Thermalization in one-dimensional anharmonic chains: the Wave Turbulence approach

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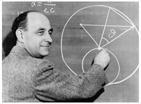
May 20, 2022

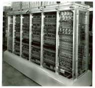
The weakly nonlinear one-dimensional chain model


Enrico Fermi (1901-1954)

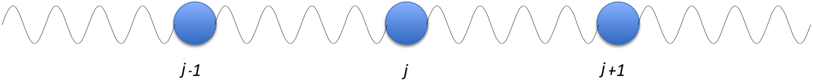

John Pasta (1909-1984)


Stanislaw Ulam (1918-1984)


Mary Tsingou-Menzel (1928-)

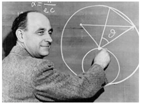

MANIAC I (1952-1957)

N equal masses connected by springs



$$F = -\kappa \Delta q$$

The weakly nonlinear one-dimensional chain model



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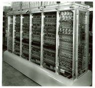

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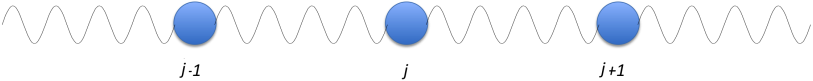
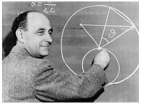


$$F = -\kappa \Delta q + \alpha \Delta q^2 + \beta \Delta q^3 + \ldots$$

The weakly nonlinear one-dimensional chain model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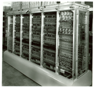
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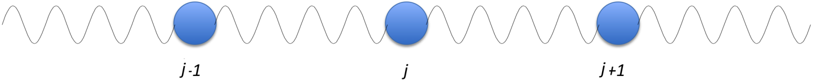


$$F = -\kappa \Delta q + \alpha \Delta q^2 + \beta \Delta q^3 + \dots$$

The Hamiltonian

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

The result expected by Fermi and collaborators

Equipartition of harmonic energy in Fourier space for large times

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

then

$$E_k = |P_k|^2 + \omega_k^2 |Q_k|^2 = const \quad (\text{in} \;\; k)$$

with

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

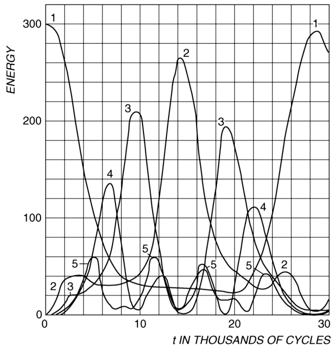
STUDIES OF NON LINEAR PROBLEMS

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.



Following up on the "little discovery"

- Soliton theory
- Theory of integrable PDEs
- Hamiltonian Chaos

Some years after FPUT: solitons and integrability in physics

In the limit of long waves (continuum limit) the α-FPUT 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)

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

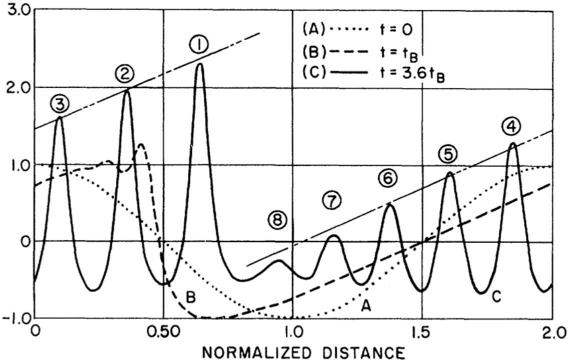
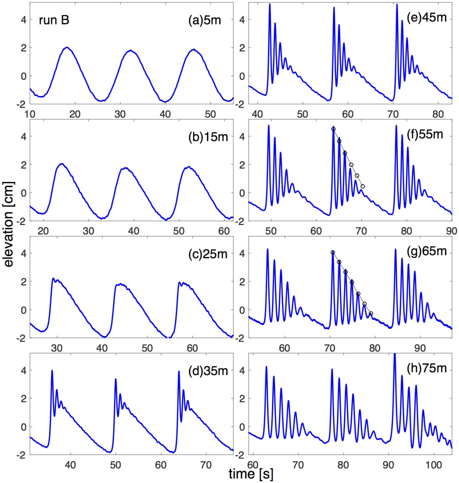


FIG. 1. The temporal development of the wave form $u(x)$.

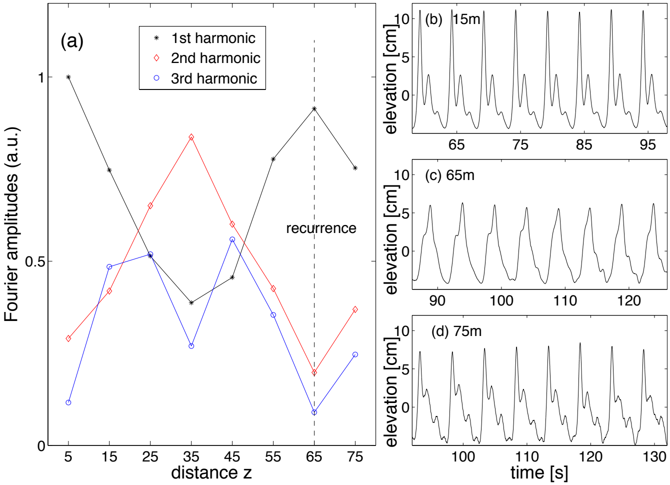
Experimental demonstration of the ZK solitons



Trillo et. al PRL 2016

The wave tank in Berlin (5 m $\times$ 90 m $\times$ 15 cm)

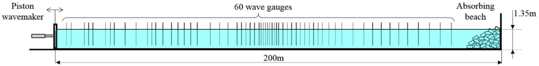
FPUT recurrence in shallow water (Trillo et. al PRL 2016)

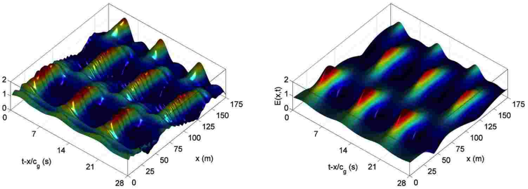


FPUT recurrence in deep water (Kimmoun et al, Sci. Reports 2016)

In the limit of narrow band process, the β-FPUT system reduces to the Nonlinear Schrödinger equation:

$$i\frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial x^2} + |\psi|^2\psi = 0$$





See new theoretical result:
Conforti, Mussot, Kudlinski, Trillo and Akhmediev, Phys Rev A 2020,
Coppini, Grinevich and Santini, Phys Rev E 2020

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.

