Thermalization and conduction in one-dimensional chains: a wave turbulence approach

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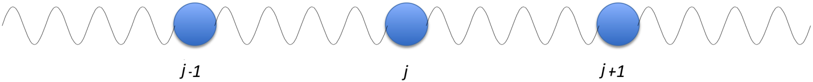
November 4, 2019

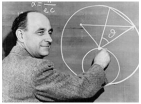
The weakly nonlinear one-dimensional chain model

N equal masses connected by a weakly nonlinear spring



The Hamiltonian

$$H = \sum_{j=1}^{N} \left[\frac{1}{2m} p_j^2 + \frac{\kappa}{2} (q_j - q_{j+1})^2 \right] + \frac{\alpha}{3} \sum_{j=1}^{N} (q_j - q_{j+1})^3 + \frac{\beta}{4} \sum_{j=1}^{N} (q_j - q_{j+1})^4 + \ldots$$

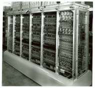


Enrico Fermi (1901-1954)

John Pasta (1909-1984)

Stanislaw Ulam (1918-1984)

Mary Tsingou-Menzel (1928-)



MANIAC I (1952-1957)

The result expected by Fermi and collaborators

Equipartition of *linear* energy in Fourier space for large times

$$Q_k = \frac{1}{N}\sum_{j=0}^{N-1} q_j e^{-i\frac{2\pi kj}{N}}, \; P_k = \frac{1}{N}\sum_{j=0}^{N-1} p_j e^{-i\frac{2\pi kj}{N}},$$

then

$$E_k = |P_k|^2 + \omega_k^2 |Q_k|^2 = const$$

with

$$\omega_k = 2\left|\sin\left(\frac{\pi k}{N}\right)\right|$$

The Los Alamos report

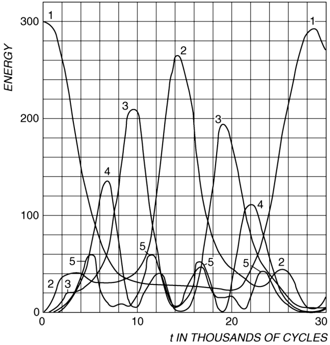
STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM

Document LA-1940 (May 1955).

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.



Following up on the "little discovery"

- Soliton theory
- Theory of integrable PDEs
- Hamiltonian Chaos

Some years after FPUT: solitons and integrability in physics

In the limit of long waves (continuum limit) the α-FPUT system reduces to the Korteweg-de Vries (KdV) equation:

$$\frac{\partial \eta}{\partial t} + \eta \frac{\partial \eta}{\partial x} + \frac{\partial^3 \eta}{\partial x^3} = 0$$

VOLUME 15, NUMBER 6 PHYSICAL REVIEW LETTERS 9 AUGUST 1965

INTERACTION OF "SOLITONS" IN A COLLISIONLESS PLASMA AND THE RECURRENCE OF INITIAL STATES

N. J. Zabusky

Bell Telephone Laboratories, Whippany, New Jersey

and

M. D. Kruskal

VOLUME 19, NUMBER 19 PHYSICAL REVIEW LETTERS 6 NOVEMBER 1967

METHOD FOR SOLVING THE KORTEWEG-deVRIES EQUATION*

Clifford S. Gardner, John M. Greene, Martin D. Kruskal, and Robert M. Miura

Plasma Physics Laboratory, Princeton University, Princeton, New Jersey

(Received 15 September 1967)

ZK showed, besides recurrence, the formation of train of solitons

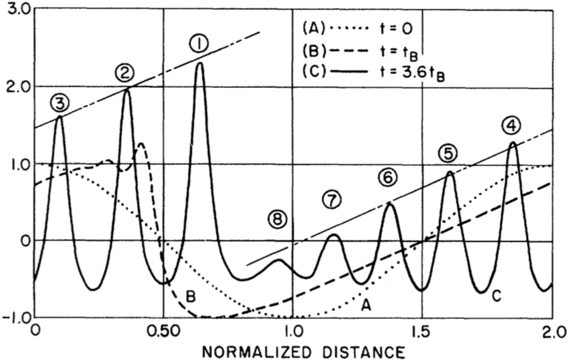
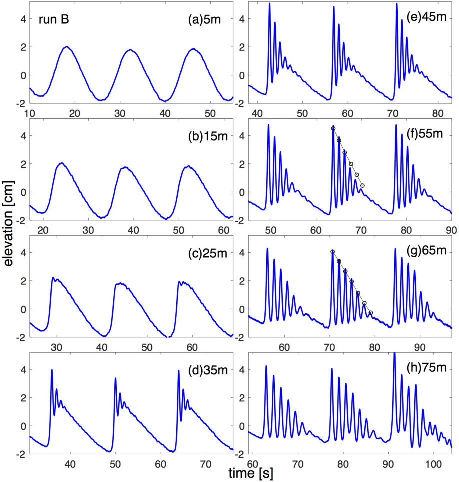


FIG. 1. The temporal development of the wave form $u(x)$.

