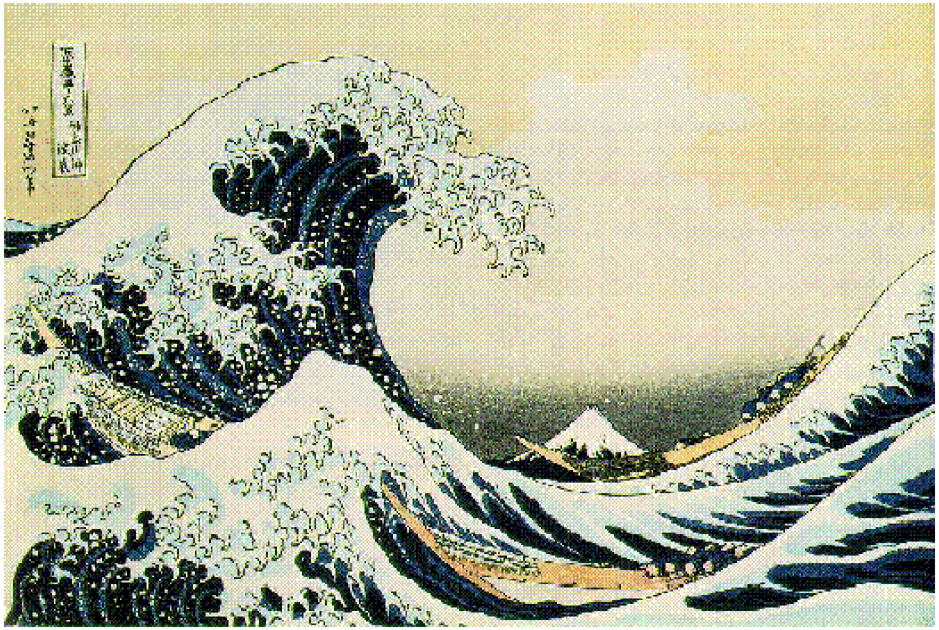
From FPU to Intrinsic Localized Modes:

An Odyssey in Nonlinear Science

David K. Campbell

Boston University



Department of Physics
University of Toronto
March 30, 2006

Outline

- Intrinsic Localized Modes: Definition and Bottom Line
- “In the beginning..” was the FPU Problem
  - FPU and Solitons—integrable vs. non-integrable
  - Quest for a continuum ϕ^4 breather—hints of a *discrete* ϕ^4 breather
- ILMs/discrete breathers in the *anti*continuum limit
  - Intuition and Theory
  - Other Historical Precursors
- Current Experimental Observations of ILMs
- Towards the future
- Summary and Conclusions

Discrete Breathers and ILMs

- Definition: an “intrinsic localized mode”—or “discrete breather”—is a *highly* spatially localized, time-periodic, stable (or at least very long-lived) excitation in a spatially extended, perfectly periodic, discrete system.

- Bottom Line: The mechanism that permits the existence of ILMs/DBs has been understood theoretically for more than a decade, following pioneering works of Sievers, Takeno, Page, Aubry, MacKay, and others. Only recently have they been observed in physical systems as distinct as charge-transfer solids, Josephson junctions, photonic structures, and micromechanical oscillator arrays.

"In the beginning…" was FPU

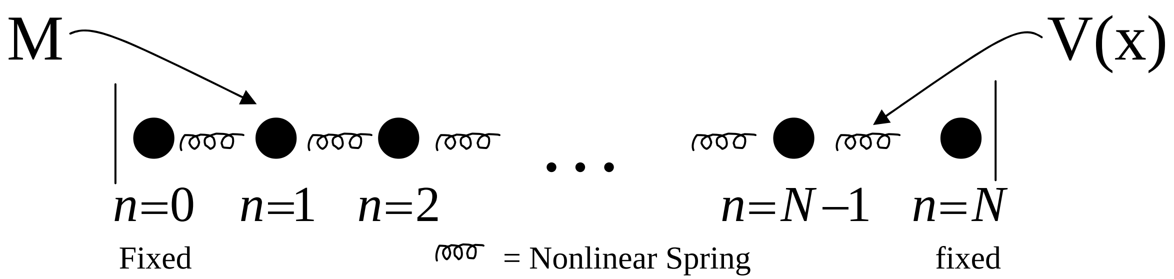
Los Alamos, Summers 1953-4 Enrico Fermi, John Pasta, and Stan Ulam decided to use the world's then most powerful computer, the

MANIAC-1

(Mathematical Analyzer Numerical Integrator And Computer)

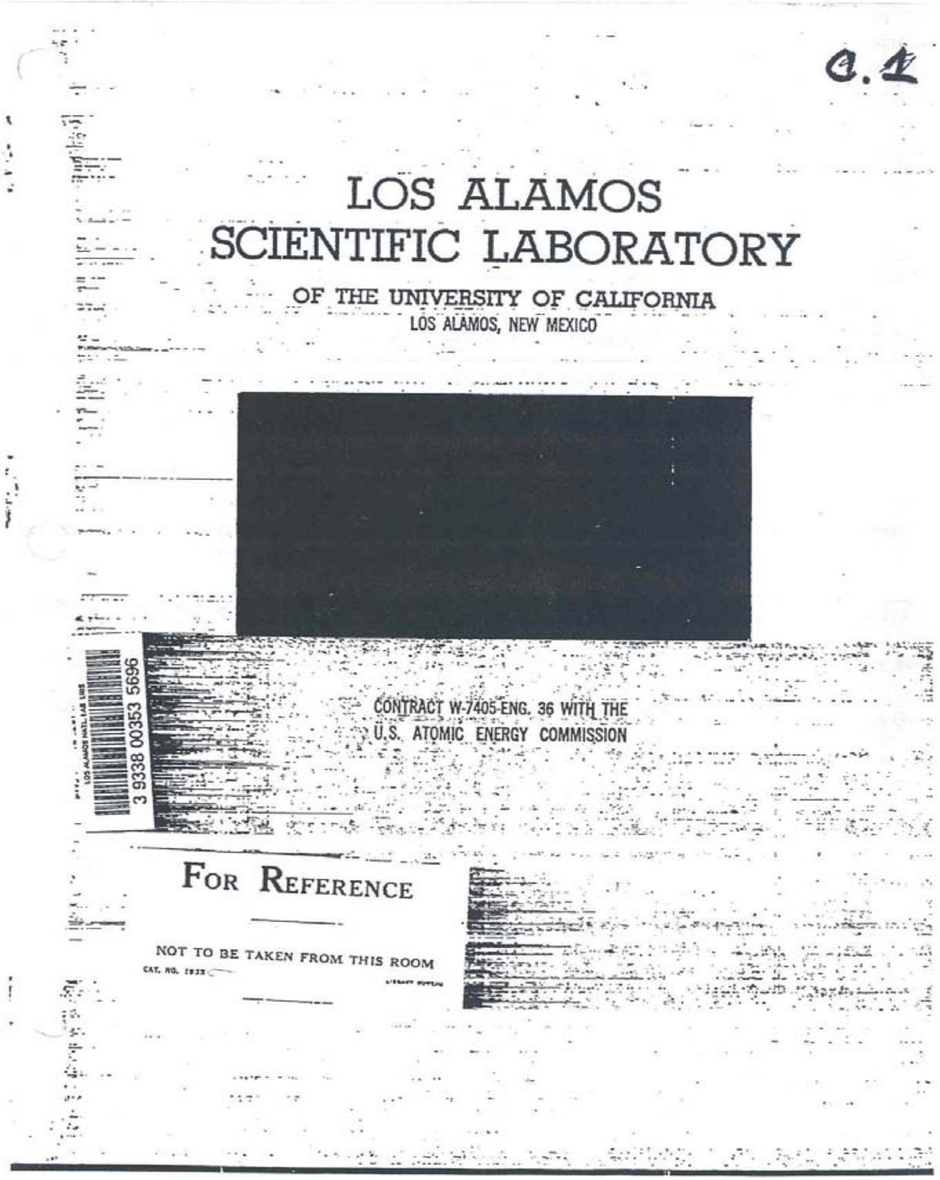
to study the equipartition of energy expected from statistical mechanics in simplest classical model of a solid: a ID chain of equal mass particles coupled by *nonlinear** springs:

*They knew linear springs could not produce equipartition



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

“In the beginning……”



c.1

LOS ALAMOS
SCIENTIFIC LABORATORY

OF THE UNIVERSITY OF CALIFORNIA
LOS ALAMOS, NEW MEXICO

[redacted]

CONTRACT W-7405-ENG. 36 WITH THE
U.S. ATOMIC ENERGY COMMISSION

Additional author ?

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

Key conclusion

ABSTRACT

A one-dimensional dynamical system of 64 particles with forces be-
en 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.

-2-

“Experimental Mathematics”: Von Neumann quote

At least an acknowledgement

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

...form, and heuristic work was performed numerically on a fast

electronic computing machine ...

behavior of such systems was ...

ing, 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.

-3-

What did FPU discover?

