Thermalisation in weakly nonlinear chains

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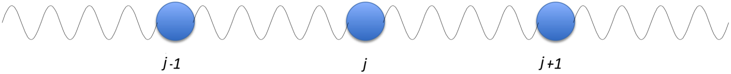


MAGIC Launch Lecture, September 30th, 2021

(based on the joint work with Miguel Onorato, Lara Vozella and Yuri V. L'vov entitled "A route to thermalisation in the α-Fermi-Pasta-Ulam(-Tsingou) system", PNAS 112, 4208-4213, 2015)

About me

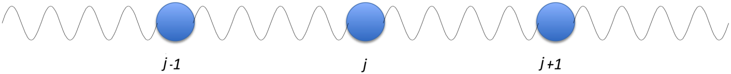
- Associate professor at the UEA School of Mathematics
- Background in physics (theoretical physics)
- Main research area is **theory and numerical simulations of quantum fluids** (MAGIC092 Introduction to superfluids and turbulence, MAGIC099 Numerical methods in Python)
- In general I am interested in the dynamics of nonlinear systems where waves/particles/excitations/coherent structures arise and interact (fluids, solids, discrete chains, ...). An example are discrete nonlinear chains
- Use theory of ODEs/PDEs, Hamiltonian & Lagrangian mechanics, statistical mechanics, nonlinear physics, fluid mechanics, turbulence, quantum mechanics, and numerical simulations

Outline of the talk

- Introduction to the Fermi-Pasta-Ulham(-Tsingou) (FPUT) model for nonlinear chains: definition and history of the model, main literature results
- The wave-wave interaction / wave turbulence approach: efficient resonant interaction assumption, *n*-wave interactions, canonical transformations, estimation of *n*-wave interaction timescales
- Numerical simulations
- Conclusions

The weakly nonlinear chain model (FPUT system)

N equal masses m, at positions q_j with $j = 1, \dots N$, connected by the identical weakly nonlinear springs with their neighbours



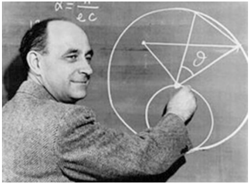
modified Hooke's law $\quad F \simeq -\Delta q(\gamma + \alpha \Delta q + \beta \Delta q^2 \dots)$

<u>The α-FPU system has equation of motion and Hamiltonian</u>

$$m\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j)\left[\gamma + \alpha(q_{j+1} - q_{j-1})\right], \quad j = 1, \dots, N$$

$$H(p,q) = \frac{1}{2}\sum_{j=1}^{N} p_j^2 + \sum_{j=1}^{N} V(q_{j+1} - q_j), \quad \text{with } V(r) = \frac{r^2}{2} + \alpha\frac{r^3}{3}$$

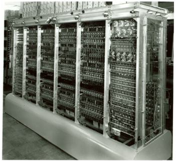
Fermi, Pasta, Ulam (and Tsingou-Menzel) in Los Alamos



Enrico Fermi (1901-1954)

John Pasta (1909-1984)

Stanislaw Ulam (1918-1984)



MANIAC I (1952-1957)

Mary Tsingou-Menzel
(1928-)

(the story of Mary Tsingou-Menzel is narrated by Thierry Dauxois in the general audience article appeared in Physics Today 56, January 2008)

Solving the linear chain model with normal modes

Assume first to consider the simple linear system, that is the harmonic chain ($\alpha = \beta = 0$). **This is fully solvable!**

Assuming periodic boundary conditions, one introduces the discrete Fourier transform and wave-action variable (normal mode)

$$Q_k = \frac{1}{N}\sum_{j=0}^{N} q_j\, e^{-i\frac{2\pi}{N}jk}\,,\;\; P_k = \dot{Q}_k\,,\;\; \omega_k = 2|\sin(\pi k/N)|\,,\;\; a_k = \frac{1}{\sqrt{2\,\omega_k}}(P_k - i\omega_k Q_k),$$

$$m\ddot{q}_j = \gamma\,(q_{j+1} + q_{j-1} - 2q_j)\,,\quad j = 1,\dots,N$$

$$\Longrightarrow \qquad i\frac{da_k}{dt} = \omega_k a_k,\quad k = -N/2+1,\dots,N/2$$

Each mode k **evolves in time independently**, $a_k(t) = a_k(t_0)e^{-i\omega_k(t-t_0)}$, that is saying that $\omega_k = 2|\sin(\pi k/N)|$ is its angular frequency

