The Fermi-Pasta-Ulam (FPU) Problem: A Watershed in Computational and Nonlinear Physics

Notes are based on a talk by Prof. David K. Campbell

ECE and Physics at Boston University

Outline

- What is the “FPU” Problem?
- FPU and Solitons
- FPU and Chaos
- FPU Today
  - The fundamentals of Statistical Mechanics
  - Anomalous Transport in Low-Dimensional Systems
  - “Discrete Breathers”/Intrinsically Localized Modes

What is the FPU Problem?

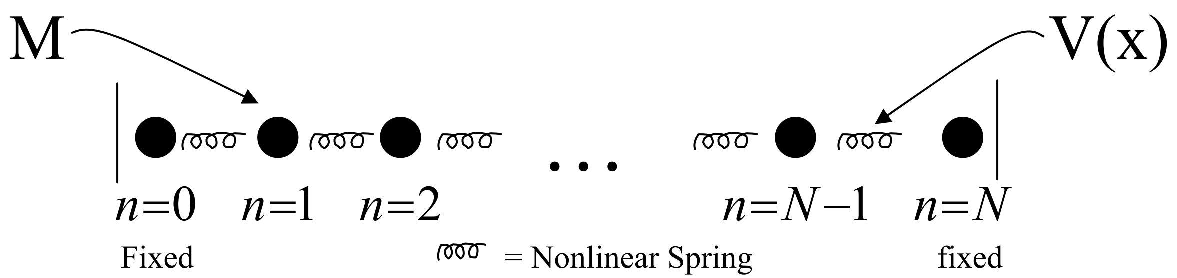
Los Alamos, Summers 1953-4 Enrico Fermi, John Pasta, and Stan Ulam decided to use the world's then most powerful computer, the

MANIAC-1

(Mathematical Analyzer Numerical Integrator And Computer)

to study the equipartition of energy expected from statistical mechanics in simplest classical model of a solid: a ID chain of equal mass particles coupled by *nonlinear** springs: (Ulam quotes)

*They knew linear springs could not produce equipartition



$$V(x) = \frac{1}{2}Kx^2 + \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4$$

C.1

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Report written:
May 1955

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LA-1940

Studies of Nonlinear Problems. I

Work done by:
E. Fermi
J. Pasta
S. Ulam
M. Tsingou

Report written by:
E. Fermi
J. Pasta
S. Ulam

The abstract

ABSTRACT

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.

The footnote

The last few examples were calculated in 1955. After the untimely death of Professor E. Fermi in November, 1954, the calculations were continued in Los Alamos.

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Abstract

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.

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“Experimental Mathematics”: Von Neumann quote

This report is intended to be the first one of a series dealing with the behavior of certain nonlinear physical systems where the non- is introduced as a perturbation to a primarily linear problem. or of the systems is to be studied for times which are long o the characteristic periods of the corresponding linear

roblems in question do not seem to admit of analytic solutions in closed form, and heuristic work was performed numerically on a fast electronic computing machine (MANIAC I at Los Alamos).* The ergodic behavior of such systems was studied with the primary aim of establishing, experimentally, the rate of approach to the equipartition of energy among the various degrees of freedom of the system. Several problems will be considered in order of increasing complexity. This paper is devoted to the first one only.

We imagine a one-dimensional continuum with the ends kept fixed and with forces acting on the elements of this string. In addition to the usual linear term expressing the dependence of the force on the displacement of the element, this force contains higher order terms. For

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*We thank Miss Mary Tsingou for efficient coding of the problems and for running the computations on the Los Alamos MANIAC machine.

Note the Error Here

the purposes of numerical work this

number of points (at most 64 in our actual computation) so that the partial differential equation defining the motion of this string is replaced by a finite number of total differential equations. We have, therefore, a dynamical system of 64 particles with forces acting between neighbors with fixed end points. If x_i denotes the displacement of the i-th point from its original position, and α denotes the coefficient of the quadratic term in the force between the neighboring mass points and β that of the cubic term, the equations were either

$$\frac{d^2xi}{dt^2} = \ddot{x}_i = (x_{i+1} + x_{i-1} - 2x_i) + \alpha\left[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2\right] \qquad (1)$$

$$i = 1, 2, \ldots 64,$$

or

$$\frac{d^2xi}{dt^2} = \ddot{x}_i = (x_{i+1} + x_{i-1} - 2x_i) + \beta\left[(x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3\right] \qquad (2)$$

$$i = 1, 2, \ldots 64.$$

α and β were chosen so that at the maximum displacement the nonlinear term was small, e. g., of the order of one-tenth of the linear term. The corresponding partial differential equation obtained by letting the number of particles become infinite is the usual wave equation plus nonlinear terms of a complicated nature.

Another case studied recently was

$$\ddot{x}_i = \delta_1(x_{i+1} - x_i) - \delta_2(x_i - x_{i-1}) + c \qquad (3)$$

where the parameters δ_1, δ_2, c were not constant but assumed different values depending on whether or not the quantities in parentheses

To Study Systematically, Start from Linear Limit

$\alpha = \beta = 0 \Rightarrow$ with $x_n = na + y_n$, a = lattice spacing

$$\boxed{\mathrm{M}\ddot{y}_n = \mathrm{K}\left(y_{n+1} + y_{n-1} - 2y_n\right)} \qquad (1)$$

Familiar (linear) "phonon" dispersion relation from solid state physics: assuming

$$\boxed{y_n = Ae^{i\left(k\cdot n\cdot a-\omega(k)t\right)}} \qquad (2)$$

Eq. (1) can be solved provided

$$\boxed{\omega(k) = 2\omega_o \sin\frac{ka}{2}} \quad , \quad \omega_o = \sqrt{\frac{\mathrm{K}}{\mathrm{M}}} \qquad (3)$$

For weak nonlinearity $\left(\alpha = \varepsilon << 1, \beta = 0\right)$

Description in terms of normal modes

$$\boxed{A_k \equiv \sqrt{\frac{2}{N}} \sum_{n=1}^{N-1} y_n \sin \frac{nak\pi}{N}}$$

Separates the problem into weakly coupled harmonic oscillators

$$\boxed{H = \frac{1}{2} \sum \dot{\mathrm{A}}_k^2 + \omega^2 \left(k\right) \mathrm{A}_\mathrm{k}^2 + \alpha \sum c_{k\ell m} \mathrm{A}_k \mathrm{A}_\ell \mathrm{A}_m}$$

For strong nonlinearity, FPU expected that whatever the initial starting point, the normal modes would share the energy equally:

??Results??

Results!!

