The β Fermi-Pasta-Ulam-Tsingou Recurrence Problem

Salvatore Pace
Boston University

(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
Document LA-1940 (May 1955).

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

Fermi-Pasta-Ulam-Tsingou (FPUT) Problem

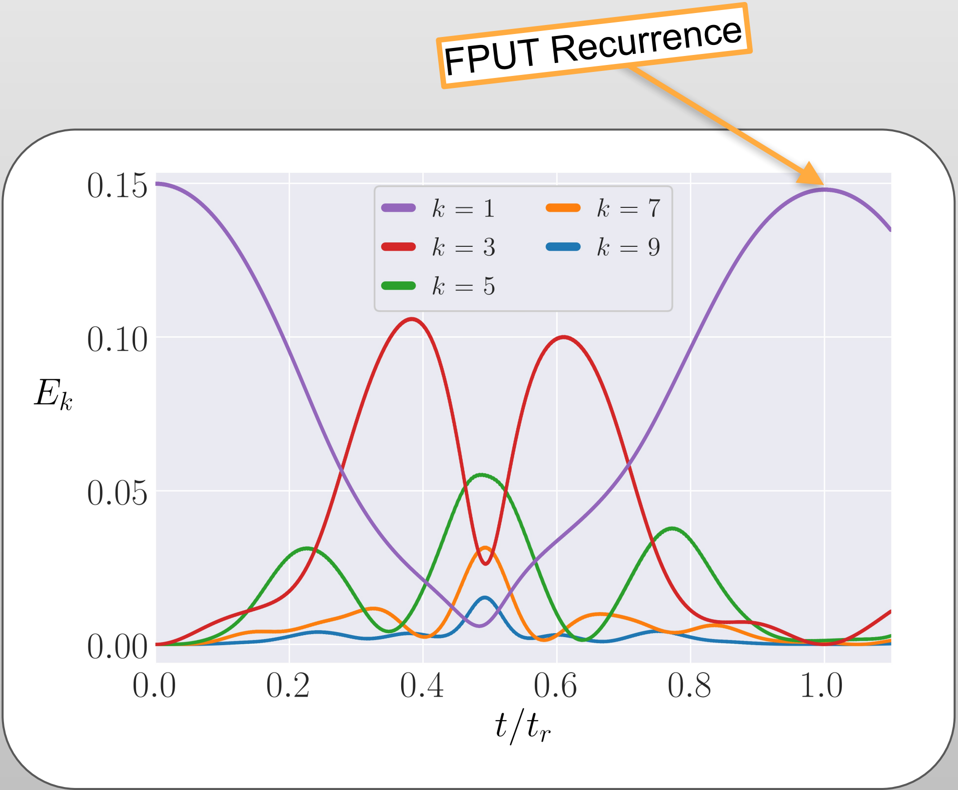
STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM
Document LA-1940 (May 1955).

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



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:

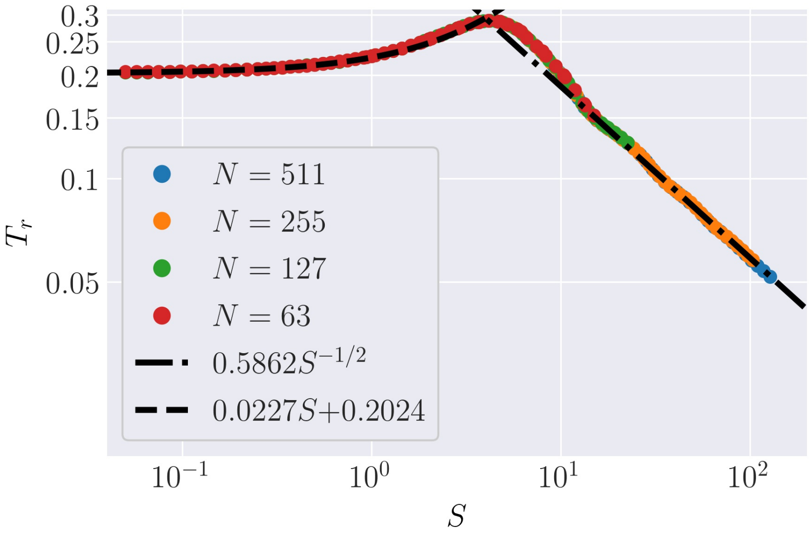
- $\omega_k = 2\sin\left(\frac{k\pi}{2(N+1)}\right)$
- $C_{kijl} = \frac{\omega_k \omega_i \omega_j \omega_l}{2(N+1)} \sum_{\pm} \left[\delta_{k,\pm j \pm l \pm m} - \delta_{k \pm j \pm l \pm m, \pm 2(N+1)}\right]$