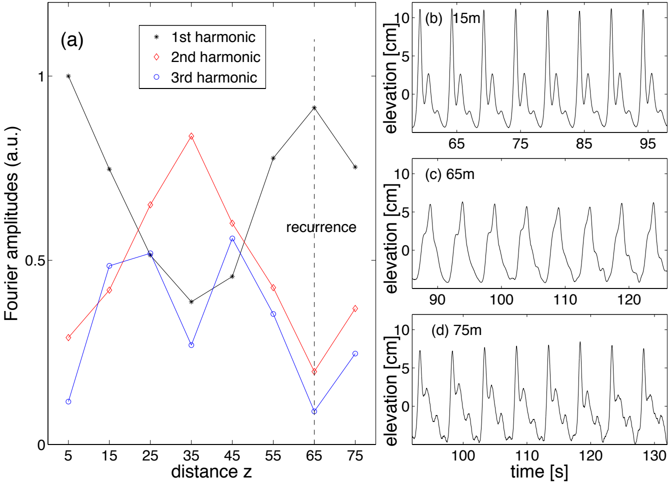
Experimental demonstration of the ZK solitons



Trillo et. al PRL 2016

The wave tank in Berlin (5 m $\times$ 90 m $\times$ 15 cm)

FPUT recurrence in shallow water (Trillo et. al PRL 2016)



Literature and reviews

Some reviews:

- Ford, J. ”The Fermi-Pasta-Ulam problem: paradox turns discovery.” Physics Reports 213.5 (1992): 271-310.
- Berman, G. P., and F. M. Izrailev. ”The Fermi-Pasta-Ulam problem: fifty years of progress.” Chaos (Woodbury, NY) 15.1 (2005): 15104
- Carati, A., L. Galgani, and A. Giorgilli. ”The Fermi-Pasta-Ulam problem as a challenge for the foundations of physics.” Chaos: An Interdisciplinary Journal of Nonlinear Science 15.1 (2005): 015105-015105.
- Weissert, Thomas P. ”The genesis of simulation in dynamics: pursuing the Fermi-Pasta-Ulam problem.” Springer-Verlag New York, Inc., 1999.
- Gallavotti, G., ed. ”The Fermi-Pasta-Ulam problem: a status report.” Vol. 728. Springer, 2008.

Open questions

… but FPU is not an integrable system…

- Does the system thermalize for arbitrary small nonlinearity?
- If yes, what is the time scale of thermalization for finite N?
- What is the thermalization time scale in the thermodynamic limit?
- How does thermalization time scale depend on the number of particles?

The models

- α-FPUT

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) + \alpha \left[(q_{j+1} - q_j)^2 - (q_{j-1} - q_j)^2 \right]$$

- β-FPUT

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) + \beta \left[(q_{j+1} - q_j)^3 - (q_{j-1} - q_j)^3 \right]$$

- Discrete Nonlinear Klein Gordon (DNKG)

$$\ddot{q}_j = (q_{j+1} + q_{j-1} - 2q_j) - q_j - g q_j^3,$$

- Toda Lattice

$$\ddot{q}_j = \frac{1}{2\alpha} \left(\exp[2\alpha(q_{j+1} - q_j)] - \exp[2\alpha(q_j - q_{j-1})] \right)$$

The linear and the weakly nonlinear regime

Linear regime

- For α-FPUT, β-FPUT, Toda

$$\omega_k = 2|\sin\left(k\pi/N\right)|$$

- For DNKG

$$\omega_k = \sqrt{1 + 4\sin\left(k\pi/N\right)^2}$$

Weakly nonlinear regime

$$\beta \sim g \sim \alpha^2 \sim \epsilon$$

Normal modes

Assuming periodic boundary conditions, we introduce the wave action variable

$$a_k = \frac{1}{\sqrt{2\omega_k}}(\omega_k Q_k + iP_k),$$

with $P_k = \dot{Q}_k$ and $\omega_k = 2|\sin(\pi k/N)|$
Because of the absence of three wave interactions, i.e.:

$$k_1 \pm k_2 \pm k_3 = 0$$
$$\omega_1 \pm \omega_2 \pm \omega_3 \neq 0$$

quadratic nonlinearity can be removed from α-FPUT and Toda.

