

THE FERMI-PASTA
ULAM-TSINGOU PROBLEM

PH4104 TERM PROJECT

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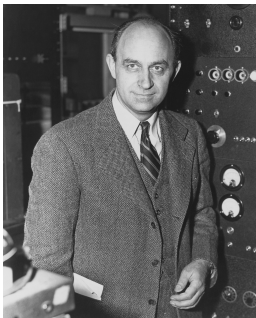
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- ▶ Conclusions

The History

1 History



(a) Enrico Fermi



(b) John Pasta



(c) Stanislaw Ulam



(d) Mary Tsingou

Figure: The Fermi-Pasta-Ulam-Tsingou Team

The History

1 History

In light of the new MANIAC (Metropolis and von Neumann Install Awful Computers) computer, Fermi, Pasta, Ulam and Tsingou[1] set out to study some physical problem using numerical simulations. They chose to study a 1D chain of particles connected by nonlinear springs. Their goal was to understand how energy would distribute among the normal modes of the system over time, expecting that the nonlinearity would lead to thermalization and equipartition of energy among the modes.

Introduction

1 History

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- ▶ Then we try to answer some questions that arise from the problem.

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- ▶ Then we try to answer some questions that arise from the problem.
- ▶ Then we try to see some possible resolutions to the problem.
- ▶ Finally, we connect the richness of this problem with statistical mechanics.

For this we will use [2] and [3] as our main references.



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The Setup

2 Problem Setup

The FPUT problem considers a one-dimensional chain of N particles connected by springs with both linear and nonlinear restoring forces. The Hamiltonian is:

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + \sum_{i=1}^N \left(\frac{1}{2}(x_{i+1} - x_i)^2 + \frac{\alpha}{3}(x_{i+1} - x_i)^3 + \frac{\beta}{4}(x_{i+1} - x_i)^4 \right)$$

where p_i is the momentum of the i^{th} particle, x_i is its position, and α, β are coefficients for the nonlinear terms.

The boundary conditions are fixed at both ends: $x_0 = x_{N+1} = 0$.

Equations of Motion

2 Problem Setup

The equations of motion derived from the Hamiltonian are given by:

$$\frac{d^2 x_i}{dt^2} = (x_{i+1} - 2x_i + x_{i-1}) + \alpha \left((x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2 \right) \\ + \beta \left((x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3 \right)$$

for $i = 1, 2, \dots, N$, with appropriate boundary conditions.

Normal Modes

2 Problem Setup

For the linear Hamiltonian (H_0) , we can express the displacements in terms of normal mode coordinates Q_k :

$$Q_k(t) = \sqrt{\frac{2}{N+1}} \sum_{j=1}^N x_j(t) \sin\left(\frac{\pi k j}{N+1}\right)$$

where $k = 1, 2, \dots, N$. Each normal mode oscillates with its own frequency ω_k :

$$\omega_k = 2 \sin\left(\frac{\pi k}{2(N+1)}\right)$$

Normal Modes

2 Problem Setup

Using the normal mode coordinates, the equations of motion for the linear system can be written as:

$$\ddot{Q}_k + \omega_k^2 Q_k = 0$$

with the k^{th} mode energy given by:

$$E_k = \frac{1}{2} \dot{Q}_k^2 + \frac{1}{2} \omega_k^2 Q_k^2$$

Thus we can decouple the oscillators in the linear case. No energy exchange between modes.

Initial Expectations

2 Problem Setup

The original Hamiltonian with linear springs (H_0) would lead to normal modes of vibration, each with a specific frequency. The expectation was that the addition of nonlinear terms (H_1) with perturbation, either α or β , would cause energy to spread out among these modes over time, leading to thermalization and equipartition of energy.

Normal Mode Energies

2 Problem Setup

For the α model, the equations of motion in terms of normal modes become:

$$\ddot{Q}_k + \omega_k^2 Q_k = -\frac{\alpha}{\sqrt{2(N+1)}} \sum_{j,l=1}^N C_{jlk} Q_j Q_l Q_m$$

where C_{jlk} are coupling coefficients that depend on the mode indices.

Similarly, for the β model, we have:

$$\ddot{Q}_k + \omega_k^2 Q_k = -\frac{\beta}{2(N+1)} \sum_{j,l,m=1}^N D_{jlmk} Q_j Q_l Q_m Q_n$$

where D_{jlmk} are the corresponding coupling coefficients.

A constant of motion is a function $F(q_i, p_i, t)$ that remains constant along the trajectories of the system in phase space for a given Hamiltonian $H(q_i, p_i, t)$. Mathematically, F is a constant of motion if its total time derivative vanishes:

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\} = 0$$

For an example, in a system with a time-independent Lagrangian, the Hamiltonian itself is a constant of motion, representing the total energy of the system.

Integrable Systems

2 Problem Setup

A Hamiltonian system with N degrees of freedom is said to be integrable if it possesses N independent constants of motion. In such systems, the equations of motion simplify significantly, and the dynamics can be described as linear motion on invariant tori in phase space.

