A route to thermalisation in the α-Fermi–Pasta–Ulam system

Miguel Onorato[1,2], Lara Vozella[1,2],
Davide Proment[3], Yuri V. L'vov[4]

[1]Dipartimento di Fisica, Università degli Studi di Torino, Italy
[2]INFN, Sezione di Torino, Italy
[3]School of Mathematics, University of East Anglia, United Kingdom
[4]Department of Mathematical Sciences, Rensselaer Polytechnic Institute, USA

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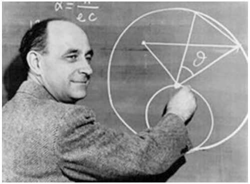
Outline of the talk

- Introduction to the FPU model: definition and history of the model, main literature, relation with the Toda lattice
- The wave-wave interaction approach: efficient resonant interaction assumption, n-wave interactions, canonical transformations, estimation of n-wave interaction timescales
- Numerical simulations: metastable states, equipartition timescale estimation
- Conclusions and open problems

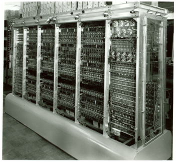
Fermi, Pasta, Ulam (and Tsingou-Menzel) in Los Alamos



Enrico Fermi (1901-1954)

John Pasta (1909-1984)

Stanislaw Ulam (1918-1984)

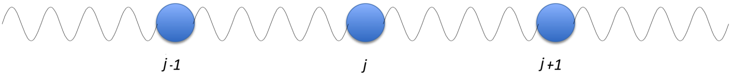


MANIAC I (1952-1957)

Mary Tsingou-Menzel
(1928-)

The weakly nonlinear chain model (FPU system)

N equal masses m connected by the same weakly nonlinear spring



$$F \simeq -\Delta q(\gamma + \alpha \Delta q + \beta \Delta q^2 \dots)$$

The α-FPU system has equation of motion and Hamiltonian

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

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

Normal modes of the non-dimensionalised α-FPU system

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

$$Q_k = \frac{1}{N}\sum_{j=0}^{N} q_j\, e^{-i\frac{2\pi}{N}jk} \quad \text{and} \quad a_k = \frac{1}{\sqrt{2\,\omega_k}}(P_k - i\omega_k Q_k),$$

with $P_k = \dot{Q}_k$, $\omega_k = 2|\sin(\pi k/N)|$ and $k = -N/2+1, \dots, N/2$

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

with the nonlinear parameter and scattering matrix are given by

$$\epsilon = \alpha\,\gamma^{1/4}/m^{3/4}\sqrt{\sum \omega_k |a_k(t_0)|^2}\,, \quad V_{1,2,3} = -\sqrt{\omega_1\omega_2\omega_3}/\left[2\sqrt{2}\,\mathrm{sign}(k_1 k_2 k_3)\right]$$

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

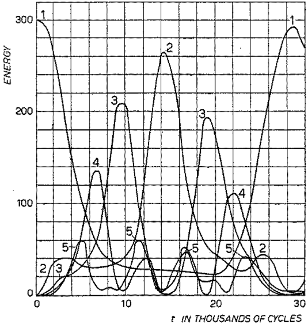
The Los Alamos report

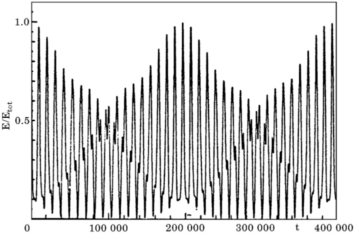
STUDIES OF NON LINEAR PROBLEMS

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.

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 (quasi-integrable system)
- statistical equilibrium (non-integrable system)

FPU can be seen as a perturbation of the integrable Toda lattice

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 is carried only by the 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 proper 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

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

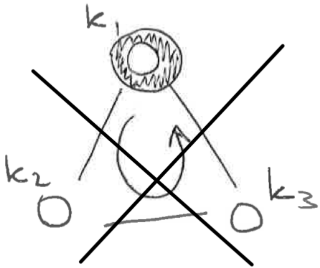
$$\begin{aligned}
\#1 \text{ term:} \quad & \delta_{1,2+3} = k_1 - k_2 - k_3\,, && \Delta\Omega^{(1)} = \omega_1 - \omega_2 - \omega_3\,.\\
\#2 \text{ term:} \quad & \delta_{1,3-2} = k_1 + k_2 - k_3\,, && \Delta\Omega^{(2)} = \omega_1 + \omega_2 - \omega_3\,.\\
\#3 \text{ term:} \quad & \delta_{1,-2-3} = k_1 + k_2 + k_3\,, && \Delta\Omega^{(3)} = \omega_1 + \omega_2 + \omega_3\,.
\end{aligned}$$

Non existence of exact triads interactions for α-FPU

Exact 3-wave resonant interactions need to satisfy

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

given $\omega_k = 2|\sin(\pi k/N)|$
and discrete modes
$k = -N/2 + 1, \ldots, N/2$



