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Advanced Workshop on Anderson Localization, Nonlinearity and Turbulence: a Cross-Fertilization

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Integrable & Chaotic Phenomena in the FPU Problem: From Stable Periodic Orbits to Diffusion in Phase Space

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Integrable & chaotic phenomena in the FPU problem: From stable periodic orbits to diffusion in phase space

Workshop: Anderson Localization, Nonlinearity and Turbulence

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University of Padova, Italy

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Joint work with with H. Christodoulidi, S. Flach and H. Skokos

OUTLINE

- Introduction
- Two models: α-FPU & Toda
- Modal energy spectrum
- Phenomenology of the energy cascade
- Diffusion of tail modes
- On the analytic side
- Conclusions

Introduction

$$H(q,p) = \sum_{n=0}^{N-1} \left[\frac{p_n^2}{2} + U(q_{n+1} - q_n) \right]$$

Fixed ends: $q_0 = q_N = p_0 = p_N = 0$.

INITIAL CONDITION:

$$q_n(0) = A \sin\left(\frac{n\pi}{N}\right) \quad , \quad p_n(0) = 0$$

corresponding to the excitation of the largest half-wavelength mode

The FPU problem consists in understanding how energy is transferred from large to small spatial scales (low to high modes), leading the system to a state of equilibrium, if any, compatible with the laws of statistical mechanics

From the FPU Los-Alamos report LA-1940 (May 1955):

- *"Instead of a gradual increase of all the higher modes, the energy is exchanged, essentially, among only a certain few. It is, therefore, very hard to observe the rate of "thermalization" or mixing in our problem, and this was the initial purpose of the calculation."*
- *"Certainly, there seems to be very little, if any, tendency towards equipartition of energy among all degrees of freedom at any given time."* [the FPU paradox]
- *"What is suggested by these special results is that in certain problems which are approximately linear, the existence of quasi-states may be conjectured."*

Two models: α-FPU and Toda

Comparison of two models:

1. $$\boxed{U_{FPU}(x) = \frac{x^2}{2} + \alpha \frac{x^3}{3}}$$ (ergodic?)
2. $$\boxed{U_{Toda}(x) = \frac{e^{2\alpha x} - 1 - 2\alpha x}{4\alpha^2}}$$ (integrable)

The two models are *close*:

$$U_{Toda}(x) = U_{FPU}(x) + O(\alpha^2 x^4) \xrightarrow{\alpha \to 0} \frac{x^2}{2}$$

Energy-amplitude relation:

$$E = H(q(0), p(0)) = \frac{\pi^2 A^2}{4N} + \underbrace{O(\alpha^2 A^4/N^3)}_{\text{Toda only}}$$

Modal energy spectrum

- Fourier coordinates: $\begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \sqrt{\frac{2}{N}} \sum_{n=1}^{N-1} \begin{pmatrix} q_n \\ p_n \end{pmatrix} \sin\left(\frac{\pi k n}{N}\right)$

- $$\boxed{H = \sum_{k=1}^{N-1} \frac{P_k^2 + \omega_k^2 Q_k^2}{2} + O(\alpha Q^3)}$$ $$\boxed{\omega_k = 2\sin\left(\frac{\pi k}{2N}\right)}$$

- modal energy spectrum (m.e.s.):

$$\boxed{E_k(t) = \frac{P_k^2(t) + \omega_k^2 Q_k^2(t)}{2} \quad vs. \quad k}$$

- We always plot a normalized m.e.s.: E_k/E vs. k

- Ergodicity would imply (almost) equipartition of the FPU E_k's on time-average:

$$\overline{E}_k(t) = \frac{1}{t}\int_{t_0}^{t} E_k(s)\, ds \stackrel{t\to+\infty}{\longrightarrow} \varepsilon \equiv \frac{E}{N}$$

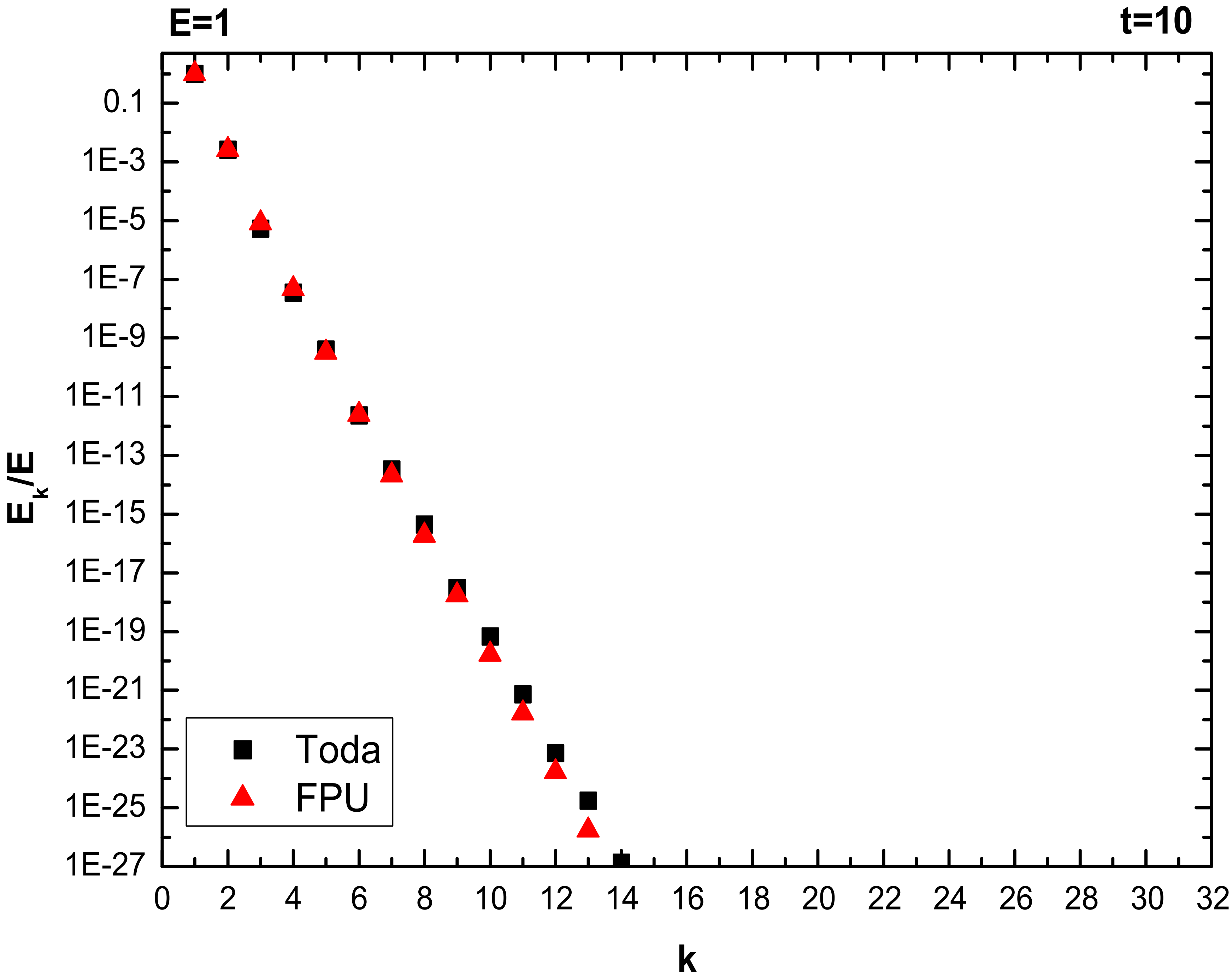
(with equipartition of r.m.s. fluctuations and much more...)

- Quasi-periodicity implies convergence of the Toda $\overline{E}_k$'s to some limit, which defines the Toda "equilibrium" state.

