Scaling of β Fermi-Pasta-Ulam-Tsingou Recurrences

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(Work in collaboration with David Campbell and Kevin Reiss)

Fermi-Pasta-Ulam-Tsingou (FPUT) Problem

STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM
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β-FPUT: $$H = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} \frac{1}{2}\left(q_{n+1} - q_n\right)^2 + \frac{\beta}{4}\left(q_{n+1} - q_n\right)^4$$

Expectation: System would thermalize and achieve energy equipartition among normal modes.

Observation: For long-wavelength, low-energy initial conditions, energy shared among only lowest normal modes and remarkable *near-recurrences* to the initial state

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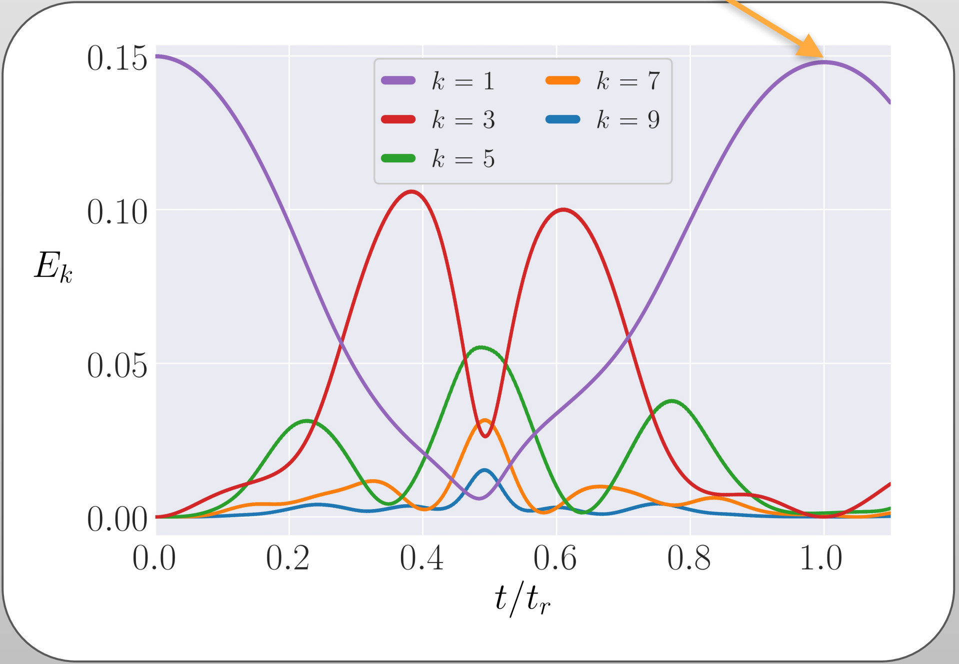
FPUT Recurrence



Results

- Rescaled FPUT recurrence time $T_r = \dfrac{t_r}{(N+1)^3}$, for large N, depend only on $S = E\beta(N+1)$
- FPUT recurrence time differs between the $\beta > 0$ and $\beta < 0$ case.
- For small $|S|$, FPUT recurrence time can be found perturbatively and found to depend only on S.
- In the "continuum limit" FPUT recurrence time is controlled by mKdV solitons.
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Numerical Determination of FPUT Recurrence Time

Define: $T_r = \dfrac{t_r}{(N+1)^3}$ and $S = E\beta(N+1)$

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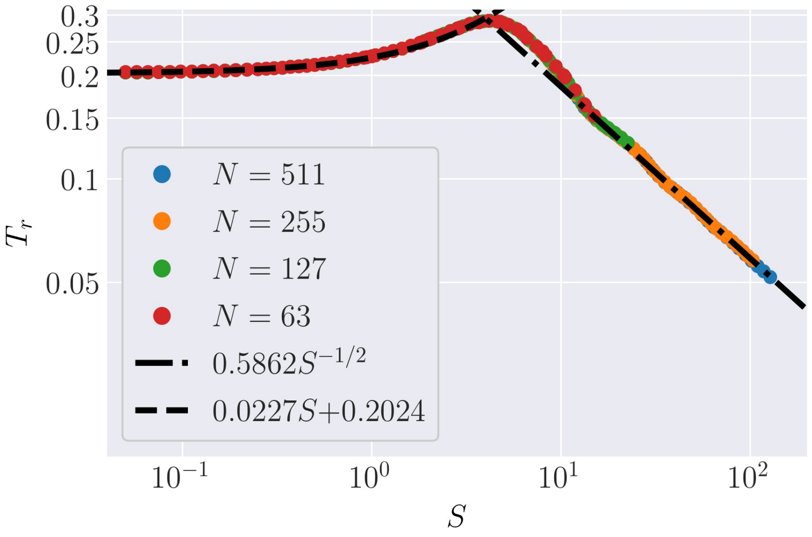
$\beta > 0$