1. Only lowest few modes excited. Note only modes 1-5
2. Recurrences

982 266. – *Studies of non Linear Problems*

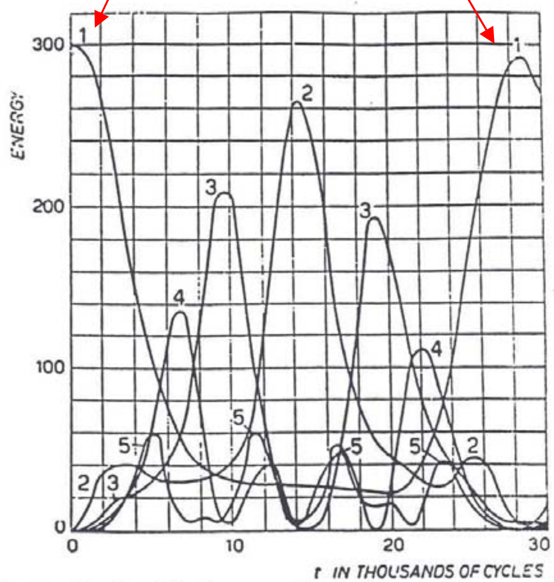


Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About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

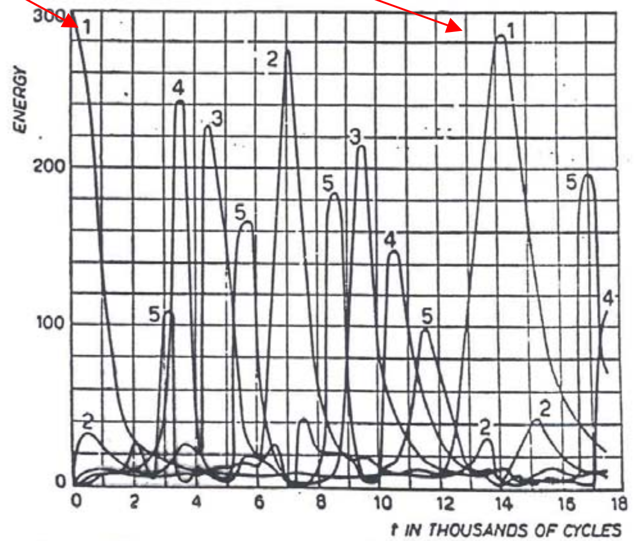
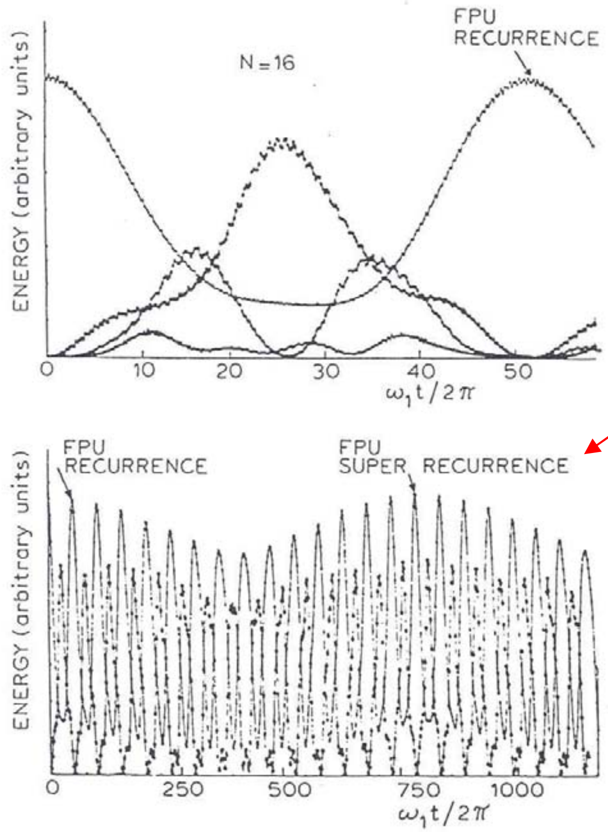


Fig. 2. – Same conditions ad fig. 1 but the quadratic term in the force was stronger. $\alpha = 1$. About 14,000 cycles were computed.

3. Superrecurrence



Now an author!

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 (Kruskal,…)used multiple scale analysis in formal continuum limit $a \to 0$ to approximate

[you will not get the whole truth here—recall advice of Mark Kac]

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

Found that for the consistency had to have $\partial y / \partial \zeta \equiv u$ satisfy KdV eqn

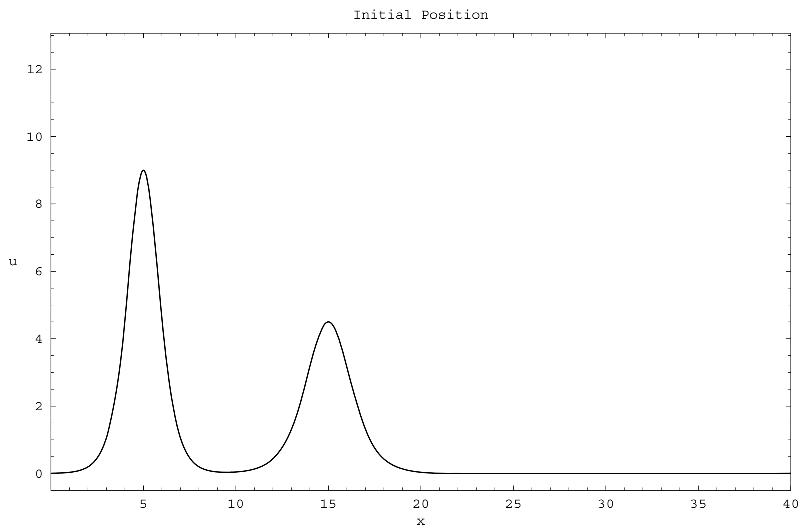
$$u_t + uu_x + u_{xxx} = 0$$

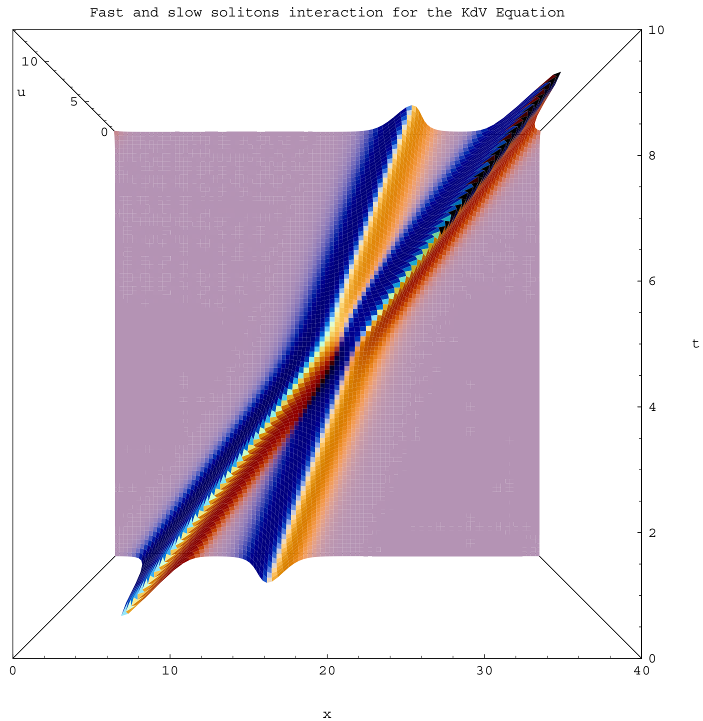
Zabusky & Kruskal (1965): "soliton"

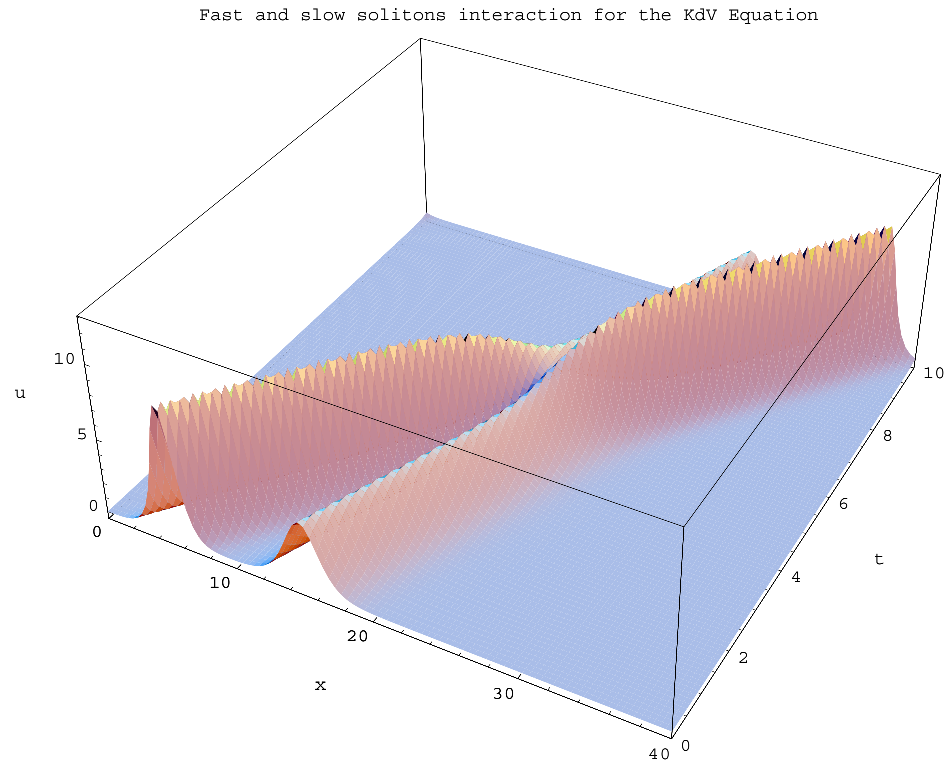
$$u(x,t) = 3\mathrm{v}\,\mathrm{sech}^2 \frac{\sqrt{\mathrm{v}}}{2}(x - \mathrm{v}t)$$