EXAMPLE

$$N = 32,\ \alpha = 0.33,\ E = E_1(0) = 1$$

$$\overline{E}_k(t)/E \text{ vs. } k \text{ at } t = 10, 10^2, \ldots, 10^8$$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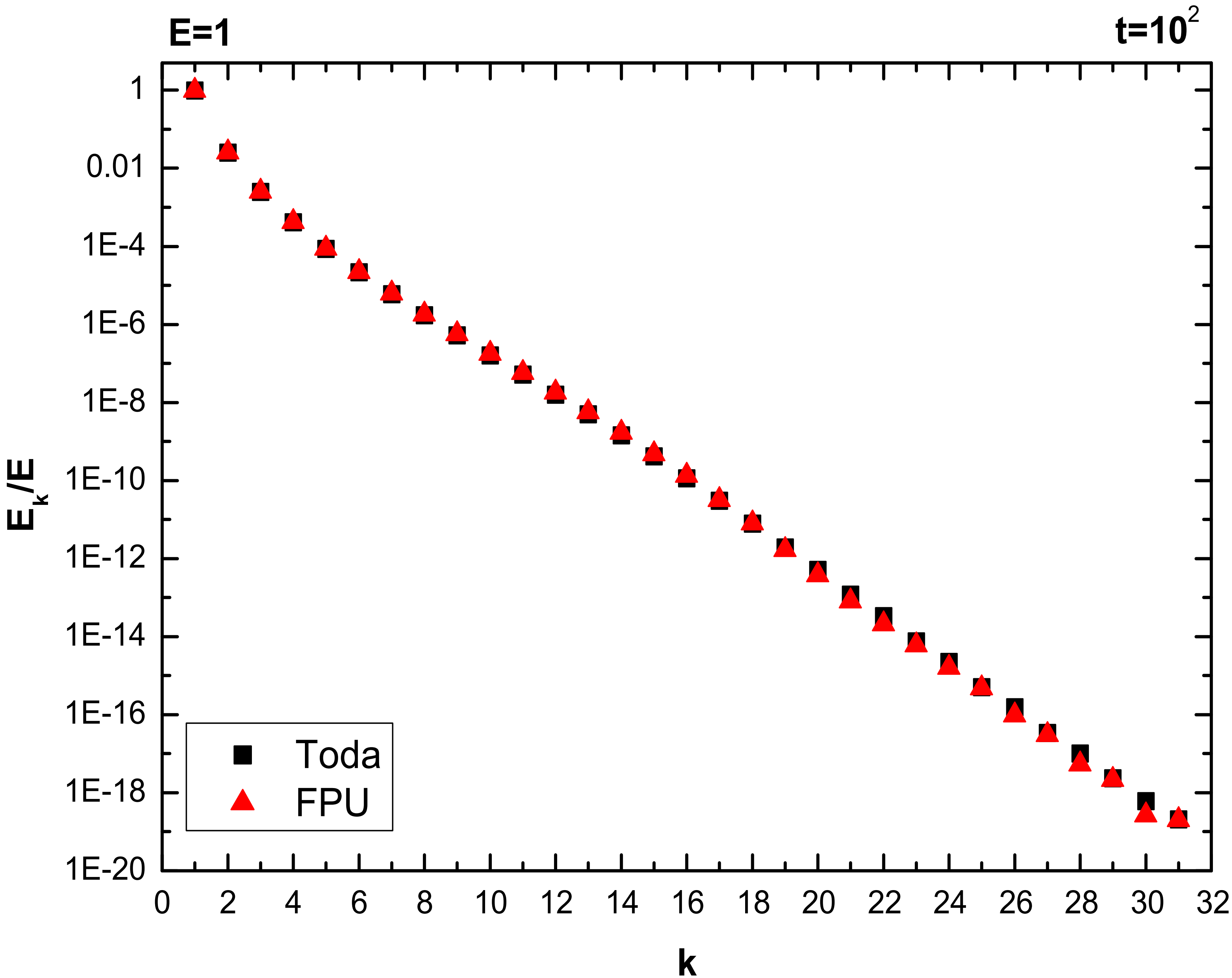
t=10
0.1
1E-3
1E-5
1E-7
1E-9
1E-11
1E-13
1E-15
1E-17
1E-19
1E-21
1E-23
1E-25
1E-27
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
E_k/E
Toda
FPU



E=1
t=10^2
E_k/E
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
1E-14
1E-16
1E-18
1E-20
0
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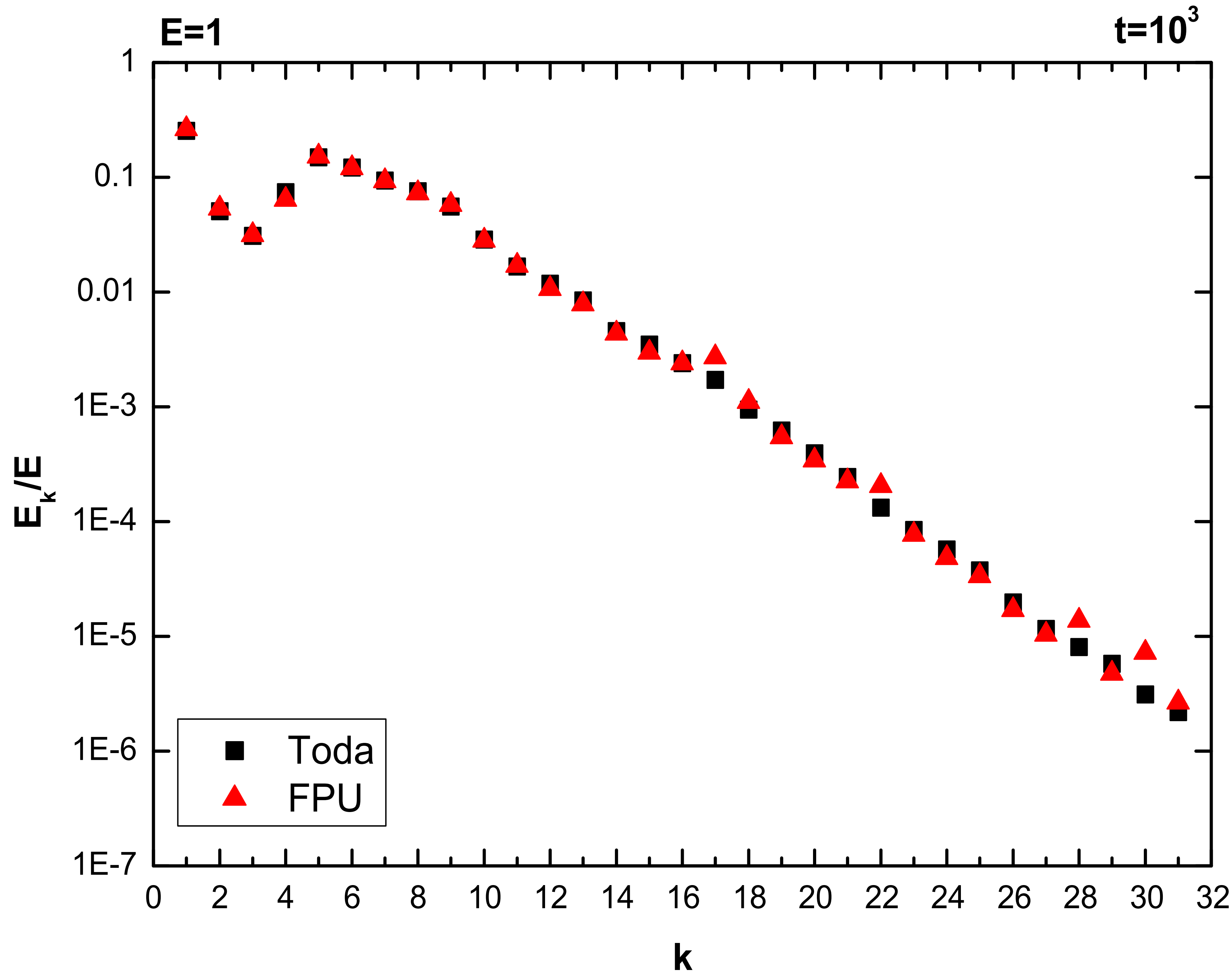
20
22
24
26
28
30
32
k
Toda
FPU