Normal modes in the α-FPU system

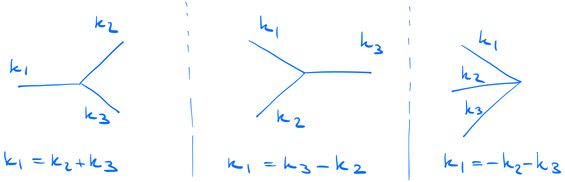
When $\alpha \neq 0$ then the evolution for the normal modes follows

$$i\frac{da_{k_1}}{dt} = \omega_{k_1} a_{k_1} + \epsilon \sum_{k_2,k_3} V_{1,2,3}\left(a_{k_2} a_{k_3} \delta_{k_1,k_2+k_3} + 2a^*_{k_2} a_{k_3} \delta_{k_1,k_3-k_2} + a^*_2 a^*_3 \delta_{k_1,-k_2-k_3} \right)$$

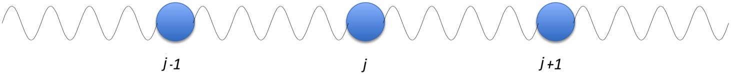
with the nonlinear parameter and scattering matrix are given by

$$\epsilon = \alpha\, \gamma^{1/4}/m^{3/4} \sqrt{\sum \omega_k |a_k(t_0)|^2}\,, \quad V_{1,2,3} = -\sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}} \Big/ \left[2\sqrt{2}\,\mathrm{sign}(k_{k_1} k_2 k_3)\right]$$

So in this case each mode k_1 interact continuously with many other modes k_2, k_3: each possible interaction is weighted by $V_{1,2,3}$ and it is non-zero provided that the Kronecker δ is non-zero

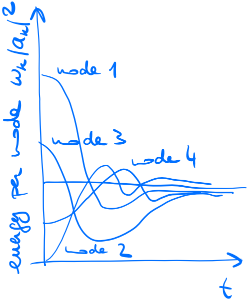


The original idea of Fermi



The α-FPUT model is the simplest toy model to study non-trivial (that is nonlinear) dynamics in solid/crystalline one-dimensional structures

- each mass is an atom and the nonlinear springs mimic the interaction with its two neighbours
- in time, nonlinear mode interactions will redistribute energy among all the modes of the system
- when (statistical) equipartition of energy has been reach the systems has thermalised, that is it can be described by some non-zero macroscopic temperature
- the approach to the thermal equilibrium can model transfer of heat into solids



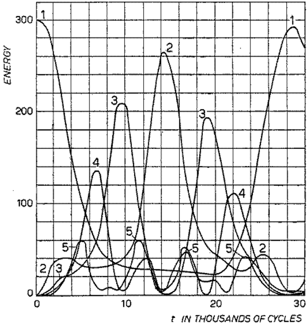
The Los Alamos report

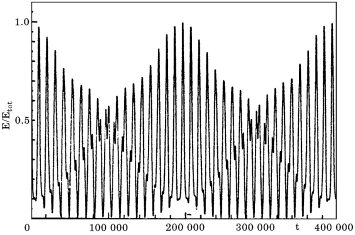
STUDIES OF NON LINEAR PROBLEMS

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.





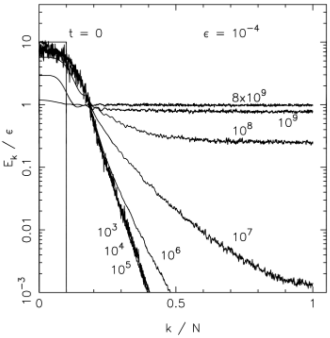
Tuck & Menzel (1972), The superperiod of the nonlinear weighted string (FPU) problem, Advances in Mathematics, 9(3), 399-407.

Review papers on the FPU system

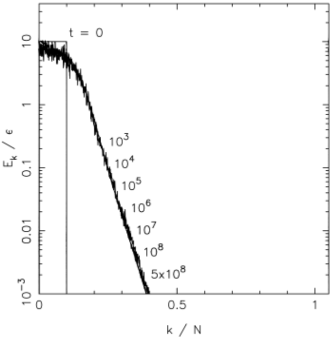
- Ford, J. "The Fermi-Pasta-Ulam problem: paradox turns discovery." Physics Reports 213.5 (1992): 271-310.
- Berman, G. P., and F. M. Izrailev. "The Fermi-Pasta-Ulam problem: fifty years of progress." Chaos (Woodbury, NY) 15.1 (2005): 15104
- Carati, A., L. Galgani, and A. Giorgilli. "The Fermi-Pasta-Ulam 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.

