FNAL
9/28/01

D K CAMPBELL

FROM FERMI-PASTA-ULAM TO SOLITONS & CHAOS

OR

FERMI & THE BIRTH OF COMPUTATIONAL PHYSICS & NONLINEAR SCIENCE

FERMI: REACH = GRASP

BREADTH OF SUBJECT: STAN ULAM

HOW TO SOLVE PROBLEM OF PRESENTATION?

MARK KAC

CHRIS QUIGG

OUTLINE

- WHAT IS THE "FPU PROBLEM"?
- FPU AND SOLITONS
- FPU AND CHAOS
- FPU TODAY: THE FUNDAMENTALS OF STAT MECH

WHAT IS THE FPU PROBLEM?

SUMMER 1954 IN LOS ALAMOS

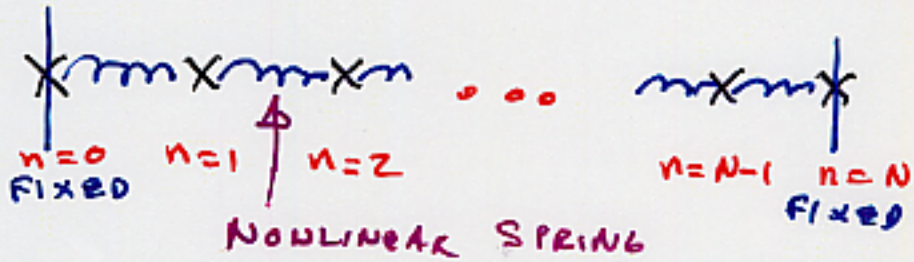
ENRICO FERMI, JOHN PASTA, STAN ULAM DECIDED TO USE THE WORLD'S THEN MOST POWERFUL COMPUTER, THE

MANIAC-1

(MATHEMATICAL ANALYZER NUMERICAL INTEGRATOR AND COMPUTER)

TO STUDY THE EQUIPARTITION OF ENERGY EXPECTED BY STATISTICAL MECHANICS BY LOOKING AT A 1D CHAIN OF EQUAL MASS PARTICLES COUPLED BY NONLINEAR* SPRINGS:

* THEY KNEW LINEAR SPRINGS COULD NOT PRODUCE EQUIPARTITION



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

2A - 2F FROM THE ORIGINAL PREPRINT

QUIZ: DETECT ANY ERRORS?

C. 19

LOS ALAMOS SCIENTIFIC LABORATORY
of the
UNIVERSITY OF CALIFORNIA

Report written:
May 1955

Report distributed:
NOV 2 1955

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

PHYSICS

LOS ALAMOS NATIONAL LABORATORY
3 9338 00353 5696

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 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.

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

The problems 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

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

the purposes of numerical work this continuum is replaced by a finite 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

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

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

or

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

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

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

NOTE THE ERROR HERE

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TO STUDY SYSTEMATICALLY, START FROM LINEAR LIMIT

$\alpha = \beta = 0 \Rightarrow$ WITH $x_n = n \cdot a + y_n$,

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

FAMILIAR (LINEAR) "PHONON" DISPERSION RELATION FROM SOLID STATE PHYSICS: ASSUMING

$$\boxed{y_n = A\, e^{i(k \cdot n \cdot a - \omega(k) t)}} \qquad (2)$$

NB: WE HAVE INTRODUCED LATTICE SPACING "a" FOR LATER PURPOSES

WE FIND THAT (1) CAN BE SOLVED PROVIDED

$$\boxed{\omega(k) = 2\omega_0 \sin \frac{ka}{2}}, \qquad \omega_0 = \sqrt{\frac{K}{M}}$$

FOR WEAK NONLINEARITY $(\alpha = \varepsilon \ll 1,\ \beta = 0)$ DESCRIPTION IN TERMS OF NORMAL MODES

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

SEPARATES THE PROBLEM INTO WEAKLY COUPLED HARMONIC OSCILLATORS

$$\boxed{H = \frac{1}{2} \sum \dot{A}_k^2 + \omega^2(k) A_k^2 + \alpha \sum C_{klm} A_k A_l A_m}$$

FOR STRONG NONLINEARITY, FPU EXPECTED THAT, WHATEVER THE INITIAL STARTING POINT, THE NORMAL MODES WOULD SHARE THE ENERGY EQUALLY:

?? RESULTS ??

ULAM QUOTE

SLIDES 3A/3B

1) ONLY LOWEST FEW MODES EXCITED !!
2) RECURRENCES !!
3) SUPERRECURRENCES !!