Integrable Systems

2 Problem Setup

More formally, a Hamiltonian $H(q_i, p_i)$ is integrable if there exists a single-valued, analytical canonical transformation to action-angle variables (J_i, θ_i) such that the Hamiltonian depends only on the action variables:

$$H = H(J_1, J_2, \dots, J_N)$$

In these variables, the equations of motion become:

$$J_i = J_{i0}, \quad \theta_i = \omega_i(J)t + \theta_{i0}$$

where $\omega_i(J) = \frac{\partial H}{\partial J_i}$ are the frequencies of the system.

Action-Angle Torus

2 Problem Setup

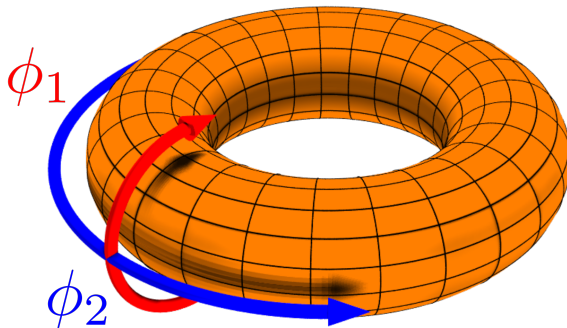


Figure: Invariant Torus in Phase Space for a system with 2 Degrees of Freedom, therefore 2 Action Variables.

A result a la Poincaré

2 Problem Setup

Consider perturbed Hamiltonians of the form:

$$H(J, \theta) = H_0(J) + \epsilon H_1(J, \theta)$$

where ϵ is a small parameter, $H_0(J)$ is integrable, and the frequencies of the unperturbed hamiltonian $\omega_i = \frac{\partial H_0}{\partial J_i}$ are functionally independent.

Poincaré's Result

Under these conditions, there exists no constant of motion $\Phi(Q_k, P_k, t)$ that is analytic in Q_k, P_k and ϵ , other than the Hamiltonian itself.

Fermi's Ergodicity Proof

2 Problem Setup

Fermi started out his career trying to prove the ergodic hypothesis. He proved that the class of Poincaré-type Hamiltonians are ergodic. Under a canonical transformation, the FPUT Hamiltonian can be expressed as a Poincaré-type Hamiltonian. Therefore, by Fermi's proof, the FPUT system is ergodic.

Energy Equipartition

2 Problem Setup

We cannot measure ergodicity directly. However, since Fermi's Proof dictates that the FPUT system is ergodic, and therefore should follow the principle of equal a priori probabilities. This would imply that over long times, the law of equipartition of energy should hold. This is how the original authors wanted to verify Fermi's proof. A more detailed explanation of this connection will be provided later in the presentation.



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The Problem

3 The Problem with The Problem

However, the numerical simulations by Fermi, Pasta, Ulam and Tsingou showed that the system did not thermalize as expected. Instead of energy spreading out evenly among all modes, it exhibited a phenomenon known as "recurrence," where the energy returned to the initially excited mode after some time.

The Plots

3 The Problem with The Problem

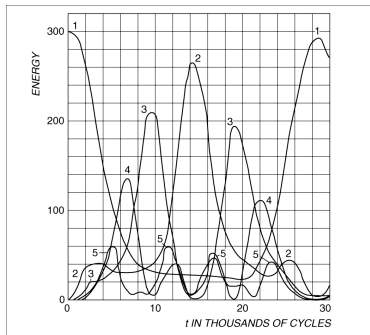


Figure: Original FPUT Simulation Results showing Recurrence Phenomenon with parameters: $N=32$, $\alpha = 0.25$, $\delta t = 1/8$ and the initial condition being the first normal mode excited. The total simulation is done over 30000 time units.



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Numerical Simulation

4 Numerical Simulation

To verify the results of Fermi, Pasta, Ulam and Tsingou, we perform our own numerical simulations of the FPUT system. We used both Euler and Velocity-Verlet integration methods to solve the equations of motion.

- ▶ The Euler method is a simple first-order method, but it can be less accurate and does not conserve energy well over long simulations.
- ▶ The Velocity-Verlet method is a second-order symplectic integrator that is more accurate and better at conserving energy in Hamiltonian systems.

Numerical Simulation

4 Numerical Simulation

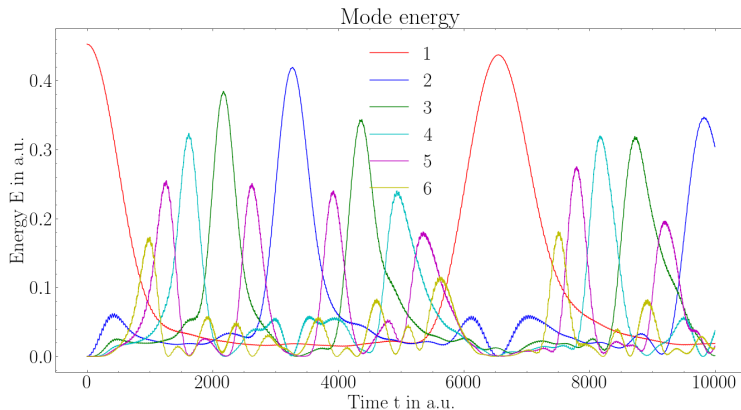


Figure: Simulation Results of the α model using Euler Method with parameters: $N=32$, $\alpha = 0.25$, $\delta t = 0.125$