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

FPUT simulation



Toda lattice simulation



- a metastable timescale is the one in which FPUT behaves essentially as an integrable system (Toda lattice)
- a second timescale is instead typical of a non-integrable dynamics and thermalisation is possible
- when does this transition occur?

The wave-wave interaction approach

Inspired by the wave turbulence theory which may be applied to any weakly nonlinear dispersive system like waves in optics, plasma, ocean, Bose-Einstein condensates [Wave Turbulence, Nazarenko (2011)]

The (long time) efficient energy transfer in the system goes only trough exact resonant *n*-wave interaction processes satisfying

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

The interaction representation

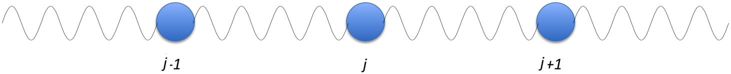
- for instance in a swing one has to push at the right resonant frequency in order to be efficient
- the same idea applies to normal modes where the nonlinear interactions are seen like a forcing term

Introduce the following rotation $a'_k(t) = a_k(t)e^{i\omega_k t}$, then

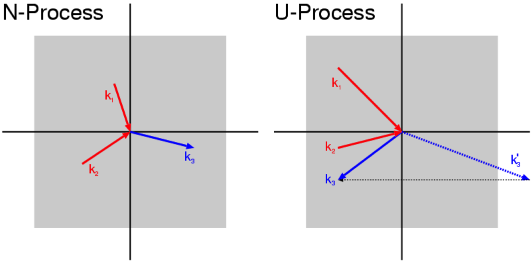
$$i\frac{da'_{k_1}}{dt} = \epsilon \sum_{k_2,k_3} V_{1,2,3} \left(a'_{k_2} a'_{k_3} e^{i\Delta\Omega^{(1)}t} \delta_{k_1,k_2+k_3} + 2\, a'^{*}_{k_2} a'_{k_3} e^{i\Delta\Omega^{(2)}t} \delta_{k_1,k_3-k_2} \right.$$
$$\left. + a'^{*}_{k_2} a'^{*}_{k_3} e^{i\Delta\Omega^{(3)}t} \delta_{k_1,-k_2-k_3} \right) ,$$

$$\begin{aligned}
\#1 \text{ term:} \quad & k_1 - k_2 - k_3 \,, \quad & \Delta\Omega^{(1)} = \omega_{k_1} - \omega_{k_2} - \omega_{k_3} \\
\#2 \text{ term:} \quad & k_1 + k_2 - k_3 \,, \quad & \Delta\Omega^{(2)} = \omega_{k_1} + \omega_{k_2} - \omega_{k_3} \\
\#3 \text{ term:} \quad & k_1 + k_2 + k_3 \,, \quad & \Delta\Omega^{(3)} = \omega_{k_1} + \omega_{k_2} + \omega_{k_3}
\end{aligned}$$

Umklapp (flip-over) scattering in crystals



Sketch of a normal process (N-process) and Umklapp process (U-process)



The (long time) efficient energy transfer in the system goes only trough exact resonant *n*-wave interaction processes satisfying

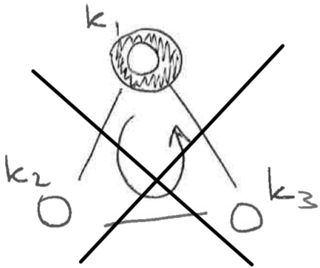
$$\begin{aligned} k_1 \pm k_2 \pm .... \pm k_n &= 0 \\ \omega(k_1) \pm \omega(k_2) \pm ... \pm \omega(k_n) &= 0 \end{aligned} \quad \Longrightarrow \quad \begin{aligned} k_1 \pm k_2 \pm .... \pm k_n &\overset{N}{=} 0 \\ \omega(k_1) \pm \omega(k_2) \pm ... \pm \omega(k_n) &= 0 \end{aligned}$$

Non-existence of 3-wave interactions for α-FPU

Exact 3-wave resonant interactions need to satisfy

$$\begin{aligned} k_1 \pm k_2 \pm k_3 &\overset{N}{=} 0 \\ \omega_1 \pm \omega_2 \pm \omega_3 &= 0 \end{aligned},$$

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



Using trigonometric identities one may show that 3-wave resonant interactions are forbidden, that is the resonant manifold is empty!