E=1
t=10^3
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
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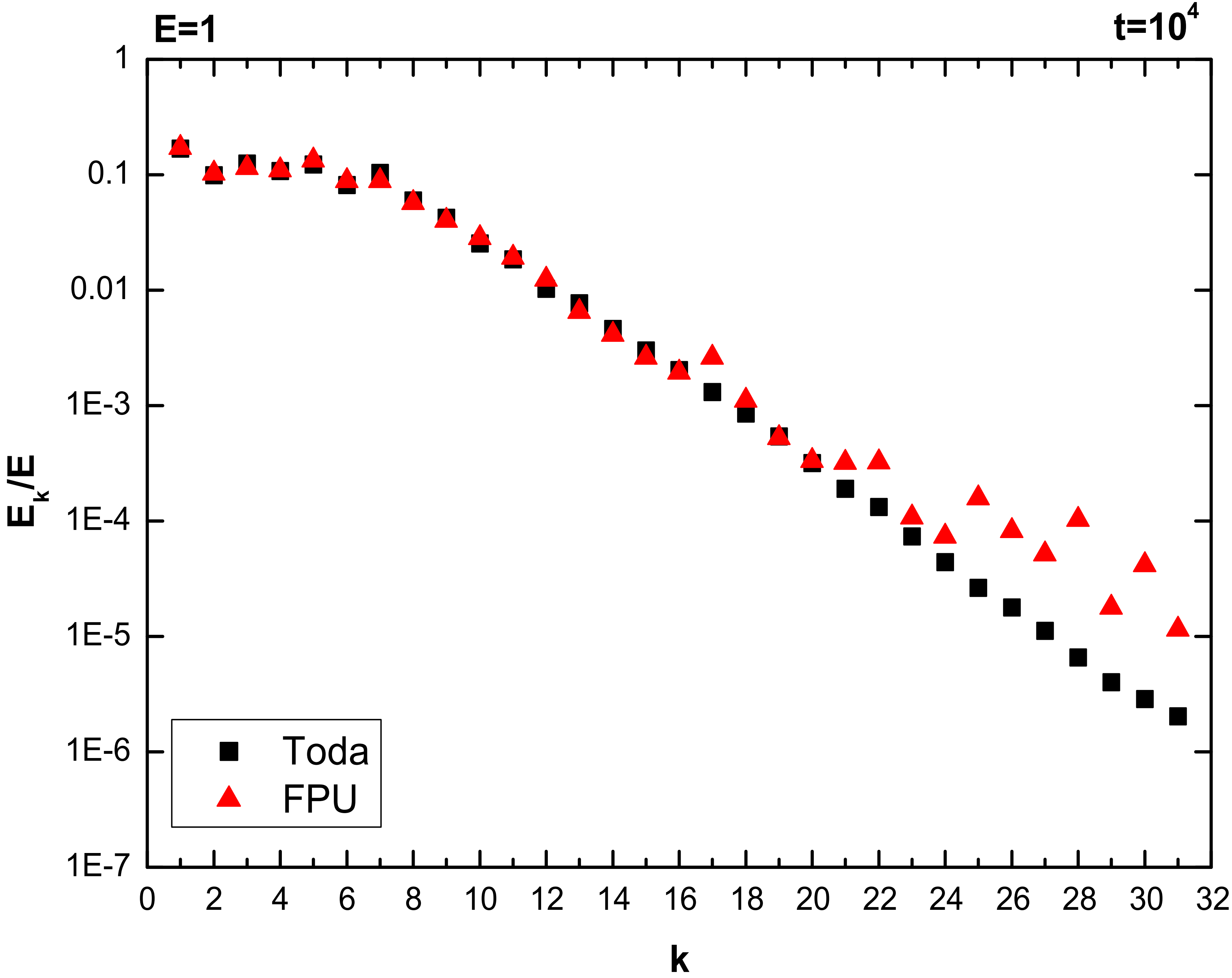
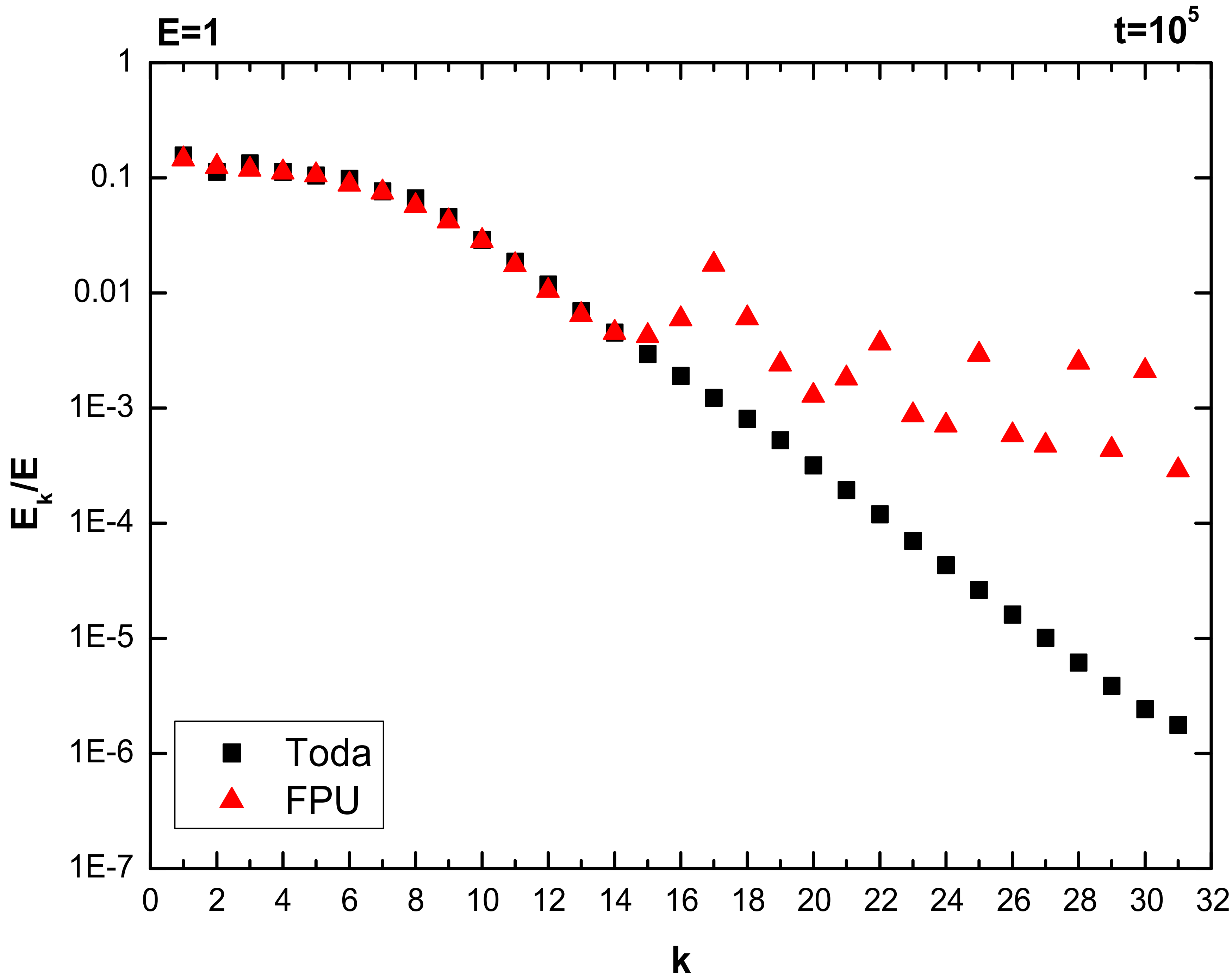
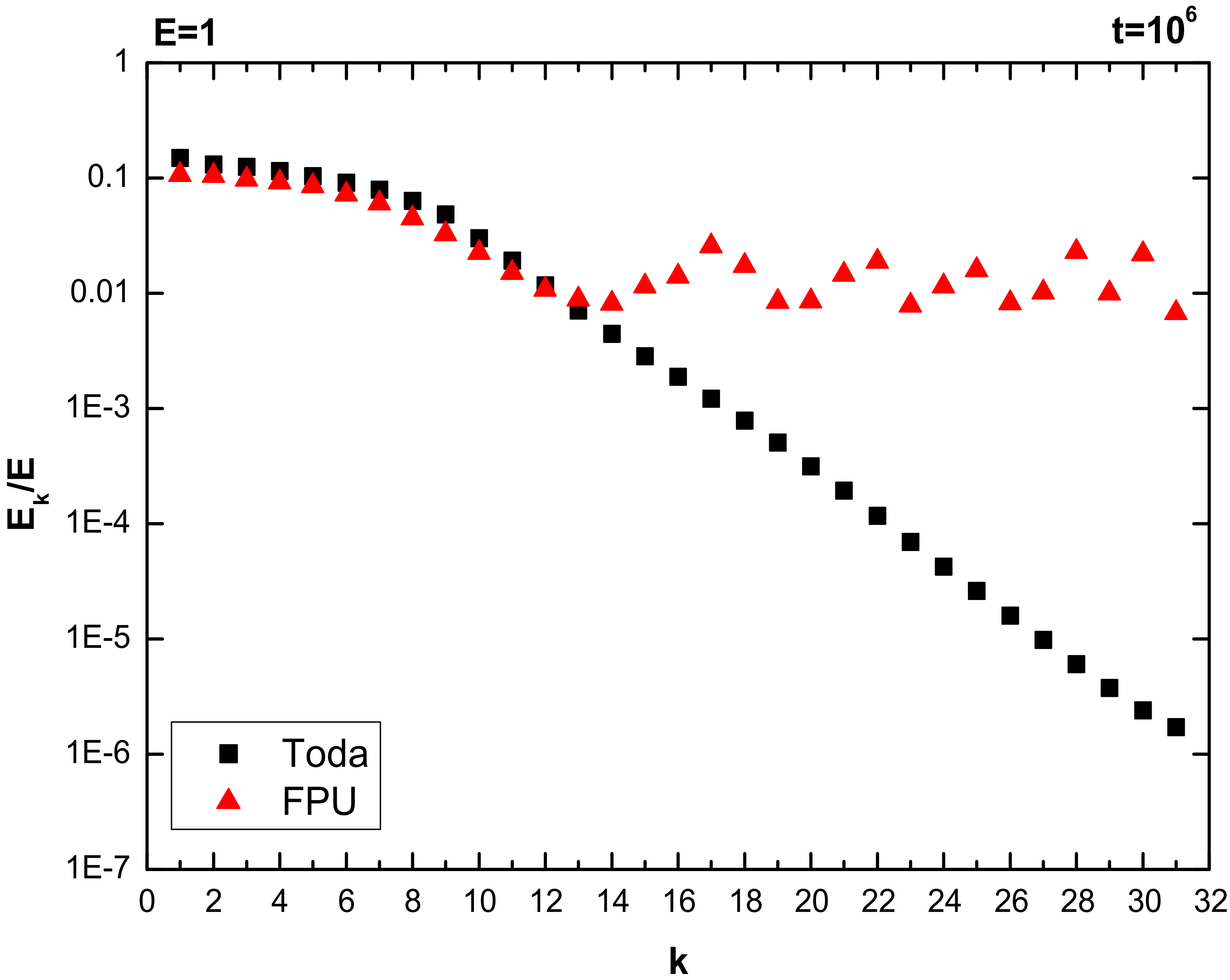
30
32
k
Toda
FPU



E=1
t=10^4
E_k/E
k
Toda
FPU
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32