Numerical Simulation

4 Numerical Simulation

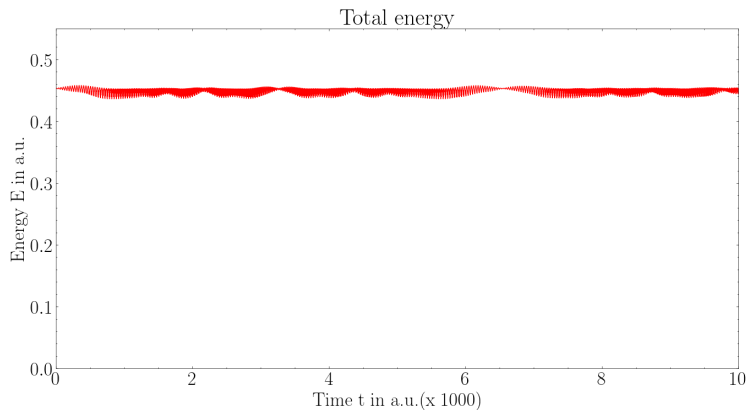


Figure: We do need to verify energy conservation in our simulations. Here is the total energy plot for the above simulation using Euler Method.

Numerical Simulation

4 Numerical Simulation

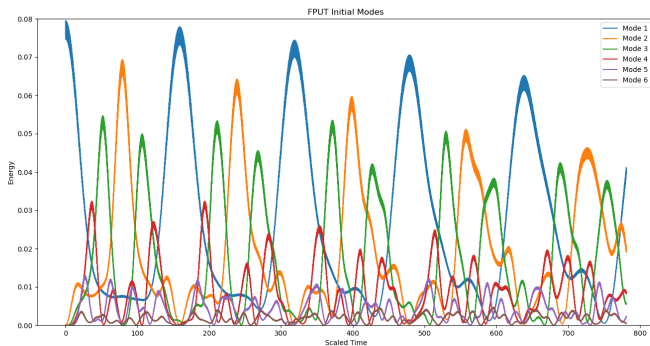


Figure: Simulation Results of the α model using Velocity-Verlet Method with parameters: $N=32$, $\alpha = 0.25$, $\delta t = 0.1$

Numerical Simulation

4 Numerical Simulation

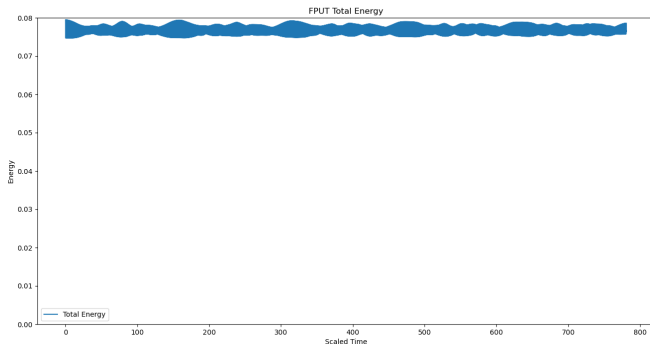


Figure: We again verify the total energy conservation in the Velocity-Verlet algorithm.



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The Fermi Problem

5 Inquisitions

- ▶ The proof by Fermi has been shown to be incorrect. Formally, there are notions of topological and metric ergodicity. Metric ergodicity is a stronger condition which implies the definition of ergodicity used in statistical mechanics.
- ▶ The experiment shows that the FPUT system does not thermalize "for certain initial conditions". How can we characterize the system?

The KAM Theorem

5 Inquisitions

KAM Theorem

Consider a Hamiltonian system with N degrees of freedom, described by action-angle variables (J_i, θ_i) . Let the Hamiltonian be given by:

$$H(J, \theta) = H_0(J) + \epsilon H_1(J, \theta)$$

- ▶ $H_0(J)$ is an integrable Hamiltonian and $H_1(J, \theta)$ is a small perturbation.
- ▶ The perturbation strength ϵ is sufficiently small (below ϵ_c)
- ▶ The frequencies of the unperturbed system satisfy,

$$\det \left(\frac{\partial^2 H_0}{\partial J_i \partial J_j} \right) = \det \left(\frac{\partial \omega_k}{\partial J_j} \right) \neq 0$$

The KAM Theorem

5 Inquisitions

KAM Theorem (contd.)

Then there exists a nowhere dense set of H_0 tori that are only slightly deformed by the perturbation. Moreover, the measure of the set of surviving tori is nearly that of the full phase space.

The completely destroyed tori of H_0 is dense in the phase space, but their total measure is small.