1.1.VI

(11A)

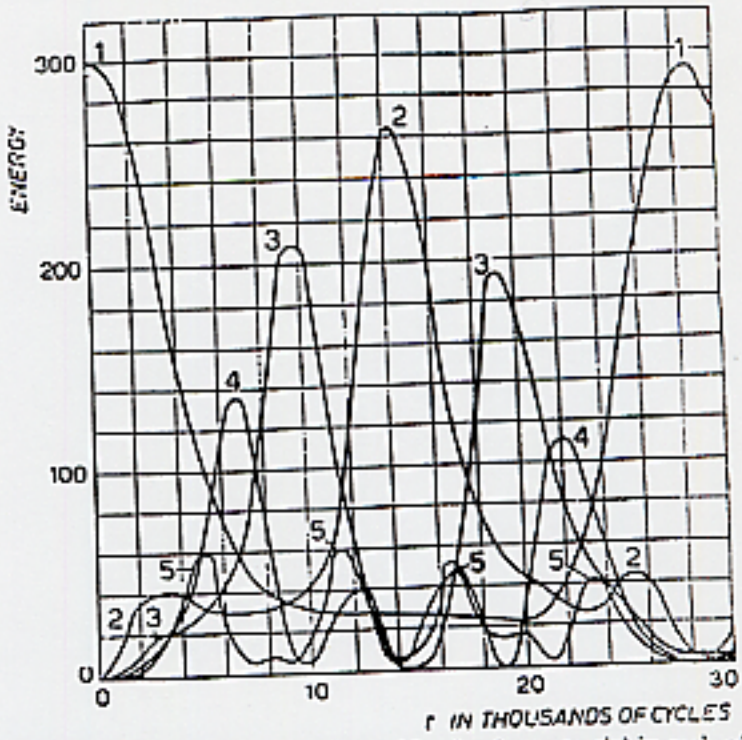


Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About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

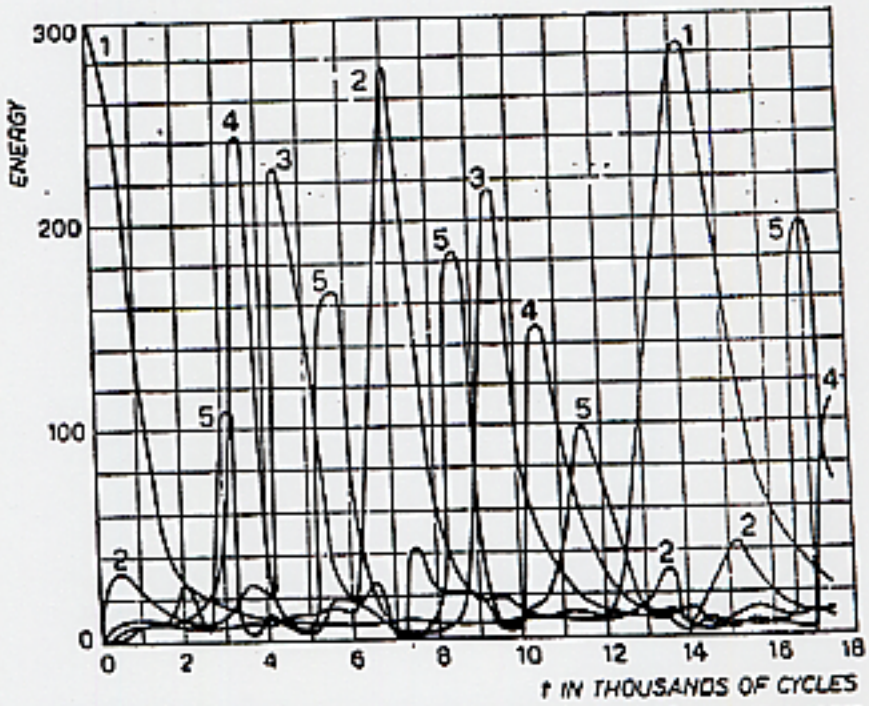


Fig. 2. – Same conditions ad fig. 1 but the quadratic term in the force was stronger. $\alpha = 1$. About 14,000 cycles were computed.