Open questions

... but FPUT is not an integrable system...

- Does the system thermalize for arbitrary small nonlinearity?
- What is the thermalization time scale in the thermodynamic limit?
- What is the time scale of thermalization for finite N?

The models

- α-FPUT

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

- β-FPUT

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

- Toda Lattice

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

The dispersion relation:

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

We assume

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

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 $\omega_k = 2|\sin(\pi k/N)|$
Because of the absence of 3-wave resonant interactions, i.e.:

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

quadratic nonlinearity can be removed from α-FPUT and Toda. The system is characterized by the existence of 4-wave resonant interactions:

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

Reduced Hamiltonian for all 3 models

$$\frac{H}{N} = \sum_{k=0}^{N-1} \omega_k |a_k|^2 + \epsilon \frac{1}{2} \sum_{k_1,k_2,k_3,k_4} T_{1,2,3,4} a_1^* a_2^* a_3 a_4 \delta_{1+2,3+4}$$

with

$$a_i = a(k_i, t), \quad T_{1,2,3,4} = T(k_1, k_2, k_3, k_4)$$

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

The reduced evolution equation:

$$i\frac{da_k}{dt} = \omega_k a_k + \epsilon \sum_{k_2,k_3,k_4} T_{1,2,3,4} a_2^* a_3 a_4 \delta_{1+2,3+4}$$

The Wave Turbulence Approach

- A statistical theory of weakly interacting dispersive waves
- Main output: the Wave Kinetic Equation
- Equilibrium and out of equilibrium stationary solutions
- The theory is based on the existence of resonances
- Application in a variety of fields as: water waves, plasma waves, BEC, elastic plates ...

Vladimir Zakharov, Dirac Medal 2003

Klaus Hasselmann, Nobel Prize 2021

The Wave Kinetic Equation

Outline of the procedure for "deriving" the WKE:

- From the normal variable a_k, move to angle-action variables $\{I_k, \theta_k\}$

$$a_k(t) = \sqrt{I_k(t)}e^{-i\theta_k(t)}$$

- Expand $I_k(t)$ and $\theta_k(t)$ in powers of ϵ
- Take averages over initial random phases and amplitudes, $\langle I_k(t)\rangle_{\{\bar{\theta}_k,\bar{I}_k\}}$
- Take the thermodynamic limit, $L \to \infty$, and define the wave action spectral density function:

$$n(k,t) := \frac{L}{2\pi}\langle I_k(t)\rangle_{\{\bar{\theta}_k(t),\bar{I}_k\}}$$

- Take the small ϵ limit

Rigorous derivation of the WKE for NLS, see Deng and Zaher arXiv:2104.11204, 2021

The WKE and its properties

$$\frac{\partial n(k_1,t)}{\partial t} = C(k_1,t)$$

$$C(k_1,t) = \epsilon^2 \int_0^{2\pi} T^2_{1,2,3,4} n_1 n_2 n_3 n_4 \left(\frac{1}{n_1} + \frac{1}{n_2} - \frac{1}{n_3} - \frac{1}{n_4}\right) \delta(\Delta k)\delta(\Delta\omega) dk_{2,3,4}$$

$$\delta(\Delta k) = \delta(k_1 + k_2 - k_3 - k_4)$$

$$\delta(\Delta \omega) = \delta(\omega(k_1) + \omega(k_2) - \omega(k_3) - \omega(k_4))$$

Conserved quantities:

$$E = \int_0^{2\pi} \omega(k) n(k,t) dk, \qquad N = \int_0^{2\pi} n(k,t) dk.$$

Existence of an H-theorem:

$$S = \int_0^{2\pi} \ln(n(k,t)) dk, \quad \text{with} \quad \frac{dS}{dt} \geq 0$$

The Rayleigh-Jeans distribution

$$dS/dt = 0 \to n(k) = \frac{T}{\omega(\kappa) - \mu}$$

Thermalization time scale: $1/\epsilon^2$

The Wave Kinetic Equation

Conserved quantities:

$$E = \int_0^{2\pi} \omega(\kappa) n(\kappa, t) d\kappa, \qquad N = \int_0^{2\pi} n(\kappa, t) d\kappa,$$

Existence of an H-theorem:

$$H = \int_0^{2\pi} \ln(n(\kappa, t)) d\kappa, \quad \text{with} \quad \frac{dH}{dt} \geq 0$$

The Rayleigh-Jeans distribution

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

Thermalization time scale: $1/\epsilon^2$

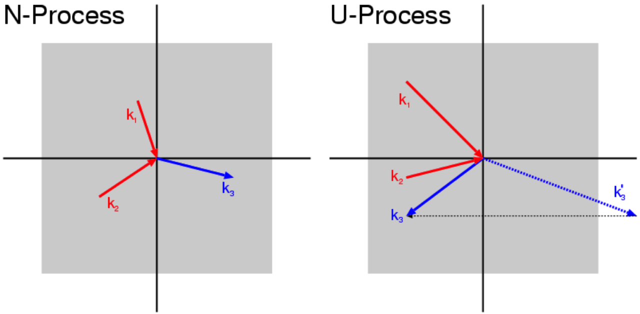
Small N regime

$\omega_k = 2|\sin(\pi k/N)|$ with $k \in \mathbb{Z}$

It can be shown that only the following interactions are possible (of Umklapp type):

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

Umklapp (flip-over) scattering



Normal process (N-process) and Umklapp process (U-process).
Example of an Umklapp scattering with $N = 32$ ($k_{max} = 16$),
$k_1 = 7$, $k_2 = 9$, $k_3 = -7$, $k_4 = 23$ → outside the Brillouin zone, therefore the wave-number is flip-over $k_4' = k_4 - N = -9$

Small N regime

For N power of 2, 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)