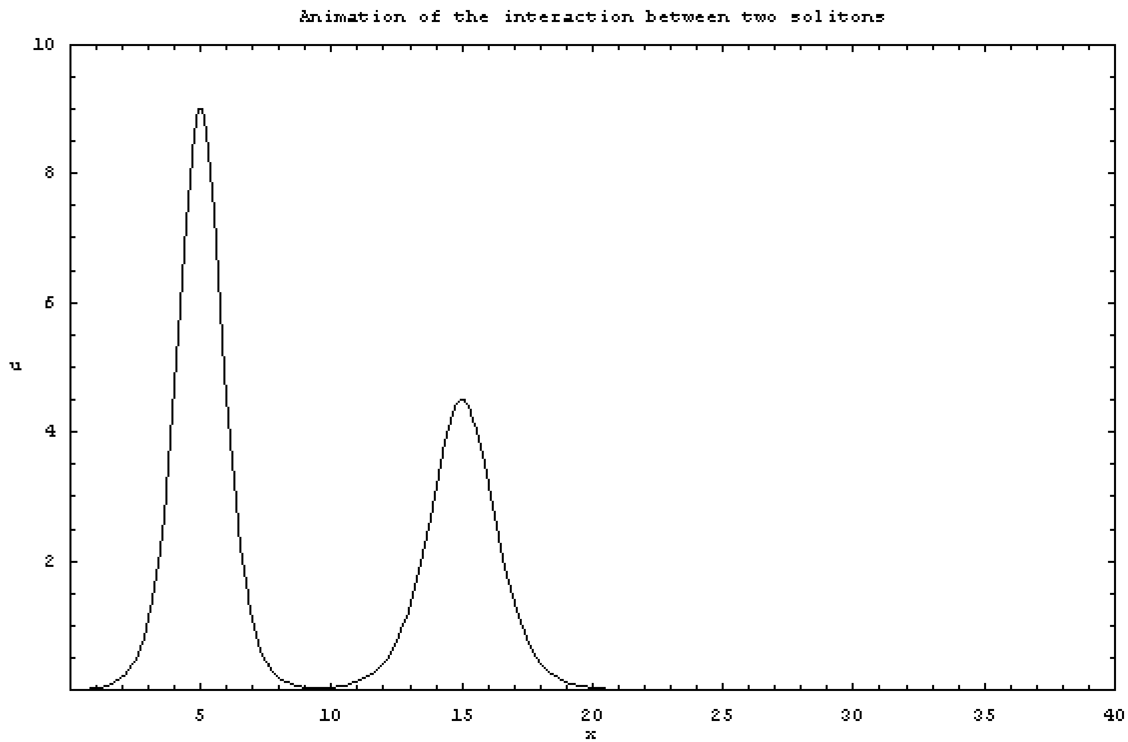
Amplitude, shape and velocity *interdependent:* characteristic of nonlinear wave—solitons *retain* identities in interactions!

Soliton collision: $V_l = 3$, $V_s=1.5$



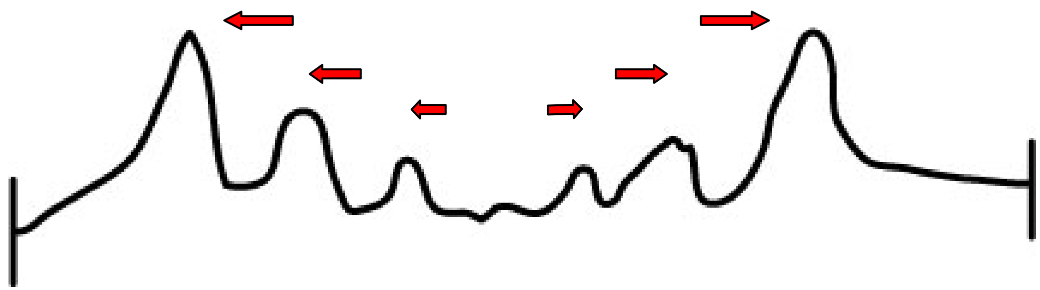





Animation of the interaction between two solitons
10
8
6
u
4
2
5
10
15
20
25
30
35
40
x

How do KdV solitons “explain” FPU recurrences?

- 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.

Integrable vs. Non-Integrable

	Equation		Solitary Wave
"S-G"	$\theta_{tt} - \theta_{xx} + \sin\theta = 0$	YES	$\theta_{s(\bar{s})} = 4\tan^{-1} e^{\pm\frac{(x-\mathrm{v}t)}{\sqrt{1-\mathrm{v}^2}}}$
" ϕ^4"	$\phi_{tt} - \phi_{xx} - \phi + \phi^3 = 0$	NO!	$\phi_{s(\bar{s})} = \pm\tanh\left(\frac{1}{\sqrt{2}}\frac{(x-\mathrm{v}t)}{\sqrt{1-\mathrm{v}^2}}\right)$

How do we know integrable from non-integrable?

Historically, combination of "experimental mathematics" (ϕ^4) and known analytic solutions (S-G), then inverse scattering transform, group theoretic structure (Kac-Moody Algebras), Painlevé test.

Does any part of hierarchy of solitons in integrable theories (S-G breather) exist in non-intergrable theories? Recall S-G breather, stable, (exponentially) localized, periodic solution

$$\theta_b(x,t) = 4\tan^{-1}\left(\frac{\varepsilon\,\sin(t/\sqrt{1+\varepsilon^2})}{\cosh([\varepsilon(x-x_0)]/\sqrt{1+\varepsilon^2})}\right),$$

Quest for a Φ^4 breather

- In late 70s-early 80s several groups took up the challenge: Does the continuum "ϕ^4" equation have a breather solution?

- Began with small amplitude, multiple scale expansion, which predicted the existence of a stable, exponentially localized breather solution

$$\phi_{SAB} = 1 + (2\varepsilon/\sqrt{3})\operatorname{sech}\xi\cos\tau - \varepsilon^2\operatorname{sech}^2\xi + \varepsilon^2/3\operatorname{sech}^2\xi\cos 2\tau +$$

$$\varepsilon^3/(6\sqrt{3})\operatorname{sech}^3\xi\cos 3\tau + \ldots\ldots$$

$$\xi = \varepsilon\sqrt{2}x/(\sqrt{(1+\varepsilon^2)}) \qquad \tau = \sqrt{2}t/(\sqrt{(1+\varepsilon^2)})$$

Localized and periodic to all orders in ε

Quest for a Φ^4 breather, cont'd

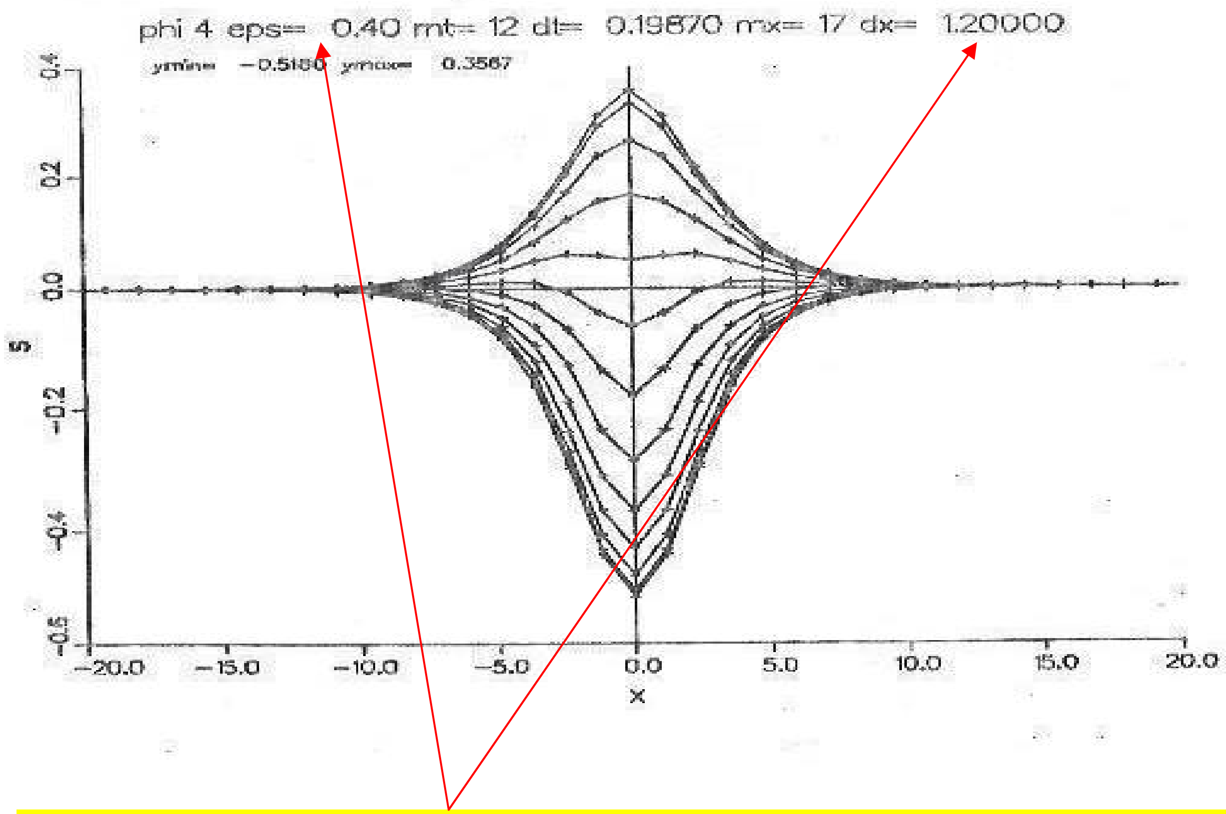
- Studied numerically model discretized in space using an iterative method that converged on solution at fixed spatial discretization and then studied (linear) stability of solution.

$$\frac{d^2\phi_n}{dt^2} - \frac{1}{(\Delta x)^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - \phi_n + \phi_n^3 = 0.$$

- Actually had to discretize in time as well to enforce periodic nature of solution—essentially studied a coupled nonlinear iterated map.