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

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

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

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

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

The reduced 4-wave FPU system

The reduced Hamiltonian results in

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

Its equation of motion is then

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

that is it model where the first nontrivial order in ϵ is given by four-wave interactions

Four-wave resonant interactions in the α-FPU

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

- NO resonant interactions for $3 \longrightarrow 1$ and $1 \longrightarrow 3$ couplings

$$\begin{array}{c} k_1 + k_2 + k_3 = k_4 \\ \omega_1 + \omega_2 + \omega_3 = \omega_4 \end{array}, \quad \begin{array}{c} k_1 = k_2 + k_3 + k_4 \\ \omega_1 = \omega_2 + \omega_3 + \omega_4 \end{array}.$$

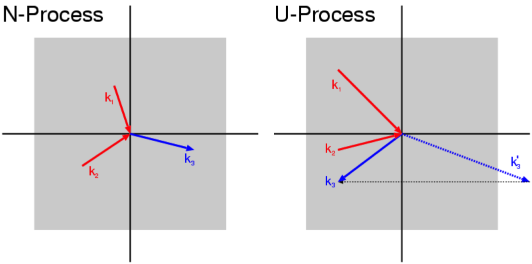
- YES, for $2 \longleftrightarrow 2$ coupling

$$\begin{array}{c} k_1 + k_2 = k_3 + k_4 \\ \omega_1 + \omega_2 = \omega_3 + \omega_4 \end{array}$$

if one considers the Umklapp scattering processes!

Umklapp (flip-over) scattering in the Brillouin zone

Sketch of a normal process (N-process) and Umklapp process (U-process) for a 3-wave interaction process



Example of an Umklapp scattering in FPU 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 mode k_4 is flipped-over to $k_4' = k_4 - N = -2$.

Four-wave resonant interactions in the α-FPU

$$\begin{array}{c} k_1 + k_2 - k_3 - k_4 \stackrel{N}{=} 0 \\ \omega_1 + \omega_2 - \omega_3 - \omega_4 = 0 \end{array},$$

where $\stackrel{N}{=}$ stands for the equality after the Umklapp process. It is possible to show that the above system has solutions for integer values of k

- *Trivial solutions*: all modes are equal to

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

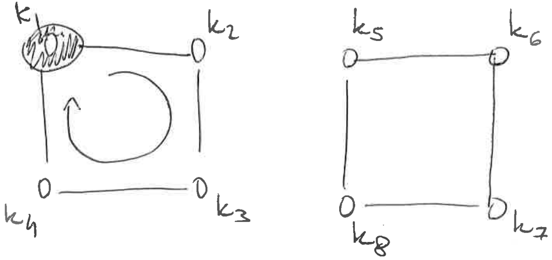
- *Nontrivial solutions*

$$\{k_1, k_2, k_3 = -k_1, k_4 = -k_2\}$$

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 Hamiltonian $\tilde{H}$ 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)]

Six-wave interactions in the α-FPU

- not possible to perform a canonical transformation to higher order because the denominators will vanishes
- check for exact resonances at higher order

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

Resonant conditions of 6-wave interactions are

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

and now non-isolated sextuples exist for integer values of k with $N = 16, 32, 64$!

Solutions of the 6-wave resonant conditions

- *Trivial solutions*:

  either all modes equal or

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

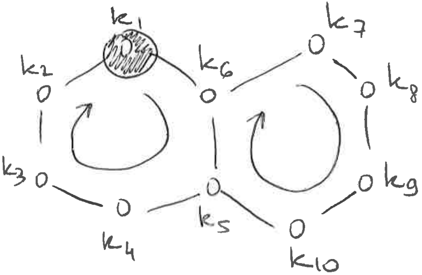
- *Nontrivial symmetric resonances*

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

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

- *Nontrivial quasi-symmetric resonances*

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



Estimation of the equipartition timescale t_{eq}

The equipartition is a statistical feature and timescale 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 wave action correlators

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

Estimation of the equipartition timescale t_{eq}

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

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

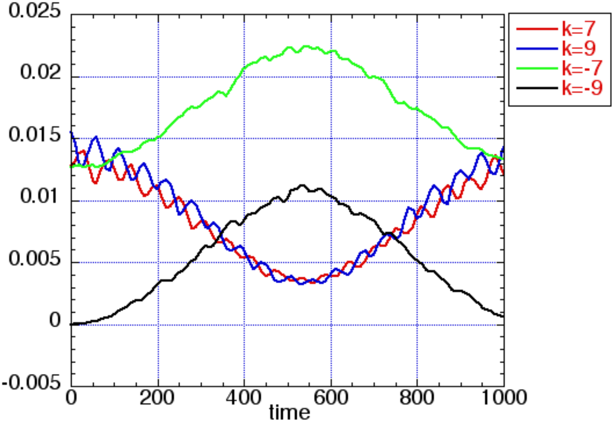
and the time of equipartition (themalisation) scales as