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

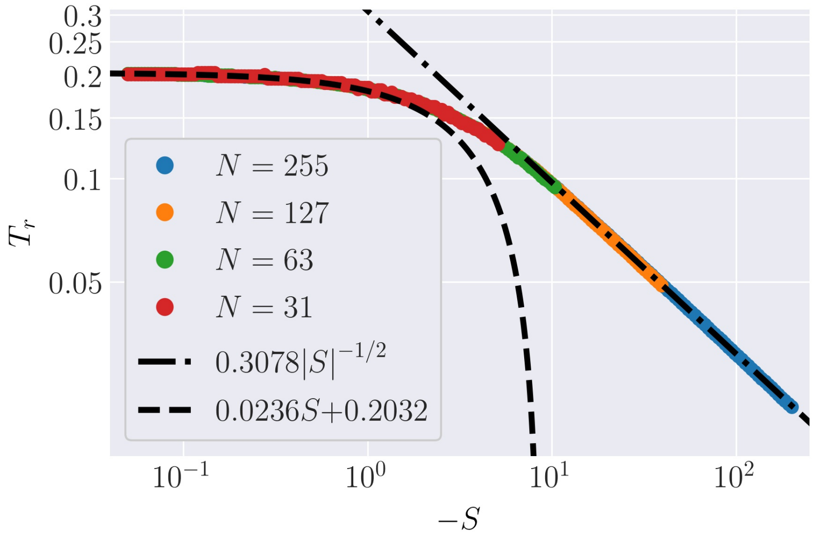
Numerical Determination of FPUT Recurrence Time

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

$\beta > 0$



$\beta < 0$



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

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

Sholl, David S., and B. I. Henry. *Physical Review A* 44.10 (1991): 6364
Sholl, David S., and B. I. Henry. *Physics Letters A* 159.1-2 (1991): 21

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

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

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

$$A_{1,1} = \frac{C_{1111}}{32\Omega_1^2}, \qquad B_{3,5} = \frac{-3C_{3311}A_{3,1}}{4\left(\Omega_3^2 - (\Omega_3 - 2\Omega_1)^2\right)},$$
$$A_{3,2} = \frac{-3C_{1111}}{4\left(\Omega_3^2 - \Omega_1^2\right)}, \qquad B_{3,6} = \frac{-3C_{3311}A_{3,1}}{\left(\Omega_3^2 - (\Omega_3 + 2\Omega_1)^2\right)},$$
$$A_{3,3} = \frac{-C_{1111}}{4\left(\Omega_3^2 - 9\Omega_1^2\right)},$$
$$A_{3,1} = -A_{3,2} - A_{3,3}, \qquad B_{5,5} = \frac{3C_{5311}A_{3,1}}{2\left(\Omega_3^2 - \Omega_5^2\right)},$$
$$B_{1,4} = \frac{-3C_{1113}A_3}{2\left(\Omega_1^2 - \Omega_3^2\right)},$$
$$B_{1,5} = \frac{-3C_{1113}A_{3,1}}{4\left(\Omega_1^2 - (\Omega_3 - 2\Omega_1)^2\right)}, \qquad B_{5,6} = \frac{3C_{5311}A_{3,1}}{4\left((\Omega_3 - 2\Omega_1)^2 - \Omega_5^2\right)},$$
$$B_{1,6} = \frac{-3C_{1113}A_{3,1}}{4\left(\Omega_1^2 - (\Omega_3 + 2\Omega_1)^2\right)}, \qquad B_{5,7} = \frac{3C_{5311}A_{3,1}}{4\left((\Omega_3 + 2\Omega_1)^2 - \Omega_5^2\right)}.$$

Sholl, David S., and B. I. Henry. *Physical Review A* 44.10 (1991): 6364
Sholl, David S., and B. I. Henry. *Physics Letters A* 159.1-2 (1991): 21