E=1
t=10^5
E_k/E
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
Toda
FPU


E=1
t=10^6
E_k/E
k
Toda
FPU
1
0.1
0.01
1E-3
1E-4
1E-5
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4
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8
10
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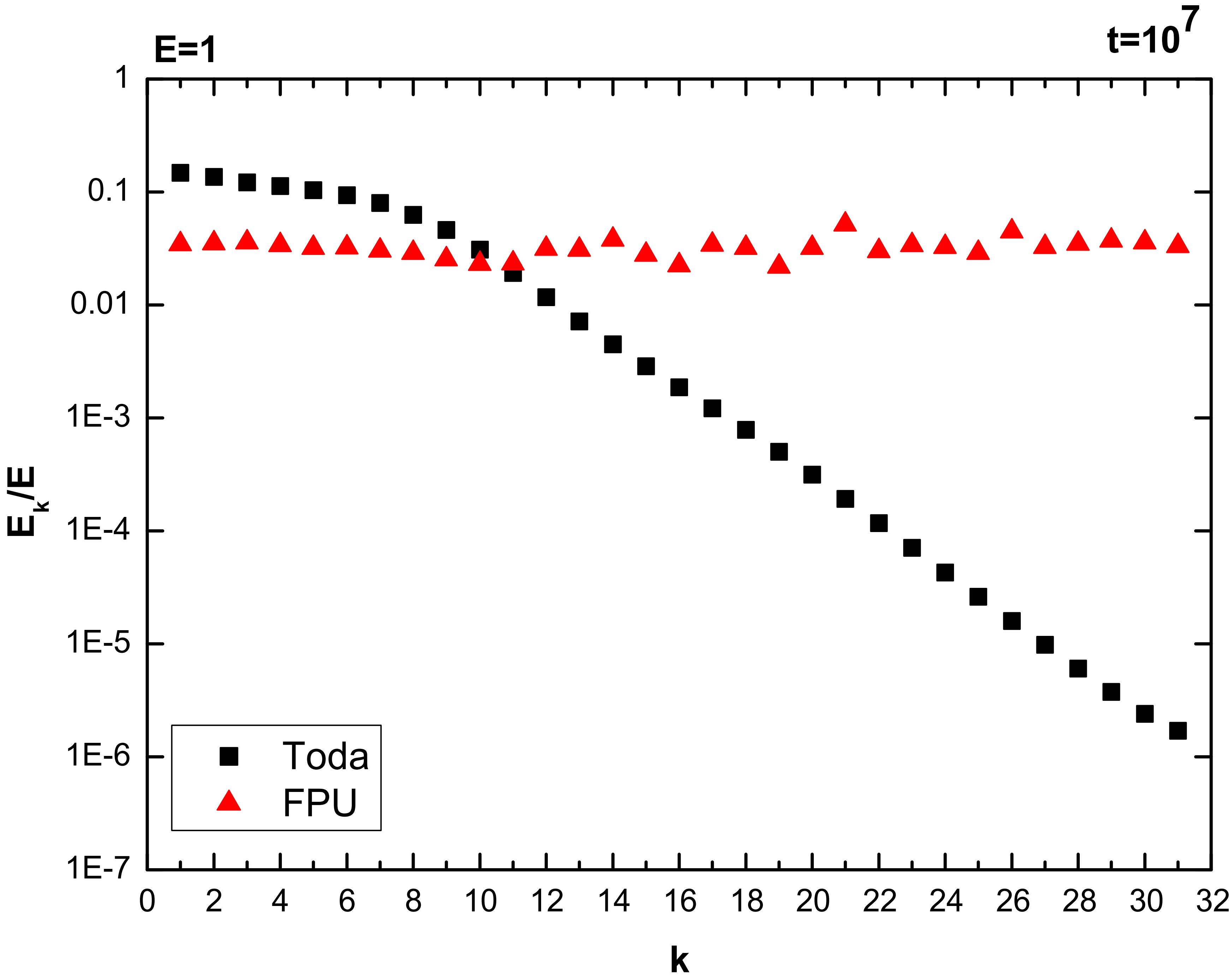
22
24
26
28
30
32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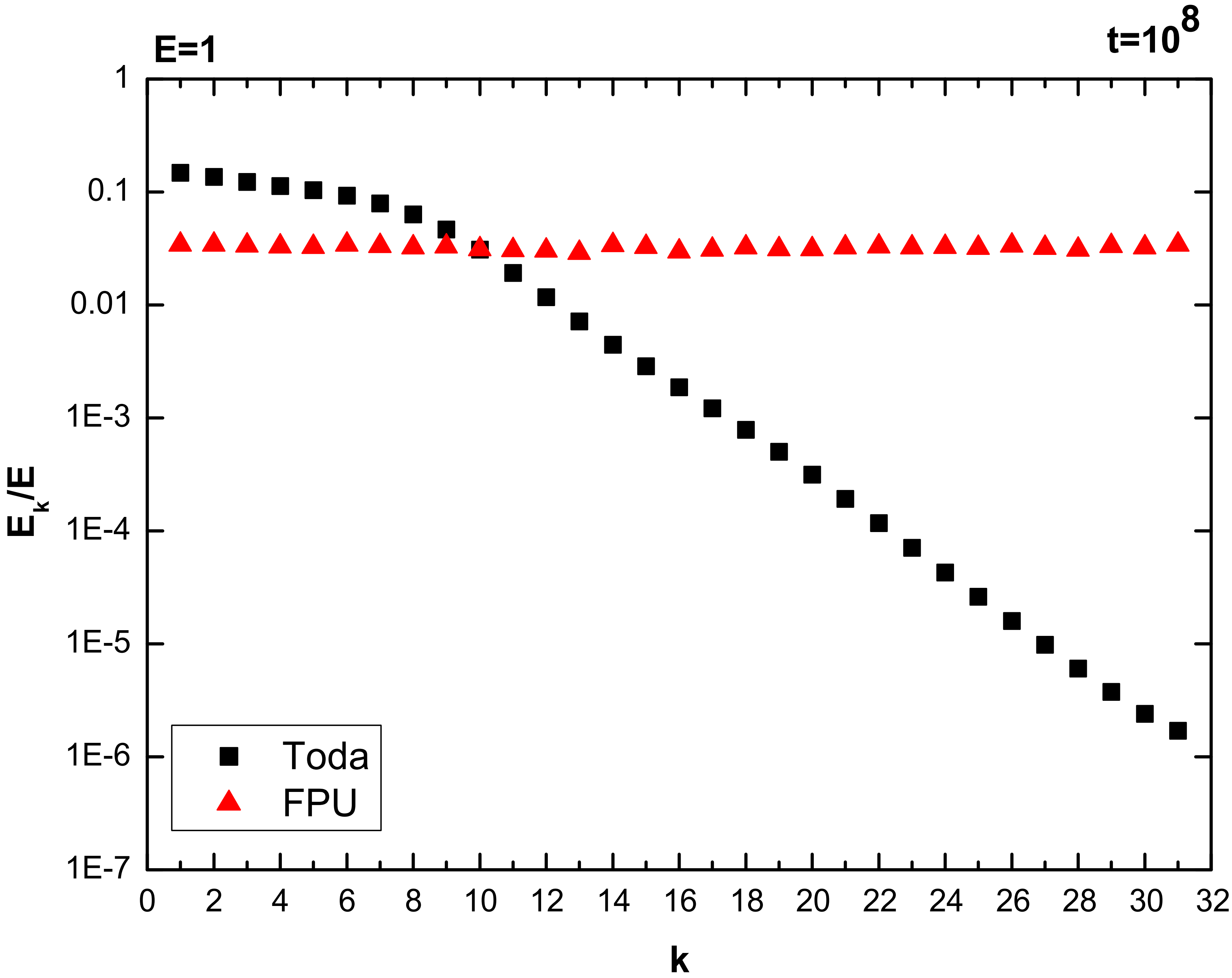
t=10^7
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
Toda
FPU


E=1
t=10^8
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
Toda
FPU

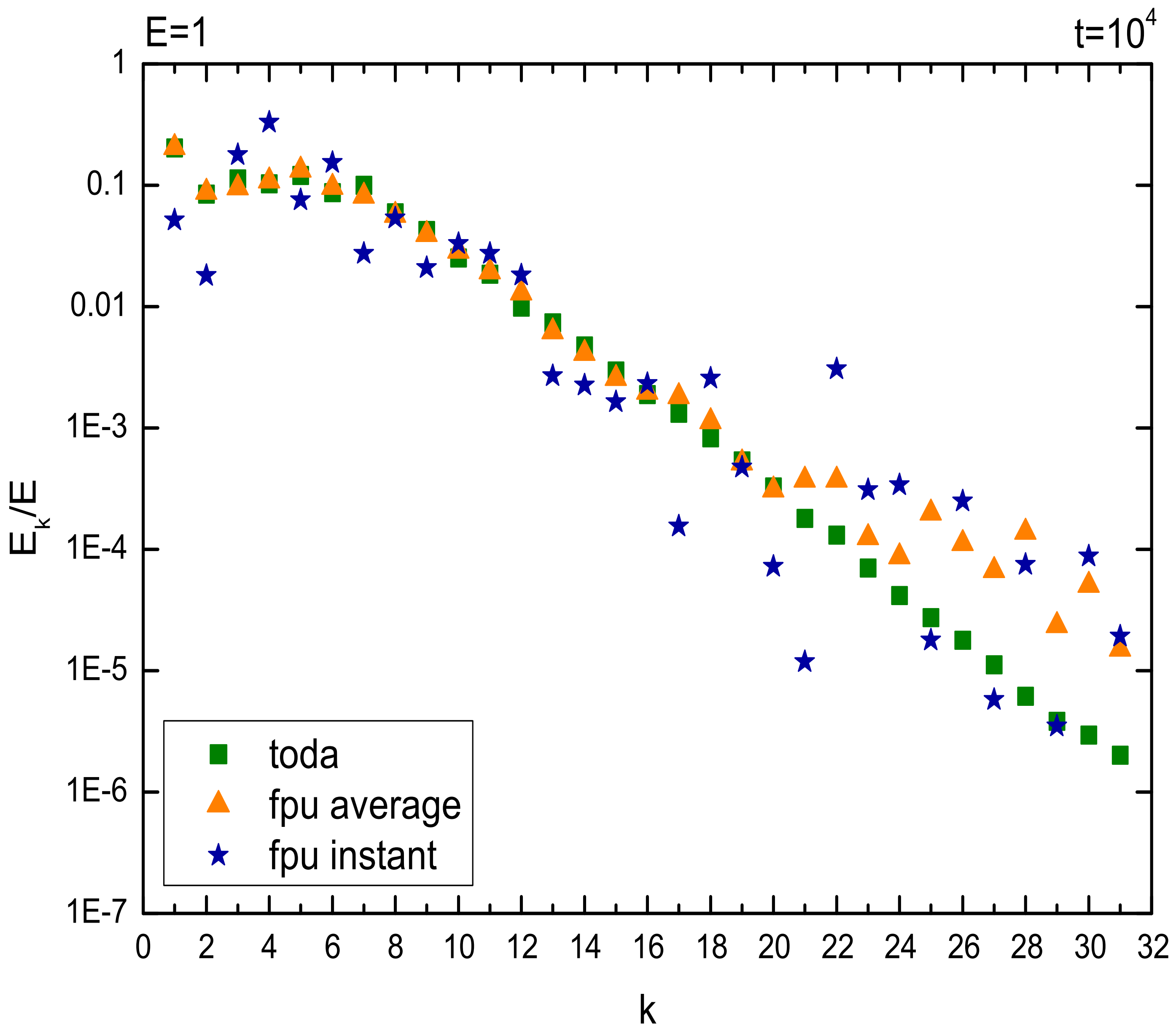
WHAT DO WE LEARN?