Removing non resonant interactions

$$\frac{H}{N} = \sum_{k=0}^{N-1} \omega_k |a_k|^2 + \epsilon \sum_{k_1,k_2,k_3,k_4} \Big[T^{(1)}_{1,2,3,4} (a_1^* a_2 a_3 a_4 + c.c.) \delta_{1-2-3-4} +$$

$$+ \frac{1}{2} T^{(2)}_{1,2,3,4} a_1^* a_2^* a_3 a_4 \delta_{1+2-3-4} + \frac{1}{4} T^{(3)}_{1,2,3,4} (a_1 a_2 a_3 a_4 + c.c.) \delta_{1+2+3+4} \Big]$$

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

$$a_1 = b_1 + \epsilon \sum_{k_2,k_3,k_4} (B^{(1)}_{1,2,3,4} b_2 b_3 b_4 \delta_{1-2-3-4} + B^{(2)}_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2-3-4} +$$

$$+ B^{(3)}_{1,2,3,4} b_2^* b_3^* b_4 \delta_{1+2+3-4} + B^{(4)}_{1,2,3,4} b_2^* b_3^* b_4^* \delta_{1+2+3+4}) + O(\epsilon^2)$$

with $B_{1,2,3,4} \simeq T_{1,2,3,4} / (\omega_1 \pm \omega_2 \pm \omega_3 \pm \omega_4)$.

Removing non-resonant four-wave interactions: the appearance six-wave interactions in the β-FPUT

- check for exact resonances at higher order

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

Resonant conditions:

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

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

$$\frac{dn_1}{dt} \sim \epsilon^4 \ldots$$

Estimation of the equipartition time scale for incoherent waves

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

$$\frac{dn_1}{dt} \sim \epsilon^2 < b_1^* b_2^* b_3^* b_4 b_5 b_6 >$$
$$\frac{d < b_1^* b_2^* b_3^* b_4 b_5 b_6 >}{dt} \sim \epsilon^2 < b_1^* b_2^* b_3^* b_4^* b_5 b_6 b_7 b_8 >$$

therefore

$$\frac{dn_1}{dt} \sim \epsilon^4 ....$$

and the time of equipartition scales as

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

Estimation of the equipartition time scale

- Thermodynamic limit: 4-wave resonant interactions

$$\mathbf{t_{eq} \sim 1/\epsilon^2}$$

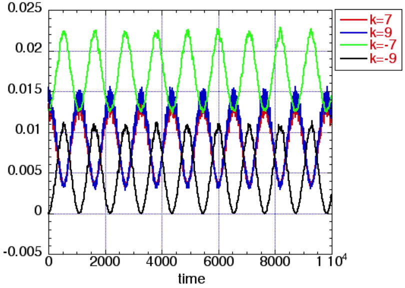
- Small N: 6-wave resonant interactions

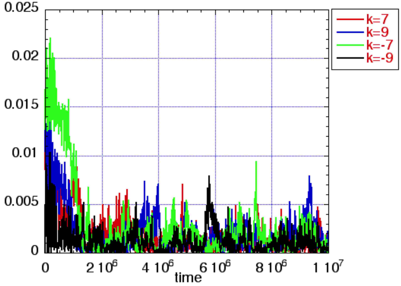
$$\mathbf{t_{eq} \sim 1/\epsilon^4}$$

Numerical simulations (symplectic integrator, H. Yoshida, 1990 Phys. Lett. A)

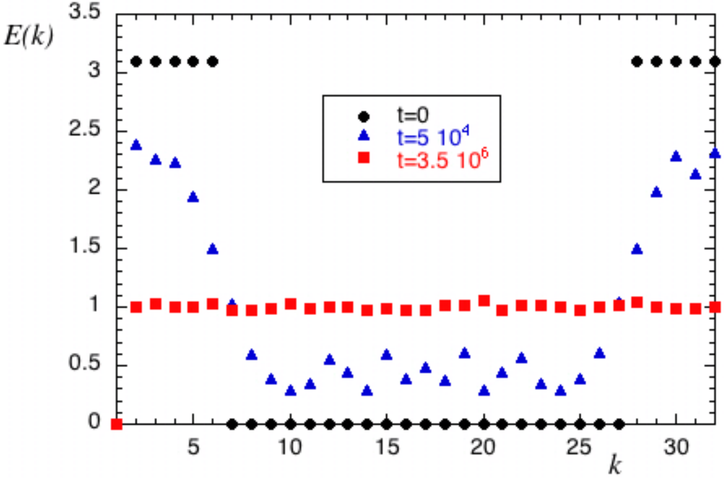
- Example of Umklapp resonance

Numerical simulations



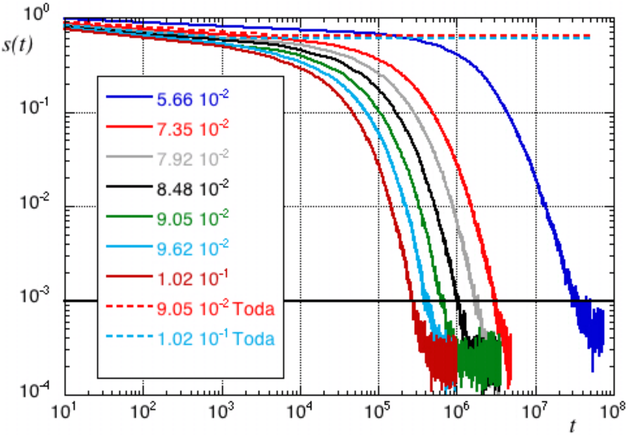


Example of thermalization for α-FPUT with $N=32$, $\epsilon = 7.3\times10^{-2}$ (1000 realizations)