1. Only lowest few modes excited!
2. Recurrences!

Note only modes 1-5

982 266. – *Studies of non Linear Problems*

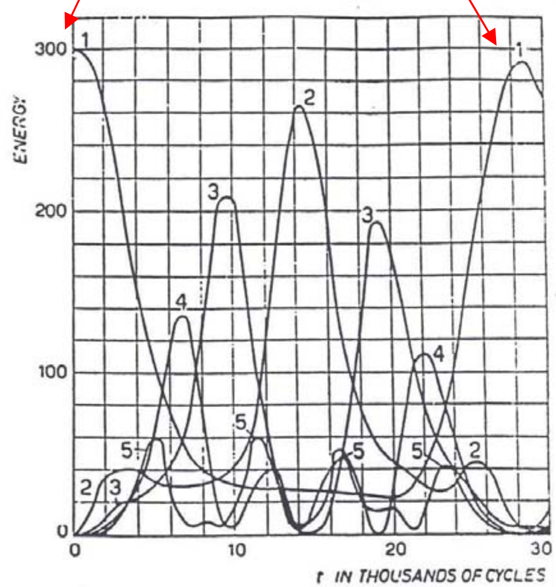


Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

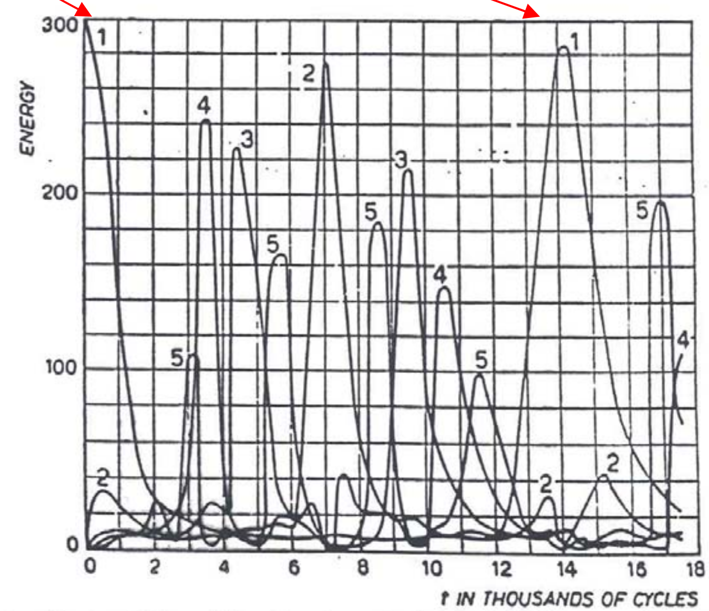


Fig. 2. – Same conditions ad fig. 1 but the quadratic term in the force was stronger. $\alpha = 1$. About 14,000 cycles were computed.

Results!!

3. Superrecurrence

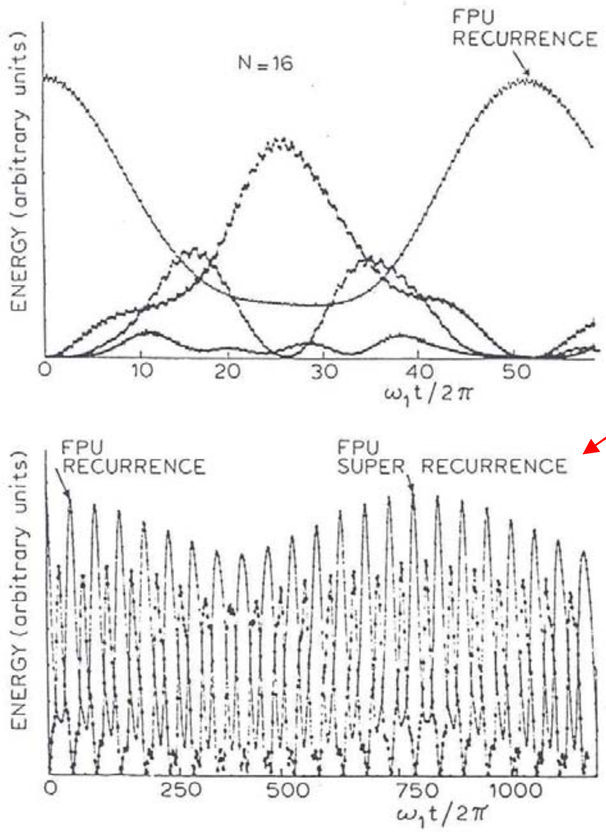


Fig. 10. In the upper part of this figure is seen the standard energy sharing between normal modes for an FPU system (here $N = 16$) integrated through one recurrence. By greatly extending the integration interval as shown in the lower figure, Tuck and Menzel [23] exposed a superperiod of recurrence. Their calculation leaves little doubt regarding almost-periodicity in the FPU motion.

FPU and Solitons

Since discrete models are harder to treat analytically than continuum theories, in the late 50s/early60s several groups used Multiple Scale Analysis in the formal continuum limit a → 0 to find

[you will not get the whole truth here]

$$y_n(t) \underset{a \to 0}{\longrightarrow} y(x = na, t) \underset{\varepsilon << 1}{\cong} y(\zeta = x - \mathrm{v}t, \varepsilon t) + 0(\varepsilon)$$

Found that for the consistency had to have

$\partial y / \partial \zeta \equiv u$ satisfy $$\boxed{u_t + uu_x + u_{xxx} = 0}$$

Kortweg – DeVries Equation

Zabusky & Kruskal (1965): "SOLITON"

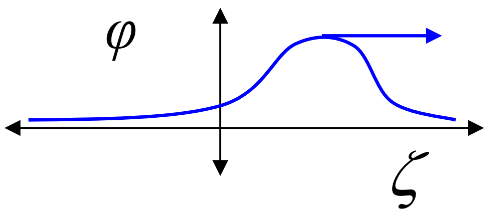
$$\boxed{u(x,t) = 3\mathrm{v}\,\mathrm{sech}^2 \frac{\sqrt{\mathrm{v}}}{2}(x - \mathrm{v}t)}$$

Amplitude, shape and velocity *interdependent:* characteristic of nonlinear wave

What is a Soliton?

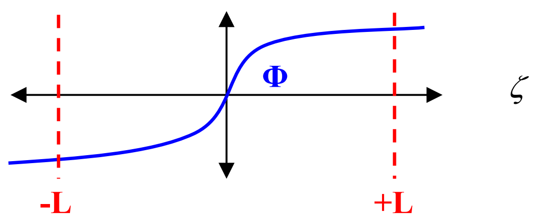
Consider continuum, wave-like motion, 1 space dimension

Definition: Solitary Wave: localized, traveling wave



$$\phi\left(\zeta = x - \mathrm{v}t\right)$$

NB: Different states allowed for $\zeta \to \pm\infty$



Localized since $\dfrac{d\phi}{d\zeta} = 0$ for $|\zeta| > L$

Definition: Soliton: Solitary wave that preserves amplitude, shape and velocity after collisions with all other waves.