Canonical transformation to introduce 4-wave interactions

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

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

The equation of motion for the (transformed) mode is then

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

that is it model at the first nontrivial order in ϵ a four-wave interaction system

4-wave interactions in the α-FPU

$$\begin{array}{r} k_1 + k_2 - k_3 - k_4 \overset{N}{=} 0 \\ \omega_1 + \omega_2 - \omega_3 - \omega_4 = 0 \end{array}, \quad \text{given } \omega_k = 2|\sin(\pi k/N)|$$

It is possible to show that the above system has solutions for integer values of k

- *Trivial solutions*: all modes are equal or

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

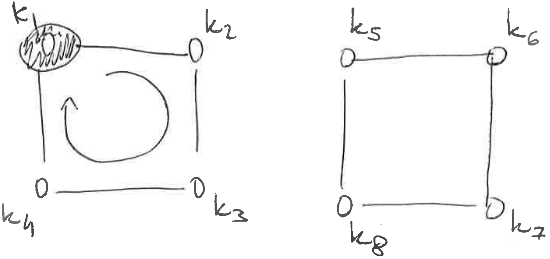
- *Nontrivial solutions*

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

with $k_1 + k_2 = mN/2$ and $m \in \mathcal{Z}$

Isolated 4-wave resonant interactions in the α-FPU

- 4-waves resonant interactions are isolated



- no efficient mixing of all modes, meaning that no thermalisation can be achieved via a 4-wave process!
- the system truncated to 4-wave interactions, that is $O(\epsilon^2)$, turns out to be integrable [Henrici & Kappeler in Commun. Math. Phys. (2008), Rink in Commun. Math. Phys. (2006)]

Next order: 6-wave interactions in the α-FPU

- *Trivial solutions*:

  either all modes equal or

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

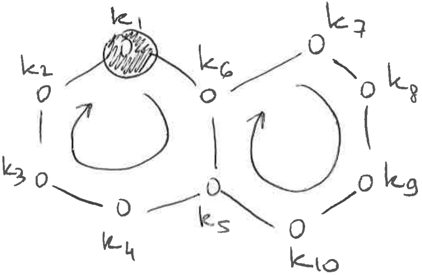
- *Nontrivial symmetric resonances*

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

  with $k_1 + k_2 + k_3 = mN/2$ and $m \in \mathcal{Z}$.

- *Nontrivial non-isolated quasi-symmetric resonances*

  $$\{k_1, k_2, k_3, -k_1, -k_2, k_3\},\ \text{with } k_1 + k_2 = mN/2 \text{ and } m \in \mathcal{Z}$$



Thermalisation timescale t_{eq}

The thermalisation timescale can be estimated from the wave turbulence theory via a kinetic equation, and depends on the number of resonantly interacting waves

$$\text{for 6-wave interactions} \implies t_{eq} \sim 1/\epsilon^8\,,$$

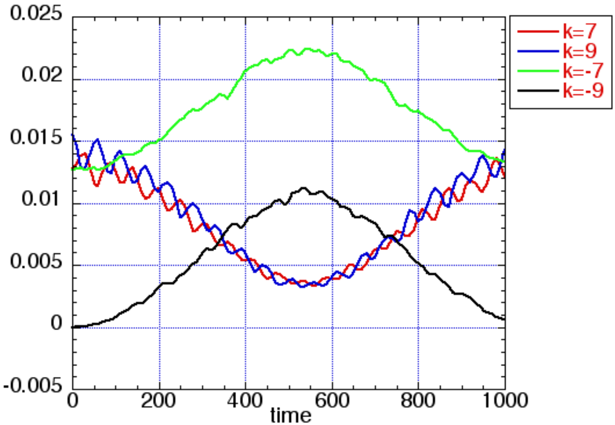
given ϵ the nonlinearity of the initial condition, $\epsilon = \alpha\,\gamma^{1/4}/m^{3/4}\sqrt{\sum \omega_k |a_k(t_0)|^2}$

How to check the thermalisation has been reached? From the kinetic equation, the **entropy function**

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

will be minimised when thermalisation is reached!