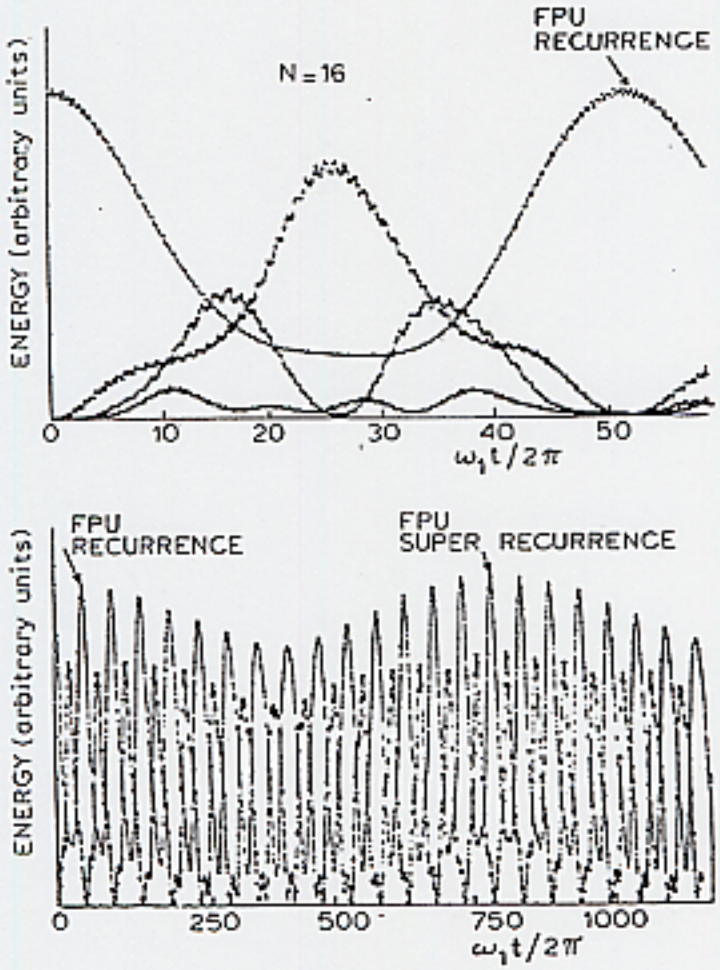


Fig. 10. In the upper part of this figure is seen the standard energy sharing between normal modes for an FPU system (here $N = 16$) integrated through one recurrence. By greatly extending the integration interval as shown in the lower figure, Tuck and Menzel [23] exposed a superperiod of recurrence. 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 LATE 50s / EARLY 60s SEVERAL GROUPS LOOKED AT THIS PROBLEM USING MULTIPLE SCALE ANALYSIS IN THE FORMAL CONTINUUM LIMIT $a \to 0$

[YOU WILL NOT GET THE WHOLE TRUTH HERE]

$$y_n(t) \xrightarrow[a \to 0]{} y(x = n \cdot a, t) \underset{\varepsilon \ll 1}{\simeq} y(\xi = x - vt, \varepsilon t) + O(\varepsilon) \cdots$$

FOUND THAT FOR CONSISTENCY HAD TO HAVE

$\partial y / \partial \xi \equiv u$ SATISFY

$$\boxed{u_t + u u_x + u_{xxx} = 0}$$

KORTEWEG - DE VRIES EQN

ZABUSKY & KRUSKAL (1965) : "SOLITON"

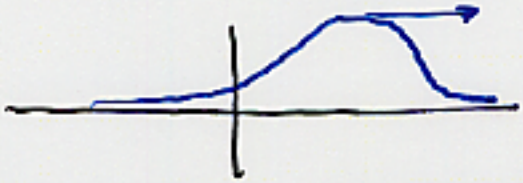
$$\boxed{u(x,t) = 3v \operatorname{sech}^2 \frac{\sqrt{v}}{2}(x - vt)}$$

NOTE THE INTERDEPENDENCE OF AMPLITUDE, SHAPE, AND VELOCITY

WHAT IS A SOLITON?

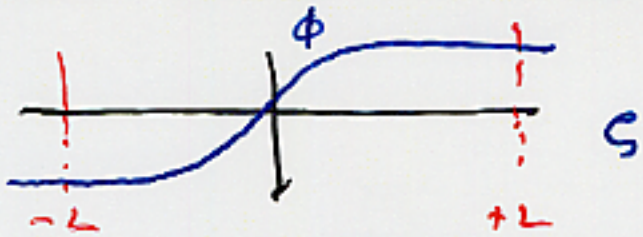
CONSIDER CONTINUUM, WAVE-LIKE MOTION, 1 SPACE DIMENSION

DEF: SOLITARY WAVE : LOCALIZED, TRAVELING WAVE



$\phi_s(\xi = x - vt)$

NB! DIFFERENT STATES ALLOWED FOR $\xi \to \pm\infty$



LOCALIZED, SINCE $\phi' = 0$ FOR $|\xi| > L$

DEF: SOLITON : SOLITARY WAVE THAT PRESERVES AMPLITUDE, SHAPE, AND VELOCITY AFTER COLLISIONS WITH ALL OTHER WAVES.