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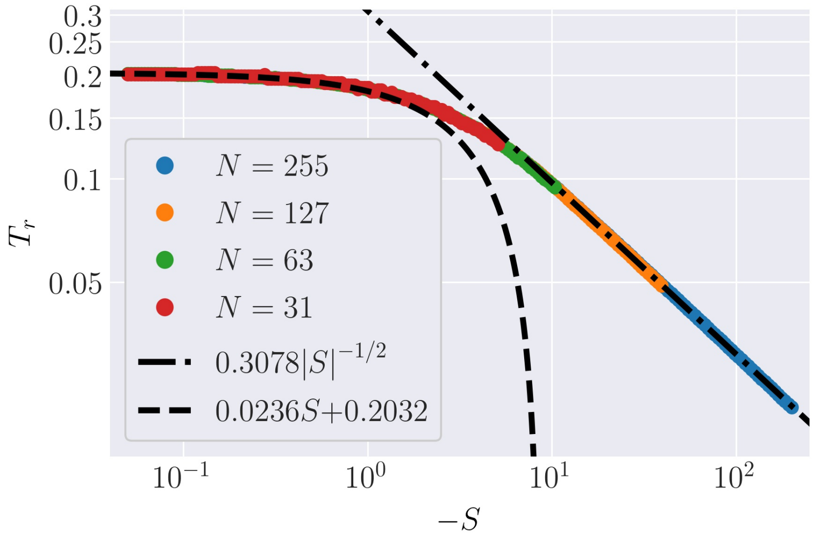

Nearly linear regime (small |S|)

From perturbation theory: $t_r = \dfrac{2\pi}{3\Omega_1 - \Omega_3}$

- Ω_k is the k^{th} perturbatively defined “nonlinear” frequency

$$T_r = \frac{864S^2 - 5376\pi^2 S + 4096\pi^4}{405S^3 + 4104\pi^2 S^2 - 4992\pi^4 S + 2048\pi^6} + \mathcal{O}(N^{-2})$$

Sholl, David S., and B. I. Henry. *Physical Review A* 44.10 (1991): 6364
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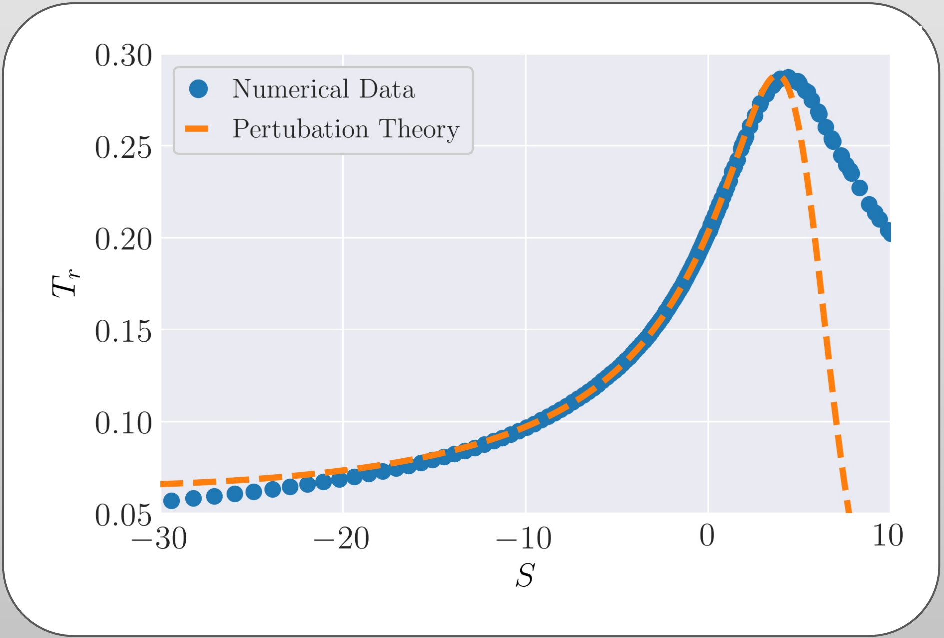

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Numerically solving continuum dynamics

- Continuum limit can be mapped onto the modified Korteweg-de Vries equation $\phi_\tau + b\phi_\xi\phi^2 + \zeta\phi_{\xi\xi\xi} = 0$
- Recurrence understand through the solitons dynamics. Agree with $T_r \propto |S|^{-1/2}$ scaling on lattice