- FPU and Toda m.e.s. almost superposed up to the time ($t \approx 10^4$) Toda m.e.s. reaches equilibrium
- The equilibrium Toda m.e.s. is exponentially localized
- FPU m.e.s. detaches from the Toda one by a slow raising of tail (high) modes, reaching equipartition at $t \approx 10^8$
- Candidate quasi-state: Toda equilibrium

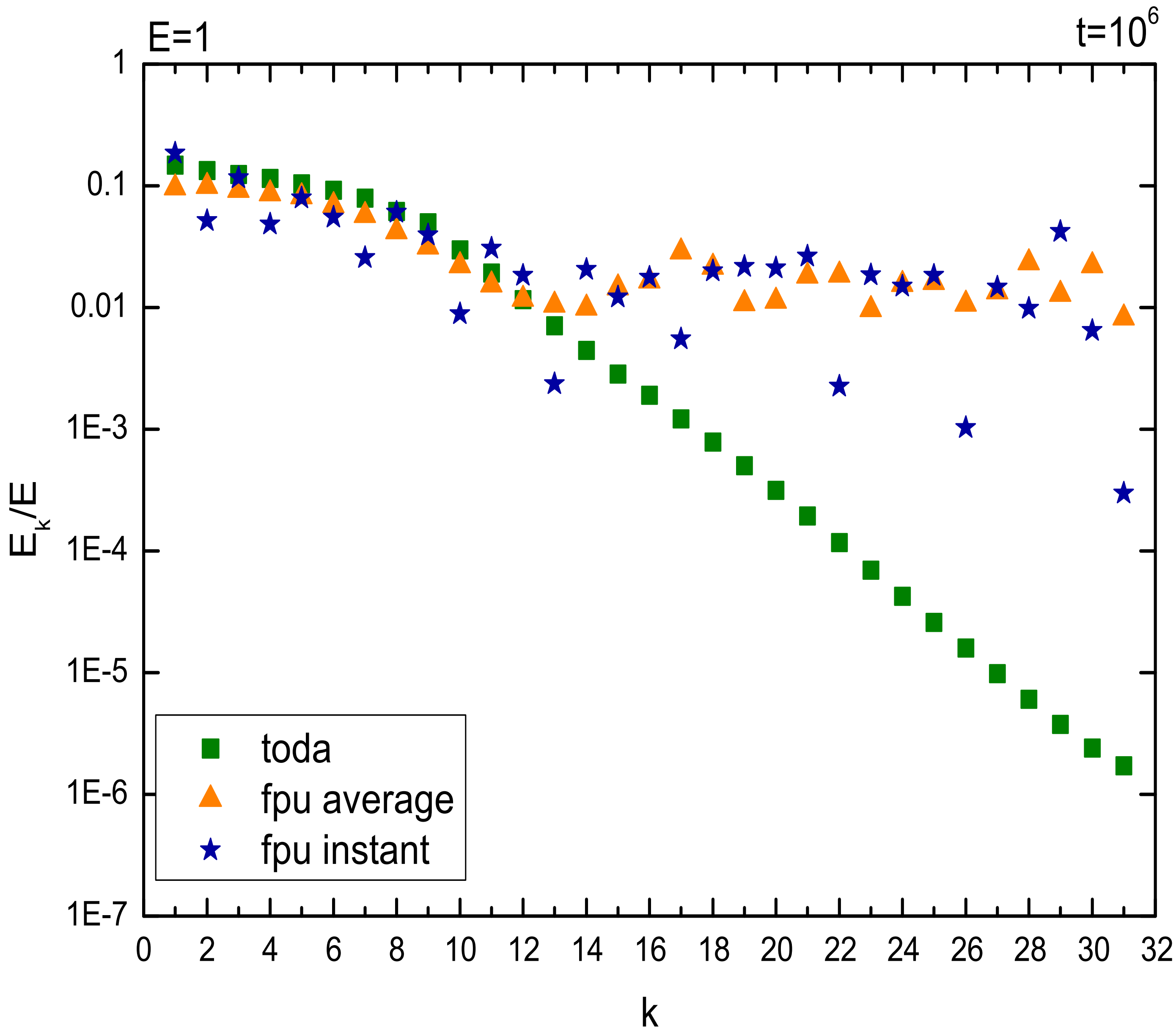
REMARKS

1. FPU typical choice was $A = 1$, i.e. $E \simeq 0.08$, with α ranging from 0.25 to 1; this can be shown to be equivalent for us to an energy ranging from $E = 0.045$ to $E = 0.72$
2. But their maximum computation time was order 10^4 to at most 10^5...!
3. To explain the FPU paradox it is necessary to see what happens at lower energies

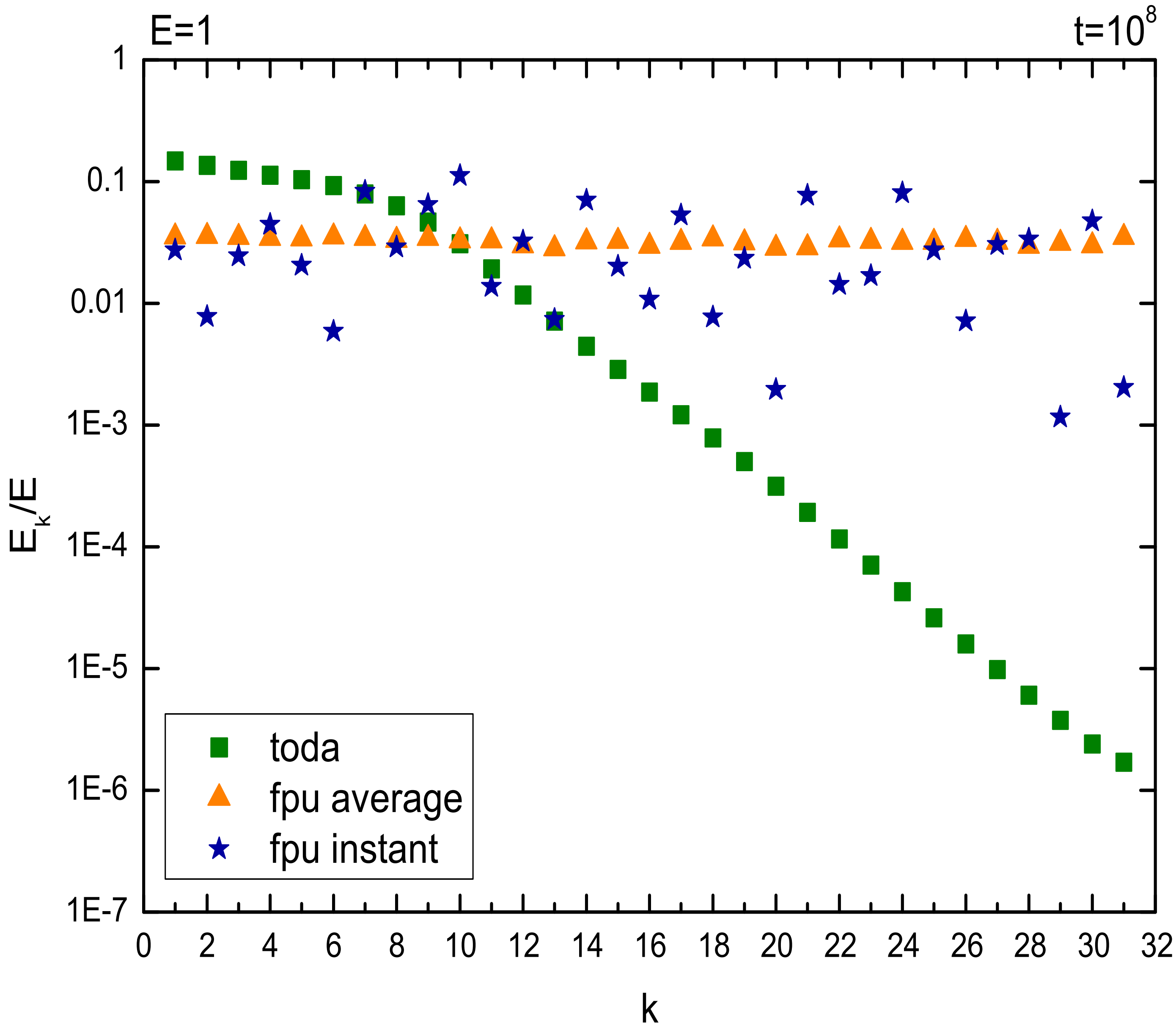
For each vale of the energy $E = 1$, $E = 0.1$, $E = 0.01$
a sequence of three snapshots of m.e.s.,
at $t = 10^4$, $t = 10^6$ and $t = 10^8$