WHERE DO SOLITONS LURK?

- LINEAR, DISPERSIONLESS WAVE EQUATIONS HAVE (TRIVIAL) SOLITON SOLUTIONS

LINEAR $\boxed{\phi_{tt} - c^2 \phi_{xx} = 0}$ 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 $\Rightarrow$

VERY BIG SURPRISE!

? WHICH EQUATIONS ?

THIS SIMPLE QUESTION SPARKED A DECADES LONG QUEST, PRETTY WELL SOLVED, TO FIND THE MYSTERY OF THE SOLITON. HERE WE GIVE CLIMPSE OF A FEW OF THE ANIMALS IN THE MATHEMATICAL SECTION OF THE SOLITON ZOO

EQUATION	SOLITARY WAVE
1) $u_t + u u_x + u_{xxx} = 0$ "KORTEWEG-DEVRIES (KdV)"	$u_s = 3v \operatorname{sech}^2 \frac{\sqrt{v}}{2}(x - vt)$
2) $i\psi_t + \psi_{xx} + k\lvert\psi\rvert^2\psi = 0$ "NONLINEAR SCHRÖDINGER"	$\psi_s = \dfrac{\psi_0 e^{i\left(\frac{v_1}{2}(x - v_2 t)\right)}}{\cosh\left[\sqrt{\frac{k}{2}}\,\psi_0 (x - v_1 t)\right]}$ $\psi_0 = \left[\dfrac{v_1(v_1 - 2v_2)}{2k}\right]^{1/2}$
3) $\theta_{tt} - \theta_{xx} + \sin\theta = 0$ "SINE-GORDON"	$\theta_{s(\bar{s})} = 4\tan^{-1} e^{\pm\frac{(x - vt)}{\sqrt{1-v^2}}}$
4) $\phi_{tt} - \phi_{xx} - \phi + \phi^3 = 0$ "ϕ^4"	$\phi_{s(\bar{s})} = \pm\tanh\left(\frac{1}{\sqrt{2}}\frac{(x - vt)}{\sqrt{1-v^2}}\right)$

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

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FERMI WAS A PHYSICIST -- WHAT ABOUT SOLITONS IN PHYSICS / NATURE ?

IN 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

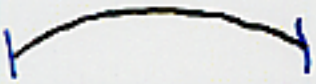
- RED SPOT OF JUPITER — 4×10^7 m
- EARTH OCEAN WAVES — 10^5 m $\rightarrow 10^2$ m
  - TSUNAMIS
  - APOLLO - SOYUZ IMAGE
  - WAUSON BEACH
- LABORATORY FLUID EXPTS — 1 m $\rightarrow 10^{-2}$ m
  - SMOKE RINGS
  - BINARY CONVECTION
- CHARGE DENSITY WAVES IN NOVEL SOLID STATE MATERIALS : $TaSe_2$ vs TaS_2 — 5×10^{-10} m
- IMPORTANT IN TECHNOLOGY $\Longrightarrow$ POLSES IN OPTICAL FIBERS — 10^{-6} m WIDE, 10^{-3} m LONG

VIDEO OF CAVITONS IN PLASMAS

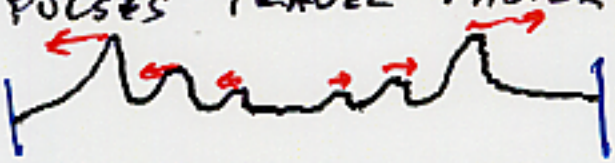
NOW CLOSE THE LOOP: HOW DO KdV SOLITONS "EXPLAIN" FPU RECURRENCES?