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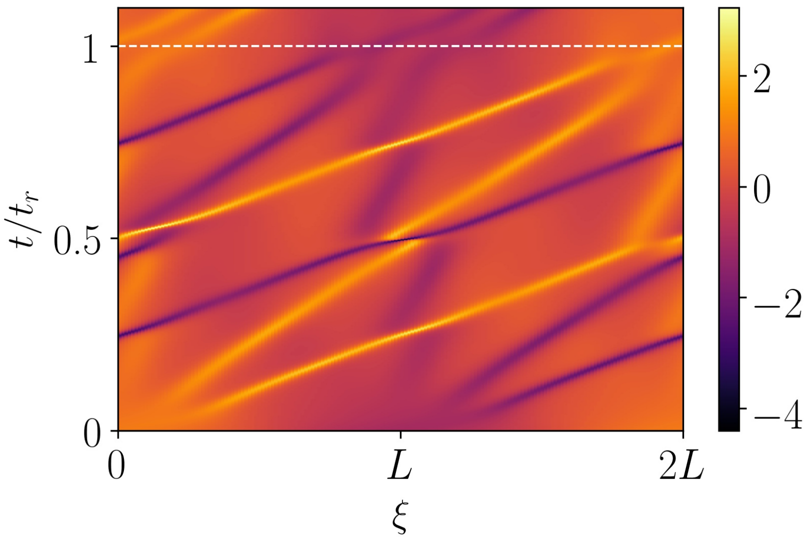

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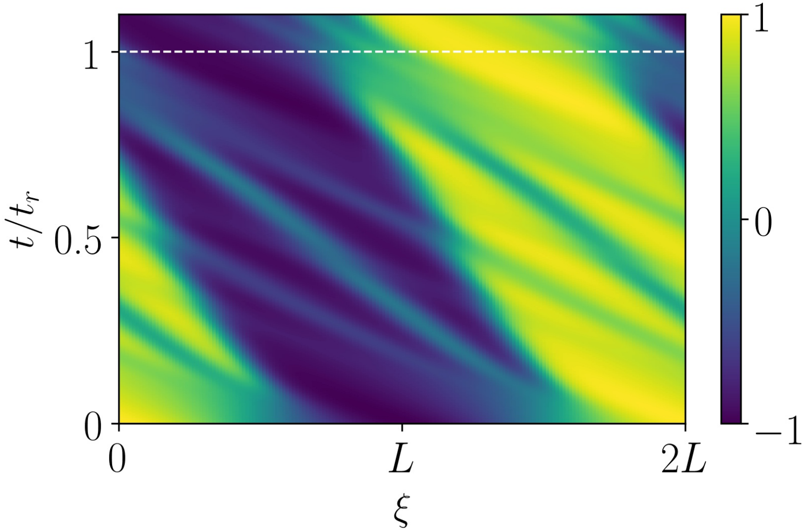

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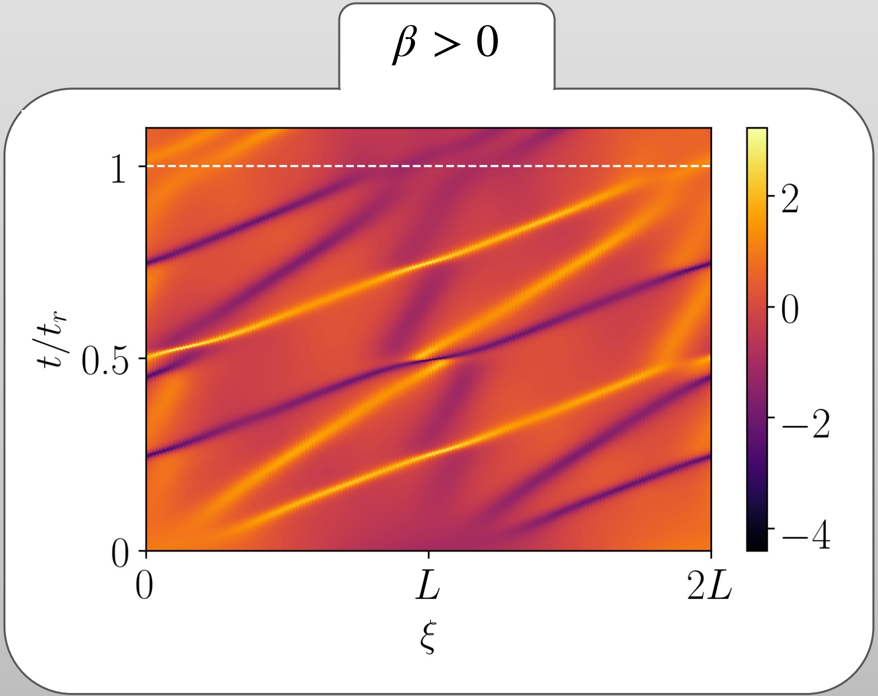