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

Numerical simulations

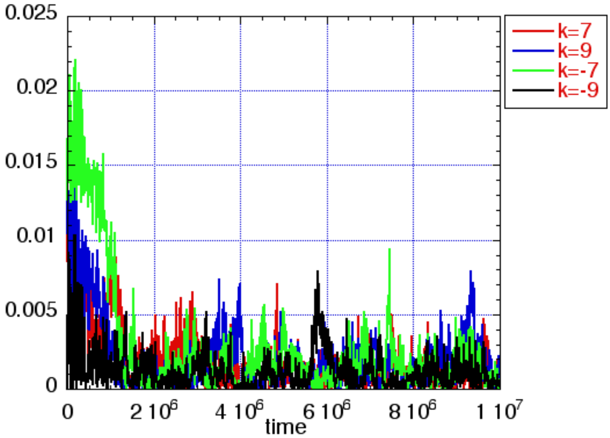
- symplectic integrator (H. Yoshida, 1990 Phys. Lett. A)
- numerical simulations with N=32 modes and $\gamma = m = 1$
- first example where the modes $k_1 = 7$, $k_2 = 9$, $k_3 = -7$ are initially perturbed
- two different initial conditions: (i) only modes $k = \pm$ have energy; (ii) modes $k = \pm 1, \pm 2, \pm 3, \pm 4, \pm 5$
- different values of ϵ to study the thermalisation time scale t_{eq}

Numerical simulations: “short” timescale



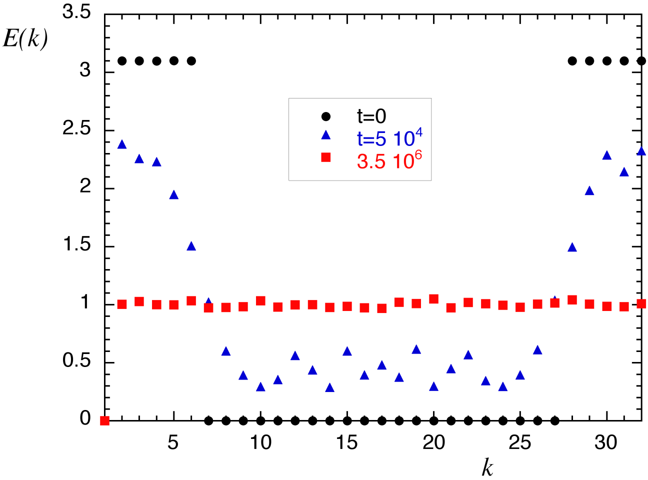
Here $\epsilon = 0.012$ and 3 modes belonging to the same quartet
are initially excited: $k_1 = 7$, $k_2 = 9$, $k_3 = -7$.
One is expecting that the Umklapp mode $k_4 = -9$ is going to be excited too.

Numerical simulations: “large” equipartition timescale



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

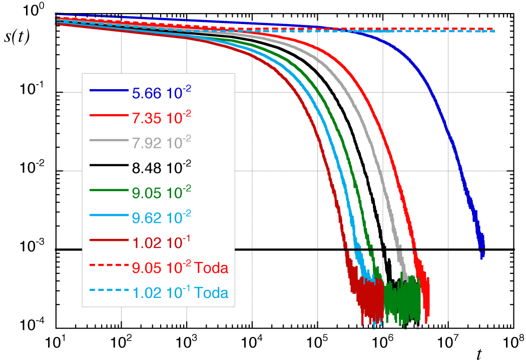
Numerical simulations: thermalisation process



Example of energy occupation of the modes at different timescales.

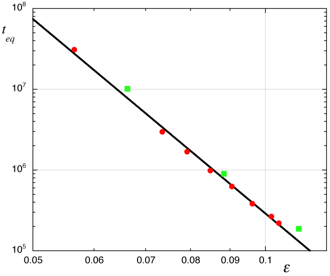
Entropy measure

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

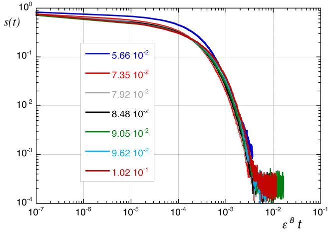


Entropy evolution for systems having different nonlinearity ϵ versus time.

Equipartition time t_{eq} and collapse of entropy curves



Red and green dots represent different perturbed initial conditions;
The straight line corresponds to power law $\propto 1/\epsilon^8$.



Entropy evolution for systems having different nonlinearities ϵ versus rescaled time $\epsilon^8 t$.

Conclusions

- resonant triads are forbidden; this implies that on the short timescale 3-wave interaction will generate a reversible dynamics
- define a suitable canonical transformation allows us to look at higher order interactions in the system which are responsible for longer timescale dynamics
- 4-wave resonant interactions exist; however, we have shown that each resonant quartet is isolated, preventing the full spread of energy across the spectrum and thermalisation
- the first significant interaction is the 6-wave one; at the timescale of these interactions one observes the thermalisation (energy equipartition phenomenon)

Open problems

- derive a rigorous kinetic equation by designing an *ad hoc* canonical transformation that is not divergent
- extend this idea to other quasi-integrable systems

Acknowledgments

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