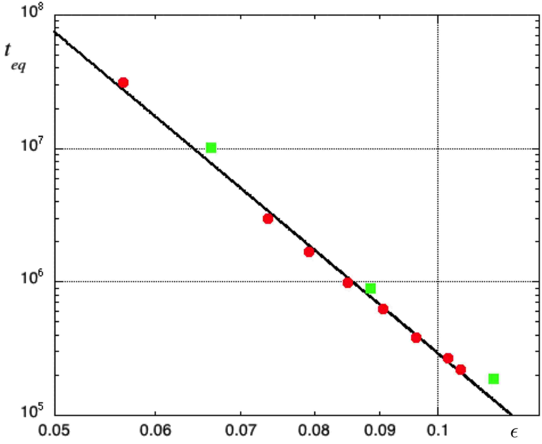


Entropy

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

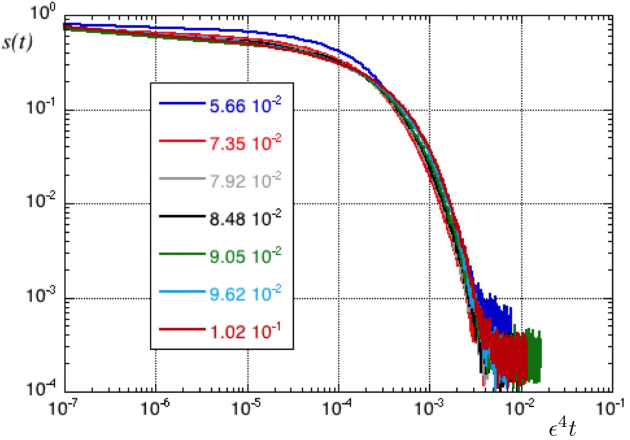


Scaling in time

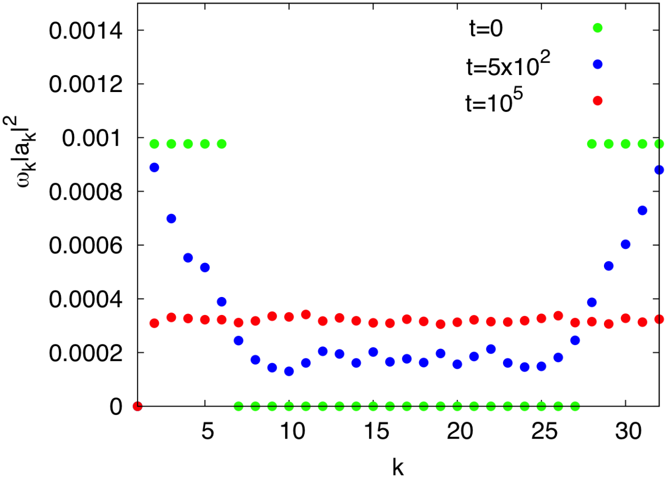


M.O, D. Proment, L. Vozella, Y. Lvov, P.N.A.S. 2015

Collapse of entropy curves

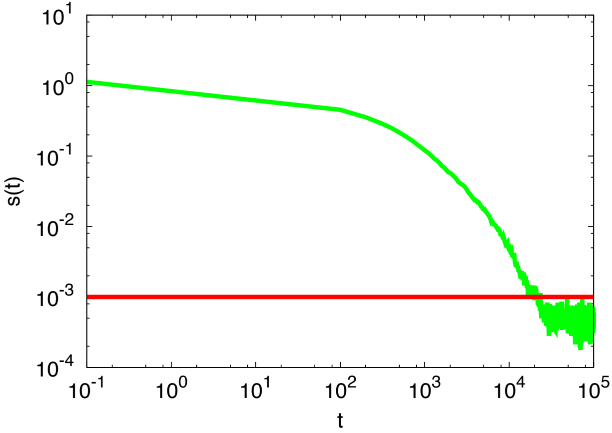


Example of equipartition: β-FPUT, $N=32$, $\epsilon = 7.05 \times 10^{-2}$

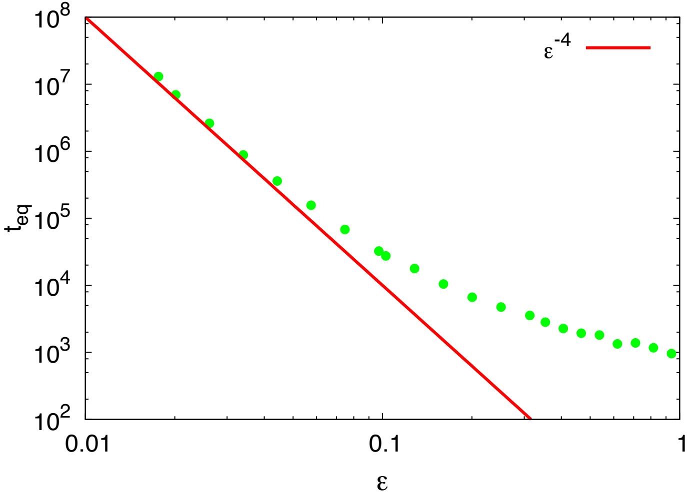


Entropy: β-FPUT, $\epsilon = 7.05 \times 10^{-2}$, $N = 32$

$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{H_0}\omega_k \langle |a_k|^2 \rangle, \quad H_0 = \sum_k \omega_k \langle |a_k|^2 \rangle$$

