamiltonian is integrable

$$H = \sum_{k_1} \omega_{k_1} |b_{k_1}|^2 + \frac{1}{2} \sum_{k_1} T_{k_1,k_1,k_1,k_1} |b_{k_1}|^2 |b_{k_1}|^2 +$$
$$+ \sum_{k_1 \neq k_2} T_{k_1,k_2,k_1,k_2} |b_{k_1}|^2 |b_{k_2}|^2 +$$
$$+ \sum_{k_1} T_{k_1,N/2-k_1,-k_1,-N/2+k_1} b^*_{k_1} b^*_{N/2-k_1} b_{-k_1} b_{-N/2+k_1}$$

This result was first obtained Henrici and Kappeler in Commun. Math. Phys. (2008) following some ideas developed by B. Rink in Commun. Math. Phys. (2006)

Six-wave interactions in the α-FPU

How to proceed?

Six-wave interactions in the α-FPU

How to proceed?

- perform a canonical transformation to higher order
- check for exact resonances at higher order

$$i\frac{db_1}{dt} = \omega_1 b_1 + \epsilon^2 \sum_{k_2,k_3,k_4} T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2,3+4} +$$
$$+ \epsilon^4 \sum W_{1,2,3,4,5,6} b_2^* b_3^* b_4 b_5 b_6 \delta_{1+2+3,4+5+6}$$

Resonant conditions:

$$k_1 + k_2 + k_3 - k_4 - k_5 - k_6 \overset{N}{=} 0$$
$$\omega_1 + \omega_2 + \omega_3 - \omega_4 - \omega_5 - \omega_6 = 0,$$

Non-isolated solutions exist for integer values of k with $N = 16, 32, 64$

Solutions of the six-wave resonant conditions

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

$$k_1 = k_4,\ k_2 = k_5,\ k_3 = k_6$$

- *Nontrivial symmetric resonances*:

$$\{k_1, k_2, k_3, -k_1, -k_2, -k_3\},$$

with $k_1 + k_2 + k_3 = mN/2$ and $m = 0, \pm 1, \pm 2, ...$

- *Nontrivial quasi-symmetric resonances*

$$\{k_1, k_2, k_3, -k_1, -k_2, k_3\},$$

with $k_1 + k_2 = mN/2$ and $m = 0, \pm 1, \pm 2, ...$

Estimation of the equipartition time scale for random waves

The equipartition is a statistical feature and time scale should be estimated from a statistical theory

$$i\frac{db_1}{dt} = \omega_1 b_1 + \epsilon^4 \sum W_{1,2,3,4,5,6} b_2^* b_3^* b_4 b_5 b_6 \delta_{1+2+3,4+5+6}$$

Introduce the following correlators

$$\langle b_1^* b_2 \rangle = n_1 \delta_{k_2,k_1}$$
$$\langle b_1^* b_2^* b_3^* b_4 b_5 b_6 \rangle = J_{1,2,3,4,5,6} \delta_{k_1+k_2+k_3,k_4+k_5+k_6}$$

Estimation of the equipartition time scale for random waves

The evolution equation for $n(k)$

$$\frac{\partial n(k_1)}{\partial t} = \epsilon^4 Im \left[\sum W_{1,2,3,4,5,6} J_{1,2,3,4,5,6} \delta_{k_1+k_2+k_3,k_4+k_5+k_6} \right]$$

with

$$Re\left[J_{1,2,3,4,5,6}\right] \sim \epsilon^4 W_{1,2,3,4,5,6}$$

Therefore

$$\frac{\partial n(k_1)}{\partial t} \sim \epsilon^8 \sum ...$$

and the time of equipartition scales as

$$\mathbf{t_{eq} \sim 1/\epsilon^8}$$

Estimation of the equipartition time scale for random waves

The equipartition is a statistical feature and time scale should be estimated from a statistical theory