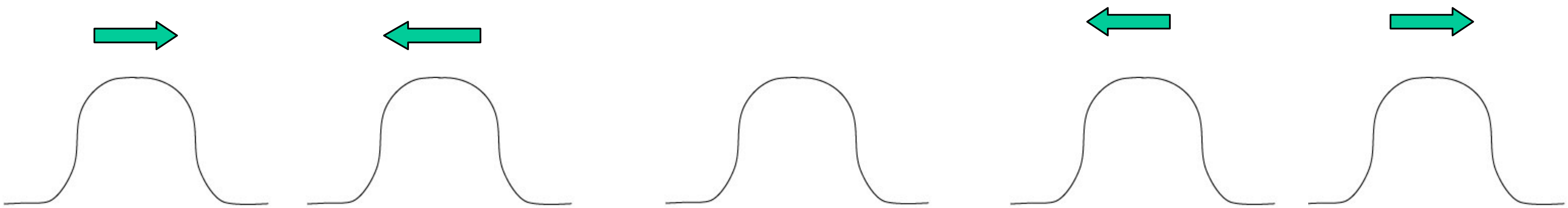
Where do Solitons Lurk?

- Linear, dispersionsless wave equations have (trivial) solitons

Linear $\phi_{tt} - c^2\phi_{xx} = 0$ Dispersionless $\omega(k) = k$

By superposition

$$\phi \equiv e^{-(x-ct)^2} + e^{-(x+ct)^2}$$



t = -T t = 0 t = +T

BUT ALSO: (some!) nonlinear, dispersive equations also have solitons
➔

VERY BIG SUPPRISE!

?Which Equations?

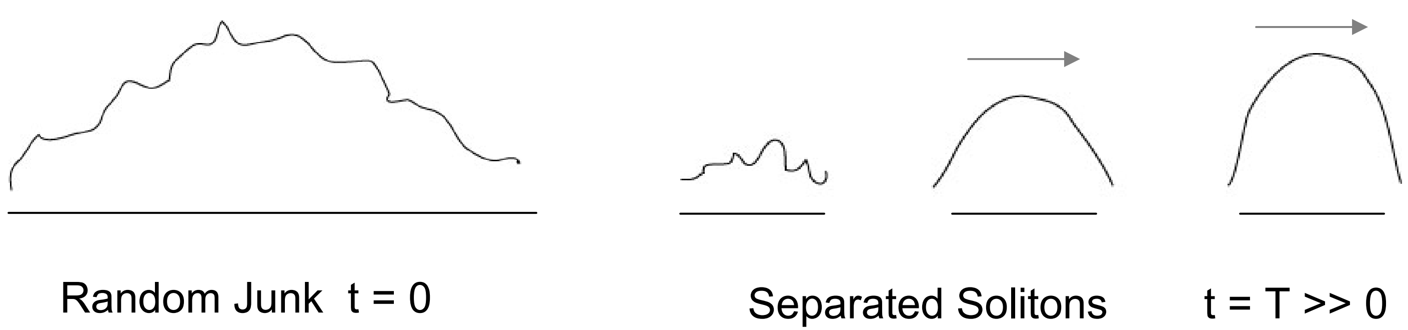
Equation		Solitary Wave
1. $u_t + uu_x + u_{xxx} = 0$	YES	$u_s = 3\mathrm{v}\,\mathrm{sech}^2 \frac{\sqrt{\mathrm{v}}}{2}\left(x - \mathrm{v}t\right)$
"Korteweg - De Vries "		
2. $i\psi_t + \psi_{xx} + k\lvert\psi\rvert^2\psi = 0$	YES	$\psi_s = \dfrac{\psi_0 e^{i\left(\frac{\mathrm{v}_1}{z}\left(x - v_2\, t\right)\right)}}{\cosh\left[\sqrt{\frac{x}{2}}\,\psi_0\left(x - \mathrm{v}_1 t\right)\right]}$ $\quad \psi_0 = \left[\dfrac{v_1(v_1 - 2v_2)}{2\mathrm{k}}\right]^{\frac{1}{2}}$
"Nonlinear Schrödinger"		
3. $\theta_{tt} - \theta_{xx} + \sin\theta = 0$	YES	$\theta_{s(\bar{s})} = 4\tan^{-1} e^{\pm\frac{(x - \mathrm{v}t)}{\sqrt{1-\mathrm{v}^2}}}$
"Sine-Gordon"		
4. $\phi_{tt} - \phi_{xx} - \phi + \phi^3 = 0$	NO!	$\phi_{s(\bar{s})} = \pm\tanh\left(\dfrac{1}{\sqrt{2}}\dfrac{(x - \mathrm{v}t)}{\sqrt{1 - \mathrm{v}^2}}\right)$
"ϕ^4"		

These solutions are clearly solitary waves, but are they solitons?

How do we know which are solitons? Historically, "experimental mathematics", then inverse scattering transform, group theoretic structure (Kac-Moody Algebras), Painlevé test.

Why are Solitons so Special?

1. That they exist at all in nonlinear equations is amazing; expect nonlinearity would destroy, particularly in view of our experience with low-dimensional dynamical systems.
2. Solitons—more generally, coherent structures—can dominate asymptotic form of solution.



Why are Solitons so Special?