The KAM Theorem

5 Inquisitions

- ▶ The KAM theorem provides a resolution to why the FPUT system does not thermalize for small perturbations. The surviving invariant tori still show signatures of integrable behavior, preventing ergodicity.
- ▶ Fermi in his proof assumed that the surface dividing the regions of phase space invariant under Hamiltonian flow, is analytic. The work by Kolmogorov, shows that these surfaces are not analytic, and are in fact "pathological monstrosities".

KAM Tori

5 Inquisitions

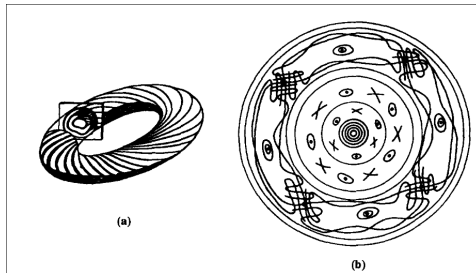


Figure: In the left is seen a set of nested tori with a cutaway showing a Poincaré surface of section. An exploded view of this surface of section is shown on the right. The circles represent preserved tori. The first signs of instability are represented by the alternating elliptic—hyperbolic pairs surrounding the origin. Moving out from the origin, one sees intersecting invariant curves in whose neighborhood lie trajectories which are realizations of random processes. But the true complexity implied by this picture is that it is replicated about each elliptic fixed point in the figure and in each replication ad infinitum. Source [2]

The Fermi Problem

5 Inquisitions

- Is the FPUT system integrable or non-integrable? Note Poincaré's result states that we can't analytically continue the constants of motion from the unperturbed system to the perturbed system. It does not say anything about introducing new constants of motion.

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The Fermi Problem

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- ▶ Does the FPUT system not thermalize at all, or does it thermalize over very long timescales?
- ▶ Does the FPUT system thermalize for certain initial conditions and not for others?
- ▶ Is the FPUT system ergodic after all?

Let's explore these questions one by one.

Is the FPUT system integrable?

5 Inquisitions

People have thought for some time that the FPUT system might be integrable after all. However, the simple answer to our question is **NO**.

- ▶ Let us consider the α model with $N = 3$ masses with periodic boundary conditions. The Hamiltonian is given by:

$$H = \sum_{i=1}^3 \frac{p_i^2}{2} + \sum_{i=1}^2 \left(\frac{1}{2}(x_{i+1} - x_i)^2 + \frac{\alpha}{3}(x_{i+1} - x_i)^3 \right)$$

- ▶ Under a simple canonical transformation, we obtain the Hénon-Heiles Hamiltonian, which is a well known non-integrable system, that exhibits chaotic behavior above a certain energy threshold.

The Hénon-Heiles System

5 Inquisitions

The Hénon-Heiles Hamiltonian is given by:

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3$$

This system was originally proposed to model the motion of a star around a galactic center. For energies above a certain threshold, the system exhibits chaotic behavior, with trajectories that are highly sensitive to initial conditions.

As a result, we get a clue that the FPUT system might be chaotic for higher perturbations or energies.

Chaos in Hénon-Heiles System

5 Inquisitions

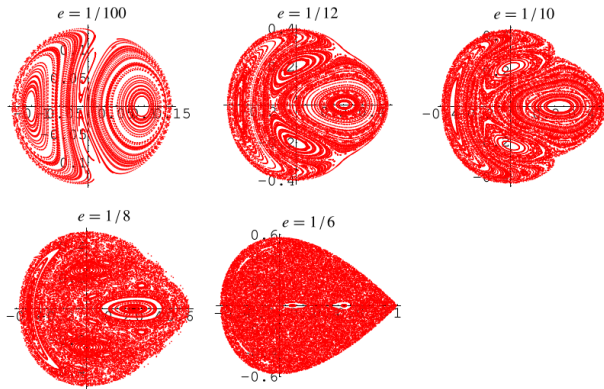
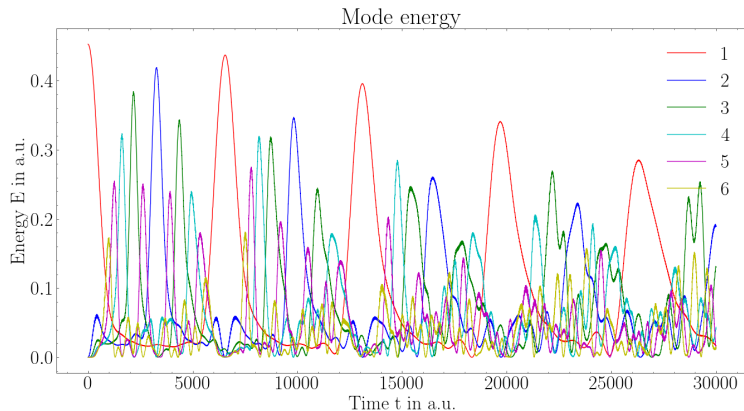


Figure: Poincaré surface of the Hénon-Heiles system showing chaotic behavior at higher energies. [4]

Does the FPUT system thermalize over long timescales?

5 Inquisitions

We see a dip in the energy of the first mode. People had conjectured that over longer timescales, the system might thermalize.