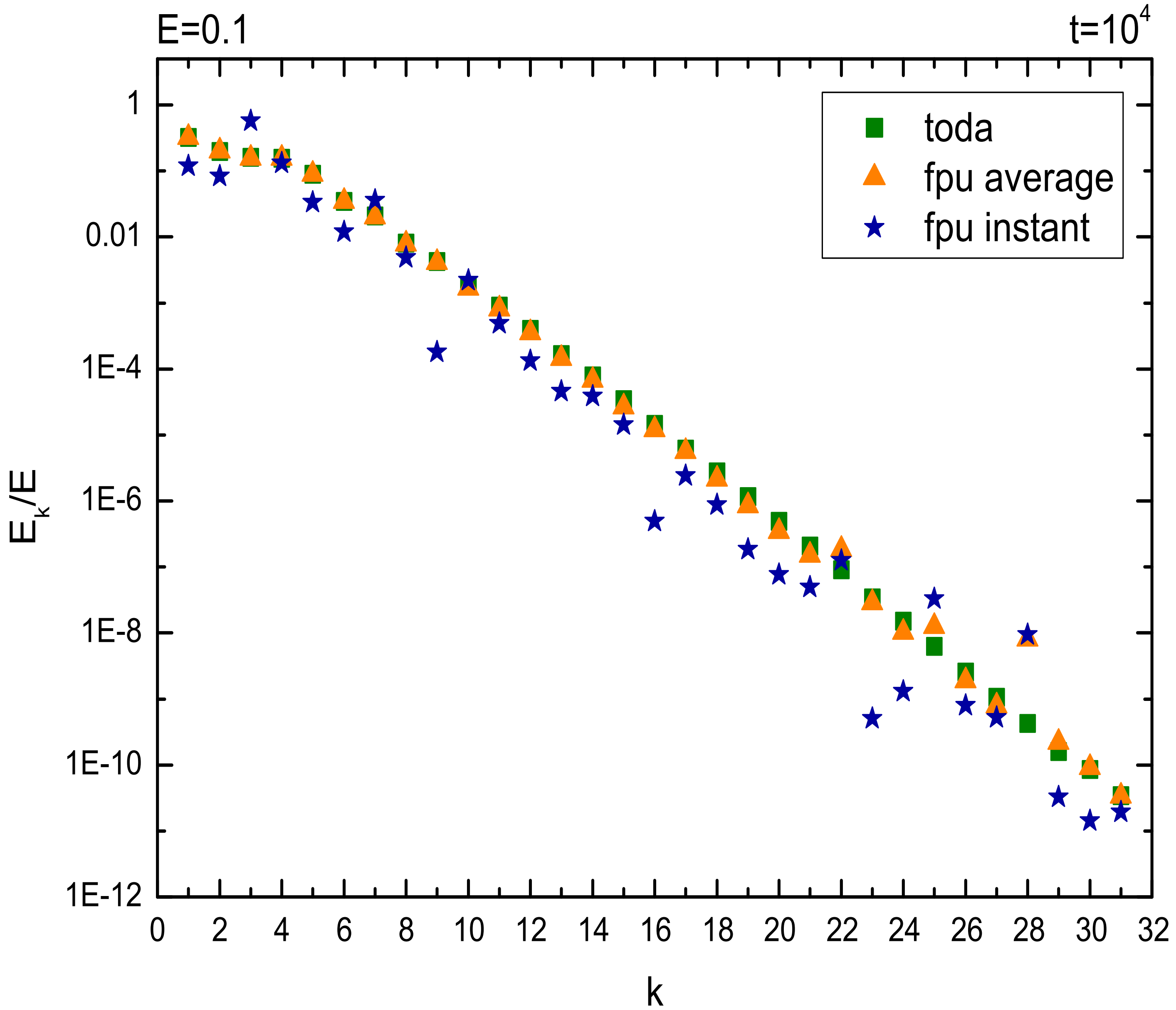
E=1
t=10^4
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
toda
fpu average
fpu instant



E=1
t=10^6
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
toda
fpu average
fpu instant



E=1
t=10^8
1
0.1
0.01
1E-3
1E-4
1E-5
1E-6
1E-7
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k
toda
fpu average
fpu instant