The evolution equation for $n(k) =< |b(k)|^2 >$

Random phase approximation

After long calculation

$$\frac{\partial n(k)}{\partial t} \sim \epsilon^8 \sum ...$$

and the time of equipartition scales as

$$\mathbf{t_{eq} \sim 1/\epsilon^8}$$

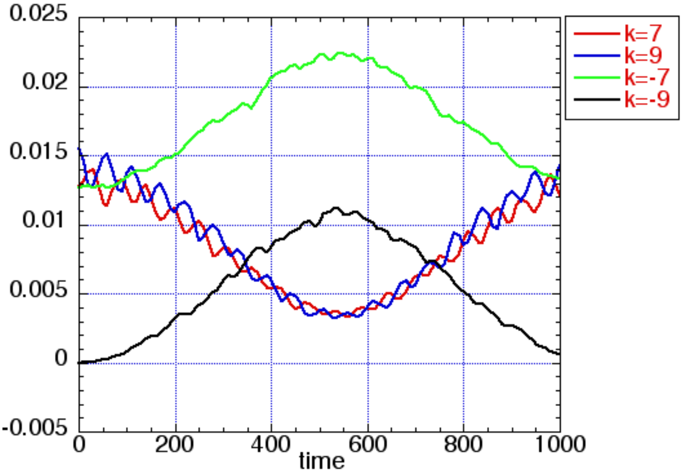
Numerical simulations

- Symplectic integrator (H. Yoshida, 1990 Phys. Lett. A)
- Numerical simulations with N=32 modes

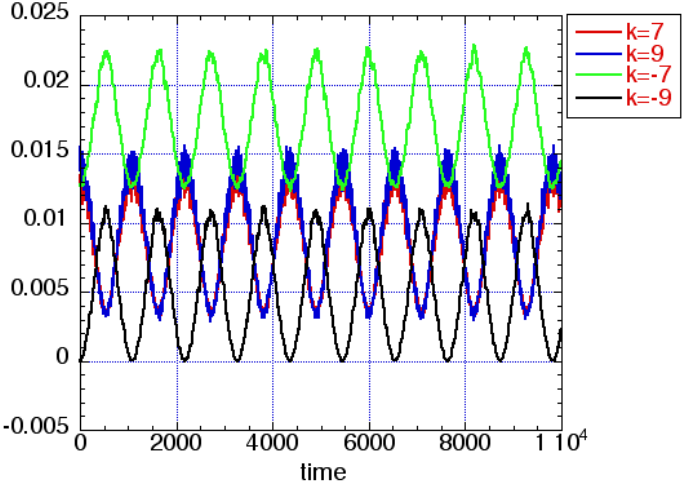
Numerical simulation

Initial condition characterized by $\epsilon = 0.012$ and 3 modes belonging to a quartet:
$k_1 = 7$, $k_2 = 9$, $k_3 = -7$, expecting $k_4 = -9$

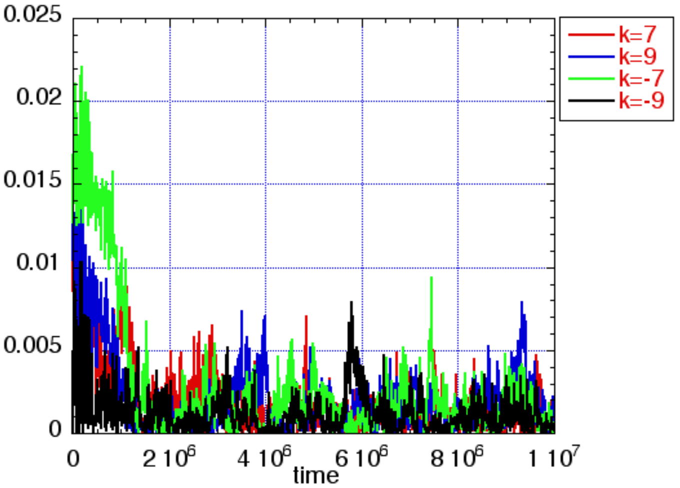
Numerical simulations: “short” time scale