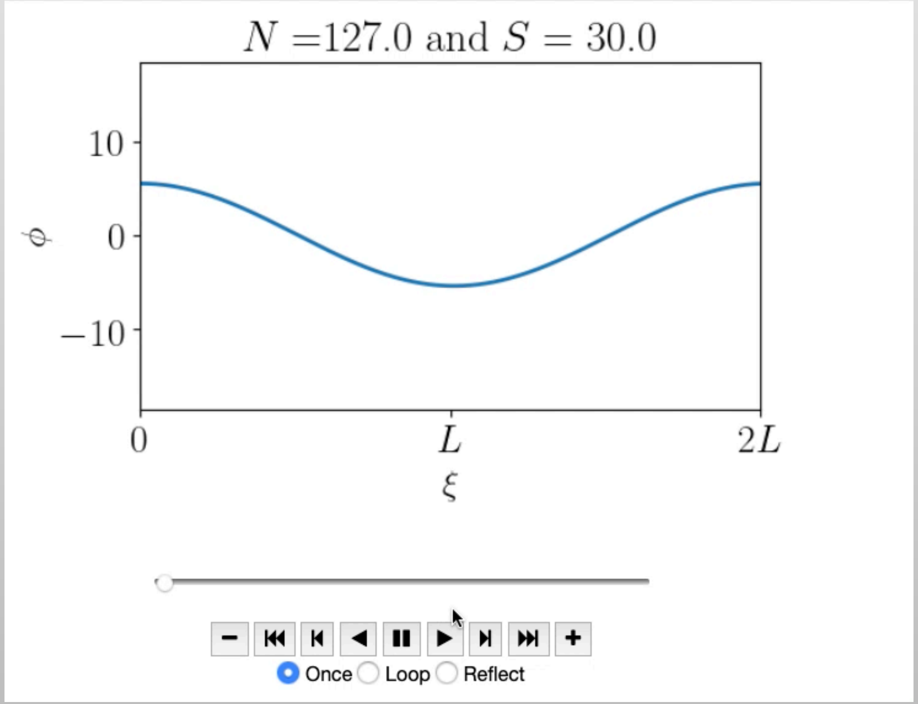

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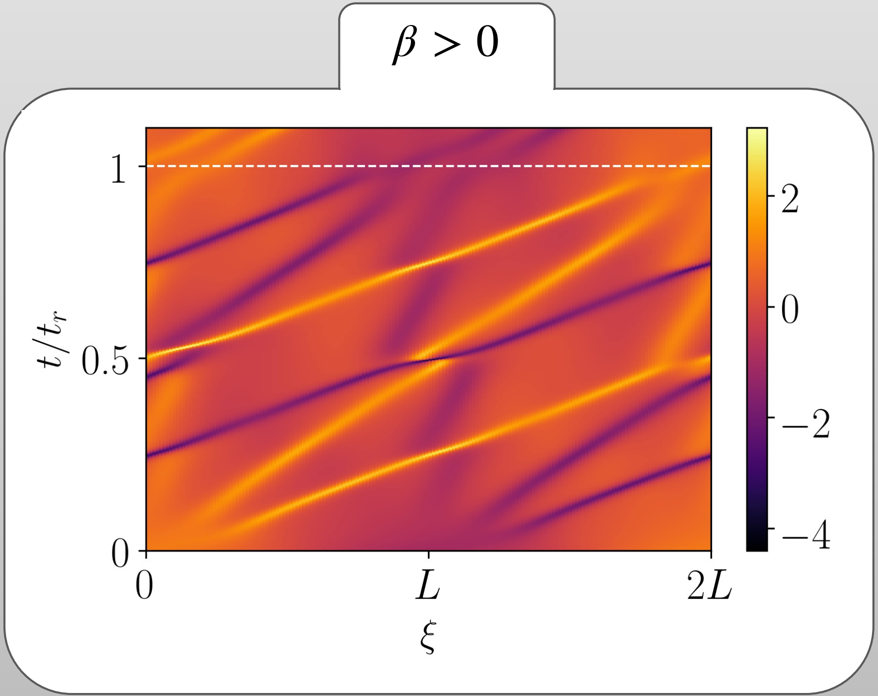