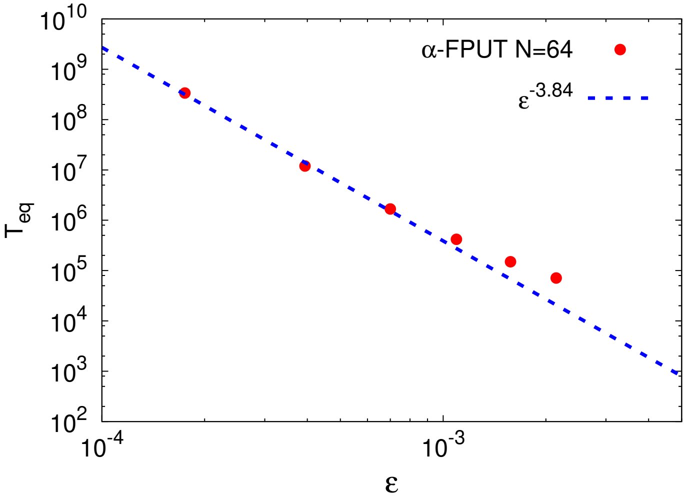


Equipartition time as a function of ϵ

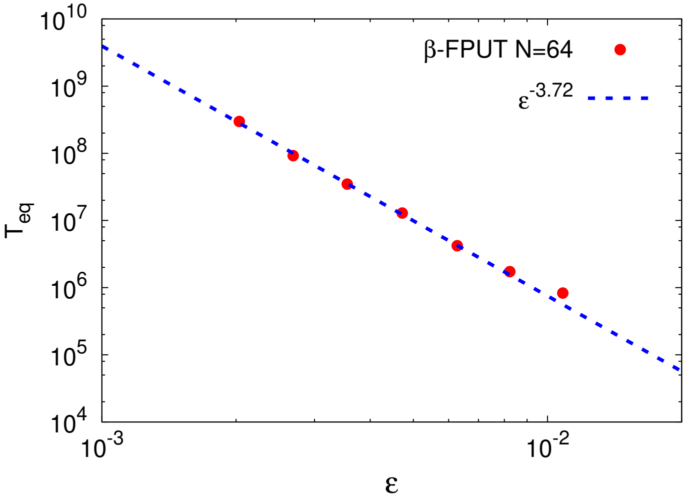


Y. Lvov, M.O., PRL 2018

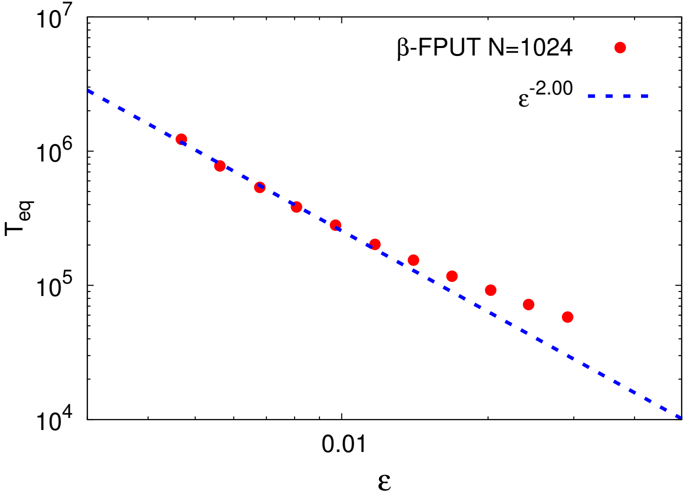
Equipartition time as a function of ϵ: $\alpha - FPUT$ N=64



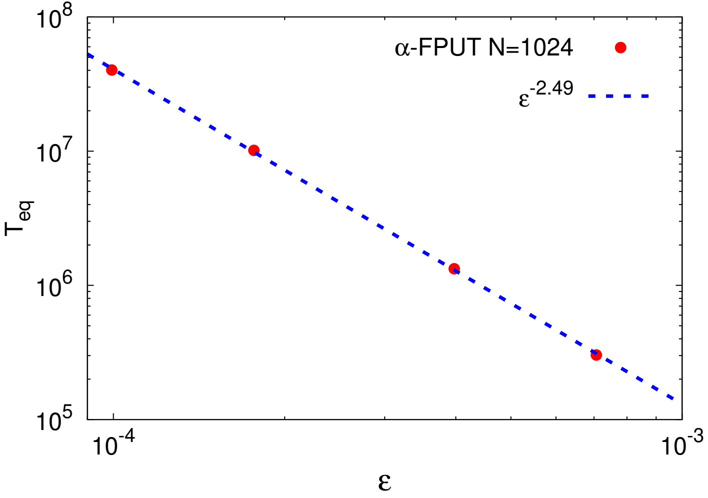
Equipartition time as a function of ϵ: $\beta - FPUT$ N=64



Equipartition time as a function of ϵ: $\beta - FPUT$ N=1024



Equipartition time as a function of ϵ: $\alpha - FPUT$ N=1024



DNKG equation: from discrete to the Large Box Limit

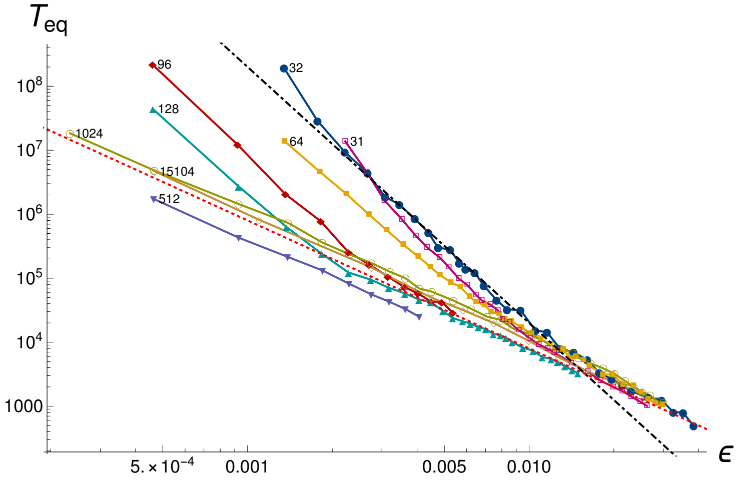
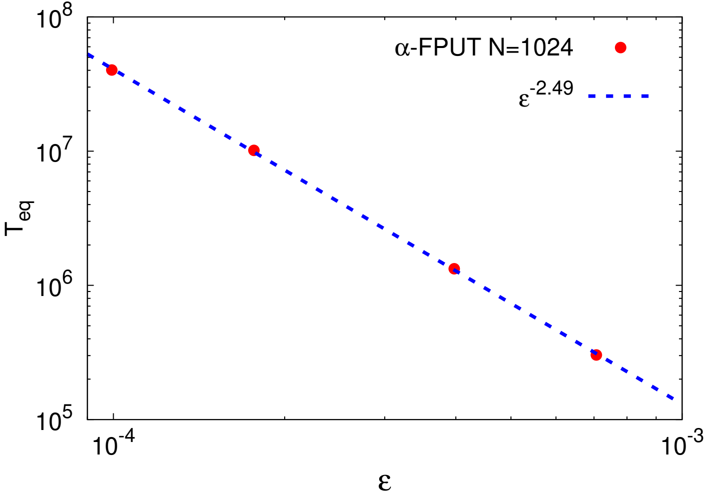


Figure: The scaling of T_{eq} on ϵ for multiple values of N, with $m = 1$ and $E = 0.1N/32$. Scaling laws ϵ^{-2} and ϵ^{-4} in red dotted and black dash-dotted lines for reference.