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 define "nonlinear" frequency
- Dropping terms $\mathcal{O}(N^{-2})$:

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

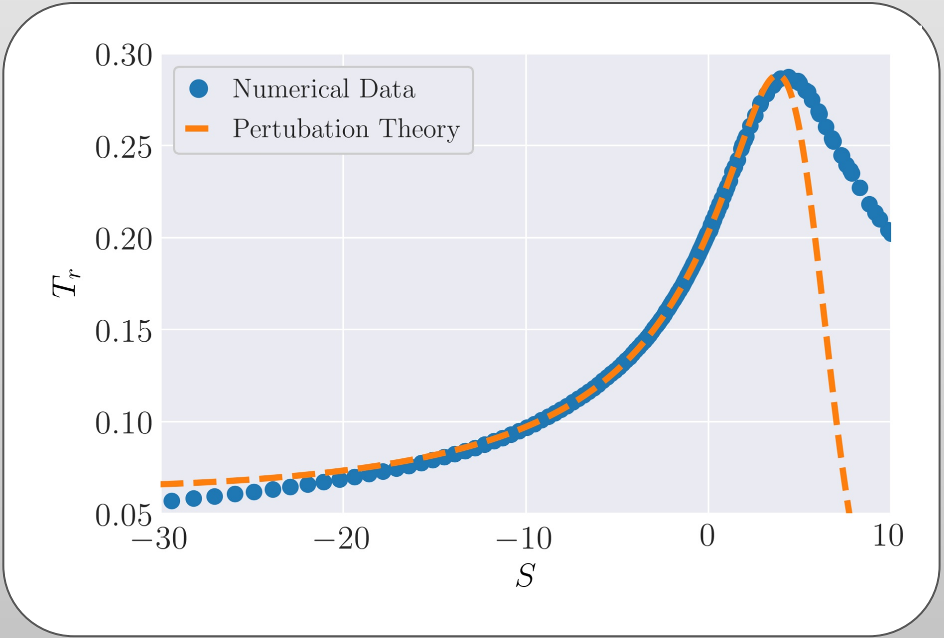
Sholl, David S., and B. I. Henry. *Physical Review A* 44.10 (1991): 6364
Sholl, David S., and B. I. Henry. *Physics Letters A* 159.1-2 (1991): 21

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 define “nonlinear” frequency
- Dropping terms $\mathcal{O}(N^{-2})$:

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



Sholl, David S., and B. I. Henry. *Physical Review A* 44.10 (1991): 6364
Sholl, David S., and B. I. Henry. *Physics Letters A* 159.1-2 (1991): 21

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 $\varepsilon = 3|\beta|a^2$, $\zeta = 1/(36|\beta|)$, $b = \mathrm{sgn}(\beta)$

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

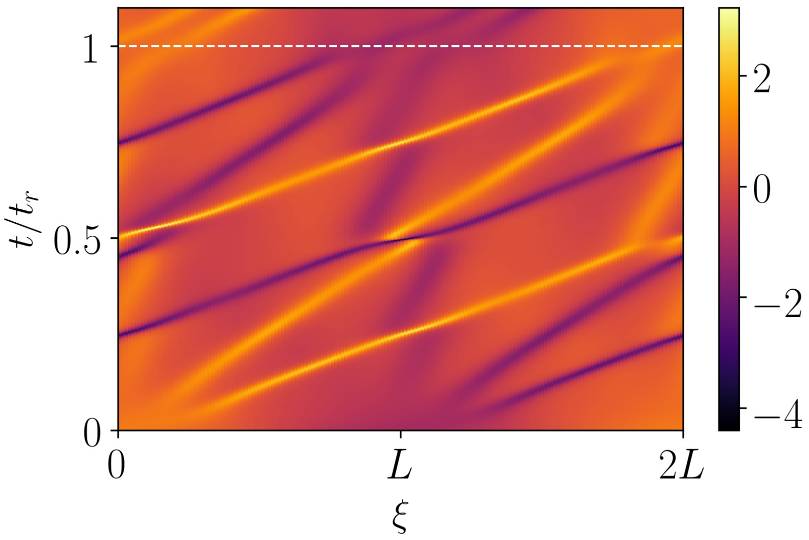
5. Let $\phi(\xi, \tau) = F_\xi(\xi, \tau)$: $\boxed{\phi_\tau + b\phi_\xi \phi^2 + \zeta \phi_{\xi\xi\xi} = 0}$ (modified Korteweg-de Vries (mKdV) equation)