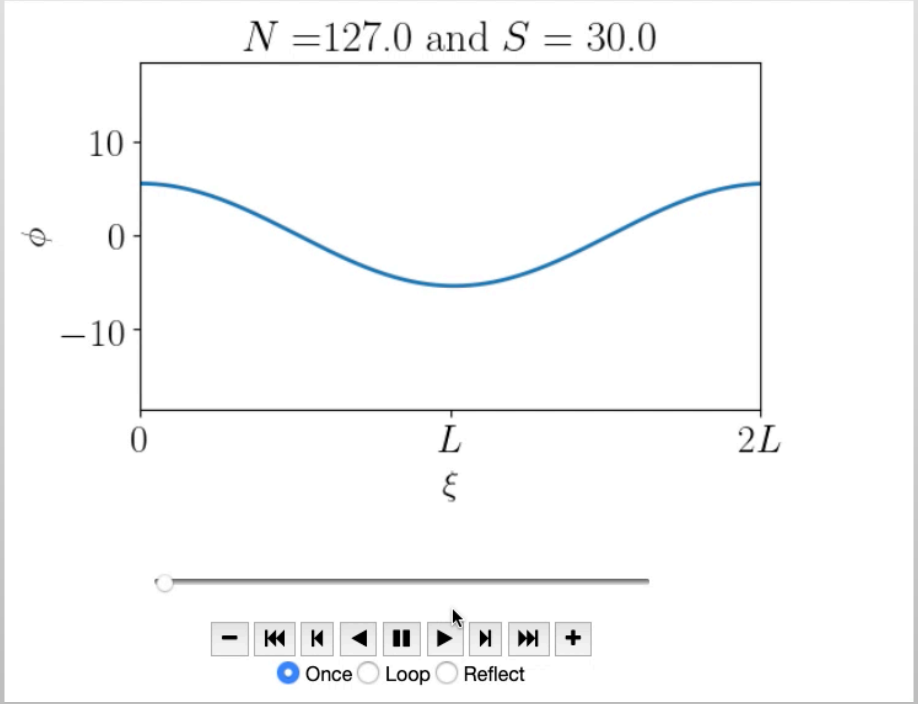

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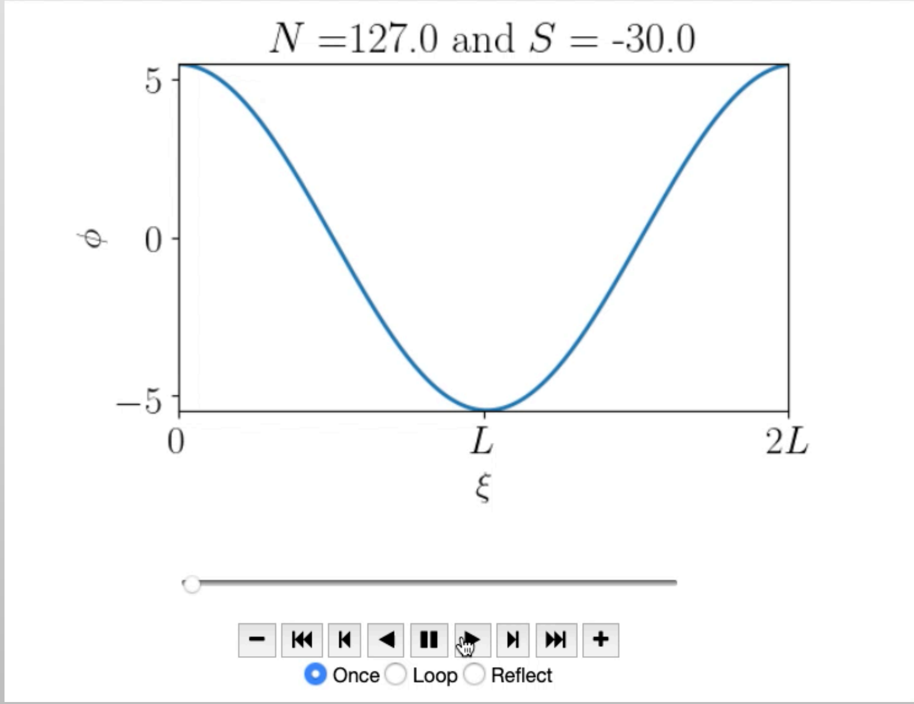