E=0.1
t=10^4
toda
fpu average
fpu instant
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
E_k/E
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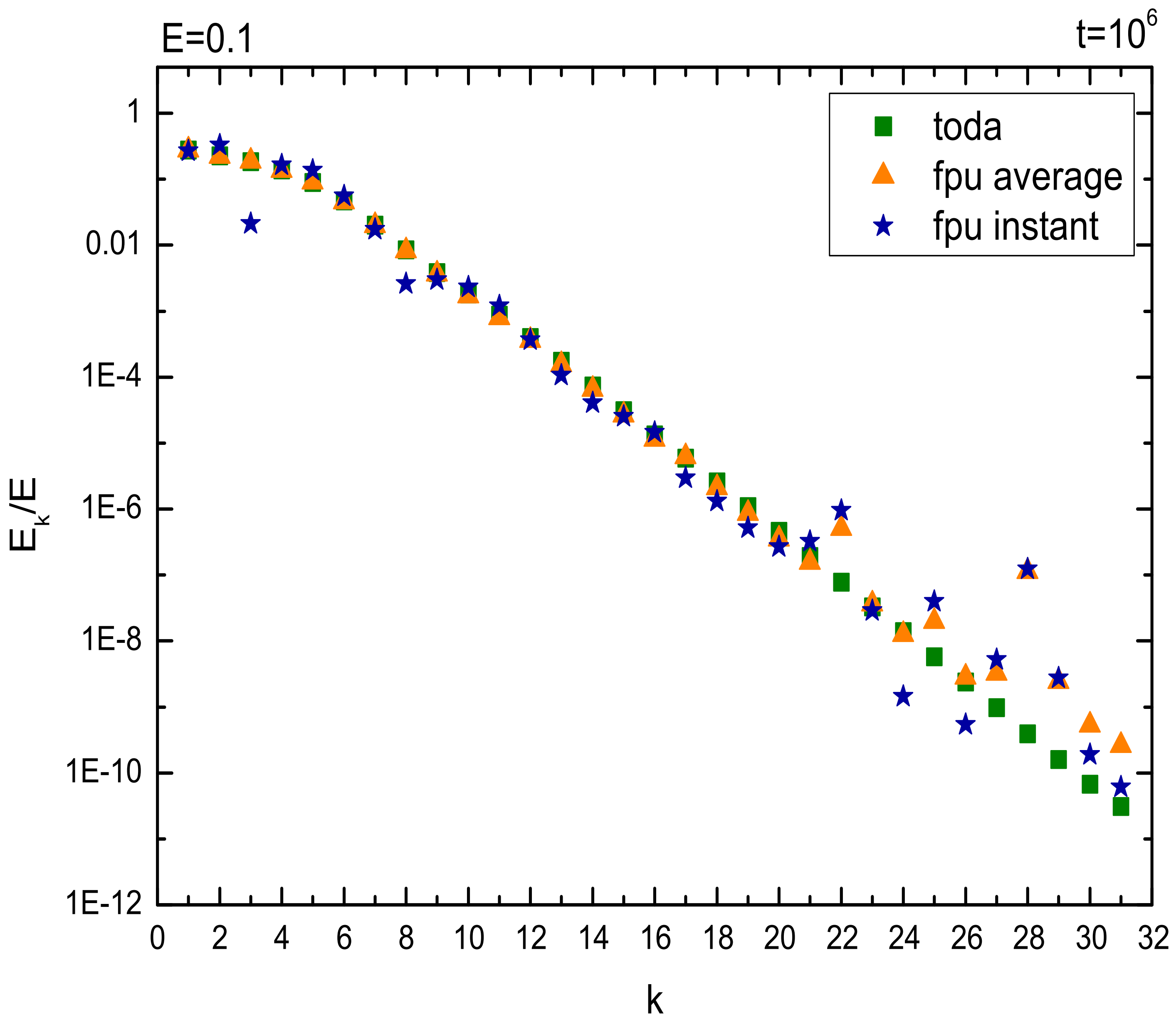
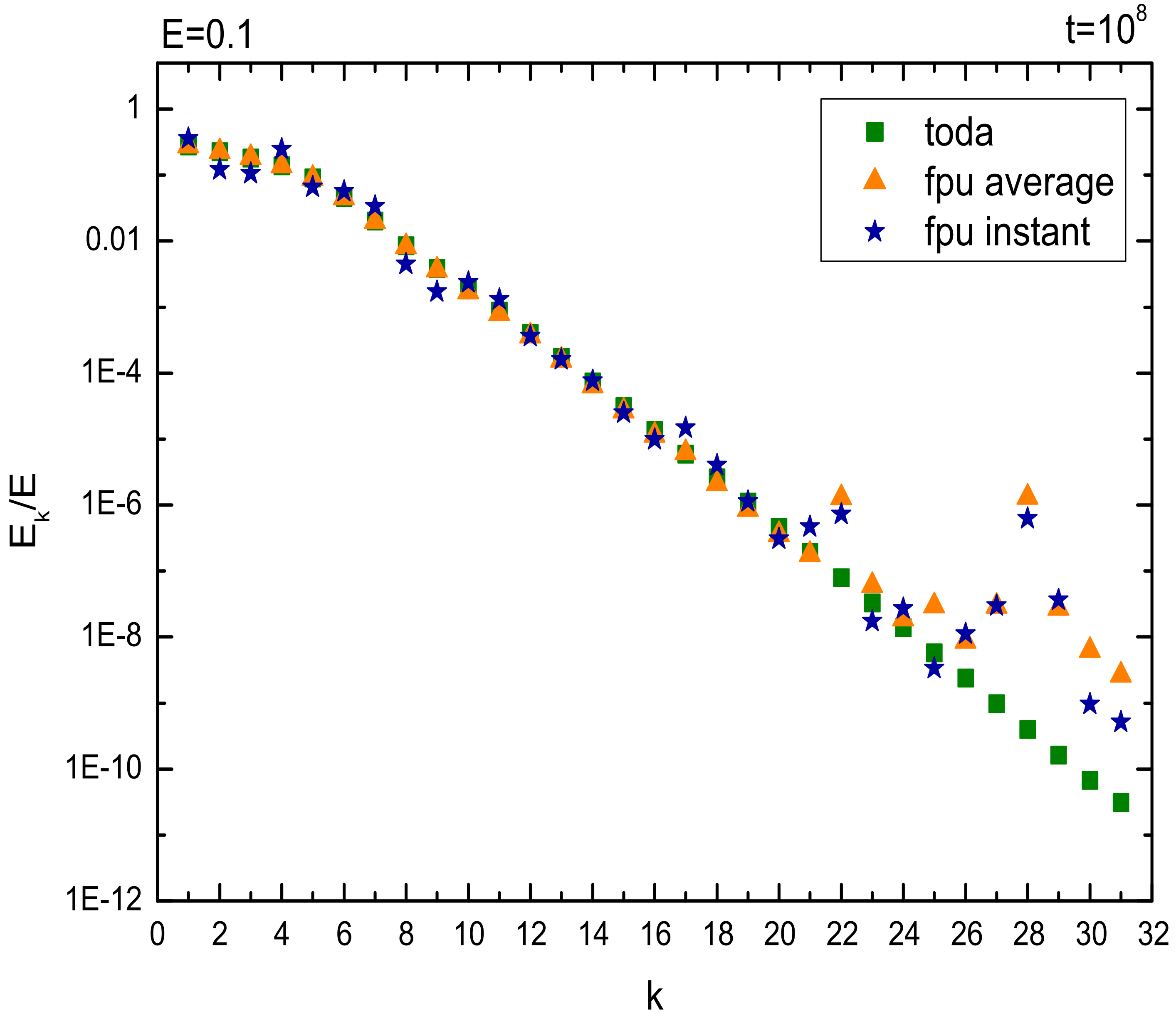
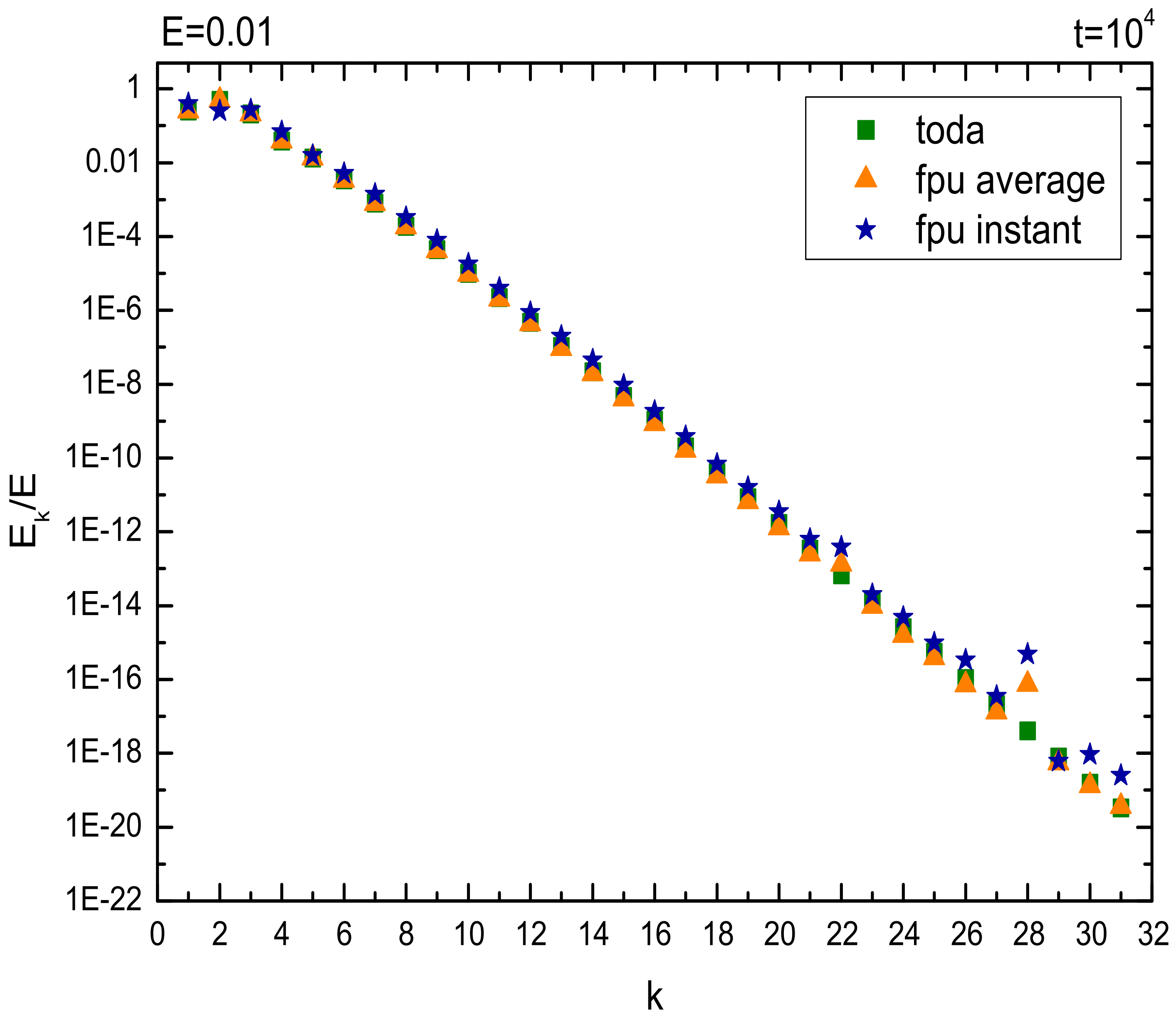
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k



E=0.1
t=10^6
toda
fpu average
fpu instant
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
E_k/E
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32
k


E=0.1
t=10^8
toda
fpu average
fpu instant
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k