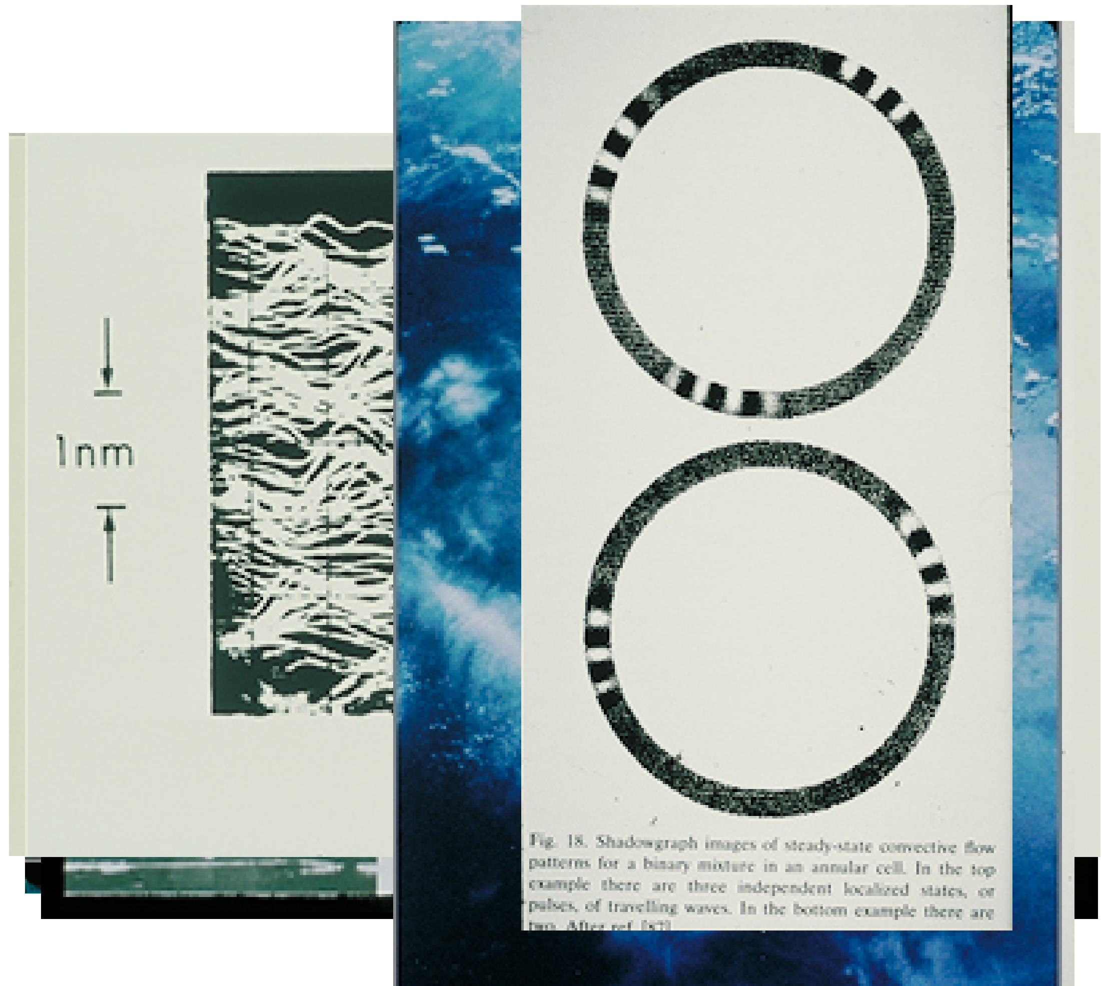
3. Many physical systems are well-approximated by soliton equations: novel starting point for pertubation theory.
    - KdV: Water waves, plasma motions, nonlinear lattices
    - NLSE: Self-focusing in laser/plasma, laser/fiber optic interactions, self-trapping in solids
    - SG: Domain walls in magnetic materials, Josephson transmission lines, model relativistic quantum field theory, key renomalization group equation
4. Conversely, soliton-like excitations are observed in all branches of physics, e.g. “Skyrmions” in nuclear and condensed matter physics, “monopoles” in particle physics, etc.
5. Deep mathematical structure
    - Infinite dimensional, completely integrable systems
    - Group theoretic/algebraic structure of conservation laws:
    - Kac – Moody algebras, Strings
    - Inverse spectral transformation/Painlevè test

Fermi was a Physicist – What About Solitons in Physics/Nature?

In the real world, don't expect exact soliton behavior: more general concept of coherent structures – persistent, localized spatial structures in extended nonlinear systems--is relevant.

Coherent Structures are observed on all scales in nature

- Red Spot of Jupiter
- Earth Ocean Waves
  - Tsunamis
  - Apollo – Soyuz image
  - Waves on a Beach
- Laboratory Fluid Expts
  - Smoke rings
  - Binary Convection
- Charge density waves in novel solid state materials
- Pulses in optical fibers

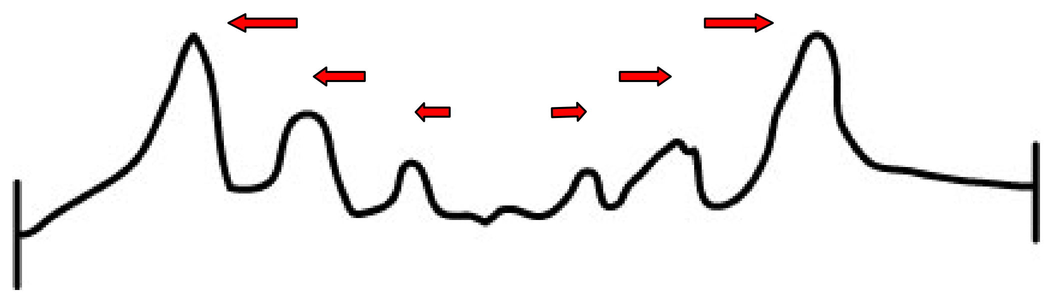


Important in Technology

Now close the loop: How do KdV solitons “explain” FPU recurrences?

Sketch of Argument:

- Initial pulse (typically low mode)  breaks up into (primarily) a few solitons. Number and size of solitons depends on initial condition. Recall larger pulses travel faster for KdV solitons.



- Solitons move with different velocities, so initial pulse spreads to other linear normal modes.

- But solitons retain their identities in collisions with each other and reflections off ends of system. Soliton velocities and length of interval L, determine frequencies will be incommensurate in general but can be approximated by rationals so that initial state will recur with period proportional to lowest common denominator.

$$\omega_i \propto v_i / L$$

$$\omega_i / \omega_j \cong \left(n / m \right)$$

- Exactness of recurrence is function of number of soliton modes and accuracy of rational approximation.

FPU and Chaos

Essence of chaos is "sensitive dependence on initial conditions" that causes nearby points in phase space to separate exponentially in time, creating orbits that wander throughout (much of) phase space $\approx$ "equipartition of energy" or ergodicity

Where is this in FPU?

First simple example of (Hamiltonian) chaos.

The "Standard" Map

$$p_{n+1} = p_n - \frac{k}{2\pi} \sin 2\pi q_n$$ Nonlinearity Parameter

(MOD 1)

$$q_{n+1} = q_n + p_{n+1}$$

n+1 necessary for Hamiltonian
(= Area preserving) map

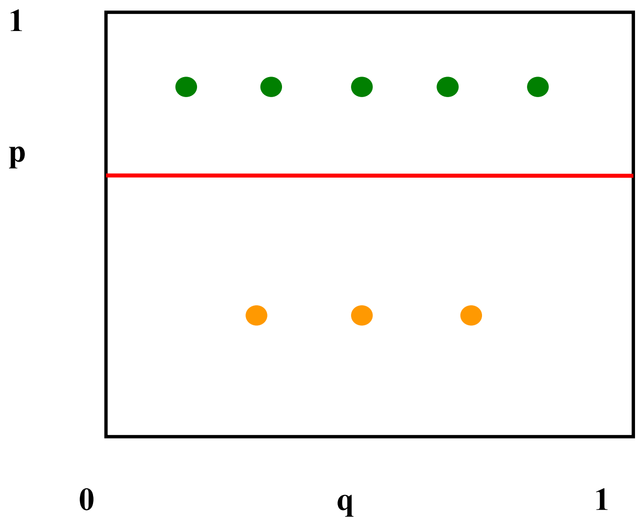
For $k = 0$ (i.e. no nonlinearity)

$$p_{n+1} = p_n \equiv p_0$$

Momentum Conserved

$$q_{n+1} = q_n + p_0$$

So orbits are straight lines of constant $p=p_o$ and q simply “rotating” around interval