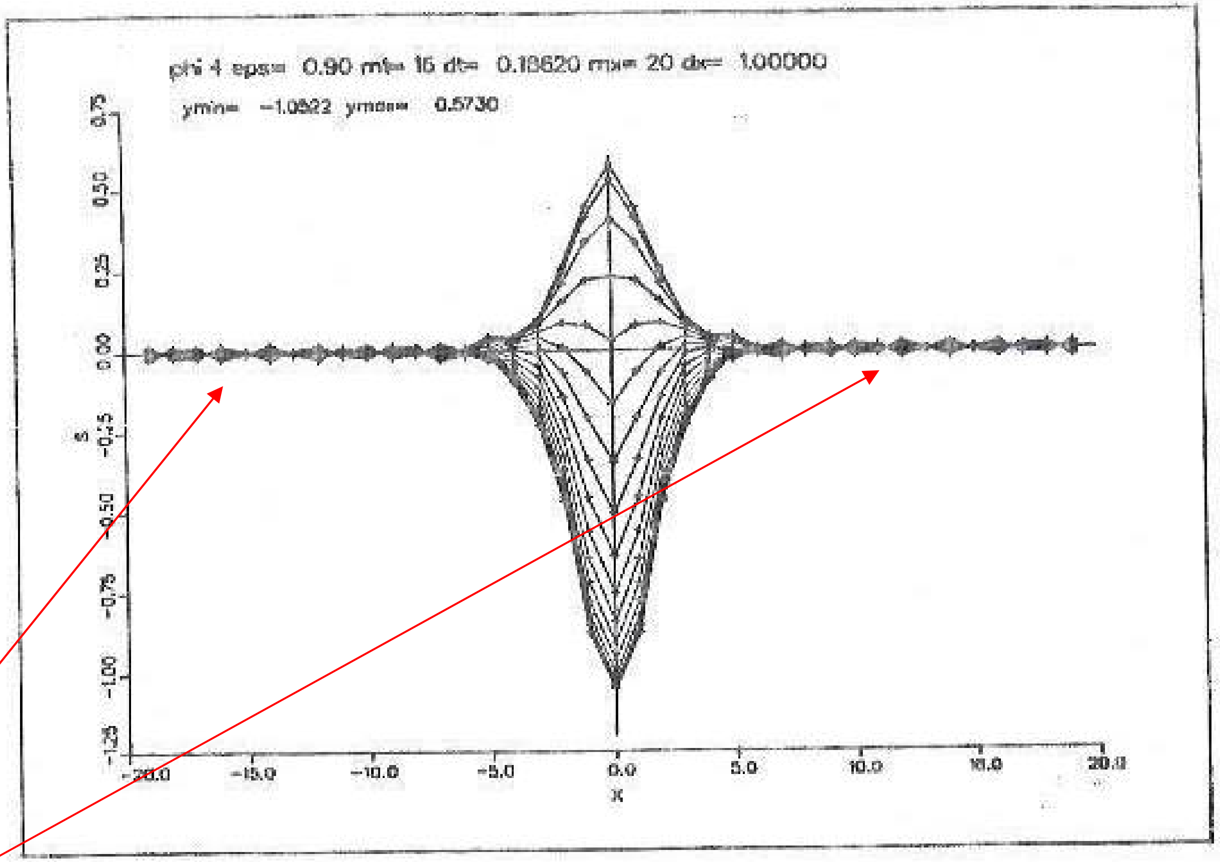
- Results on next several slides

Site-centered localized "breather"



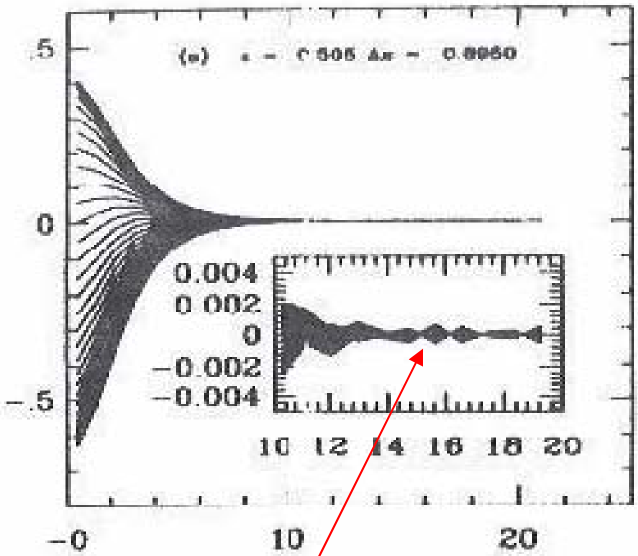
Note values of parameters and apparent localization

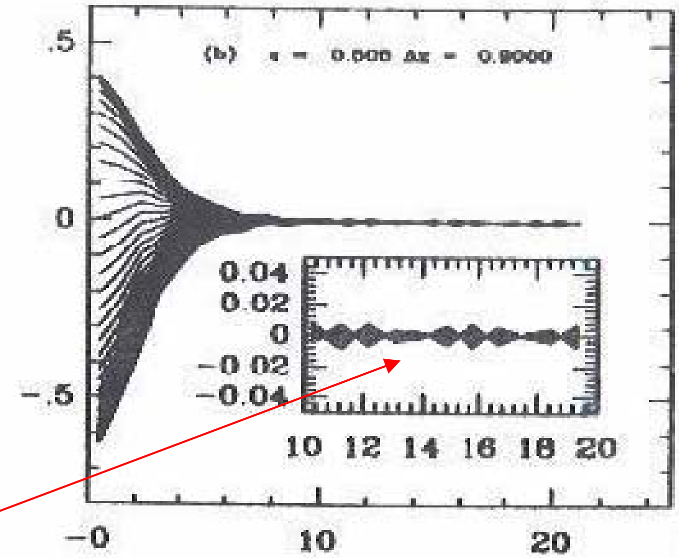
SC, nonlocalized breather—"nanopteron"



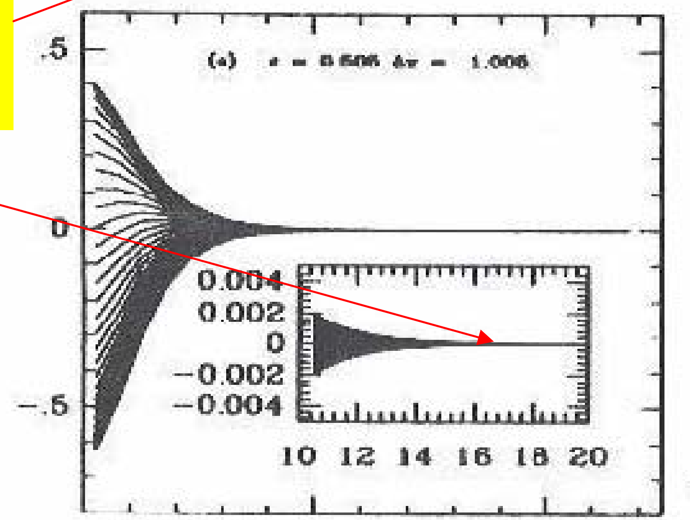
"Wings" reflect coupling to small (linear) oscillations—solution is not localized

