The Fermi-Pasta-Ulam problem

The birth of nonlinear physics and dynamical chaos

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SUMMARY

- The Fermi-Pasta-Ulam experiment on MANIAC at LANL in 1955
- The ergodic hypothesis
- The 32-atom-fixed-end chain: linear and nonlinear springs
- Conclusions
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The FPU experiment

- 1D chain of particles with nearest neighbor interactions
- Particles are connected with springs that have a linear and a weakly nonlinear component
- Particles were given an initial displacement according to a fundamental mode (or a superposition of modes) of the linear system
- Newton’s equations of motion would then be integrated on the computer MANIAC (i.e., an MD simulation)
Implementation details

- All atoms have a unit mass and the elastic constant has been taken one, as in the original experiment.
- Two models are usually considered in the literature: the \( \alpha \)- and \( \beta \)- model.

\[
\begin{align*}
\ddot{x}_n &= (x_{n+1} - 2x_n + x_{n-1}) + \alpha[(x_{n+1} - x_n)^2 - (x_n - x_{n-1})^2] \\
\ddot{x}_n &= (x_{n+1} - 2x_n + x_{n-1}) + \beta[(x_{n+1} - x_n)^3 - (x_n - x_{n-1})^3]
\end{align*}
\]
The equations of motion have been integrated with a second order scheme (Velocity Verlet) and a fourth order scheme (Forest-Ruth)

In the absence of nonlinear forces, the normal modes can be expressed as a Fourier representation of the displacements. For example for fixed ends:

\[ Q_k(t) = \sqrt{\frac{2}{N}} \sum_{n=1}^{N} x_n(t) \sin \frac{\pi kn}{N} \]

\[ E_k = \frac{1}{2} (\dot{Q}_k^2 + \omega_k^2 Q_k^2) \]
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The ergodic hypothesis

- Stated by Ludwig Boltzmann in 1871, it is at basis of statistical mechanics (or is it?)
- The hypothesis: given sufficient time, the dynamical trajectory of a system will visit all microstates consistent with the applied constraints
- Assuming the ergodicity of the system, then the phase average of a function defined over phase space is the same as its time average
- FPU believed that a 32 particle system would reveal ergodic behavior, provided that the nonlinearity is not extremely small: to the great surprise of FPU, the result was the opposite!
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Simulation results

- The ends of the chain are kept fixed: only sinusoidal modes are normal modes for the linear chain (i.e. no nonlinearity present)
- Only the ground mode \((k = 1)\) was excited and numerical experiments were performed varying \(\beta \in \{0.3, 1, 3\}\)
Simulation results: $\beta = 0.3$
Simulation results: $\beta = 1$
Simulation results: $\beta = 3$
The FPU paradox

- The first attempts to explain the FPU paradox questioned the accuracy of the numerics.
- A fourth order integration scheme (the Forest-Ruth algorithm) has been implemented.
The FPU paradox: the threshold of stochasticity

- Many studies therefore demonstrated that the FPU could not be trivialized accusing the low accuracy of the integration scheme employed by FPU.
- A successful approach to resolve the paradox is due to Chirikov: he introduced the notion of stochasticity (or dynamical chaos).
- He found analytically a stochastic threshold, above which the FPU system was shown to behave in accordance with the original expectations of FPU, revealing strong statistical properties, such as energy equipartition among the linear modes.
Simulation results: three modes $(k = 1, 3, 5)$ are excited and $\beta = 0.003$
Simulation results: three modes \((k = 1, 3, 5)\) are excited and \(\beta = 0.03\).
The threshold of stochasticity

- When higher modes are initially excited, the FPU system is above the threshold of stochasticity, therefore lower values for $\beta$ are necessary to reveal a stochastic behavior of the system.

- This can be shown analytically (Chirikov, 1959)

\[
3\beta_{cr} \frac{E}{N} \approx 3 \sqrt{\frac{\Delta k}{k}}
\]
The threshold of stochasticity

- The FPU was then explained. The original simulations were performed by FPU for the lowest value of $k = 1$
- For that value of $k$, only strong perturbations (nonlinearity) could reveal a non-recurrent behavior
- Indeed, the nonlinear energy in numerical studies of FPU had never exceeded 10% the total energy, therefore the system was well below the stochasticity border
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- Simulations to study the FPU problems have been run.
- Increasing the order of accuracy of the integration schemes adopted does not prove successful in explaining the FPU paradox: Velocity Verlet (2° order) and Forest-Ruth (4° order) have been implemented and revealed that the recurrent/non-recurrent behavior is determined by intrinsic properties of the FPU system.
- The stochasticity threshold successfully explains the behavior of the FPU, revealing a dependence of the stochastic behavior (ergodicity) on the initial conditions.
- The criterion due to Chirikov has shown that when the system is excited in higher modes, lower values of the nonlinearity parameter $\beta$ are necessary to trigger a chaotic behavior (dynamical chaos).
References

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- Chirikov B. V., *A universal instability of many-dimensional oscillator systems*, Physics Reports (Review Section of Physics) 52, No. 5 (1979), 263-379
Questions?