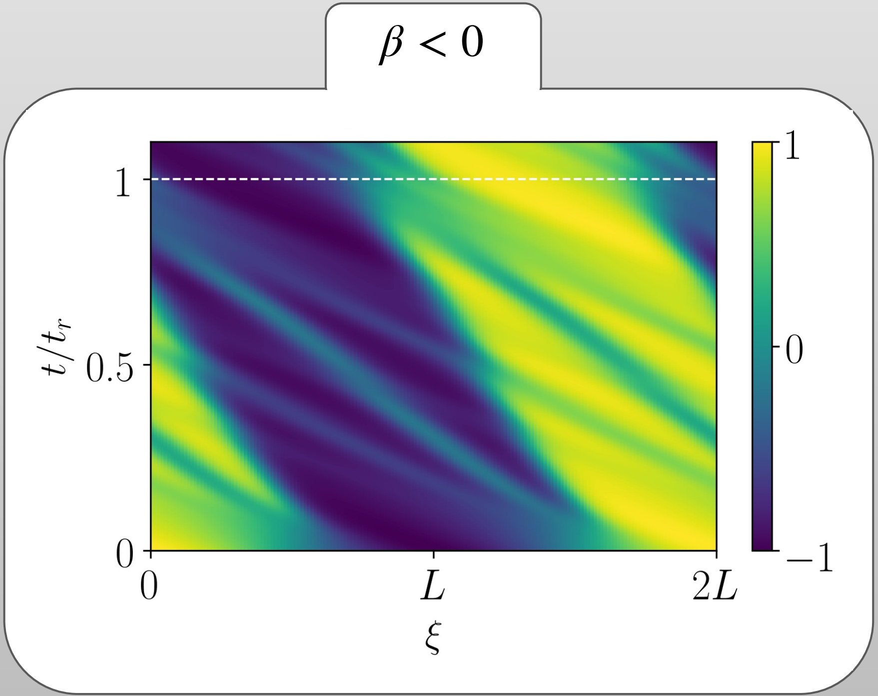

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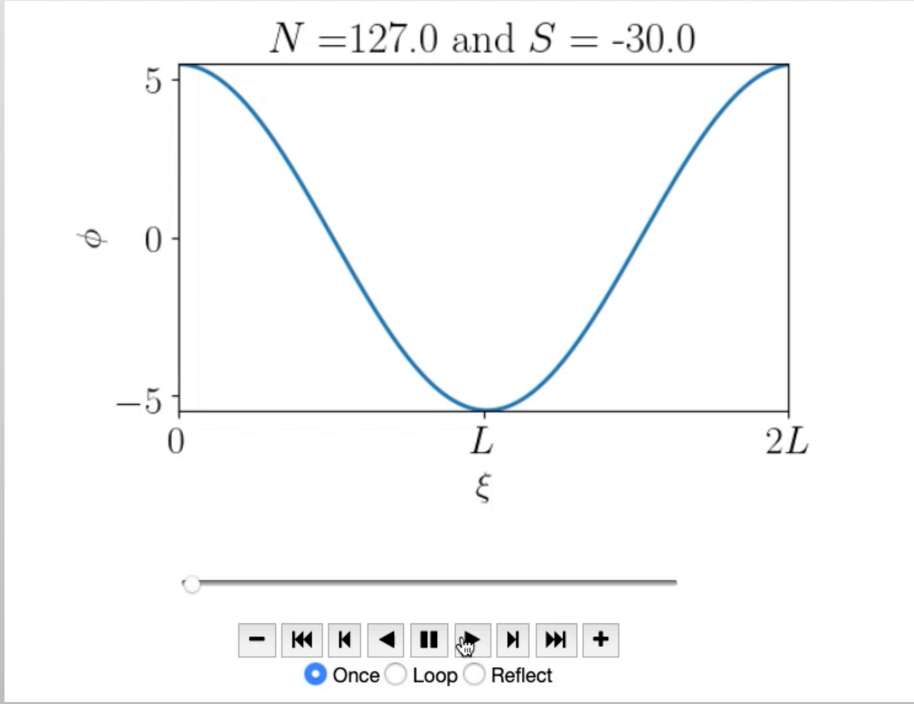

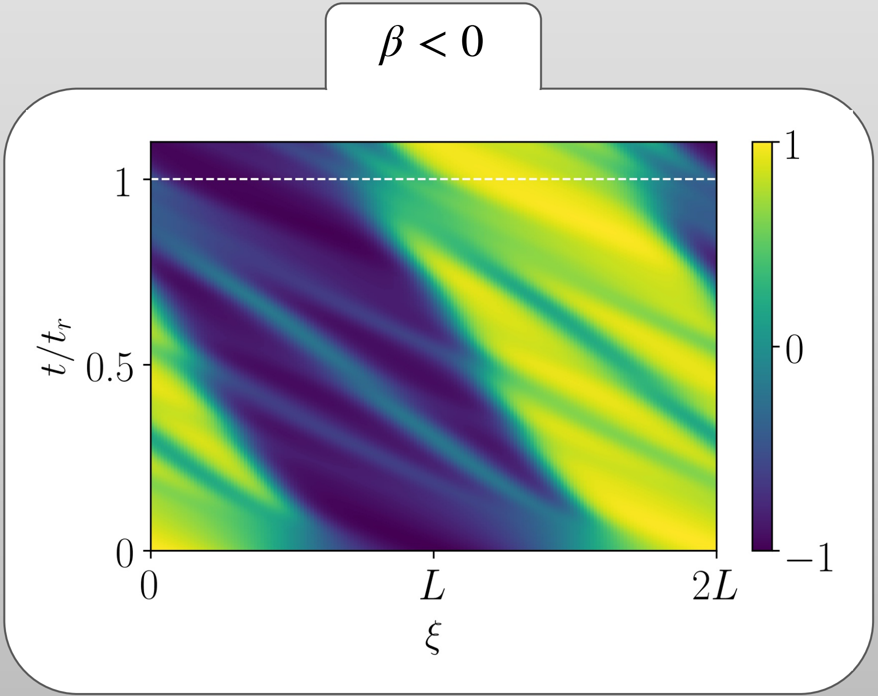

Highly nonlinear regime (large |S|)

- From soliton dynamics, neglecting soliton-soliton interactions: $\tau_r = \frac{(b+3)}{2}\frac{L}{\Delta v}$
- Approximately solve for the eigenvalues, E_n
  - $$T_r = \frac{\sqrt{6}}{\pi}\left|S\right|^{-1/2} \quad (\beta > 0)$$
  - $$T_r = \frac{3\sqrt{2}}{\pi\sqrt{12|S| + \pi\sqrt{6|S|}}} \quad (\beta < 0)$$