Behavior as Δ x => 0





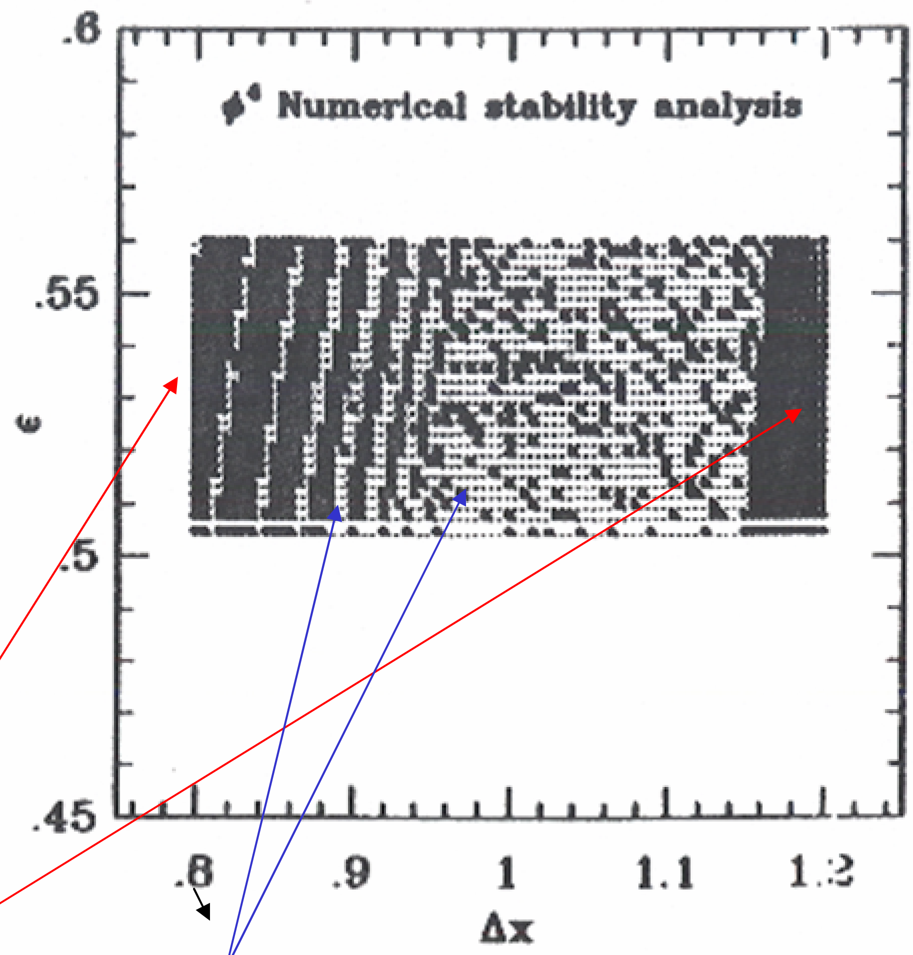
Solution delocalizes as Δ x => 0



Hints of a discrete Φ^4 breather

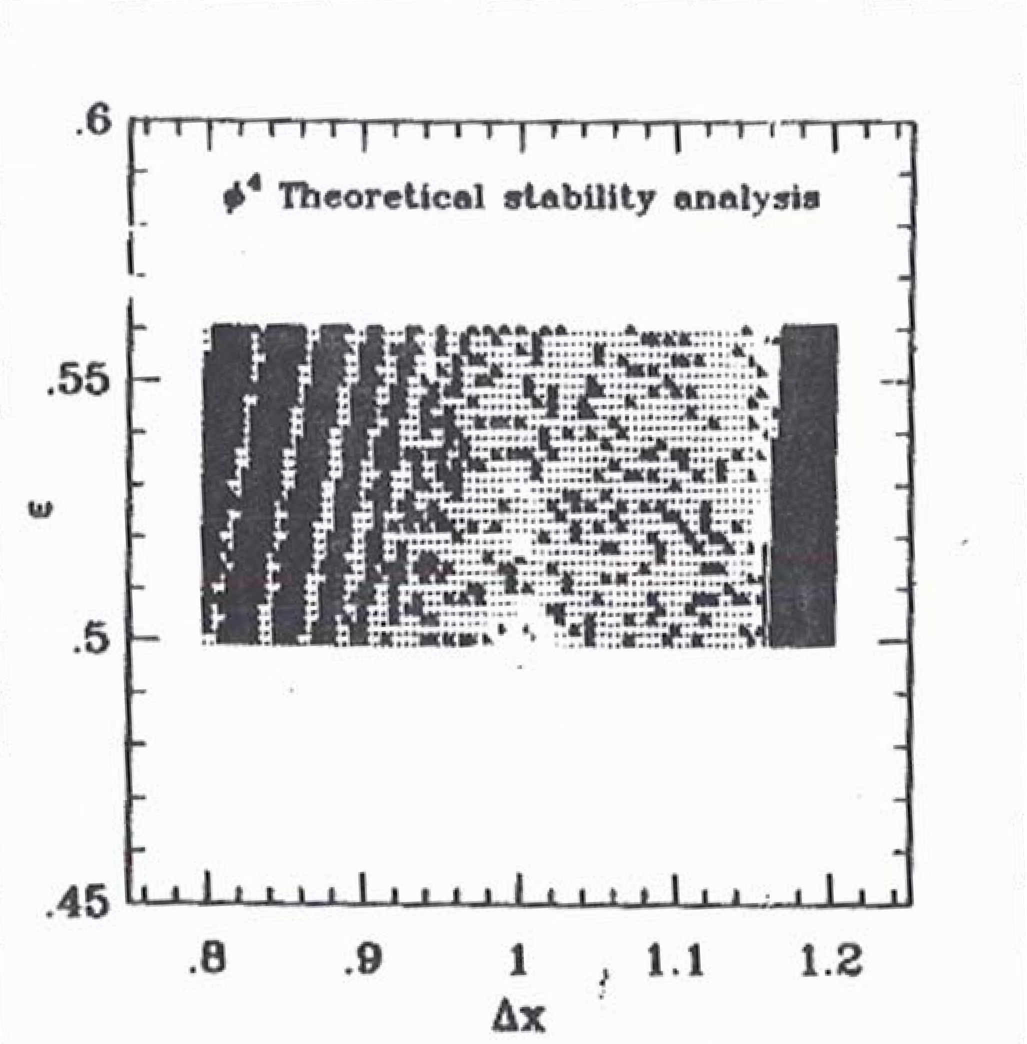
- Numerics could not resolve $\Delta x \Rightarrow 0$ behavior, but suggested that for any given ε, at finite $\Delta x > \Delta x_0$, there existed stable, localized "*discrete*" ϕ^4 breathers. For $\Delta x < \Delta x_0$, the breathers had extended oscillatory tails, became "nanopterons".
- Numerical studies of stability of the discrete breathers as functions of Δx and ε showed a complex pattern of stable and unstable regions. Detailed results are shown on next slide for particular region of parameter space.
- A theoretical analysis based on a resonance between the second harmonic of the breather frequency, 2 ωB, and the linear phonon of the same frequency predicts the stability regions shown in the second slide. The results are in close agreement.

Discrete ϕ^4 Breather stability region: numerics



Black=unstable, "white"=stable, where points indicate discrete grid of calculation

Discrete ϕ^4 Breather stability region: theory



Black=unstable, “white”=stable, where points indicate discrete grid of calculation

Fate of the continuum ϕ^4 breather

- Segur and Kruskal showed that the small amplitude expansion is only *asymptotic* and terms "beyond all orders" (*i.e.*, of the form $\exp(-1/\varepsilon)$) render the putative ϕ^4 breather unstable to "decay" into spatially extended linear excitations (phonons), leading to a "nanopteron". Leading term is coupling to second harmonic of breather, consistent with numerics.

$$\phi_{True} = \phi_{SAB} + c_1 \exp^{-(c_2/\varepsilon)} [\cos (k_{2B}\, x) - \omega_{2B}\, t)] + \ldots\ldots.$$

where $k_{2B} = \sqrt{(\omega_{2B}{}^2 - 1)}$

"beyond all orders"

- Stability of SG breather is now rigorously known to be result of the "complete integrability" of the SG equation ("true" soliton equation) and it is unique among continuum theories—all other putative breathers do decay by emitting phonons with frequencies that are harmonics of the breather frequency.

ILMs: Intuition and Theory

- Consider diatomic molecule modeled as two coupled *anharmonic* oscillators:
  - *anharmonic* = nonlinear => frequency depends on amplitude of motion, $\omega(A)$: familiar from plane pendulum, where frequency *decreases* with amplitude
- Consider "anti-continuum" limit of no coupling:
  - Trivial to "localize" excitation on one of oscillators only; frequency of oscillation depends on amplitude ~ energy
- Consider weak coupling:
  - Imagine one oscillator highly excited, other weakly excited. Frequencies are very different. Suppose

    $\omega(A_1) / \omega(A_2) \neq p/q$—i.e., frequencies are *incommensurate*. Then there are no possible resonances between oscillators, and energy transfer must be very difficult, if even possible.
- Can formalize heuristic argument via KAM Theorem

ILMs: Intuition and Theory

Choose our favorite discrete ϕ^4 model as example.

$$\frac{d^2\phi_n}{dt^2} - \frac{1}{(\Delta x)^2}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) - \phi_n + \phi_n^3 = 0.$$

- "Quartic" double-well oscillator $\phi_n(t)$ at each site (n) of infinite "lattice": minimum of potential at $\phi_n = 1$

- Coupling ~ $1/(\Delta x)^2$

Key point

- Spectrum of *linear* oscillations about minimum $\phi_n = 1$ is $\omega_q^2 = 2 + (2/\Delta x)^2 \sin^2(q/2)$, a *band*, bounded from above and below—*upper cut-off from discreteness*.

ILMs: Intuition and Theory

For nonlinear oscillations about minimum in quartic oscillator, frequencies *decrease* with amplitude, so one can create a nonlinear localized mode with frequency ω_b *below* the linear spectrum.

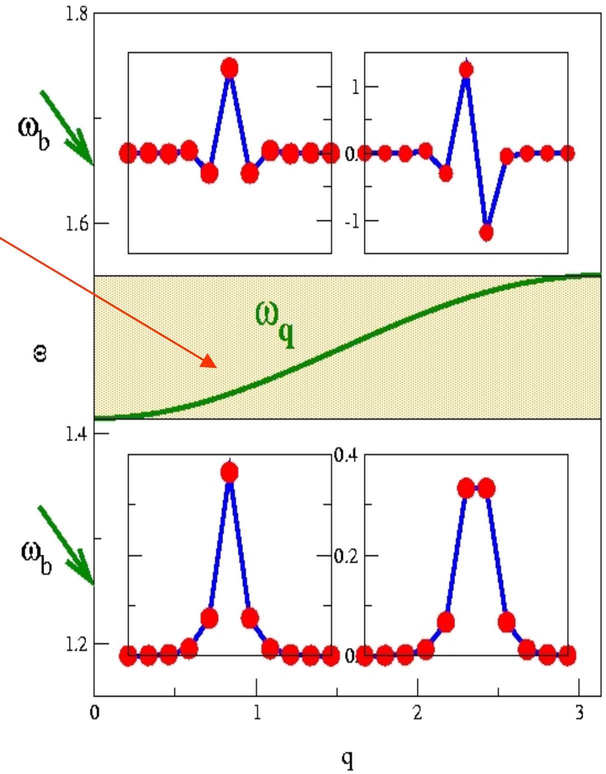
If Δx is large enough, so coupling ~ $1/(\Delta x)^2$ is small, the band of excitations $\omega_q^2 = 2 + (2/\Delta x)^2 \sin^2(q/2)$ is very narrow, so that the second harmonic of ω_b can lie *above* top of band. *Thus there can be no (linear) coupling of local mode to extended states and it is (linearly) stable.*

ILMs: Intuition and Theory

Figure shows linear band (yellow) with energy-momentum dispersion relation (green curve)

$$\omega_q^2 = 2 + (2/\Delta x)^2 \sin^2(q/2)$$

for Δx =10. The isolated localized mode frequencies, ω_b , are shown for the types of ILMs shown in the top and bottom panels. Note that ILMs can occur both *above* and *below* the linear band—those above have an optical character (adjacent particles out of phase) , whereas those below have an acoustic character (adjacent particles in phase). There are many ILMs—only four are shown here.



ILMs: Intuition and Theory

- Rigorous results based on “anti-continuum” limit establish existence of, and can be used to construct, ILMs/DBs in wide variety of lattice systems in any spatial dimension.
- ILMs can propagate along lattices, can be generated by thermal fluctuations, and can be quantized.
- ILMs act as strong, frequency dependent scatterers of linear modes.