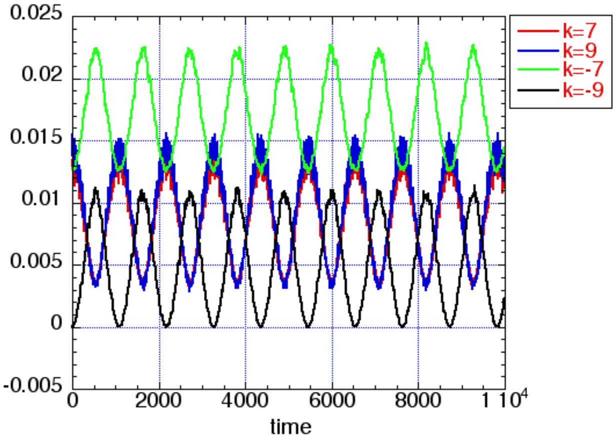
Numerical simulations: "short" timescale



Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.

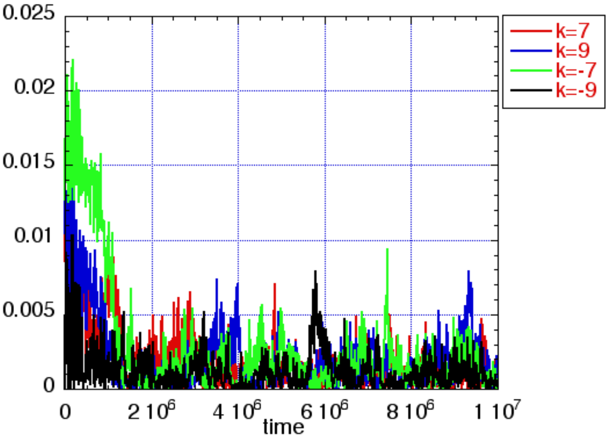
One is expecting that the Umklapp mode $k_4 = -9$ is going to be excited too.

Numerical simulations: 4-wave interactions



Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.

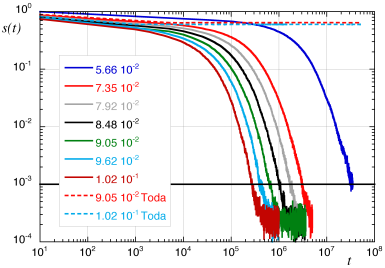
Numerical simulations: "long" thermalisation timescale



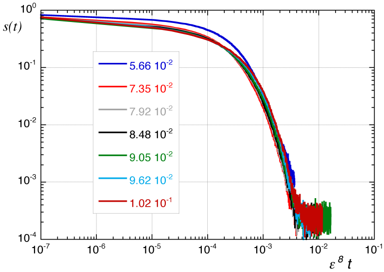
Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.

Entropy measure and thermalisation time $t_{eq} \sim 1/\epsilon^8$

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



Entropy evolution for different nonlinearities ϵ vs. time t



Entropy evolution for different nonlinearities ϵ vs. rescaled time $\epsilon^8 t$

(averaging 1,000 realisations with initial conditions having the same wave mode amplitudes but phases uniformly distributed)

Conclusions

- resonant 3-wave interactions are forbidden; this implies that on the short timescale 3-wave interactions will generate a reversible dynamics
- via a canonical transformation, 4-wave resonant interactions exist; however, we have shown that each resonant quartet is isolated, preventing the full energy transfer between all modes, therefore thermalisation
- the first significant interactions are 6-wave interactions; at this timescale one finally observes thermalisation

Further comments

- despite being a simple toy model, the seminal FPUT work has triggered a lot of new maths and physics research (MAGIC021 Nonlinear Waves, MAGIC083 Integrable Systems, MAGIC022 Dynamical Systems, MAGIC090 Introduction to Continuum Mechanics)
- it is always a good idea to revisit an "old problem" from a different perspective!
- weird physics appears in reduced dimensions, for example one-dimensional chains exhibit anomalous heat diffusion and ballistic transfer [Physical Review Letters 125, 024101 (2020)], and current experiments in nano-physics detect these phenomena [Nature Reviews Physics 3, 555-569 (2021)]

Thanks for your attention!

(based on the joint work with Miguel Onorato, Lara Vozella and Yuri V. L'vov entitled "A route to thermalisation in the α-Fermi-Pasta-Ulam(-Tsingou) system", PNAS 112, 4208-4213, 2015)