Super Period

5 Inquisitions

The super period was first observed by Tuck and Tsingou(then Menzel) in 1972.

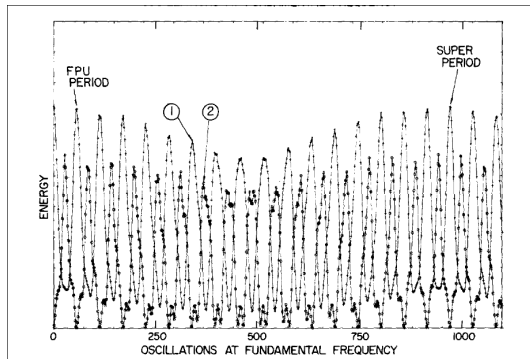


Figure: Original Tuck and Tsingou simulation showing super period of recurrence. The super period is approximately 52 times the normal recurrence period. [5]

Super Period

5 Inquisitions

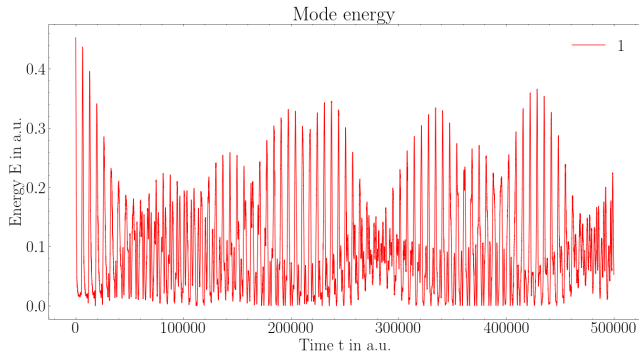


Figure: Very long time simulation of the α model using the Euler Method. We almost see a super period of recurrence, after which the energy returns to the first mode almost completely. Here, we notice a problem with the Euler method, as the total energy is not conserved well enough over such long timescales.

Super Period

5 Inquisitions

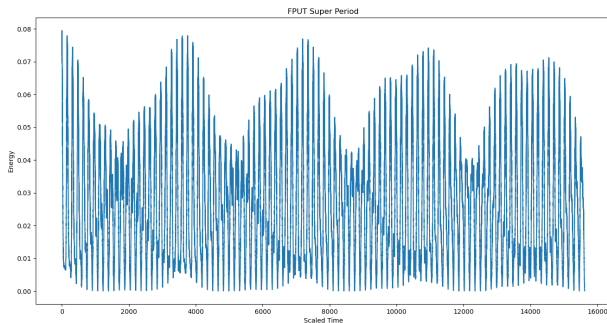


Figure: Very long time simulation of the α model using the Velocity-Verlet Method. We almost see a super period of recurrence, after which the energy returns to the first mode almost completely. Here, we notice that the total energy is conserved much better over such long timescales.

Super Period

5 Inquisitions

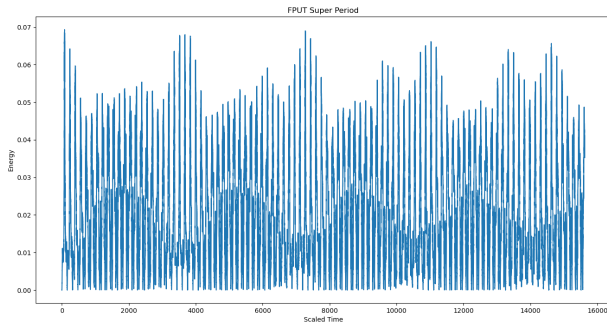


Figure: A super period is also observed in the second mode energy.

Does the FPUT system thermalize at longer times?

5 Inquisitions

There have been some studies that suggest that the FPUT system might thermalize over extremely long timescales. Similar to glassy behavior in condensed matter systems, the FPUT system might be stuck in a metastable state for long times before eventually reaching thermal equilibrium.

Does the FPUT system thermalize for certain initial conditions?

5 Inquisitions

- ▶ KAM theorem hints that for small perturbations, there are invariant tori that survive. Therefore, for initial conditions lying on these tori, the system will not thermalize.

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- ▶ The original FPUT paper considers two models, the α and β models, with certain initial conditions.

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- ▶ The original FPUT paper considers two models, the α and β models, with certain initial conditions.
- ▶ Israilev and Chirikov showed for the β model, the initial conditions lie below the stochasticity threshold for the respective models, explaining the lack of thermalization.

Chirikov Criterion

Consider the β model with N masses. Let us assume fixed boundary conditions. Also assume that the initial value problem is just the k th mode excited. The stochasticity threshold for a mode number k is given by:

$$3\beta_s \left(\frac{\partial x}{\partial z} \right)_m^2 \approx \begin{cases} \frac{3}{k}, & \text{if } k \ll N \\ \frac{3\pi^2}{N^2} \left(\frac{k}{N} \right)^2, & \text{if } N - k \ll N \end{cases}$$

Chirikov Criterion

5 Inquisitions

- ▶ There is region of conditions where due to the KAM theorem, the system does not thermalize. This criterion is a property of a lot of other systems as well. The system here exhibits **Kolmogorov Stability**.