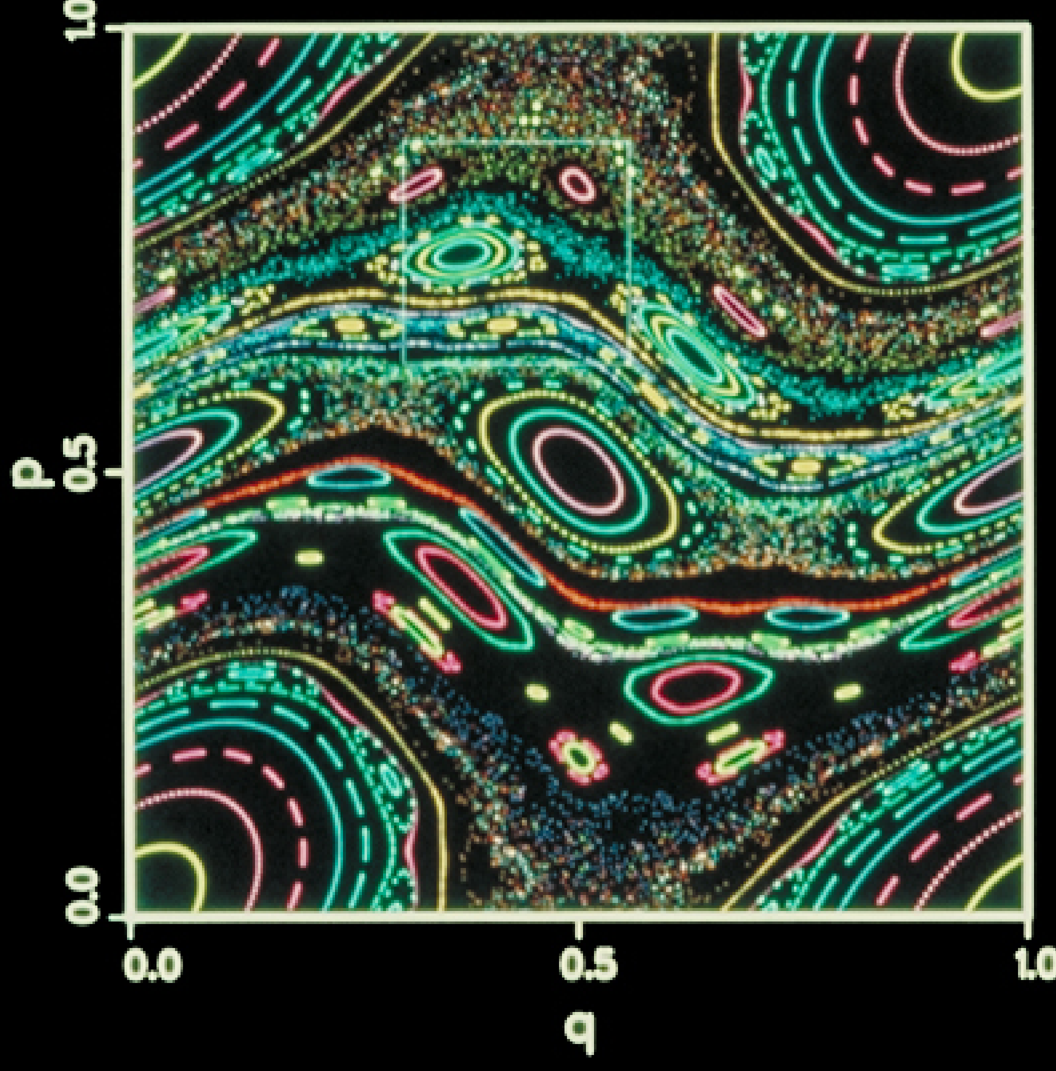
$p_0 = 4/5,\ q_0 = 0.1$

$p_0 = 1/\sqrt{2},\ q_0 =$ arbitrary