Same (approximate) Hamiltonian for all 4 models

$$\frac{H}{N} = \sum_{k=0}^{N-1} \omega_k |a_k|^2 + \epsilon \sum_{k_1,k_2,k_3,k_4} \Big[T^{(1)}_{1,2,3,4} (a_1^* a_2 a_3 a_4 + c.c.) \delta_{1-2-3-4} +$$
$$+ \frac{1}{2} T^{(2)}_{1,2,3,4} a_1^* a_2^* a_3 a_4 \delta_{1+2-3-4} + \frac{1}{4} T^{(3)}_{1,2,3,4} (a_1 a_2 a_3 a_4 + c.c.) \delta_{1+2+3+4} \Big]$$

with

$$\delta_{1\pm2\pm3\pm4} = \delta(k_1 \pm k_2 \pm k_3 \pm k_4), \quad a_i = a(k_i, t), \qquad T_{1,2,3,4} = T(k_1, k_2, k_3, k_4)$$

$\epsilon \sim \beta \sim g \sim \alpha^2$

Starting point for statistical theory (see Nazarenko 2011)

The thermodynamic limit

$$N \to \infty, \quad L \to \infty \quad \text{with} \quad \frac{L}{N} = \Delta x = const$$

Then the dispersion relations become:

$$\omega_\kappa = 2|\sin(\kappa/2)|, \quad \omega_\kappa = \sqrt{1 + 4\sin(\kappa/2)^2}$$

with $\kappa \in \mathbb{R}$. The following 4-wave resonant interactions are satisfied:

$$\kappa_1 + \kappa_2 - \kappa_3 - \kappa_4 = 0$$
$$\omega_1 + \omega_2 - \omega_3 - \omega_4 = 0$$

Standard Wave Turbulence can be developed

The Wave Kinetic Equation

- Look for an evolution equation for the correlator
  $< a(\kappa_i, t)a(\kappa_j, t)^* >= n_i \delta(\kappa_i - \kappa_j)$
  with $n_i = n(\kappa_i, t)$
- Assume random initial phases and amplitudes

$$\frac{\partial n(\kappa_1, t)}{\partial t} = J(\kappa_1, t)$$

$$J(\kappa_1, t) = \epsilon^2 \int_0^{2\pi} T^2_{1,2,3,4} n_1 n_2 n_3 n_4 \left(\frac{1}{n_1} + \frac{1}{n_2} - \frac{1}{n_3} - \frac{1}{n_4} \right) \delta(\Delta\kappa)\delta(\Delta\omega) d\kappa_{2,}$$

$$\delta(\Delta\kappa) = \kappa_1 + \kappa_2 - \kappa_3 - \kappa_4$$

$$\delta(\Delta\omega) = \omega(\kappa_1) + \omega(\kappa_2) - \omega(\kappa_3) - \omega(\kappa_4)$$

The Wave Kinetic Equation

Conserved quantities:

$$E = \int_0^{2\pi} \omega(\kappa) n(\kappa, t) d\kappa, \qquad N = \int_0^{2\pi} n(\kappa, t) d\kappa,$$

Existence of an H-theorem:

$$H = \int_0^{2\pi} \ln(n(\kappa, t)) d\kappa, \quad \text{with} \quad \frac{dH}{dt} \leq 0$$

The Rayleigh-Jeans distribution

$$dH/dt = 0 \rightarrow n(k, t) = \frac{T}{\omega(\kappa) + \mu}$$

Thermalization time scale: $1/\epsilon^2$

Small N regime

$\omega_k = 2|\sin(\pi k/N)|$ with $k \in \mathbb{Z}$

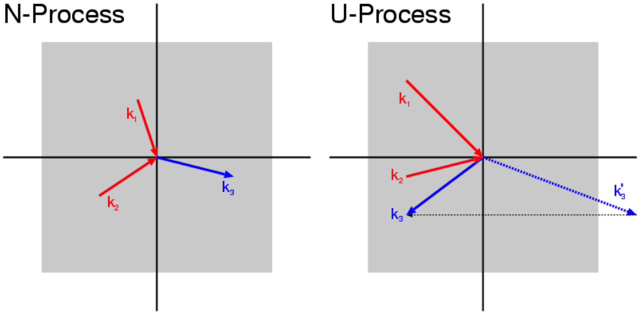
$$k_1 \pm k_2 \pm k_3 \pm k_4 = 0 \pmod N$$