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- ▶ The criterion shows that very high nonlinear couplings are required for thermalization when low frequency modes are excited initially.
- ▶ For higher modes and large N , the threshold is much lower, and thermalization can occur for smaller nonlinear couplings.



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Which neighbour is Integrable?

6 Resolutions??

This energy recurrence phenomenon is explained by the fact that there is an integrable Hamiltonian in the neighbourhood of the FPUT system. (We can map a Hamiltonian to a space where this sentence makes perfect sense). That cannot be the linear model, since the Poincare surfaces of the FPU are quite different from that of the linear one. In the quest for finding a suitable candidate, two of them have been the leading candidates,

1. The KdV equation.
2. The toda Lattice

We shall look at the connection to the KdV equation in more detail.

Integrable Approximation

6 Resolutions??

The FPUT system can be regarded a discrete approximation to the integrable Korteweg-de Vries (KdV) equation. Let's see how. We shall consider the α model for simplicity.

The connection to the KdV equation is a tiny bit technical, so bear with me. We will show that the naive approach to the continuum limit does not work, and leads to unphysical results. We follow the approach by [7].

The FPUT equations of motion for the α model with arbitrary m and k are given by:

$$m\ddot{x}_i = k(x_{i+1} - 2x_i + x_{i-1})(1 + \alpha(x_{i+1} - x_{i-1}))$$

We approximate the spring mass system as a continuous string of length L . Let the equilibrium positions of the masses be given by $x_i^0 = ih$, where $h = L/(N + 1)$ is the spacing between masses.

- ▶ ρ is the density of the string.
- ▶ Then $m = \rho h$.
- ▶ Let κ denotes the Young's modulus for the string (i.e., the spring constant for a piece of unit length)
- ▶ Then $k = \kappa/h$ will be the spring constant for a piece of length h .

Defining $c = \sqrt{\kappa/\rho}$ we obtain,

$$\ddot{x}_i = c^2 \frac{(x_{i+1} - 2x_i + x_{i-1}))}{h^2} (1 + \alpha(x_{i+1} - x_{i-1}))$$

Let $u(x, t)$ be the function measuring the displacement of the string from equilibrium at position x and time t . Let us analyse for one particular $x = x_i$ Then,

- ▶ $x_i(t) = u(x, t)$
- ▶ $x_{i+1}(t) = u(x + h, t)$
- ▶ $x_{i-1}(t) = u(x - h, t)$

Naive Approach

6 Resolutions??

- We can see that $\ddot{x}_i = u_{tt}(x, t)$. Using Taylor series expansion about x , we have,

$$\frac{(x_{i+1} - 2x_i + x_{i-1}))}{h^2} = u_{xx}(x, t) + u_{xxxx}(x, t)\frac{h^2}{12} + O(h^4)$$

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- Similarly,

$$\alpha(x_{i+1} - x_{i-1}) = (2\alpha h)u_x(x, t) + \frac{2\alpha h^3}{6}u_{xxx}(x, t) + O(h^5)$$

Naive Approach

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$$\frac{(x_{i+1} - 2x_i + x_{i-1}))}{h^2} = u_{xx}(x, t) + u_{xxxx}(x, t)\frac{h^2}{12} + O(h^4)$$

- Similarly,

$$\alpha(x_{i+1} - x_{i-1}) = (2\alpha h)u_x(x, t) + \frac{2\alpha h^3}{6}u_{xxx}(x, t) + O(h^5)$$

- We arrive at,

$$\left(\frac{1}{c^2}\right)u_{tt} - u_{xx} = \epsilon u_x u_{xx} + O(h^2)$$

where $\epsilon = 2\alpha h$.

The Problem with the Naive approach

6 Resolutions??

- We obtain the PDE,

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- ▶ This happens over a characteristic time scale t_s which is found to be much smaller than the recurrence time observed in the FPUT simulations.
- ▶ This is unphysical, since the FPUT system with small nonlinearity does not exhibit such shock formation.

The KZ approach

6 Resolutions??

To resolve this issue, we follow the approach by Zabusky and Kruskal.

- ▶ The correct approach is to keep higher order terms in the Taylor series expansion.

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- ▶ We now differentiate w.r.t. x and define $w = u_x$, to obtain,

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- ▶ This is known as the Boussinesq equation. This admits wave like solutions that do not form shocks, these are periodic water waves.

KZ approach

6 Resolutions??

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KZ approach

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- ▶ Note that for small values α and h , the wave like solutions should qualitatively behave like solutions to the linear wave equation.
- ▶ In general, the solutions will be superpositions of right and left moving waves. Here, these two cases are treated differently.
- ▶ To be specific, let us consider only right moving waves. We would like to look for solutions, such that behave more and more like right moving waves for longer and longer times as $\alpha, h \rightarrow 0$.

A bit of math

6 Resolutions??

- Suppose that $y(\xi, \tau)$ is a smooth function of two real variables ξ, τ such that the map $\tau \mapsto y(\cdot, \tau)$ is uniformly continuous from $\mathbb{R}$ to $L^2(\mathbb{R})$ with the sup norm.