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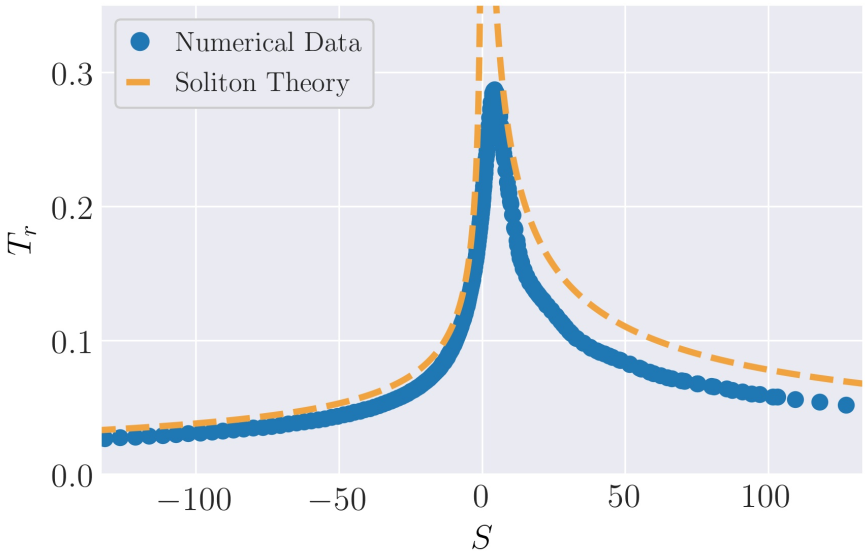

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Recap

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Thank You!

David Campbell

Kevin Reiss

Normal Mode Coordinates

Normal Mode Canonical Transformation: $$\begin{bmatrix} q_n \\ p_n \end{bmatrix} = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \begin{bmatrix} Q_k \\ P_k \end{bmatrix} \sin\left(\frac{nk\pi}{N+1}\right)$$

Hamiltonian becomes: $$H = \sum_{k=1}^{N} \frac{P_k^2}{2m} + \frac{\omega_k^2 Q_k^2}{2} + \frac{\beta}{4} \sum_{i,j,l=1}^{N} C_{kijl} Q_k Q_i Q_j Q_l$$ with:

- $$\omega_k = 2\sin\left(\frac{k\pi}{2(N+1)}\right)$$
- $$C_{kijl} = \frac{\omega_k \omega_i \omega_j \omega_l}{2(N+1)} \sum_{\pm} \left[\delta_{k,\pm j \pm l \pm m} - \delta_{k \pm j \pm l \pm m, \pm 2(N+1)}\right]$$

Equations of motion: $$\ddot{Q}_k + \omega_k^2 Q_k = -\sum_{i,j,l=1}^{N} C_{kijl} Q_i Q_j Q_l$$

Motivation for T definition

Expanding Sholl and Henry's perturbative result:

$$t_r = \left.\frac{2\pi}{3\Omega_1 - \Omega_3}\right|_{\beta=0} = \frac{2\pi}{3\omega_1 - \omega_3}$$

$$= \frac{\pi}{3\sin\left(\frac{\pi}{2(N+1)}\right) - \sin\left(\frac{3\pi}{2(N+1)}\right)}$$

$$= \frac{2(N+1)^3}{\pi^2} + \frac{N+1}{4} + \mathcal{O}\left(\frac{1}{N+1}\right)$$

Large N: $t_r \sim (N+1)^3$

Lin, C. Y., C. G. Goedde, and S. Lichter. *Physics Letters A* 229.6 (1997): 367-374.

Motivation for S definition

β-FPUT: $H = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} \frac{1}{2}\left(q_{n+1} - q_n\right)^2 + \frac{\beta}{4}\left(q_{n+1} - q_n\right)^4$

Rescale $(q_n, p_n) \rightarrow \left(\frac{q_n}{\sqrt{\beta}}, \frac{p_n}{\sqrt{\beta}}\right)$ and the Hamiltonian becomes $H\beta = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} \frac{1}{2}\left(q_{n+1} - q_n\right)^2 + \frac{1}{4}\left(q_{n+1} - q_n\right)^4$

Thus we had $S = E\beta(N+1)^C$ and numerically found the data to collapse when $C = 1$.

Shifted Frequency Perturbation Theory

Expand: $Q_k = \sum_{j=0}^{\infty} \beta^j Q_{k,j}$

Define: $\Omega_k^2 \equiv \omega_k^2 + \sum_{j=1}^{\infty} \beta^j \mu_{k,j}$

Replace ω_k in the normal modes equation of motion with Ω_k

- $\ddot{Q}_k + \Omega_k^2 Q_k = - \sum_{i,j,l=1}^{N} C_{kijl} Q_i Q_j Q_l$

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$$
\begin{aligned}
\mu_{1,1} &= \frac{3}{4} C_{1111}, \\
\mu_{1,2} &= -\frac{3}{4} C_{1111} A_{1,1} + \frac{3}{4} C_{1,1,1,3} \left(3A_{3,2} + A_{3,3}\right), \\
\mu_{3,1} &= \frac{3}{2} C_{3311}, \\
\mu_{3,2} &= \frac{3}{4A_{3,1}} \left[C_{3111} \left(2B_{1,4} + B_{1,5} + B_{1,6}\right) \right. \\
&\qquad + C_{3311} \left(B_{3,5} + B_{3,6} - 4A_{3,1} A_{1,1}\right) \\
&\qquad \left. + C_{3115} \left(2B_{5,5} + B_{5,6} + B_{5,7}\right) \right], \\
\mu_{5,1} &= \frac{3}{2} C_{5511}.
\end{aligned}
$$