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

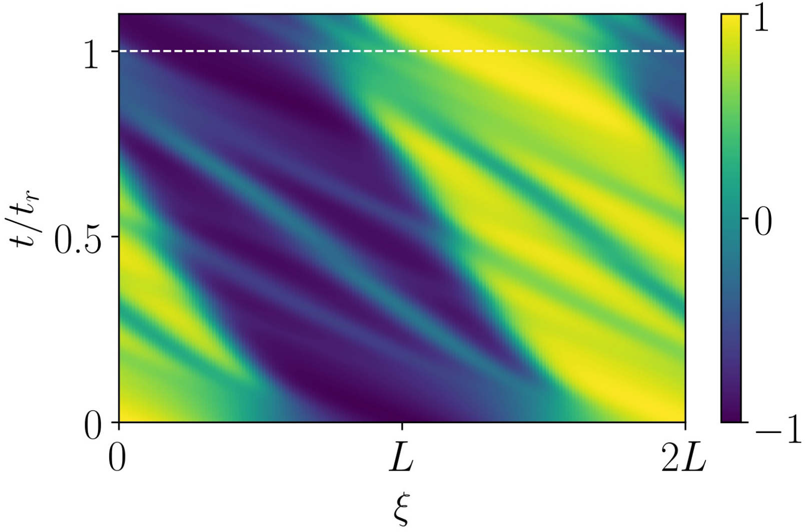
Numerically solving continuum dynamics

- 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

$\beta > 0$



$\beta < 0$



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
  - $\pm i\left(\psi_\pm\right)_\xi - \frac{i\phi}{\sqrt{6b\zeta}}\psi_\mp = \sqrt{E}\psi_\pm$

[45] T. Aktosun, Inverse Scattering Transform and the Theory of Solitons, pp. 771–782. New York, NY: Springer New York, 2011.

- Can show that the change in the speed of two consecutive noninteracting solitons is
  - $\Delta v = 4\zeta\left|E_{n+1} - E_n\right|$

Highly nonlinear regime (large |S|)

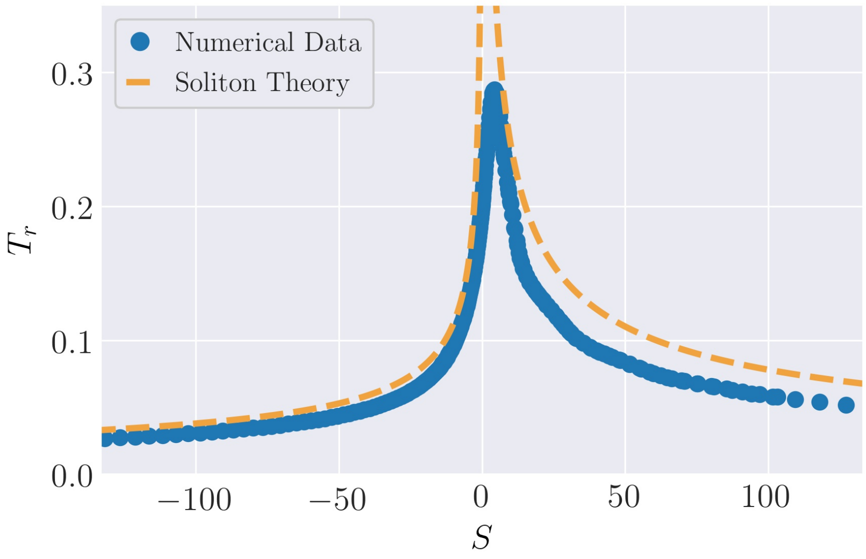
M. Toda, Physics Reports, vol. 18, no. 1, pp. 1–123, 1975.

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

Highly nonlinear regime (large |S|)

M. Toda, Physics Reports, vol. 18, no. 1, pp. 1–123, 1975.

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



Recap

- Rescaled FPUT recurrence time, 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.
- For large $|S|$, FPUT recurrence time can be estimated from the mKdV solution velocities.

Thank You!

David Campbell

Kevin Reiss