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- ▶ Then for $|t - t_0| < T = \delta(\alpha hc)$, $|\alpha hc(t - t_0)| < \delta$. Therefore,

$$\|y(x - ct, \alpha hct) - y(x - ct, \alpha hct_0)\|_{L^2} < \epsilon \quad \forall \quad \xi \in \mathbb{R}$$

where $x = \xi + ct$.

KZ approach

6 Resolutions??

- To interpret this physically, the function $u(x, t) = y(x - ct, \alpha hct)$ uniformly approximates the right moving wave $u^0(x, t) = y(x - ct, \alpha hct_0)$ over the time interval $|t - t_0| < T$.

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- ▶ To restate this, $u(x, t) = y(x - ct, \alpha hct)$ is approximately a right moving wave whose shape gradually changes over time.

KdV Equation

6 Resolutions??

- We now substitute $w(x, t) = y(x - ct, \alpha hct)$ into the (KZ) equation, and divide by $-2\alpha h$.

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- ▶ We then define $\delta = \lim_{h \rightarrow 0} \sqrt{\frac{h}{24\alpha}}$. This also means that $\alpha h = O(h^2)$.
- ▶ In this limit, we obtain the celebrated Korteweg-de Vries Equation by taking $v(\xi, \tau) = y_{\xi}(\xi, \tau)$:

$$v_{\tau} + vv_{\xi} + \delta^2 v_{\xi\xi\xi} = 0$$

We begin by making the substitutions, $\xi = x - ct$ and $\tau = \alpha hct$. Then we have,

$$\frac{\partial^k}{\partial x^k} = \frac{\partial^k}{\partial \xi^k} \quad ; \quad \frac{\partial}{\partial t} = -c \frac{\partial}{\partial \xi} + \alpha hc \frac{\partial}{\partial \tau}$$

$$\frac{\partial^2}{\partial t^2} = c^2 \frac{\partial^2}{\partial \xi^2} - 2\alpha hc^2 \frac{\partial^2}{\partial \xi \partial \tau} + (\alpha hc)^2 \frac{\partial^2}{\partial \tau^2}$$

Our wave operator reduces to

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} = -2\alpha h \frac{\partial^2}{\partial \xi \partial \tau} + (\alpha h)^2 \frac{\partial^2}{\partial \tau^2}$$

Connection to Solitons

6 Resolutions??

- ▶ In their seminal 1965 paper, Zabusky and Kruskal performed numerical simulations of the KdV equation and discovered solitons, which are stable, localized wave packets that maintain their shape while traveling at constant speed.
- ▶ They then observed how solitons interfere with each other, and found that they pass through each other without changing shape.
- ▶ Using this connection to solitons, they gave a phenomenological explanation for the recurrence phenomenon observed in the FPUT system.
- ▶ We now see how these solitons arise in the KdV equation, from a small section of the report [8].

Solitons

6 Resolutions??

- Initially, the first two terms of the KdV equation dominate and the classical overtaking phenomenon occurs; that is, u steepens in regions where it has a negative slope. (Due to the first two terms being similar to the inviscid Burgers equation)

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- ▶ Second, after u has steepened sufficiently, the third term becomes important and serves to prevent the formation of a discontinuity.
- ▶ Instead, oscillations of small wavelength (of order δ) develop on the left of the front. The amplitudes of the oscillations grow and finally each oscillation achieves an almost steady amplitude (which increases linearly from left to right) and has a shape almost identical to that of an individual solitary-wave solution of the KdV equation.

Solitons

6 Resolutions??

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- ▶ Thus, the solitons spread apart. Because of the periodicity, two or more solitons eventually overlap spatially and interact nonlinearly. Shortly after the interaction, they reappear virtually unaffected in size or shape.
- ▶ In other words, solitons "pass through" one another without losing their identity.
- ▶ Here we have a nonlinear physical process in which interacting localized pulses do not scatter irreversibly.

Soliton formation

6 Resolutions??

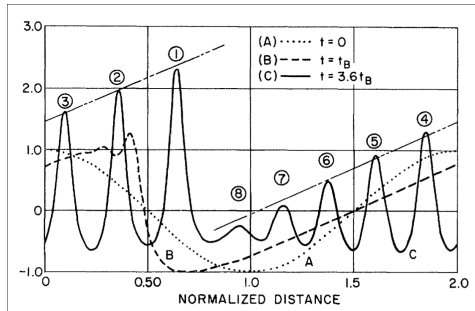


Figure: The dashed line is the initial condition, a half cosine wave. At an intermediate time step (B) we see the steepening of the front of the wave. Then at longer (C) times, there is development of oscillations of smaller wavelength near the front of the wave.

They explained the recurrence phenomenon on an FPUT system with periodic boundary conditions. These solitons arise and interfere periodically, leading to the recurrence of the initial state after some time.

Note that these derivation also agrees with the Chirikov criterion. The KdV approximation is valid for small nonlinearity, which is precisely the regime where the stochasticity threshold is high, preventing thermalization.