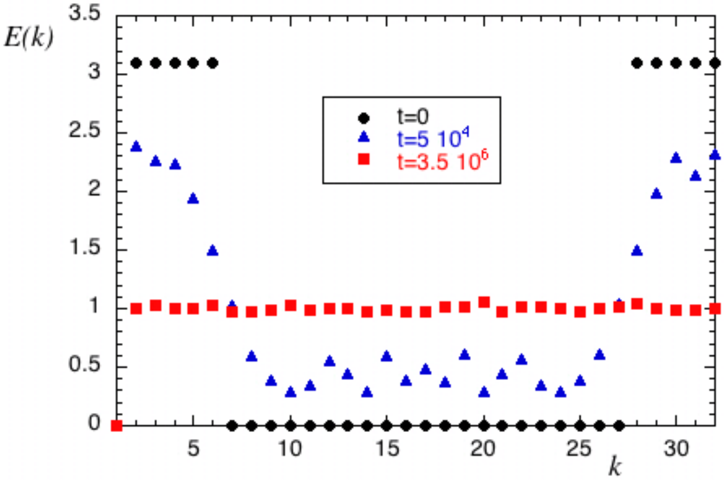
Numerical simulations: four wave interactions



Numerical simulations: "large" time scales - transition to chaotic state

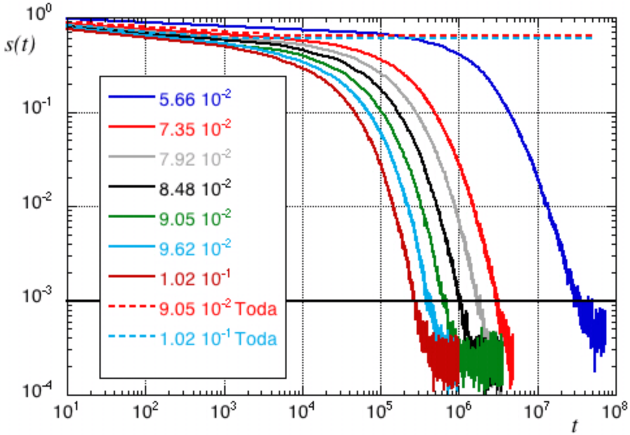


Numerical simulations: thermalization

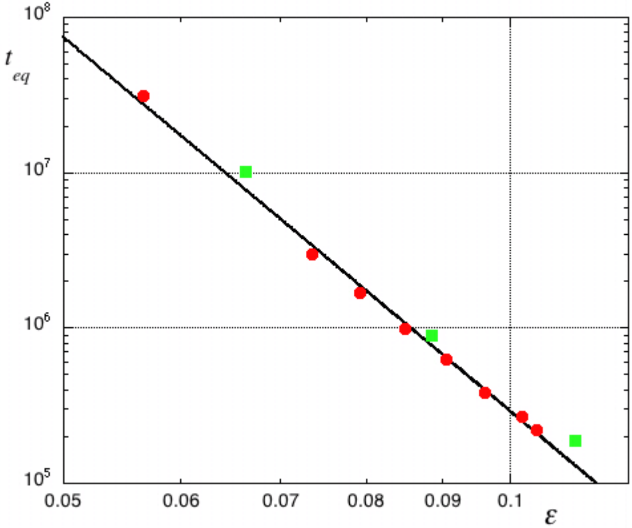


Entropy

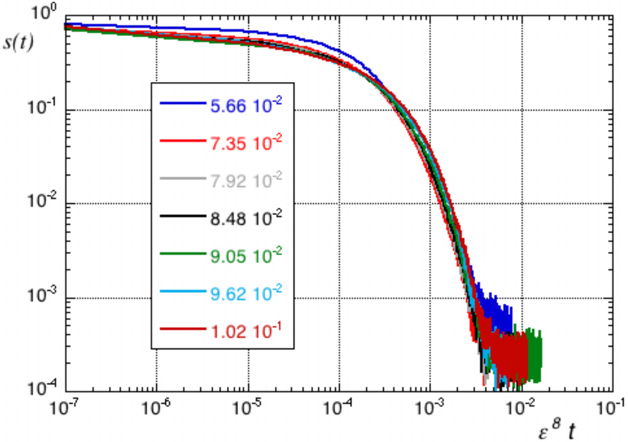
$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{E_{tot}} \omega_k \langle |a_k|^2 \rangle, \quad E_{tot} = \sum_k \omega_k \langle |a_k|^2 \rangle$$



Scaling in time



Collapse of entropy curves



E. Fermi with E. Amaldi in Varenna, 1954

The Thermodynamic Limit

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

Then the 4-wave equation of motion becomes:

$$i\frac{\partial b_1}{\partial t} = \omega_1 b_1 + \epsilon^2 \int T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2,3+4} dk_2 dk_3 dk_4$$

Exact 4-wave resonant interactions exist and are not isolated.