Historical Precursors

- Continuum breathers in non-integrable theories: "been there, done that"

- Defect vs. Self-Trapped Modes—Bloch's theorem implying only extended ("band") states in perfect solids is avoided *if* the lattice is deformable—Landau (1933) first recognized possible existence of a self-trapped "polaron" excitation. Modeled by "Discrete Nonlinear Schrödinger Equation"

$$i\frac{d\psi_n}{dt} + J(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \kappa|\psi_n|^2\psi_n = 0,$$

NB: 1) Think of |Ψ|2 as a strongly localized potential—relation to defect states and Anderson localization.

2) Form of nonlinearity implies trivial example of ILM/DB—amplitude-independent frequency solutions exist.

Historical Precursors

- Quantum ILMs in Small Molecules —already in 1920s chemists realized that anharmonicity in vibrational potential in molecules could lead to the localization of highly excited (*i.e*., many-quanta) vibrational modes. Frequencies of these localized modes are "red-shifted" from expected values based on simple multiples of fundamental phonon frequency. These "quantum ILMs" are predicted (and observed) in benzene and are long-lived (but not infinitely stable).

Current Experiments: Solids

Natural lattice structure of solids suggests ILMs should be found here, likely in quantum version. Observed redshift of Raman modes in charge transfer solid PtCl can be explained by assuming ILM formed as shown in Figure (from Kladko *et al*.).

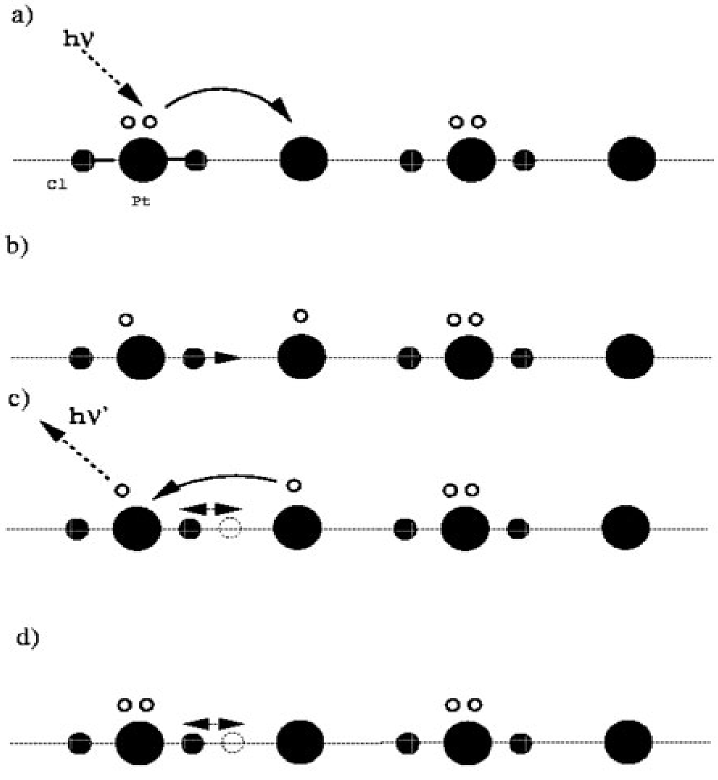
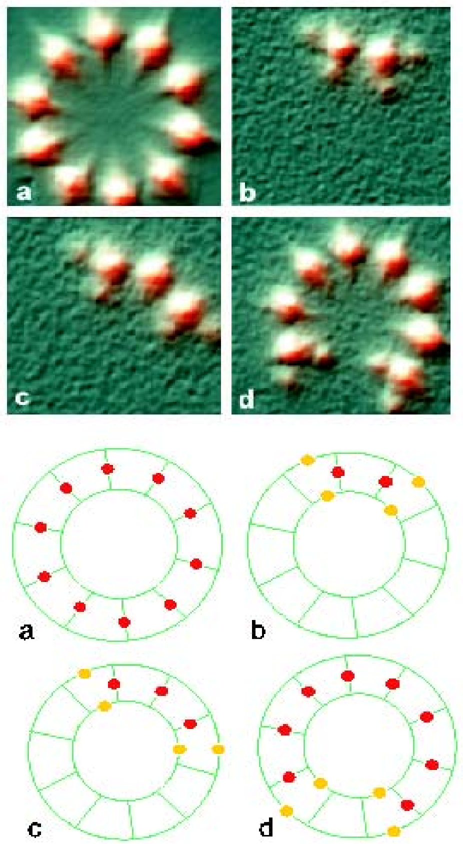


Fig. 1

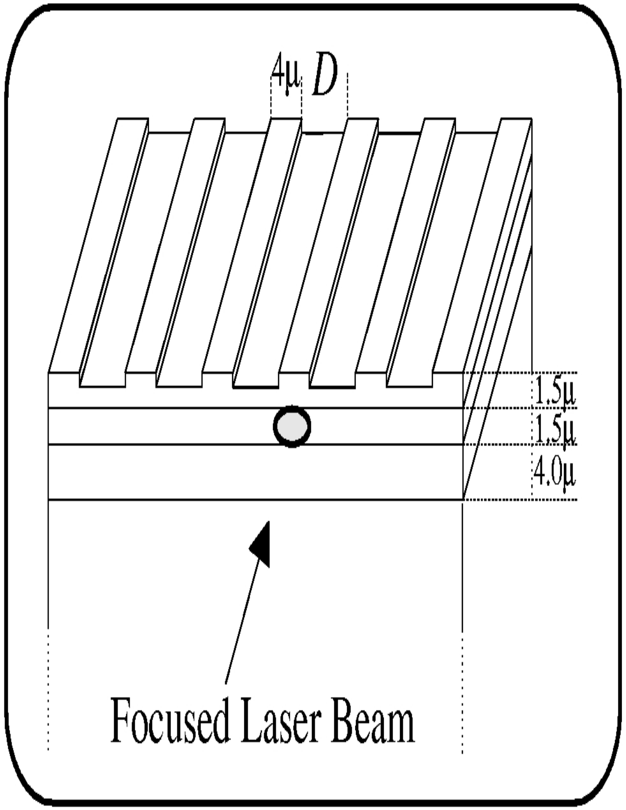
Current Experiments: Josephson Junctions

In an annular Josephson Junction ladder driven by a DC current, ILMs appear as localized normal junctions in the otherwise superconducting annular ladder. The red and yellow images in the experiment (sketched below for clarity) correspond to different values of the voltage drop across the resistive states. (From A. Ustinov et al)



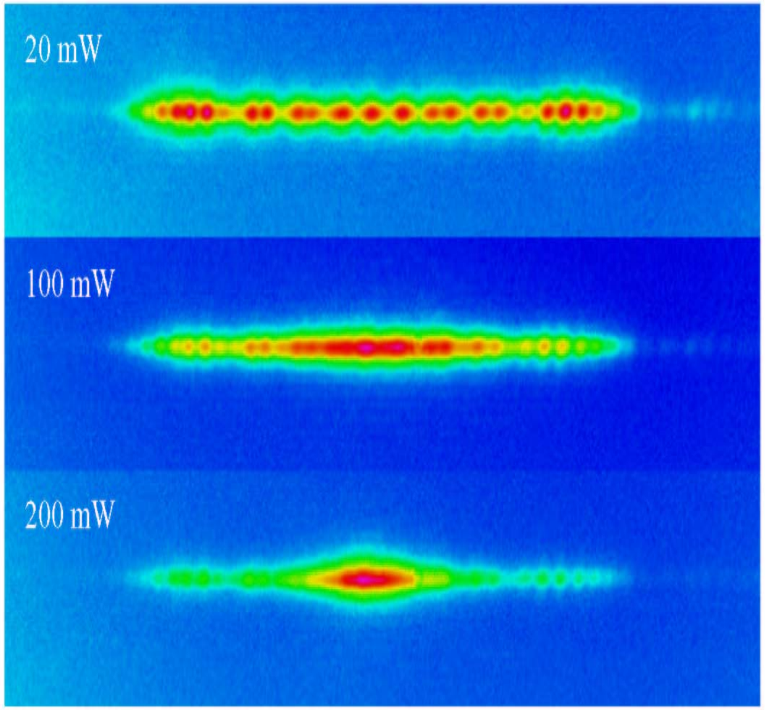
Current Experiments: Optical Waveguides

Schematic view of an optical waveguide array created by patterning a layered semiconductor, showing the rough dimensions of the system. Note that the input laser beam can be focused on a single element of the array, creating an initially spatially localized excitation, which then propagates toward the output facet at the back of the array. (From Eisenberg et al).



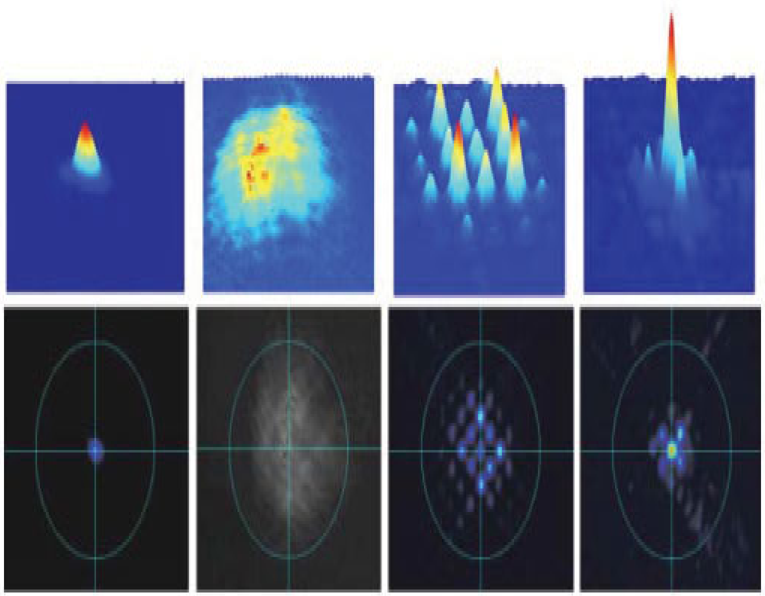
Current Experiments: Optical Waveguides

Edge-on view of the output facet of the coupled optical waveguide array shown on previous slide. The input pulse is localized at the center of the array. At low power, pulses propagate linearly and “diffract” across entire array. At intermediate power, nonlinear effects induce some localization. At high power, the pulse remains truly localized and is an example of an ILM in these systems. (From Eisenberg et al).