Toda Lattice

6 Resolutions??

The N-particle Toda lattice also serves as a leading candidate as an integrable Hamiltonian in the neighbourhood of the FPUT lattice.

$$H = \frac{1}{2} \sum P_k^2 + \frac{1}{2} \left(\sum e^{(Q_k - Q_{k-1})} \right)$$

where the index k runs from 1 to N and we impose periodic boundary conditions $Q_{N+1} = Q_1$. The Toda lattice can be in a sense, the discretized form of the KdV equation.

One can show that the Toda Lattice is completely integrable using LAX pairs.



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- ▶ Conclusions

Statistical mechanics has been one the most successful theories in physics. It provides a microscopic explanation for macroscopic thermodynamic phenomena, for widely different systems.

Even after more than a century after Boltzmann's pioneering work, the foundations of statistical mechanics are still not quite rigourously justified. Some of them include what the thermodynamic limit really means, whether the free energy functionals are well defined at that limit, why do these systems thermalize, and most importantly, the **ergodic hypothesis**.

Statistical Mechanics

7 Connection to Statistical Mechanics

One might think it would be too naive to apriori expect equipartition of energy in a slightly perturbed system. But if we establish a connection between ergodicity and the basic building block of statistical mechanics, the **principle of equal a priori probabilities**, we can see why the FPUT problem is so rich in its physical implications.

7 Connection to Statistical Mechanics

Section 7.1

Ergodicity

The Ergodic Hypothesis

7 Connection to Statistical Mechanics

Ergodic Hypothesis

Over long periods of time, the time spent by a system in some region of the phase space of microstates with the same energy is proportional to the volume of this region, i.e., all accessible microstates are equally probable over a long period of time.

This is a restatement of the hypothesis that Boltzmann used to derive the microcanonical ensemble and the law of equipartition of energy. Let's see a heuristic proof of this statement.

The Ergodic Hypothesis

7 Connection to Statistical Mechanics

Consider a system with Hamiltonian $H(q_i, p_i)$ and total energy E .

- Let us discretize the phase space into small cells of volume ΔV_Γ .

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- ▶ Therefore, the probability of finding the system in that cell, in our long time observation is given by:

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- ▶ Taking the limit $\Delta V_\Gamma \rightarrow 0$, we obtain the probability density function:

$$dP = \rho(q_i, p_i) dV_\Gamma \propto dV_\Gamma$$

The Principle of Equal A Priori Probabilities

7 Connection to Statistical Mechanics

Principle of Equal A Priori Probabilities

In an isolated system in equilibrium, all accessible microstates corresponding to one macrostate are equally probable.

This principle is the cornerstone of statistical mechanics. It allows us to derive the microcanonical ensemble and subsequently other ensembles.

A misconception

7 Connection to Statistical Mechanics

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- ▶ Therefore, our energy hypersurface will be further constrained to a submanifold defined by $\Phi(p_i, q_i) = \phi_0$.
- ▶ So the probability density function will be given by:

$$dP \propto \delta(H(p_i, q_i) - E) \delta(\Phi(p_i, q_i) - \phi_0) dV_\Gamma$$

- ▶ We need to ensure that there are no additional constants of motion other than the Hamiltonian itself, to obtain the microcanonical ensemble.

The return of Poincaré

7 Connection to Statistical Mechanics

Recall that Poincaré's result states that for perturbed Hamiltonians of that form, there exists no constant of motion $\Phi(Q_k, P_k, t)$ that is analytic in Q_k, P_k and ϵ , other than the Hamiltonian itself.

This motivated Fermi's proof to show that those Hamiltonians are ergodic.

The Ergodic Hypothesis

7 Connection to Statistical Mechanics

The Ergodic hypothesis also helps us understand systems and their validity in the real world. This relates time averages to ensemble averages.

$$\overline{A} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T A(q(t), p(t)) dt = \langle A \rangle = \int A(q, p) \rho(q, p) dV_{\Gamma}$$

For real systems, we can only measure time averages. The ergodic hypothesis allows us to equate these to ensemble averages, which are easier to compute theoretically. A proof of this hypothesis still eludes us. There have been some system specific proofs, by von Neumann and Birkhoff, but a general proof is still unknown.

Section 7.2

Energy Equipartition

Energy Equipartition

7 Connection to Statistical Mechanics

The principle of equal a priori probabilities leads to the law of equipartition of energy. This is a fairly standard derivation. One can look at any statistical mechanics textbook for details, for example [9].

Since equipartition of energy is a direct consequence of the principle of equal a priori probabilities, FPUT decided to test this as a signature of ergodicity in their system.



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Conclusions

8 Conclusions

The foundations of statistical mechanics are still not completely rigourously justified. Khinchin [10] and Ruelle [11] have a lot of opinions and criticisms about these foundations. The FPUT problem is a classic example that highlights the subtleties involved in these justifications. It launched the fields of studying solitons and chaos theory.

Moreover, FPUT forever pioneered the usage of computers in physics research.

Thank You!

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Q&A

Thank you for listening!
Your feedback will be highly appreciated!