$$
\begin{aligned}
A_{1,1} &= \frac{C_{1111}}{32\Omega_1^2}, & B_{3,5} &= \frac{-3C_{3311} A_{3,1}}{4\left(\Omega_3^2 - (\Omega_3 - 2\Omega_1)^2\right)}, \\
A_{3,2} &= \frac{-3C_{1111}}{4\left(\Omega_3^2 - \Omega_1^2\right)}, & B_{3,6} &= \frac{-3C_{3311} A_{3,1}}{\left(\Omega_3^2 - (\Omega_3 + 2\Omega_1)^2\right)}, \\
A_{3,3} &= \frac{-C_{1111}}{4\left(\Omega_3^2 - 9\Omega_1^2\right)}, & & \\
A_{3,1} &= -A_{3,2} - A_{3,3}, & B_{5,5} &= \frac{3C_{5311} A_{3,1}}{2\left(\Omega_3^2 - \Omega_5^2\right)}, \\
B_{1,4} &= \frac{-3C_{1113} A_3}{2\left(\Omega_1^2 - \Omega_3^2\right)}, & & \\
B_{1,5} &= \frac{-3C_{1113} A_{3,1}}{4\left(\Omega_1^2 - (\Omega_3 - 2\Omega_1)^2\right)}, & B_{5,6} &= \frac{3C_{5311} A_{3,1}}{4\left((\Omega_3 - 2\Omega_1)^2 - \Omega_5^2\right)}, \\
B_{1,6} &= \frac{-3C_{1113} A_{3,1}}{4\left(\Omega_1^2 - (\Omega_3 + 2\Omega_1)^2\right)}, & B_{5,7} &= \frac{3C_{5311} A_{3,1}}{4\left((\Omega_3 + 2\Omega_1)^2 - \Omega_5^2\right)}.
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The β-FPUT Chain in the Continuum Limit

1. Equations of Motion: $\ddot{q}_n = q_{n+1} + q_{n-1} - 2q_n + \beta\left[\left(q_{n+1} - q_n\right)^3 - \left(q_n - q_{n-1}\right)^3\right]$

2. Let $q_n(t) \equiv q(na, t)$ & Expand $q_{n\pm1}(t) = q \pm a q_x + \frac{a^2}{2} q_{xx} \pm \frac{a^3}{6} q_{xxx} + \frac{a^4}{24} q_{xxxx}$

3. Find: $\ddot{q} = a^2\left(q_{xx} + b\varepsilon\left(q_x\right)^2 q_{xx} + \zeta\varepsilon q_{xxxx}\right)$ with $\varepsilon = 3|\beta|a^2$, $\zeta = 1/(36|\beta|)$, $b = \text{sgn}(\beta)$

4. Let: $q(x,t) \sim F(\xi, \tau)$ where $\xi = x - at$ and $\tau = \frac{\varepsilon a t}{2}$

5. Let $\phi(\xi,\tau) = F_\xi(\xi,\tau)$: $\boxed{\phi_\tau + b\phi_\xi\phi^2 + \zeta\phi_{\xi\xi\xi} = 0}$ (modified Korteweg-de Vries (mKdV) equation)

N.J. Zabusky *Nonlinear partial differential equations*. Academic Press, 1967

Finding Soliton Velocities

- Rewrite mKdV equation in the Lax pair formalism: $\phi_\tau + b\phi_\xi\phi^2 + \zeta\phi_{\xi\xi\xi} = 0 \implies \mathscr{L}_\tau = \left[\mathscr{A}, \mathscr{L}\right]$
  - $\mathscr{L} \equiv i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \partial_\xi - \frac{i\phi}{\sqrt{6b\zeta}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
  - $\mathscr{A} \equiv -4\zeta \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \partial_\xi^3 - b \begin{pmatrix} \phi^2 & -\phi_\xi\sqrt{6b\zeta} \\ \phi_\xi\sqrt{6b\zeta} & \phi^2 \end{pmatrix} \partial_\xi - \frac{b}{2} \begin{pmatrix} 2\phi\phi_\xi & -\phi_{\xi\xi}\sqrt{6b\zeta} \\ \phi_{\xi\xi}\sqrt{6b\zeta} & 2\phi\phi_\xi \end{pmatrix}$
- Eigenvalue equation $\mathscr{L}\overrightarrow{\psi} = \sqrt{E}\,\overrightarrow{\psi}$ is a 1+1 dimensional Dirac equation
  - $\pm i \left(\psi_\pm\right)_\xi - \frac{i\phi}{\sqrt{6b\zeta}}\psi_\mp = \sqrt{E}\psi_\pm$
- Can show that the change in the speed of two consecutive noninteracting solitons is
  - $\Delta v = 4\zeta \left| E_{n+1} - E_n \right|$