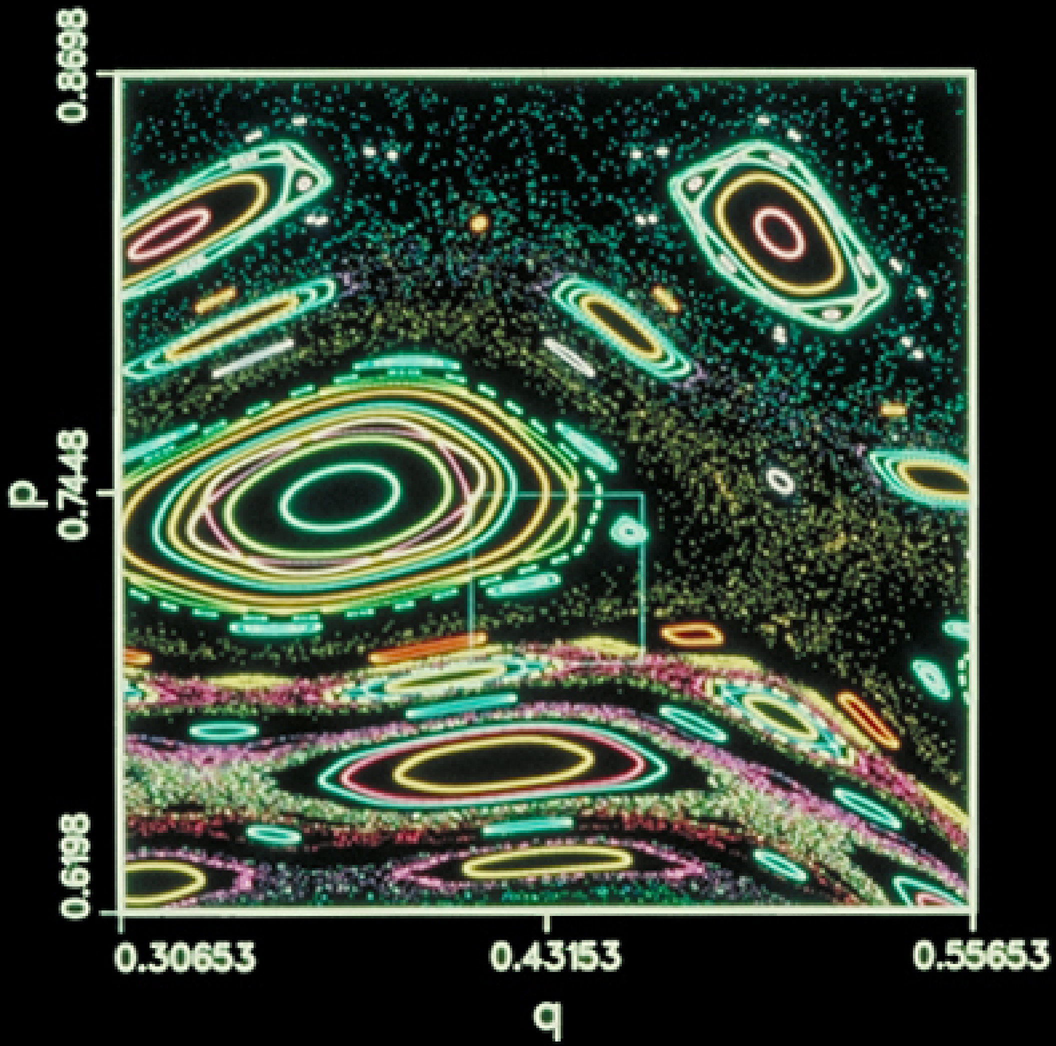
$p_0 = 1/3,\ q_0 = 0.5$

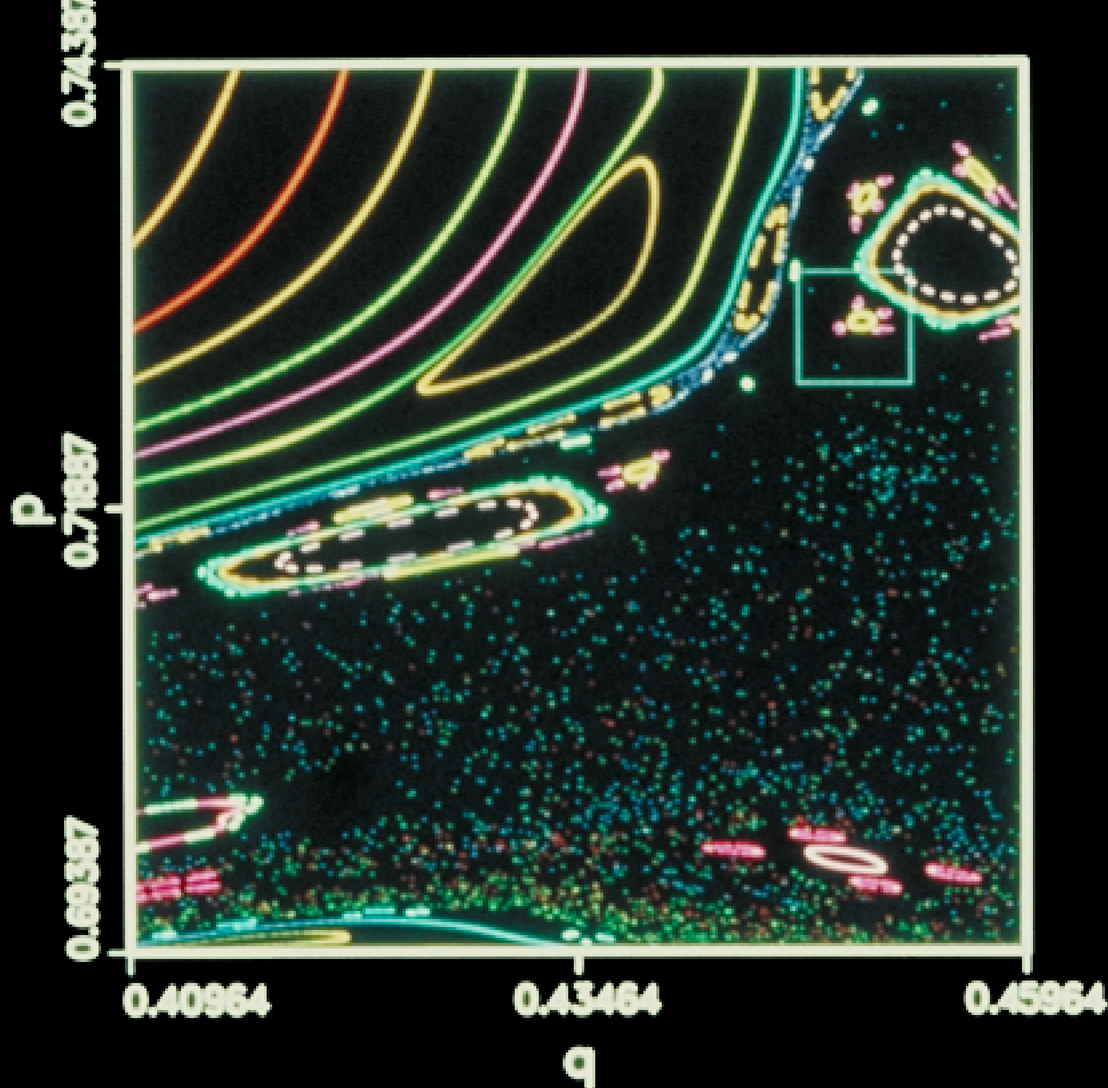
What about $k \neq 0$? => Chaos !