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



- 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 OF ENDS OF SYSTEM. SOLITON VELOCITIES & LENGTH OF INTERVAL, L, DETERMINE FREQUENCIES $\omega_i \propto v_i/L$: ω_i'S WILL BE INCOMMENSURATE IN GENERAL BUT CAN BE APPROXIMATED BY RATIONALS $\omega_i/\omega_j \cong (n/m)_{ij}$ SO THAT INITIAL STATE WILL RECUR WITH PERIOD $\propto$ LOWEST COMMON DENOMINATOR

$\Rightarrow$ EXACTNESS OF RECURRENCE IS FUNCTION OF NUMBER OF SOLITON MODES AND ACCURACY OF RATIONAL APPROXIMATION

FPU AND CHAOS

RECALL THAT ESSENCE OF CHAOS IS "SENSITIVE DEPENDENCE ON INITIAL CONDITIONS" WHICH CAUSES NEARBY POINTS IN PHASE SPACE TO SEPARATE EXPONENTIALLY IN TIME, CREATING ORBITS THAT WANDER THROUGHOUT (MUCH OF) PHASE SPACE ≈ ? "EQUIPARTITION OF ENERGY / ERGODICITY"?

? WHERE IS THIS IN FPU? FIRST CONSIDER SIMPLE EXAMPLE OF (HAMILTONIAN) CHAOS

THE "STANDARD" MAP

NONLINEARITY PARAMETER

$$p_{n+1} = p_n - \frac{k}{2\pi}\sin 2\pi q_n \quad (\text{MOD } 1)$$

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

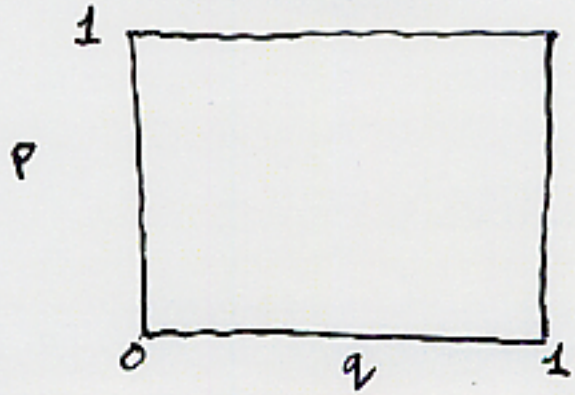
NB: n+1 NECESSARY FOR HAMILTONIAN (= AREA PRESERVING) MAP

FOR $k=0$ (i.e., NO NONLINEARITY)

$$p_{n+1} = p_n \equiv p_0 \qquad \text{MOMENTUM CONSERVED}$$

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

SO ORBITS ARE STRAIGHT LINES OF CONSTANT $p = p_0$ AND q SIMPLY "ROTATING" AROUND INTERVAL



WHAT ABOUT $k \neq 0$? CHAOS S9A–S9F

CHAOTIC ORBITS ≈ "CANTOR DUST"

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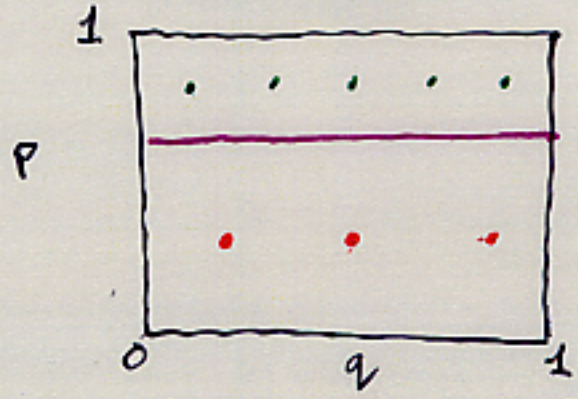

$p_0 = 4/5$, $q_0 = .1$

$p_0 = 1/\sqrt{2}$

$p_0 = \frac{1}{3}$ $q_0 = 1/2$

WHAT ABOUT $k \neq 0$? CHAOS S9A–S9F

CHAOTIC ORBITS ≈ "CANTOR DUST"