$$\omega_1 \pm \omega_2 \pm \omega_3 \pm \omega_4 = 0$$

It can be shown that only the following interactions are possible (of Umklapp type):

$$k_1 + k_2 - k_3 - k_4 = 0 \pmod N$$
$$\omega_1 + \omega_2 - \omega_3 - \omega_4 = 0$$

Umklapp (flip-over) scattering



Normal process (N-process) and Umklapp process (U-process).
Example of an Umklapp scattering with $N = 32$ ($k_{max} = 16$),
$k_1 = 7$, $k_2 = 9$, $k_3 = -7$, $k_4 = 23$ $\rightarrow$ outside the Brillouin zone, therefore the wave-number is flip-over $k_4' = k_4 - N = -9$

Small N regime

For N power of 2, the above system has solutions for integer values of k:

- *Trivial solutions*: all wave numbers are equal or

$$k_1 = k_3,\ k_2 = k_4, \quad \text{or} \quad k_1 = k_4,\ k_2 = k_3$$

- *Nontrivial solutions*:

$$\{k_1, k_2; k_3, k_4\} = \left\{k_1, \frac{N}{2} - k_1; N - k_1, \frac{N}{2} + k_1\right\}$$

  with $k_1 = 1, 2, \dots, \lfloor N/4 \rfloor$

However....

- Four-waves resonant interactions are isolated
- No efficient mixing (and thermalization) can be achieved via a four-wave resonant process (for weak nonlinearity)

Removing non resonant interactions

$$\frac{H}{N} = \sum_{k=0}^{N-1} \omega_k |a_k|^2 + \epsilon \sum_{k_1,k_2,k_3,k_4} \left[T^{(1)}_{1,2,3,4} (a_1^* a_2 a_3 a_4 + c.c.) \delta_{1-2-3-4} + \right.$$

$$\left. + \frac{1}{2} T^{(2)}_{1,2,3,4} a_1^* a_2^* a_3 a_4 \delta_{1+2-3-4} + \frac{1}{4} T^{(3)}_{1,2,3,4} (a_1 a_2 a_3 a_4 + c.c.) \delta_{1+2+3+4} \right]$$

Eliminate the non-resonant terms from the Hamiltonian using a near-identity (canonical) transformation from $\{ia, a^*\}$ to $\{ib, b^*\}$

$$a_1 = b_1 + \epsilon \sum_{k_2,k_3,k_4} (B^{(1)}_{1,2,3,4} b_2 b_3 b_4 \delta_{1-2-3-4} + B^{(2)}_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2-3-4} +$$

$$+ B^{(3)}_{1,2,3,4} b_2^* b_3^* b_4 \delta_{1+2+3-4} + B^{(4)}_{1,2,3,4} b_2^* b_3^* b_4^* \delta_{1+2+3+4}) + O(\epsilon^2)$$

with $B_{1,2,3,4} \simeq T_{1,2,3,4} / (\omega_1 \pm \omega_2 \pm \omega_3 \pm \omega_4)$.

Removing non-resonant four-wave interactions: the appearance six-wave interactions in the β-FPUT

- check for exact resonances at higher order

$$i\frac{db_1}{dt} = \omega_1 b_1 + \epsilon \sum_{k_2,k_3,k_4} T_{1,2,3,4} b_2^* b_3 b_4 \delta_{1+2-3-4} +$$
$$+ \epsilon^2 \sum W_{1,2,3,4,5,6} b_2^* b_3^* b_4 b_5 b_6 \delta_{1+2+3-4-5-6}$$

Resonant conditions:

$$k_1 + k_2 + k_3 - k_4 - k_5 - k_6 = 0 \pmod{N}$$
$$\omega_1 + \omega_2 + \omega_3 - \omega_4 - \omega_5 - \omega_6 = 0$$

Non-isolated solutions exist for integer values of k with arbitrary N.