Conclusions

- The unfinished work of Fermi in Los Alamos triggered new science
- Wave Turbulence theory is an extremely interesting framework for studying interacting waves
- The FPUT system, despite its apparent simplicity, still needs a lot of work for being fully understood

Equipartition time as a function of ϵ: $\alpha - FPUT$ N=1024



Estimation of the frequency shift and broadening

$$i\frac{da_1}{\partial t} = \omega_1 a_1 + \epsilon \sum_{2,3,4}^{N-1} T_{1,2,3,4} a_2^* a_3 a_4 \delta_{1,2}^{3,4}$$

$$a_k = \sqrt{I_k}\phi_k \quad \text{with} \quad \phi_k = \exp[-i\theta_k]$$

$$\frac{d\theta_1}{\partial t} = \omega_1 + \epsilon \sum_{k_i} T_{1,2,3,4} \frac{\sqrt{I_2 I_3 I_4}}{\sqrt{I_1}} \Re[\phi_1^* \phi_2^* \phi_3 \phi_4] \delta_{1,2}^{3,4}$$

Using Wick decomposition we get:

$$\tilde{\omega}_k = \langle \frac{d\theta_k}{dt} \rangle = \omega_k + 2\epsilon \sum_l T_{k,l,k,l} I_l - \beta T_{k,k,k,k} I_k$$

$$\Gamma_k = \sqrt{\langle \left(\frac{d\theta_k}{\partial t} - \tilde{\omega}_k \right)^2 \rangle} = \sqrt{5}\epsilon \sum_l T_{k,l,k,l} I_l$$

DNKG simulations: the Entropy

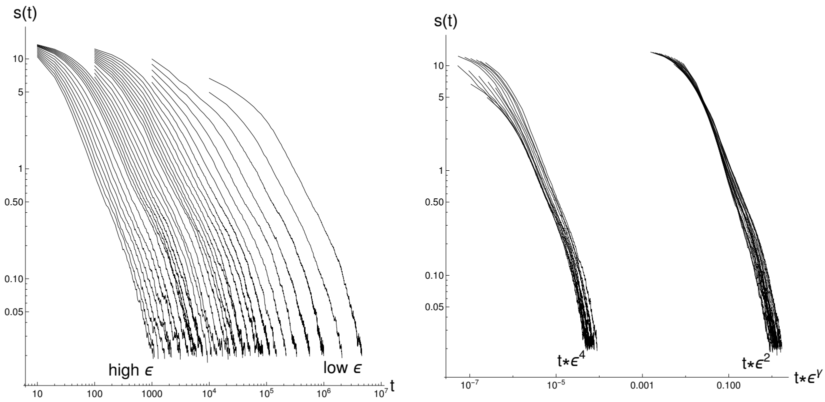


Figure: The entropy curves are naturally ordered from left to right for decreasing ϵ, with values in the range $0.002 \sim 0.03$ for $N = 64$. On the right, the same curves with rescaled time: the two regimes $T_{eq} \propto \epsilon^{-2}$ and $T_{eq} \propto \epsilon^{-4}$ are highlighted by scaling the time either by ϵ^2 or by ϵ^4

DNKG simulations: frequency mismatch

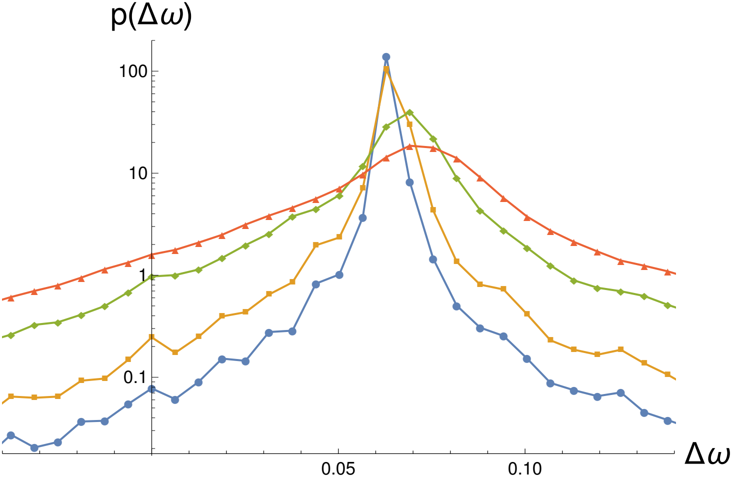


Figure: The dispersion of the frequency mismatch $\Delta\omega$, renormalized as a probability, for a $2 \to 2$ resonance with $N = 32$ and $k = \{1, -15, -11, -3\}$, with $\epsilon \simeq$ 0.0026 (●), 0.0052 (■), 0.0144 (♦), 0.023 (▲).

DNKG equation: from discrete to the Large Box Limit

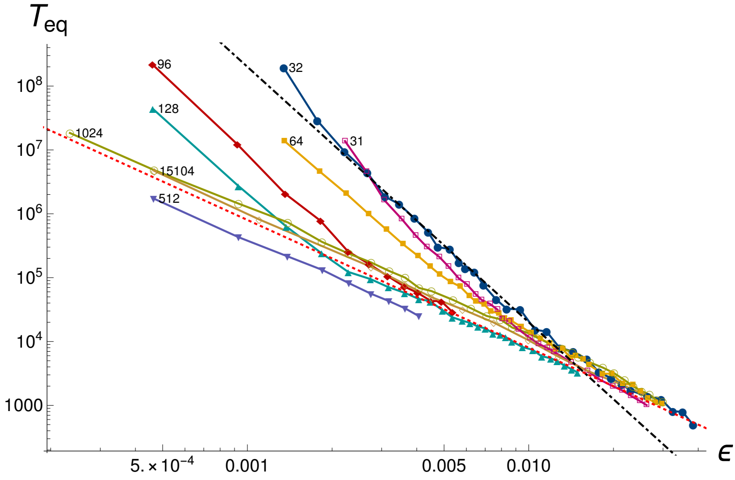
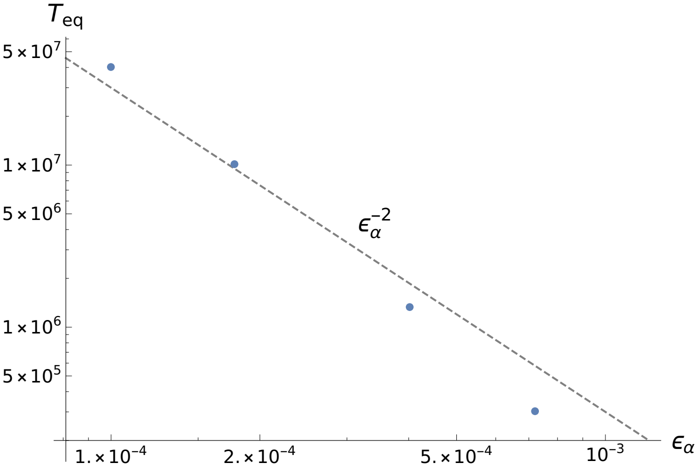
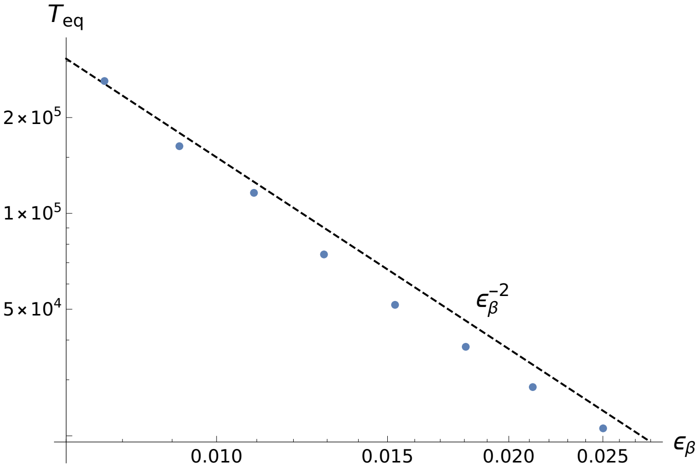