No need to go to higher order in wave interaction!

The Wave Kinetic Equation

- Look for an evolution equation for the correlator $< b(\kappa_i, t) b(\kappa_j, t)^* >= n(\kappa_i, t)\delta(\kappa_i - \kappa_j)$
- BBGKY hierarchy: need of a clousure
- Assume quasi-gaussian approximation (Wick's decomposition)

$$\frac{\partial n_1}{\partial t} = 4\pi\epsilon^4 \int T^2_{1,2,3,4} n_1 n_2 n_3 n_4 \left(\frac{1}{n_1} + \frac{1}{n_2} - \frac{1}{n_3} - \frac{1}{n_4} \right) \delta(\Delta\kappa)\delta(\Delta\omega) d\kappa_{2,3,4}$$

$$\delta(\Delta\kappa) = \kappa_1 + \kappa_2 - \kappa_3 - \kappa_4$$
$$\delta(\Delta\omega) = \omega(\kappa_1) + \omega(\kappa_2) - \omega(\kappa_3) - \omega(\kappa_4)$$

The Wave Kinetic Equation

Conserved quantities:

$$E = \int \omega(\kappa) n(\kappa, t) d\kappa, \qquad N = \int n(\kappa, t) d\kappa, \qquad P = \int \kappa n(\kappa, t) d\kappa \tag{3}$$

Existence of an H-theorem:

$$H = \int \ln(n(\kappa, t)) d\kappa \tag{4}$$

$$\frac{dH}{dt} \leq 0 \tag{5}$$

The Rayleigh-Jeans distribution

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

where constants T and μ have the meaning of temperature and chemical potential.

Conclusions

- Resonant triads are forbidden; this implies that on the short time scale three-wave interaction will generate a reversible dynamics
- A suitable canonical transformation allows us to look at higher order interactions in the system which are responsible for longer time scale dynamics
- Four-wave resonant interactions exist; however, we have shown that each resonant quartet is isolated, preventing the full spread of energy across the spectrum and thermalization

Conclusions

- The first significant interaction is the six-wave one; on the time scale of these interactions, one possibly may observed the equipartition phenomenon
- In the thermodynamic limit a wave kinetic equation can be built and thermodynamic solution can be found analytically

The End

Prospectives

- Increasing the level of nonlinearity may lead to a different dynamics because of the presence of quasi-resonances
- Nonlinear frequency renormalization, quasi-resonances and its relation to the stochastic threshold is the subject of current investigation
- Numerical simulations are being performed in order to check the time scales
- Thermodynamic limit
- Check scaling with ϵ and N

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N} V(q_{i+1} - q_i),$$

- α-FPU model:

$$V(r) = \frac{r^2}{2} + \alpha\frac{r^3}{3}$$

- Toda Lattice (Flaschka 1974, Henon 1974, Manakov, 1974):

$$V(r) = V_0(e^{\lambda r} - 1 - \lambda r), \qquad V_0,\ \lambda \quad \text{free} \quad \text{parameters}$$

For the particular choice

$$V_0 = \frac{1}{4\alpha^2}, \qquad \lambda = 2\alpha$$

the Toda potential is tangent to the FPU one

$$V(r) = \frac{1}{2}r^2 + \alpha\frac{1}{3}r^3 + \frac{1}{6}\alpha^2 r^4 + \ldots \tag{6}$$

Fundamental difference between FPU and Toda Lattice

The reduced Hamiltonian

$$\tilde{H} = \sum_{k_1} \omega_1 |b_1|^2 + \frac{1}{2}\epsilon^2 \sum_{k_1,k_2,k_3,k_4} T_{1,2,3,4} b_1^* b_2^* b_3 b_4 \delta_{1+2,3+4} + O(\epsilon^3)$$

The equation of motion

$$i\frac{db_1}{dt} = \omega_1 b_1 + \epsilon^2 \sum_{k_2,k_3,k_4} T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2,3+4} + O(\epsilon^3)$$

For the Toda Lattice it is possible to show that the $T_{1,2,3,4}$ is identically zero on the resonant manifold. Same result holds for any wave-wave interaction up to infinity!!