$$\frac{dn_1}{dt} \sim \epsilon^4 \ldots$$

Estimation of the equipartition time scale for incoherent waves

Look for the evolution equation of $< b(k_i,t)b(k_j,t)^* >= n(k_i,t)\delta_{i-j}$

$$\frac{dn_1}{dt} \sim \epsilon^2 < b_1^* b_2^* b_3^* b_4 b_5 b_6 >$$
$$\frac{d < b_1^* b_2^* b_3^* b_4 b_5 b_6 >}{dt} \sim \epsilon^2 < b_1^* b_2^* b_3^* b_4^* b_5 b_6 b_7 b_8 >$$

therefore

$$\frac{dn_1}{dt} \sim \epsilon^4 \ldots.$$

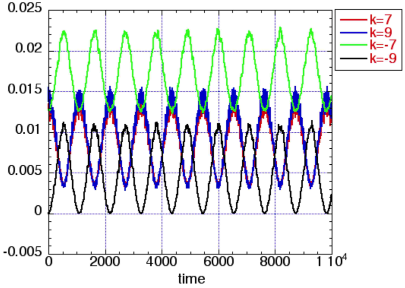
and the time of equipartition scales as

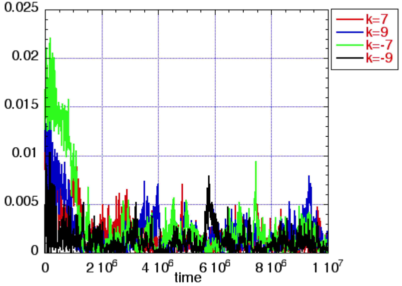
$$\mathbf{t_{eq} \sim 1/\epsilon^4}$$

Numerical simulations (Symplectic integrator (H. Yoshida, 1990 Phys. Lett. A))

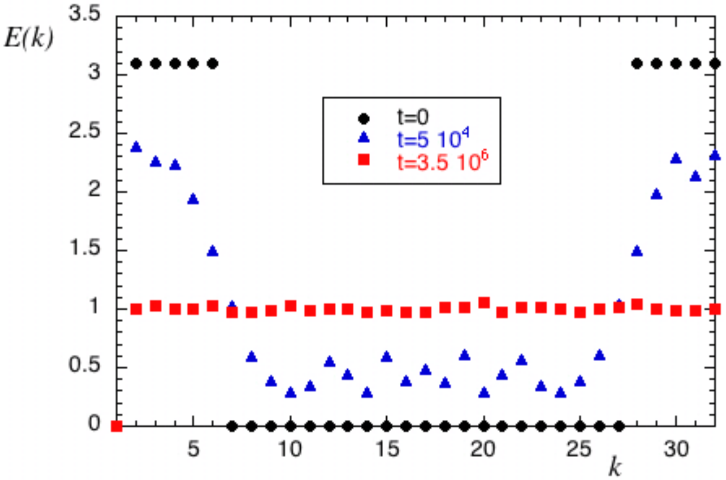
- Example of Umklapp resonance

Numerical simulations



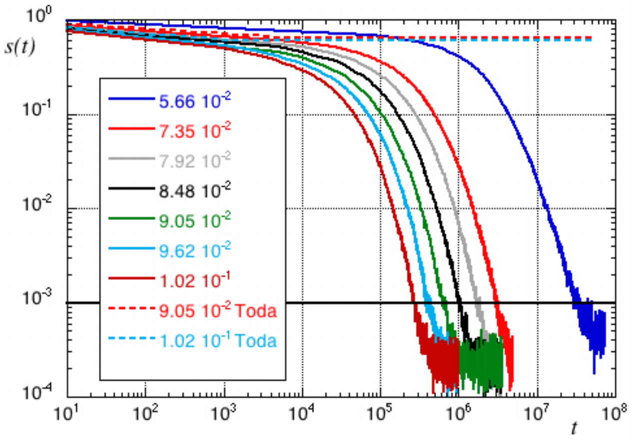


Example of thermalization for α-FPUT with N=32, $\epsilon = 7.3 \times 10^{-2}$ (1000 realizations)