Figure: The scaling of T_{eq} on ϵ for multiple values of N, with $m = 1$ and $E = 0.1N/32$. Scaling laws ϵ^{-2} and ϵ^{-4} in red dotted and black dash-dotted lines for reference.

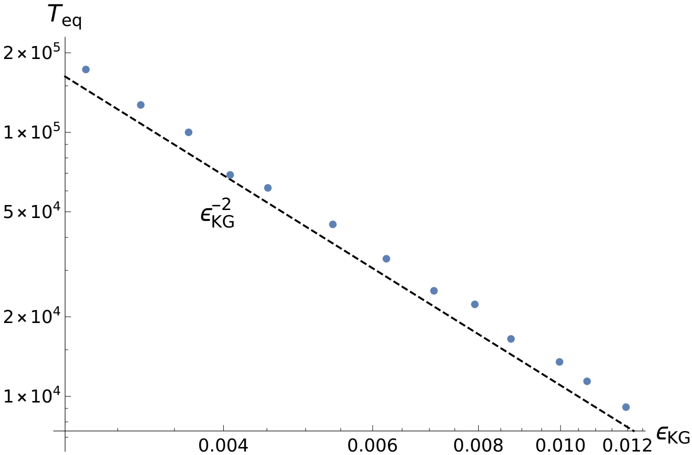
The thermodynamic limit: α-FPU



The thermodynamic limit: β-FPU



The thermodynamic limit: DNKG



Conclusions

- The FPUT/DNKG systems thermalize for arbitrary small nonlinearity
- 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

E. Fermi with E. Amaldi in Varenna, 1954

ETC 2019

17th European Turbulence Conference

Deadlines

Opening of abstract submissions:
October 20, 2018

Deadline for abstract submissions:
January 31, 2019

Notification of acceptance:
April 2, 2019

Opening of registrations:
April 2, 2019

Deadline for early bird registration: May 5, 2019

EUROPEAN MECHANICS SOCIETY — POLITECNICO DI TORINO — UNIVERSITÀ DEGLI STUDI DI TORINO

TORINO • Italy **3-6 September 2019**

CALL FOR ABSTRACTS

Newsletter No. 1 • October 2018

The 17th EUROPEAN TURBULENCE CONFERENCE (ETC17) is pleased to release its Call for Abstracts.

The deadline for the submission of abstracts is **January 31, 2019**.
All available details, including the list of the invited speakers can be found on the conference website ***www.etc17.it***.

We look forward to welcoming you to ETC17 in Torino, Italy, from 3 to 6 September 2019.

On behalf of the Organizing and Scientific Committees
Guido Boffetta, Daniela Tordella, Miguel Onorato

Topics

- *Acoustics of Turbulent Flows*
- *Instability, Transition and Control of Turbulent Flows*
- *Intermittency and Scaling*
- *Boundary Free Turbulence*
- *Wall Bounded Turbulence*
- *Fluid-structure Interaction*
- *Turbulent Convection*
- *Stratified Flows*
- *Rotating Flows*
- *Compressible Flows*
- *Non-Newtonian Flows*
- *Multiphase Flows*
- *Reacting Flows*
- *Wave Turbulence*
- *Wave-Turbulence Interactions*
- *Geophysical and Astrophysical Turbulence*
- *Two-dimensional Turbulence*
- *Turbulence, Waves and Instabilities in Plasmas*
- *Vortex Dynamics and Structure Formation*
- *Quantum and Superfluid Turbulence*
- *Turbulent Transport, Dispersion and Mixing*
- *Complex and Active Particles*
- *Numerical Methods and Data Analysis*

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The End

Dependence of the thermalization time scale on the number of particles work in progress in collaboration with M. Bustamante

Consider a general process that converts S waves into T waves with $S + T = M$

$$k_1 + \ldots + k_S = k_{S+1} + \ldots + k_{S+T} \pmod{N}$$
$$\zeta^{k_1} + \ldots + \zeta^{k_S} = \zeta^{k_{S+1}} + \ldots + \zeta^{k_{S+T}}$$

with

$$\zeta = \exp\left(\frac{i\,\pi}{N}\right)$$

The unknowns are the integers $k_1, \ldots, k_M$, satisfying $1 \leq k_j \leq N - 1$ for all $j = 1, \ldots, M.$, i.e. Diophantine equation.

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.