The next images show behavior for $k = 1.1$



1.0
p
0.5
0.0
0.0
0.5
1.0
q


0.8698
p
0.7448
0.6198
0.30653
0.43153
0.55653
q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0.69387
p
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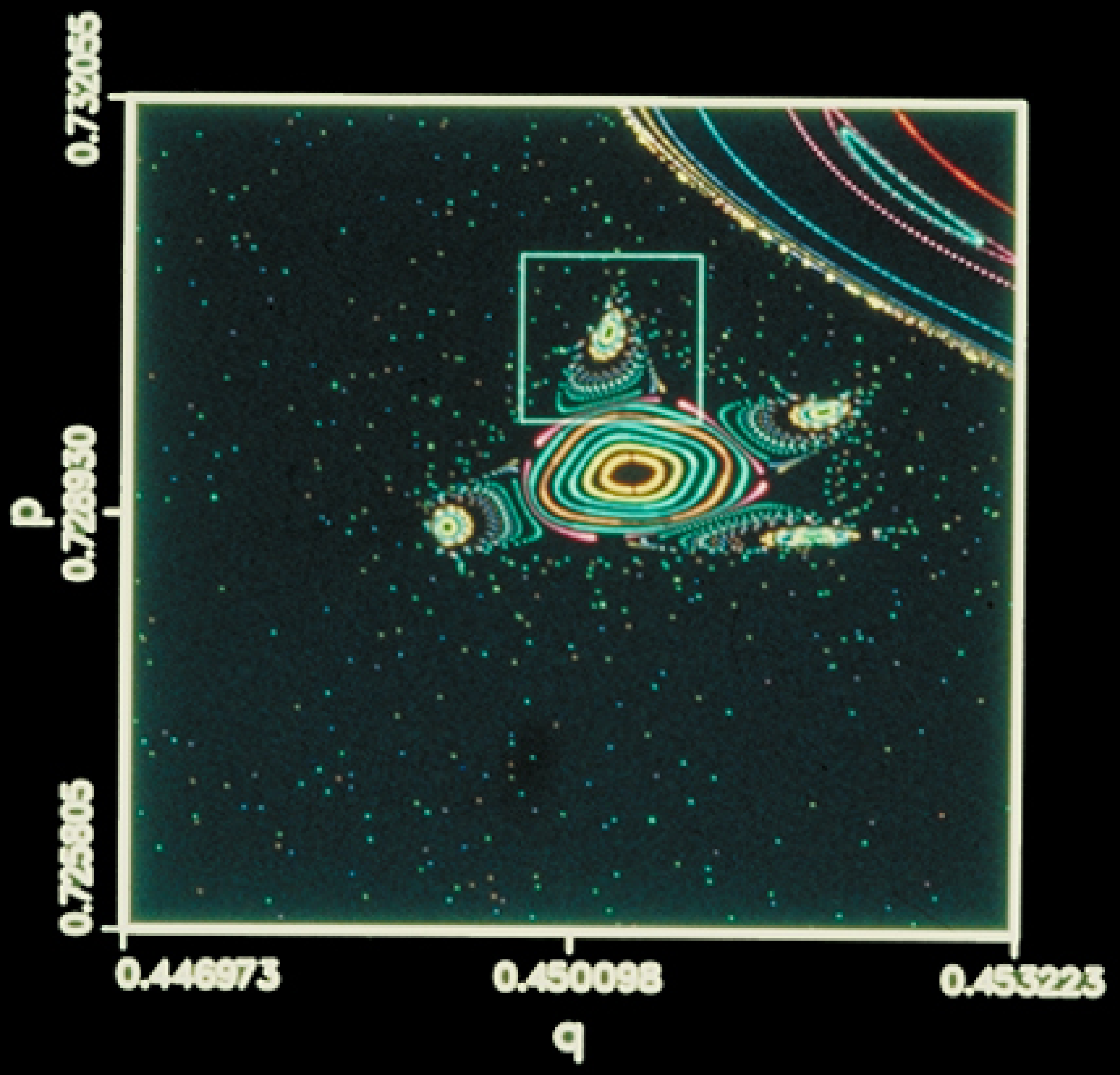
0.43464
0.45964
q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0.725805
p
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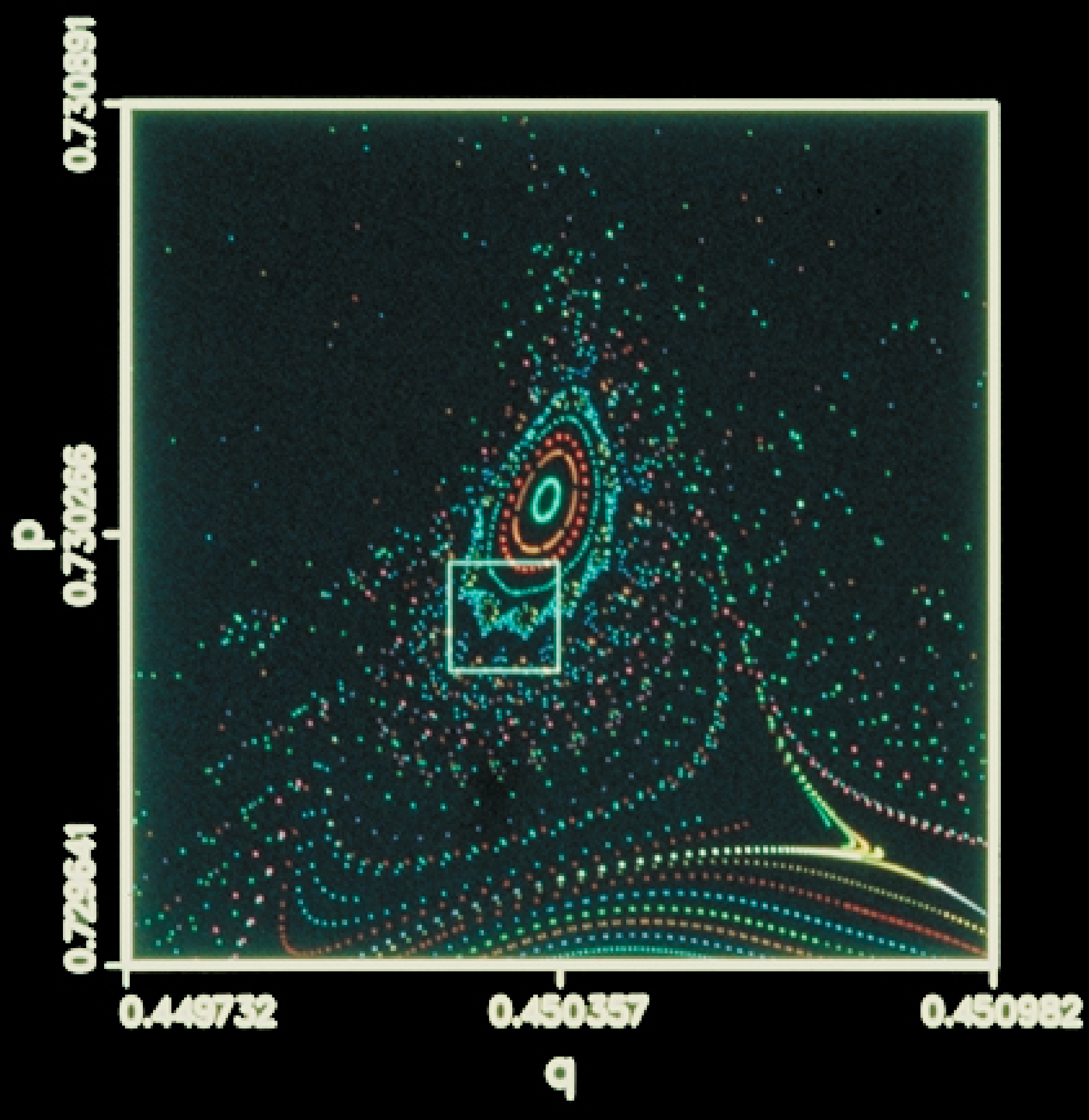
0.450098
0.453223
q