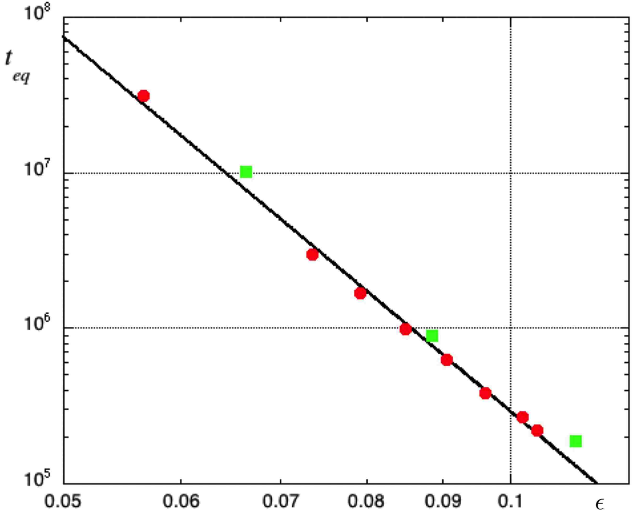


Entropy

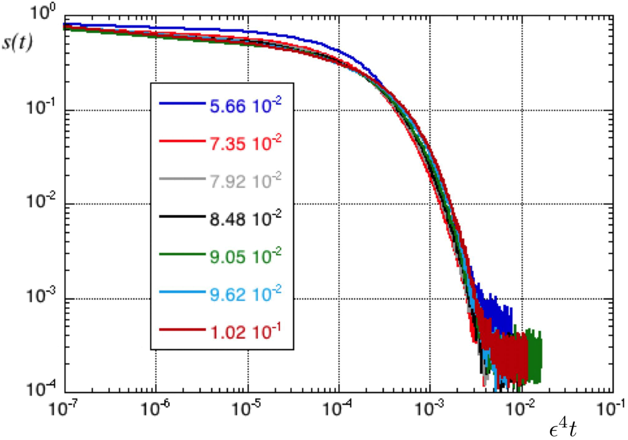
$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{E_{tot}} \omega_k \langle |a_k|^2 \rangle, \quad E_{tot} = \sum_k \omega_k \langle |a_k|^2 \rangle$$