Many thanks to Massimo Cencini and Filippo De Lillo for suggestions and fruitful discussions

The Nonlinear Schrödinger equation in the α-FPUT system

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

Assuming narrow-band process, the NLS equation is obtained:

$$i\left(\frac{\partial b}{\partial t} + c_g \frac{\partial b}{\partial x}\right) = \mu \frac{\partial^2 b}{\partial x^2} + \nu |b|^2 b$$

with

$$\mu = -\frac{1}{2}\frac{d^2\omega}{d\kappa^2} > 0, \quad \nu = \epsilon^2 T_{\kappa_0,\kappa_0,\kappa_0,\kappa_0} < 0$$

The dynamics is de-focussing (also for π mode); no modulational instability in the α-FPUT

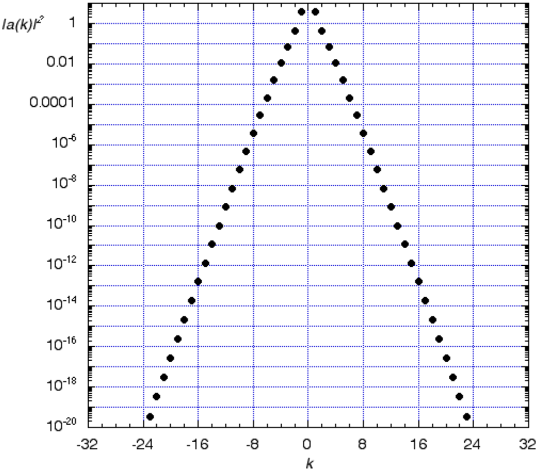
The physical interpretation of the canonical transformation

The original field a_k can be considered as a superposition of *free* and *bound* modes:

- free modes obey the linear dispersion relation and their dynamics is ruled by variable b_k
- bounds modes are constructed from free modes using the canonical transformation; for each free mode there are many bound modes that do not interact

A numerical example with 64 masses

$b_k = b_0(\delta_{k,1} + \delta_{k,-1})$



The second-order Stokes wave solution of the α-FPUT

Consider the original variable in terms of the canonical transformation:

$$q_j(t) = i \sum_k \left[\frac{a_k}{\sqrt{2\omega_k}} e^{i2\pi jk/N} - c.c. \right],$$

Assume that free modes are characterized by $b(k,t) = |\bar{b}| \delta_{k,k_0} e^{-i(\omega_{k_0} t - \phi_{k_0})}$

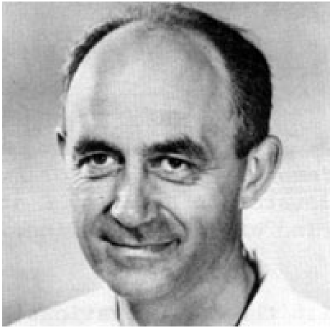
$$q_j(t) = A \sin(\theta) + \epsilon B \sin(2\theta) + O(\epsilon^2)$$

with $\theta = 2\pi k_0 j/N - \omega_0 t + \phi_{k_0}$,
$A = -2|\bar{b}|/\sqrt{2\omega_{k_0}}$,
$B = 2V_{2k_0,k_0,k_0}\sqrt{2\omega_{k_0}}|\bar{b}|^2/(-4\omega_{k_0}^2 + \omega_{2k_0}^2)$

FPUT 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)

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)

Four-wave resonant interactions in the α-FPUT

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

It is possible to show that for $N = 16,\ 32,\ 64$ 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 $m = 0, \pm 1, \pm 2, \dots$

Four-wave resonant interactions in the α-FPUT

- 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)

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
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- Weissert, Thomas P. "The genesis of simulation in dynamics: pursuing the Fermi-Pasta-Ulam problem." Springer-Verlag New York, Inc., 1999.
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E. Fermi with E. Amaldi in Varenna, 1954

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

Fundamental difference between FPUT 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!!

The α-FPUT and Toda Lattice

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

- α-FPUT model:

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

- Toda Lattice:

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

For the particular choice

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

the Toda potential is tangent to the FPUT one

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

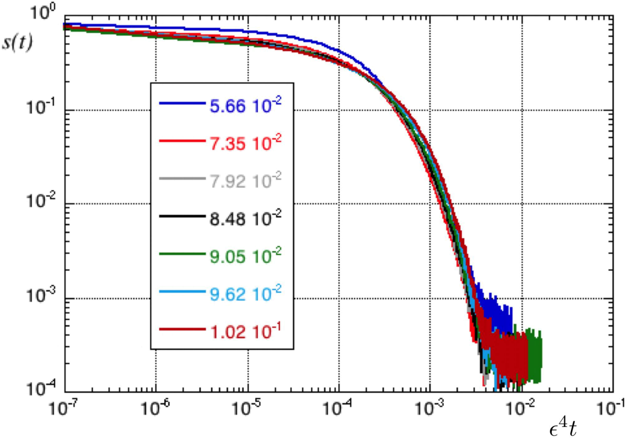
The wave-wave interaction approach

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

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

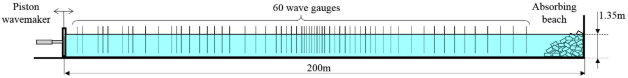
Collapse of entropy curves

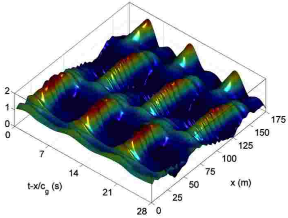


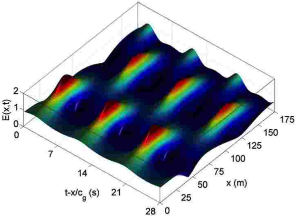
FPUT recurrence in deep water (Kimmoun et al, Sci. Reports 2016)

In the limit of narrow band process, the β-FPUT system reduces to the Nonlinear Schrödinger equation:

$$i\frac{\partial\psi}{\partial t}+\frac{\partial^2\psi}{\partial x^2}+|\psi|^2\psi=0$$







Recent numerical work on α-FPUT

CHAOS **21**, 043127 (2011)

The two-stage dynamics in the Fermi-Pasta-Ulam problem: From regular to diffusive behavior

A. Ponno,[1,a)] H. Christodoulidi,[1,b)] Ch. Skokos,[2,c)] and S. Flach[2,d)]
[1]*Università degli Studi di Padova, Dipartimento di Matematica Pura e Applicata, Via Trieste 63, 35121 Padova, Italy*
[2]*Max Planck Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany*

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

- metastable
- statistical equilibrium