Current Experiments: Photonic Lattices

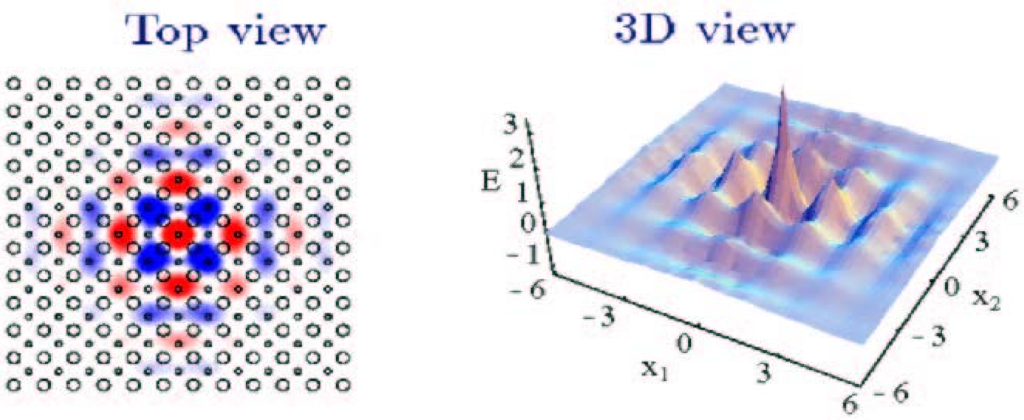
A two-dimensional ILM forming in a photonic lattice created by optical induction in a crystal with photorefractive properties. A second laser beam provides the input (shown in (a), which is centered on a single “site” in the photonic lattice. Panel (b) shows the linear “diffraction” output that occurs in the absence of the photonic lattice; panel (c) shows the behavior at weak nonlinearity; panel (d) shows an ILM at strong nonlinearity. (From H. Martin et al)



(a) (b) (c) (d)

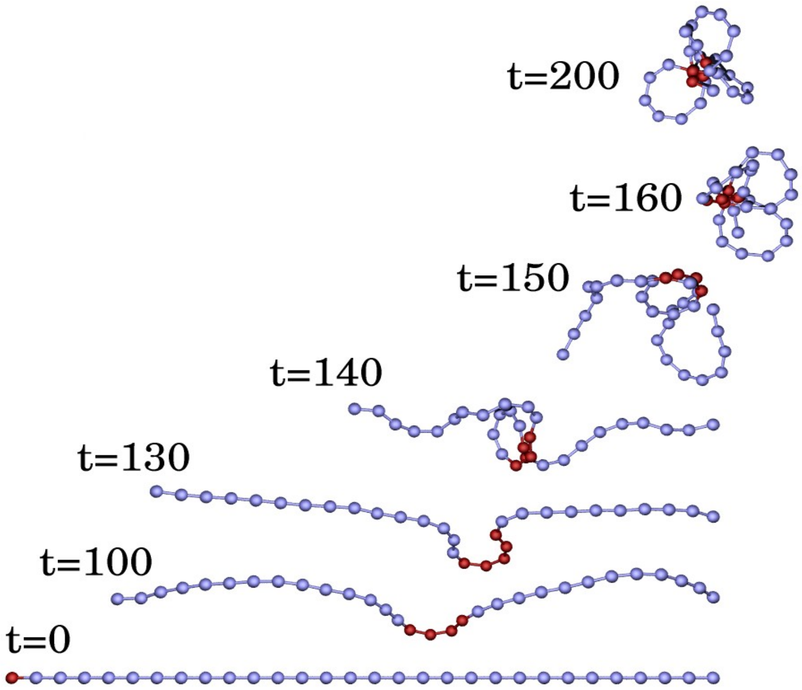
Toward the Future

Theoretical prediction of ILMs in a regular 2D lattice of rods of two different types of semiconductors. One type of rod has very weak nonlinear optical properties, whereas the other is strongly nonlinear. (From Mingaleev et al)



Towards the Future

Theoretical prediction of biopolymer folding nucleated by ILM. ILMs have been suggested as the mechanisms for the “unzipping” of DNA, as well as for the transport and storage of energy in biopolymers. Theoretical results suggest that ILMs in these systems can arise both from thermal fluctuations and from local excitation, such as by an STM tip. (From Mingaleev et al).



Towards the Future

- ILMs are more ubiquitous and robust cousins of solitons and thus will appear in still wider range of physical systems.
- ILMS may play important roles in advanced photonic switching devices, in energy transport and storage processes in biopolymers, in “unzipping” of DNA and in folding of proteins.
- The future is now! Recent predictions and observations of individual ILMs being created and destroyed in 1D AFM and in ultra-cold atoms, as well as proof of “q-breathers” in FPU itself and a proposal to observe ILMs in macromolecules with STM highlight the interest in the topic.

Summary and Conclusions

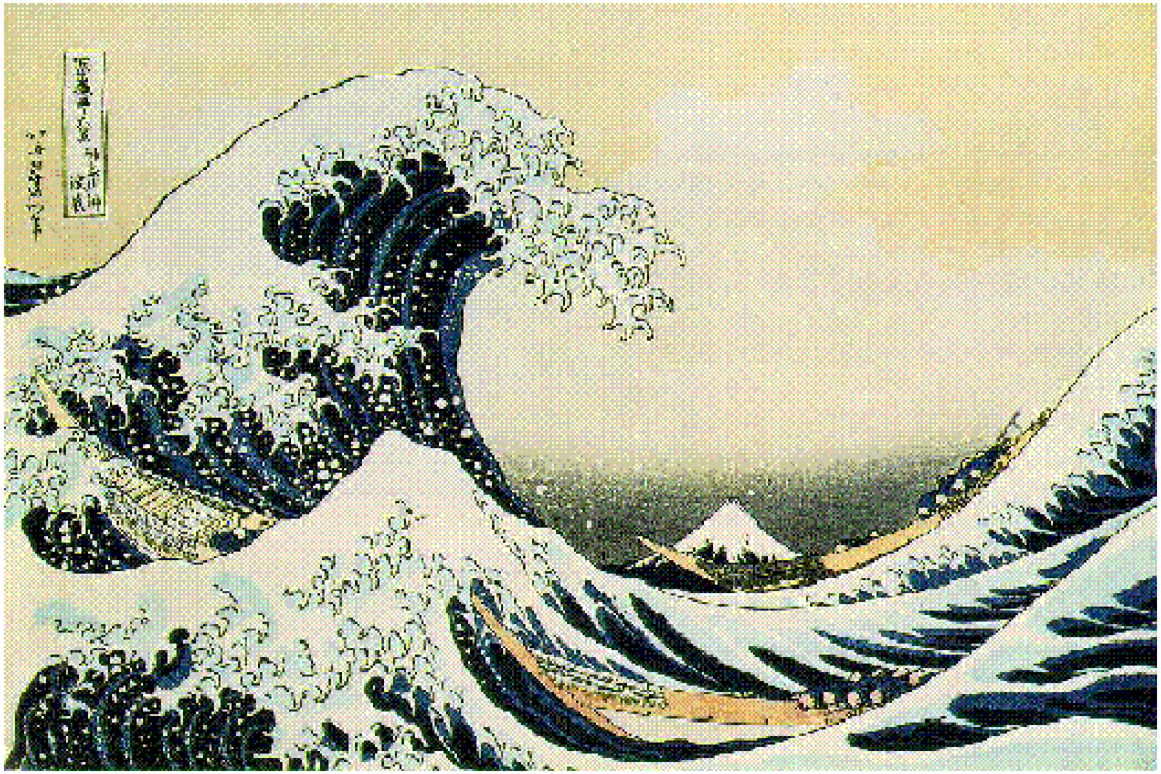
- Odyssey from FPU to ILMs followed a remarkable course
    - FPU recurrences to KdV solitons
    - Sine-Gordon vs. ϕ^4—continuum breathers?
    - Numerics of (widely) extended discrete breathers in ϕ^4
    - Anti-continuum limit and highly localized ILMs/DBs

•ILMs are ubiquitous in nonlinear discrete systems, independent of spatial dimension

- Experimental Observations of ILMs

Epilogue on FPU

FPU was a watershed problem: it led to solitons and ILMs, but also to chaos, and deep insights into the fundamentals of statistical mechanics, anomalous transport, and energy localization. It was, as Fermi once remarked, quite a "little discovery."



A Few References

David K. Campbell, Sergej Flach, and Yuri S. Kivshar, "Localizing Energy Through Nonlinearity and Discreteness," pp. 43-49, *Physics Today* (January 2004).