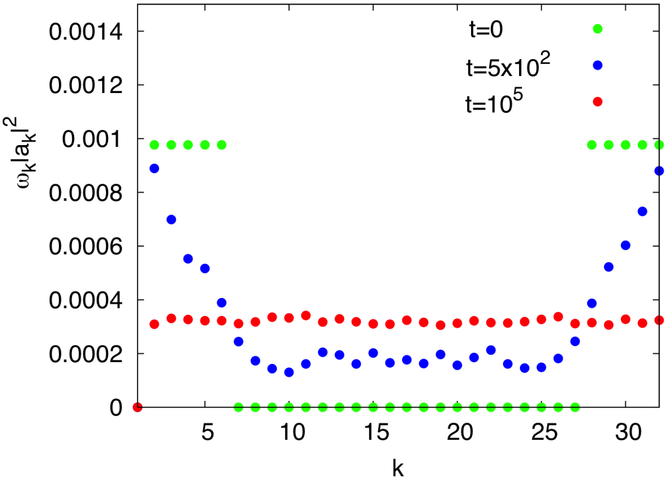
Scaling in time



Collapse of entropy curves

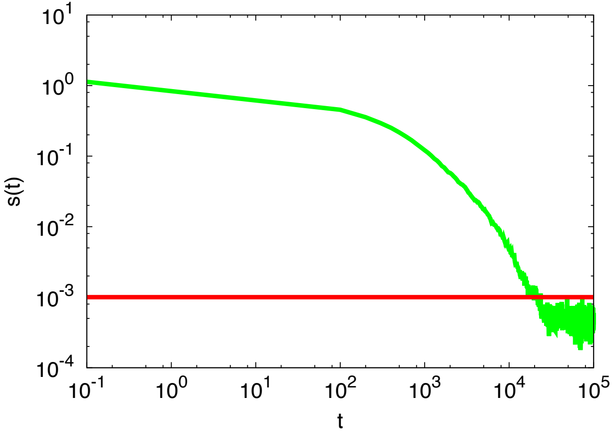


Example of equipartition: β-FPUT, N=32, $\epsilon = 7.05 \times 10^{-2}$

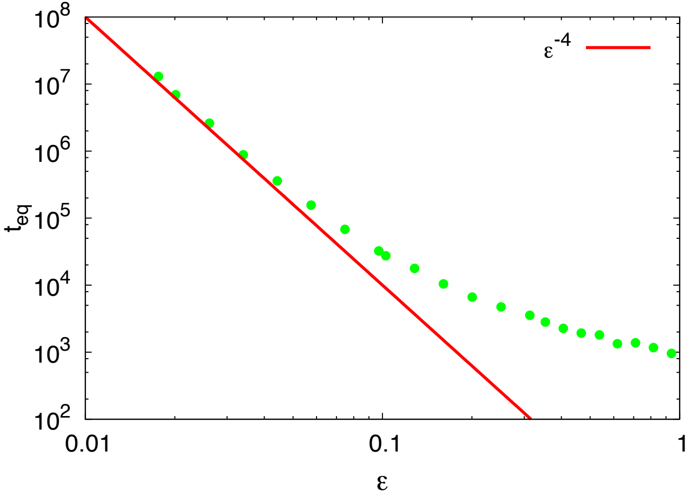


Entropy: β-FPUT, $\epsilon = 7.05 \times 10^{-2}$, $N = 32$

$$s(t) = \sum_k f_k \log f_k \quad \text{with} \quad f_k = \frac{N-1}{H_0}\omega_k \langle |a_k|^2 \rangle, \quad H_0 = \sum_k \omega_k \langle |a_k|^2 \rangle$$



Equipartition time as a function of ϵ



DNKG equation: from discrete to the Large Box Limit

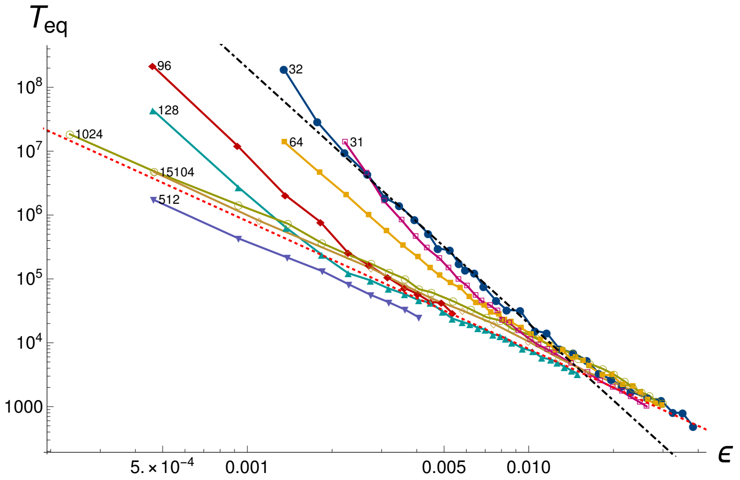
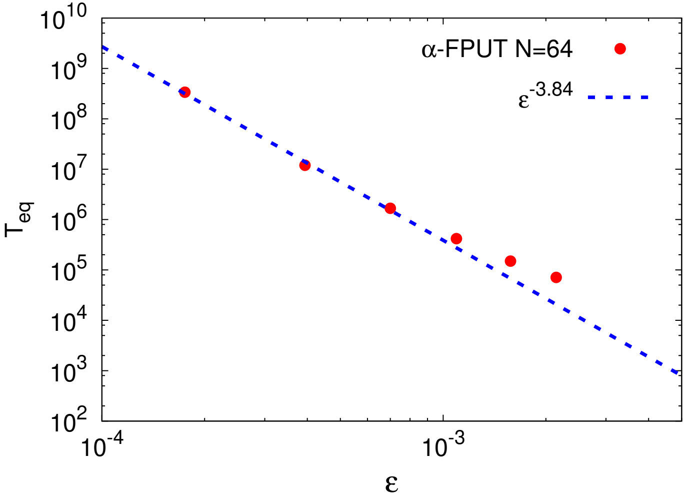
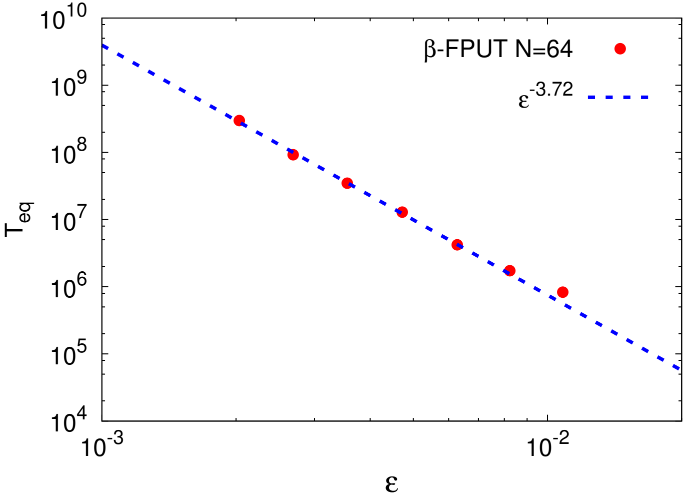


Figure: The scaling of T_{eq} on ϵ for multiple values of N, with $m = 1$ and $E = 0.1N/32$. Scaling laws ϵ^{-2} and ϵ^{-4} in red dotted and black dash-dotted lines for reference.