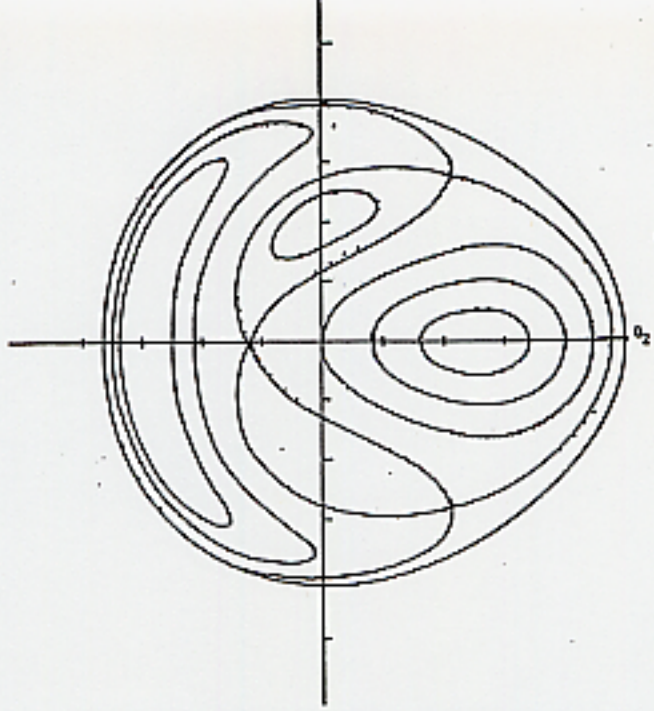

Fig. 11. The first of three figures which originally appeared in the celebrated paper by Hénon and Heiles [24]. Here we see a plot of the Poincaré surface of section for the Hénon–Heiles conservative system at system energy $E = 1/12$. Curves appear to exist everywhere in the permitted area, indicating possible integrability.

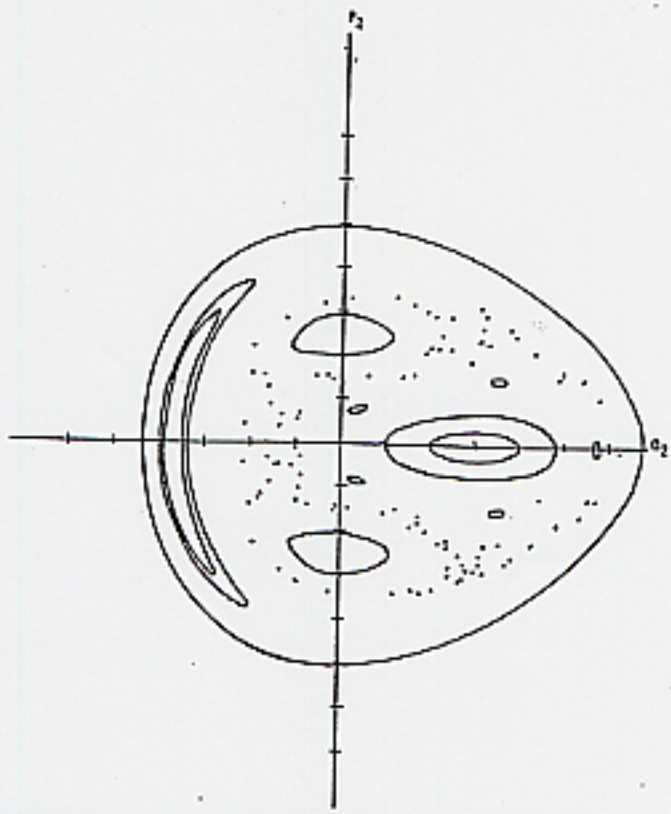

Fig. 12. The genuine surprise provided by the Hénon–Heiles calculations first appeared in this figure for $E = 1/8$. All this "random splatter" of dots was generated by a single orbit. All hope of integrability now disappears. Indeed, since Hénon and Heiles demonstrated the sensitive dependence of orbits lying in this "splatter" region, this figure provides an early illustration of the transition to chaos in a Hamiltonian system with only two degrees of freedom.

⊙ 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 ; eg

IS THERE A CRITICAL ENERGY / PARTICLE ABOVE WHICH EQUIPARTITION WILL OCCUR ?

IF SO, HOW DOES $\varepsilon_c(N_0) \equiv \left[E_{crit}/N\right]\Big|_{N_0}$ BEHAVE AS $N_0 \to \infty$? DOES $\varepsilon_c(N_0) \to 0$? $\to \varepsilon_c(\infty) \neq 0$?

ANSWER STILL UNKNOWN

CAN 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 NOR SUFFICIENT FOR NORMAL CONDUCTIVITY.

BOTTOM LINE: FPU WAS A WATERSHED PROBLEM, A CLASSIC EXAMPLE OF FERMI'S IMPACT: IT LED TO SOLITONS, TO CHAOS, AND IS STILL LEADING TO DEEPER INSIGHTS INTO THE FUNDAMENTALS OF STATISTICAL MECHANICS. NEARLY 50 YEARS AFTER IT WAS POSED AND FIRST STUDIED, FPU IS STILL VERY MUCH ALIVE AND KICKING. IT WAS INDEED A SURPRISING "LITTLE DISCOVERY"