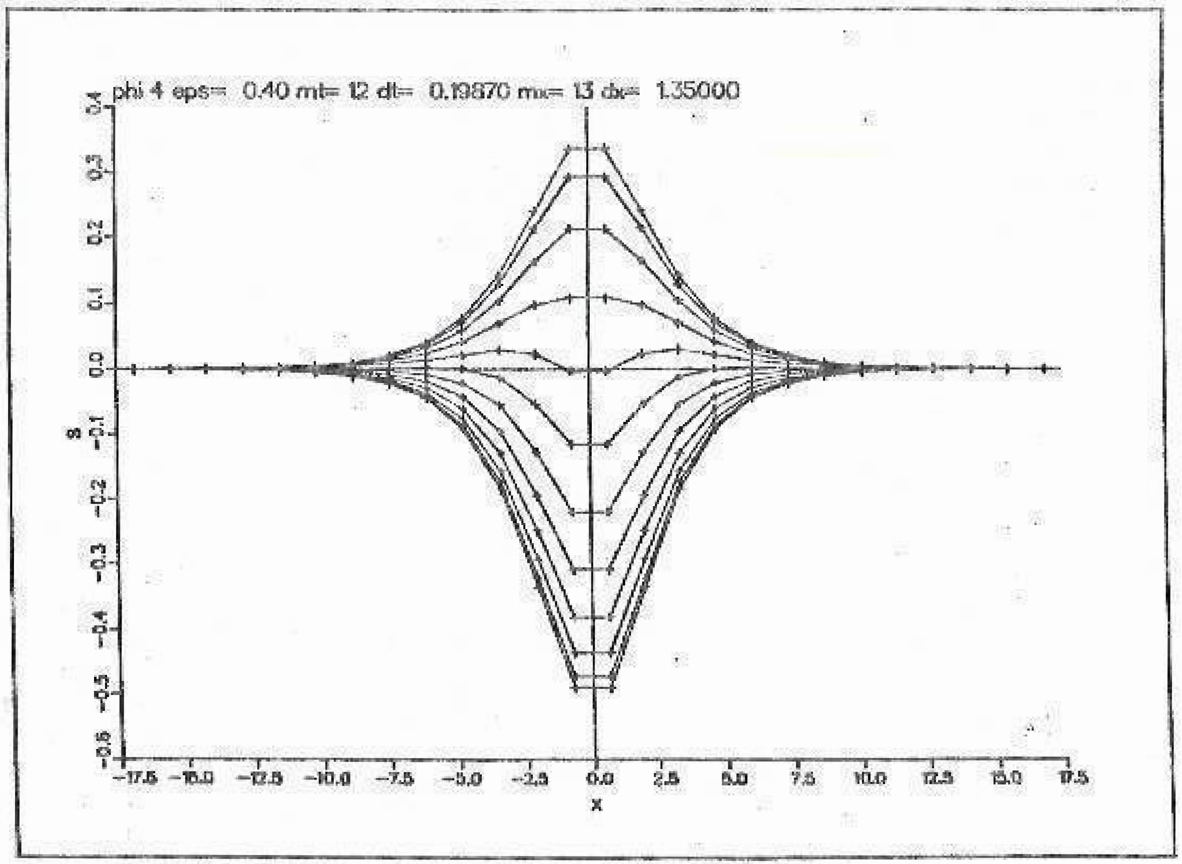
David K. Campbell and Michel Peyrard, pp.305-334 in "Chaos and Order in nonintegrable model field theories," CHAOS/XAOC Soviet American Perspectives in Nonlinear Science, American Institute of Physics (1992).

Harvey Segur and Martin Kruskal, "Nonexistence of Small-Amplitude Breather Solutions in ϕ^4 Theory," *Phys. Rev. Lett*. **58**, 747-750 (1987).

Chaos **13**, #2 Focus Issue: "Nonlinear Localized Modes: Physics and Applications," Yuri Kivshar and Sergej Flach, guest editors.

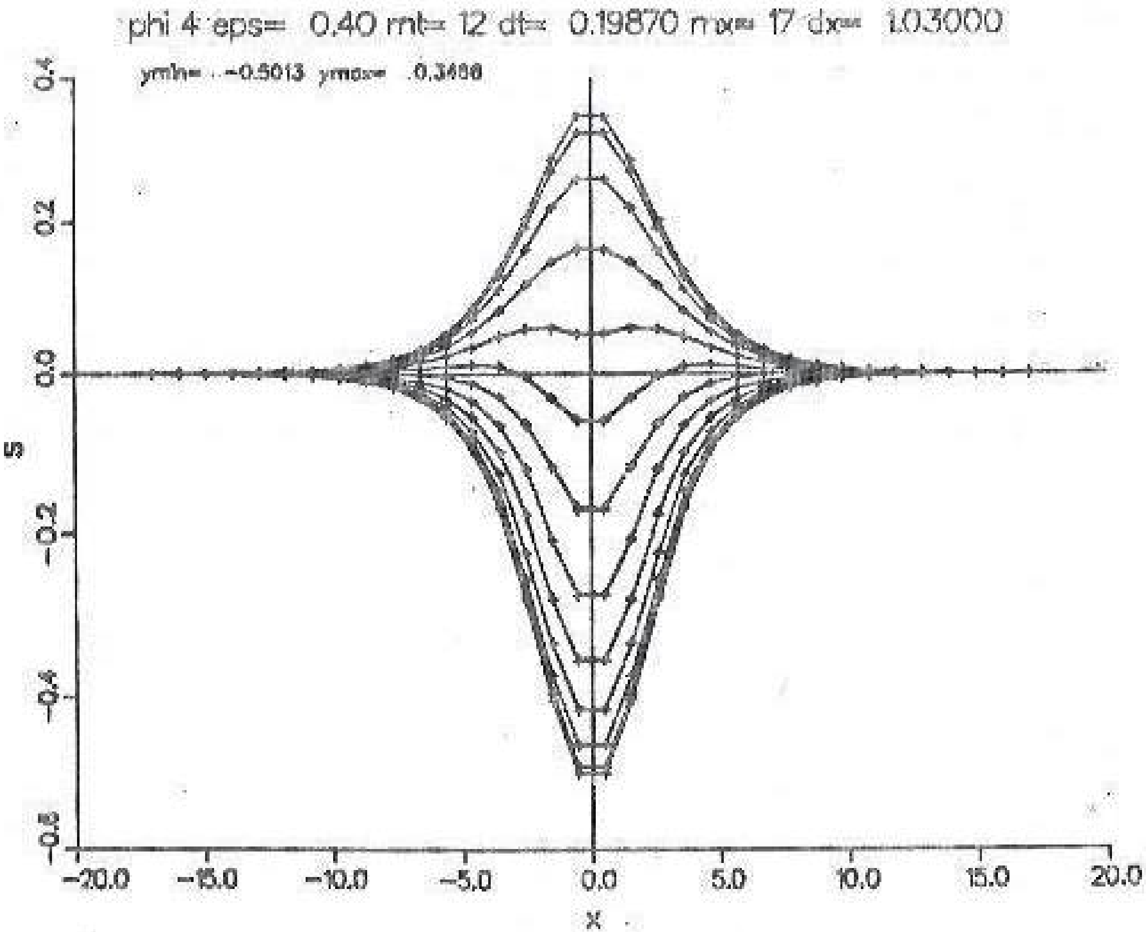
Chaos **15** # 1 Focus Issue: "The Fermi-Pasta-Ulam Problem—The First 50 Years," David Campbell, Philippe Rosenau, and George Zaslavsky, guest editors.

Intersite-centered localized "breather"



Note values of parameters and apparent localization

Intersite-centered non-localized breather



For this smaller value of Δx, “breather” acquires oscillating tail

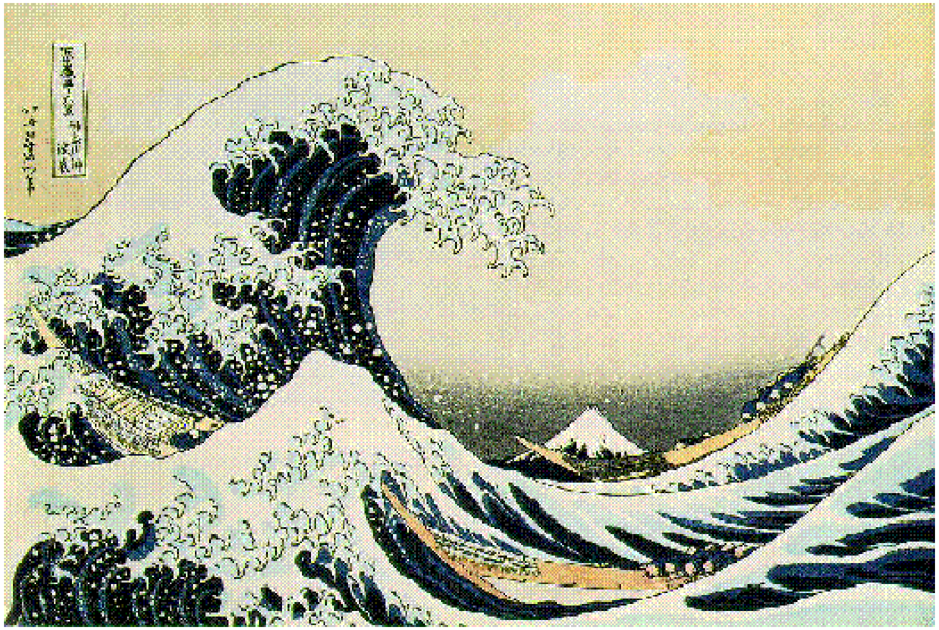
Things to Change for Houston/Ariz

- Have cut two Peyrard figures—show only 1 localized, 1 nanopteron, and the delta x => 0 results, plus the coupling to two phonons and stability regions—done 8/15/05
- Move ILM definition and bottom line to start—then go back to FPU— done 8/15/05
- Try to add some of the simulations of sine-Gordon, or something dynamical—either old movies or new stuff from Mathematica—done 10/18/05
- Fix animation on several of the slides!!
- Update latest stuff on ILMs—include new experiments
- Include q breathers as “final solution” to FPU results

From FPU to Intrinsic Localized Modes:

An Odyssey in Nonlinear Science

David K. Campbell
Boston University



Department of Physics
University of Houston
October 25, 2005

BU College of Engineering
BOSTON UNIVERSITY

Note the Error Here

the purposes of numerical work this c 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

-4-