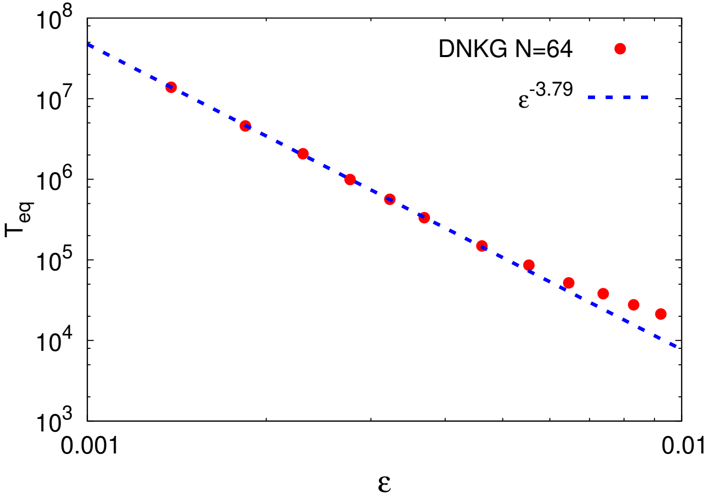
Equipartition time as a function of ϵ: $\alpha - FPUT$ N=64



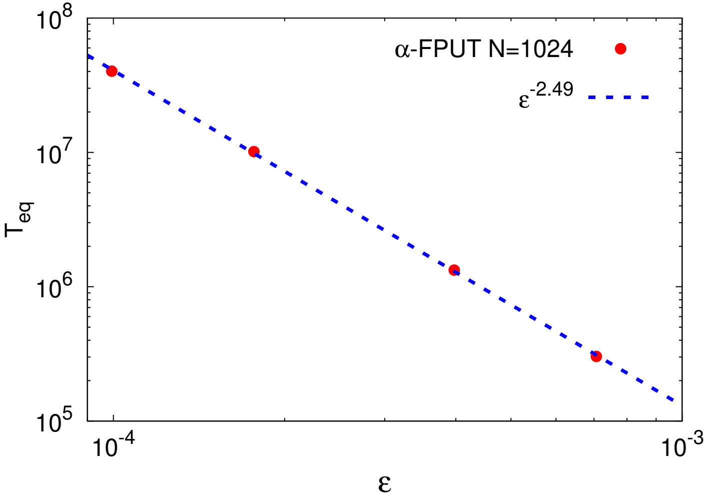
Equipartition time as a function of ϵ: $\beta - FPUT$ N=64



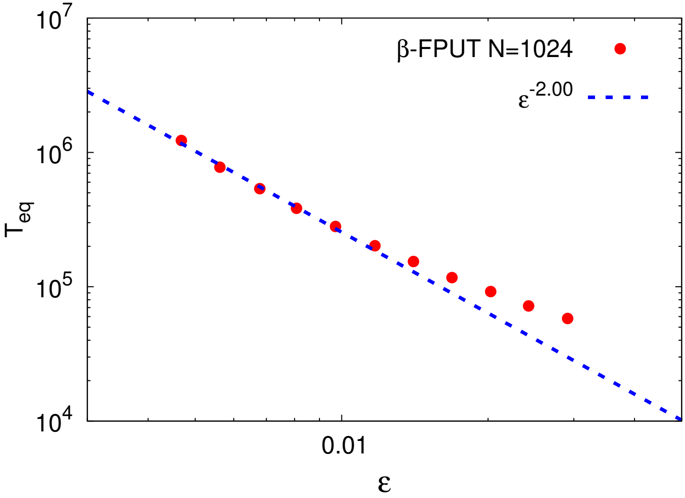
Equipartition time as a function of ϵ: $NLKG$ N=64



Equipartition time as a function of ϵ: $\alpha - FPUT$ N=1024



Equipartition time as a function of ϵ: $\beta - FPUT$ N=1024



Equipartition time as a function of ϵ: $NLKG$ N=1024