0.730891
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0.729641
p
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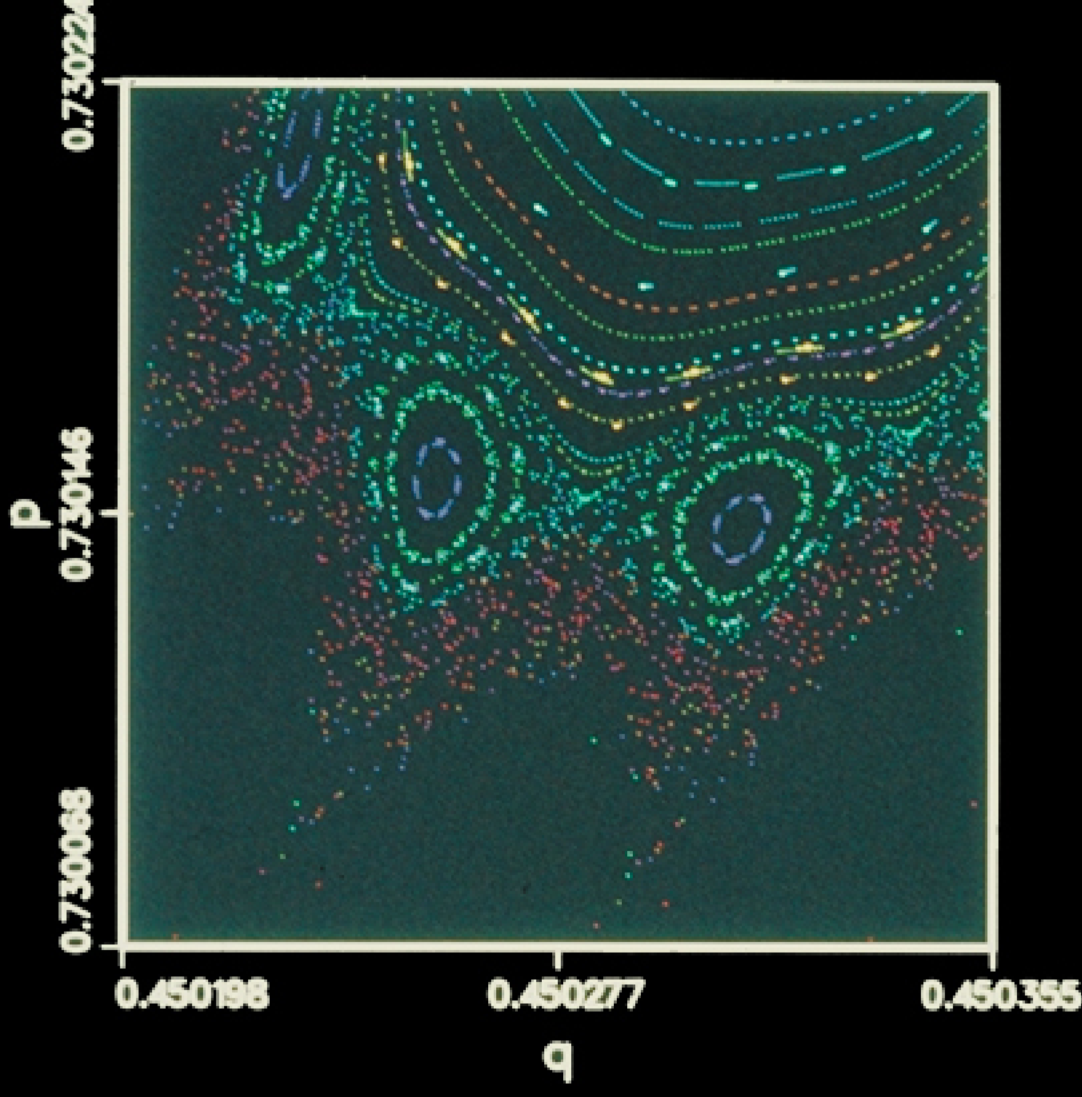
0.450982
q


0.730224
0.730146
0.730068
p
0.450198
0.450277
0.450355
q

Are there Chaos in FPU

- The answer is yes
- Detailed analysis, see reference books

FPU Today: The Fundamentals of Statistical Mechanics

Today FPU-like systems are still being studied extensively to gain insights into the nature of phase space, equipartition, and (near equilibrium) transport: e.g.

Are there permanently stable soliton-like solutions in FPU?

Is there a critical energy/particle above which equipartition will occur? If so, how does

$$\varepsilon_c(N_0) \equiv \left\lfloor Ecrit \middle/ N \right\rfloor\Big|_{N_0}$$

behave as $N_0 \to \infty$

Does $\varepsilon_c(N_0) \to 0$ $\qquad \to \varepsilon_c(\infty) \neq 0$

Answers still unknown in general !!!

See

G. Friesecke and R. Pego, "Solitary Waves in FPU Lattices: II. Linear Implies Nonlinear Stability," *Nonlinearity* **15** 1343-1359 (2002).

and

L. Casetti et al., "The Fermi-Pasta-Ulam Problem Revisited: Stochasticity thresholds in Hamiltonian systems, *Phys Rev E* **55**, 6566-6574 (1997).

FPU Today: Anomalous Transport in Low-Dimensional Systems

Do FPU like systems exhibit normal heat transport/ thermal conductivity? Relation of chaos to normal conductivity?

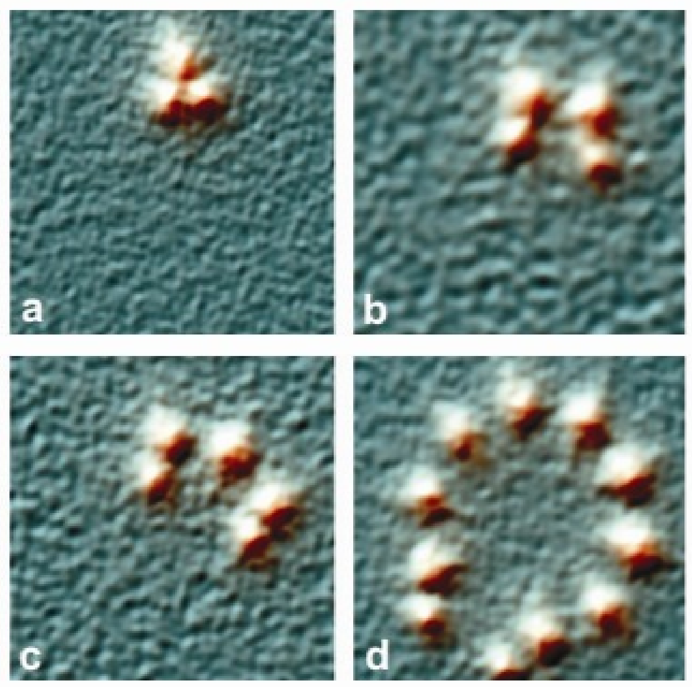
Answer recently discovered, No, to first question, for second question, chaos is neither necessary for non-sufficient for normal conductivity.

See T. Prosen and DKC, "Momentum Conservation Implies Anomalous Energy Transport in 1D Classical Lattices," ***Phys. Rev. Lett*****. 84 (2000).**

FPU Today: “Discrete Breathers”/Intrinsically Localized Modes

Nonlinear effects in lattice nonlinear systems, both classical and quantum, can produce stable, localized modes, with implications for inhomogeneous melting, energy storage, and transport.

Recent observations in Josephson Junction Ladders:



See P. Binder and A. V. Ustinov, “Exploration of a rich variety of breather modes in Josephson junction ladders,” *Phys. Rev. E* **66** 016603 (2002).

Bottom Line

FPU was a watershed problem: it led to solitons, to chaos, and is still leading to deeper insights into the fundamentals of statistic mechanics, anomalous transport, and energy localization. As we approach its 50th anniversary, the FPU problem is still very much alive and kicking. It was indeed a surprising

"Little Discovery."