E=0.01
t=10^4
toda
fpu average
fpu instant
E_k/E
k
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
1E-14
1E-16
1E-18
1E-20
1E-22
0
2
4
6
8
10
12
14
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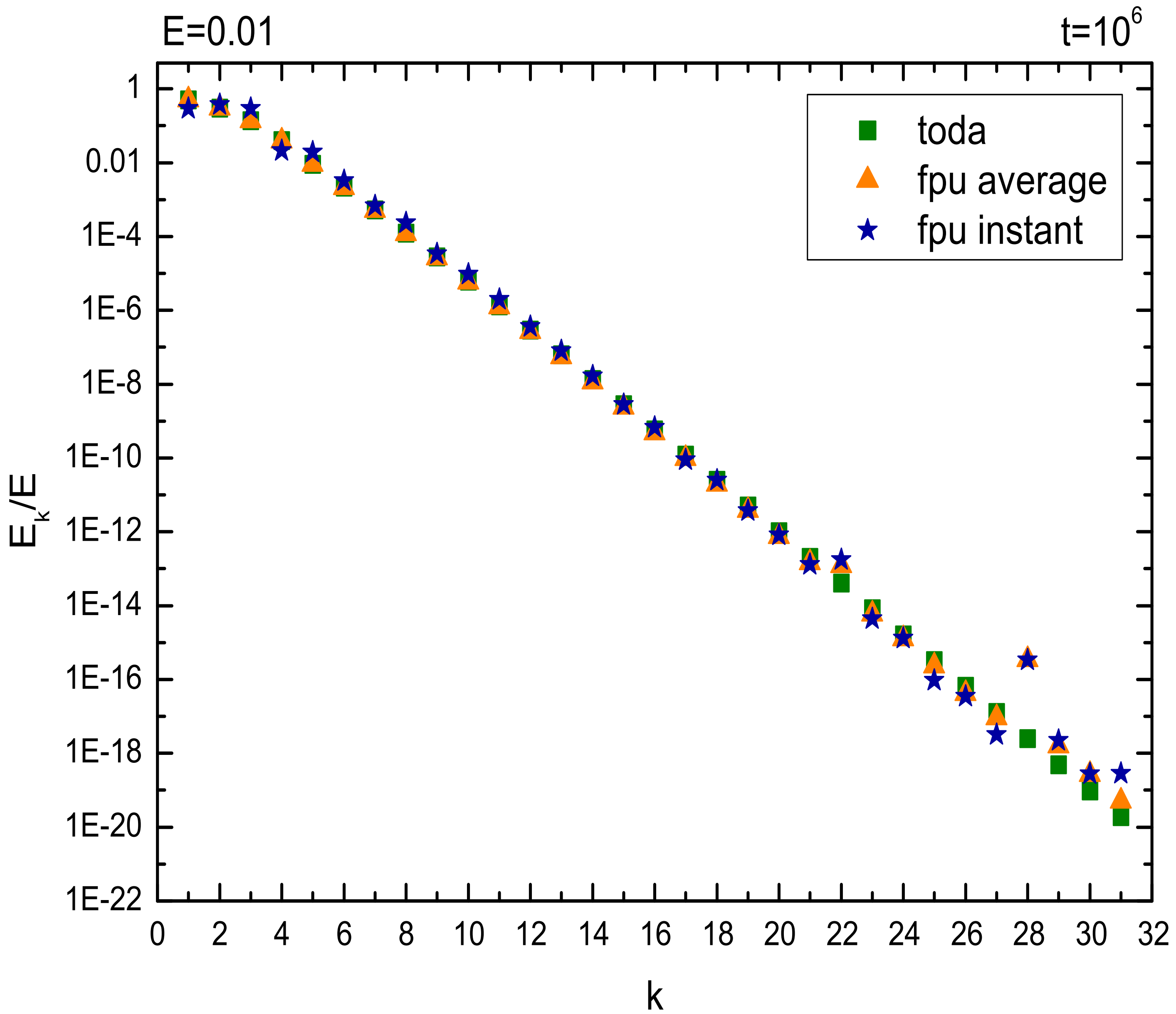
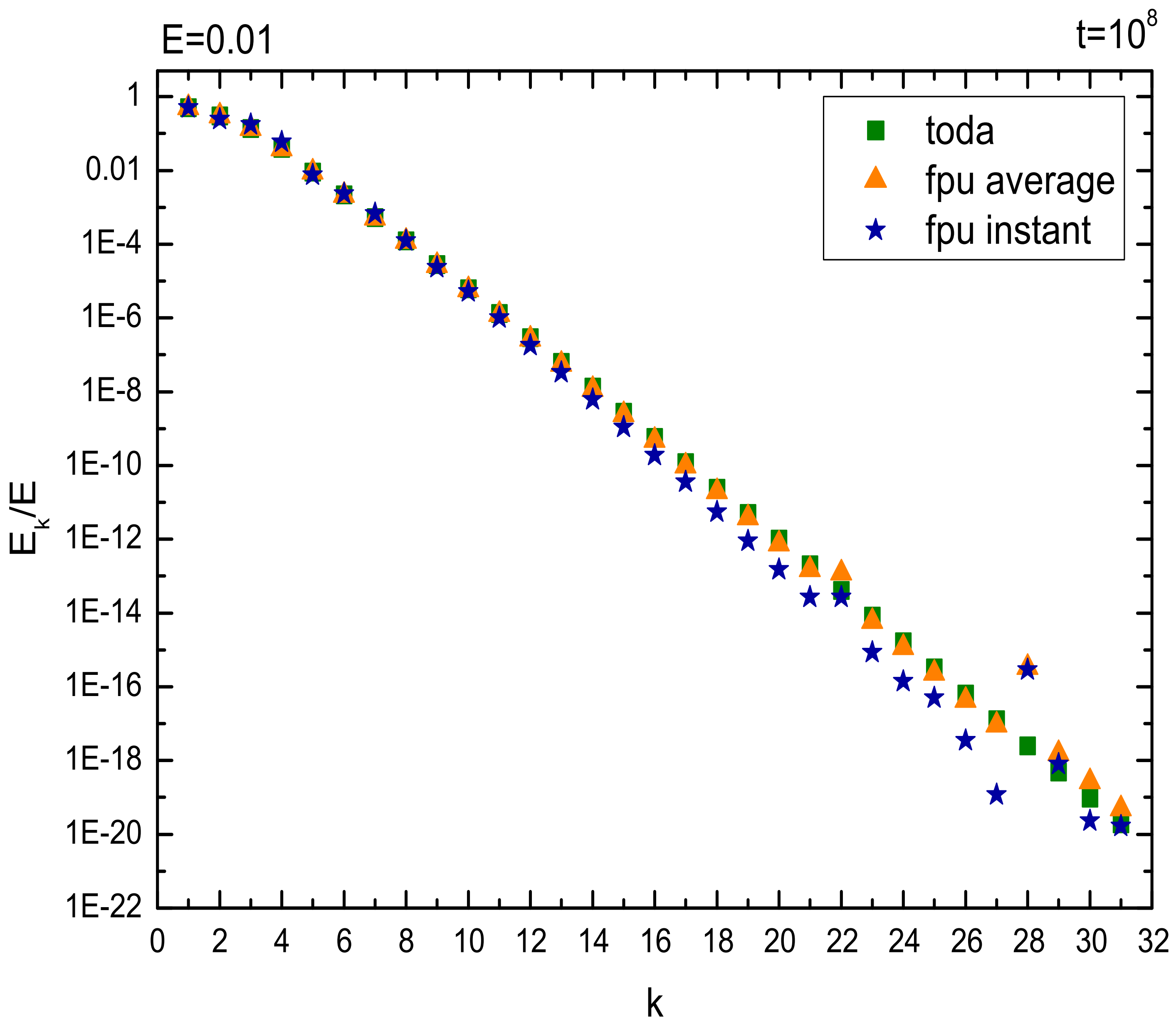
18
20
22
24
26
28
30
32


E=0.01
t=10^6
toda
fpu average
fpu instant
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
1E-14
1E-16
1E-18
1E-20
1E-22
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k



E=0.01
t=10^8
toda
fpu average
fpu instant
1
0.01
1E-4
1E-6
1E-8
1E-10
1E-12
1E-14
1E-16
1E-18
1E-20
1E-22
E_k/E
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k

A first list of conclusions

1. The FPU quasi-state is the Toda equilibrium state:
   a signature of closeness to integrability
2. The FPU paradox appears when the FPU time-scale to equipartition is
   1. much longer than the Toda equilibration time-scale
   2. longer than the (present & personal) computational time limit
3. One has to understand the raising of FPU m.e.s. tail
4. Necessary to invent a way of estimating the time-scale to equipartition when it is too long to be actually measured

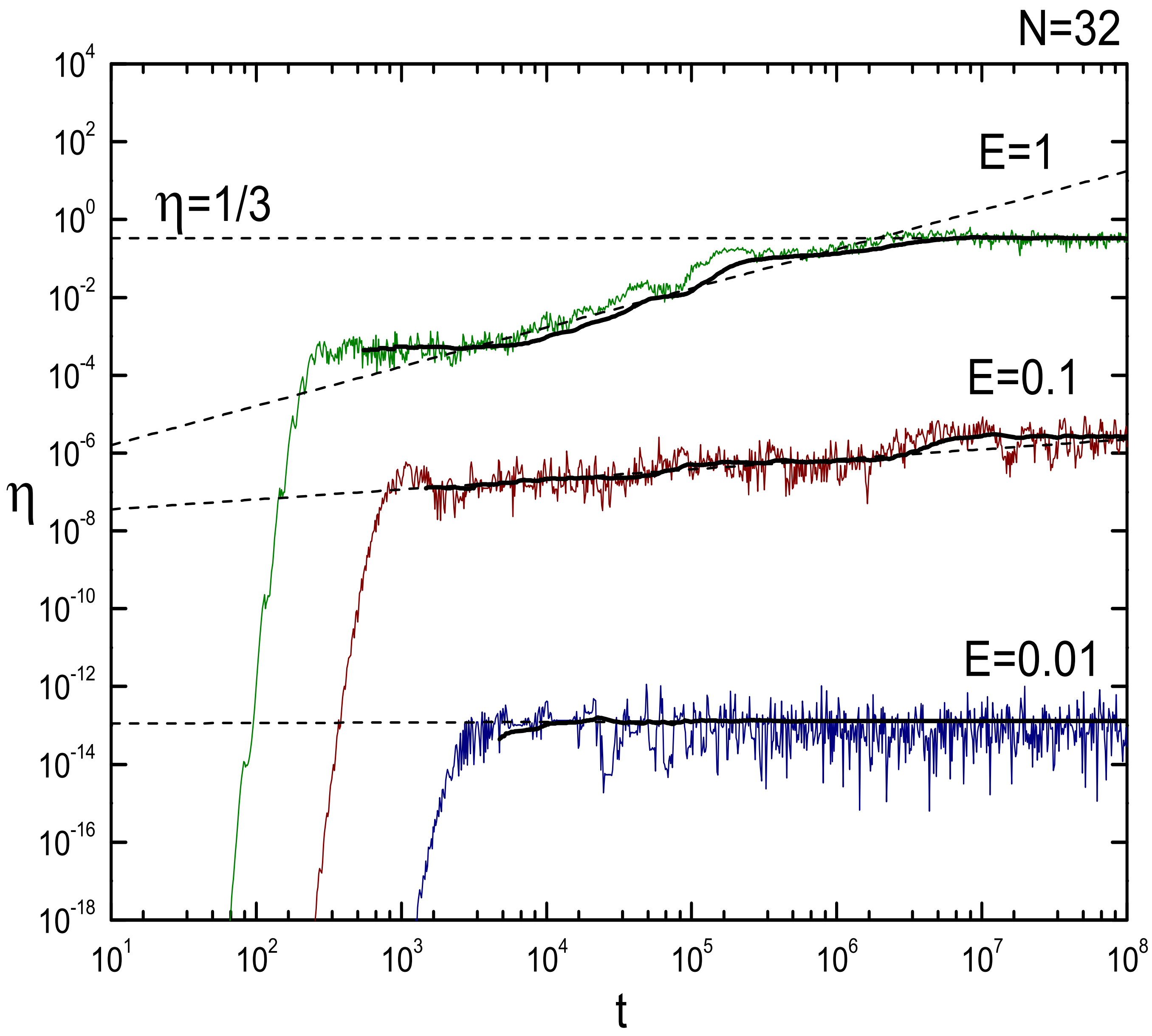
Diffusion of tail modes

- Numerical outcome: the way to equipartition in FPU is characterized by a diffusive growth of the tail modes:

$$\boxed{\eta(t) \equiv \frac{\sum_{k=22}^{31} E_k(t)}{E} \sim D\ t^{\gamma}}$$

- Both D and γ depend on E (and N)
- $\overline{\eta} \rightarrow 1/3$ approaching equipartition
- The process defines a time-scale to equipartition

$$\boxed{T^{eq} = (3D)^{-1/\gamma}}$$



N=32
E=1
E=0.1
E=0.01
η=1/3
η
t
10^4
10^2
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-14
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10^-18
10^1
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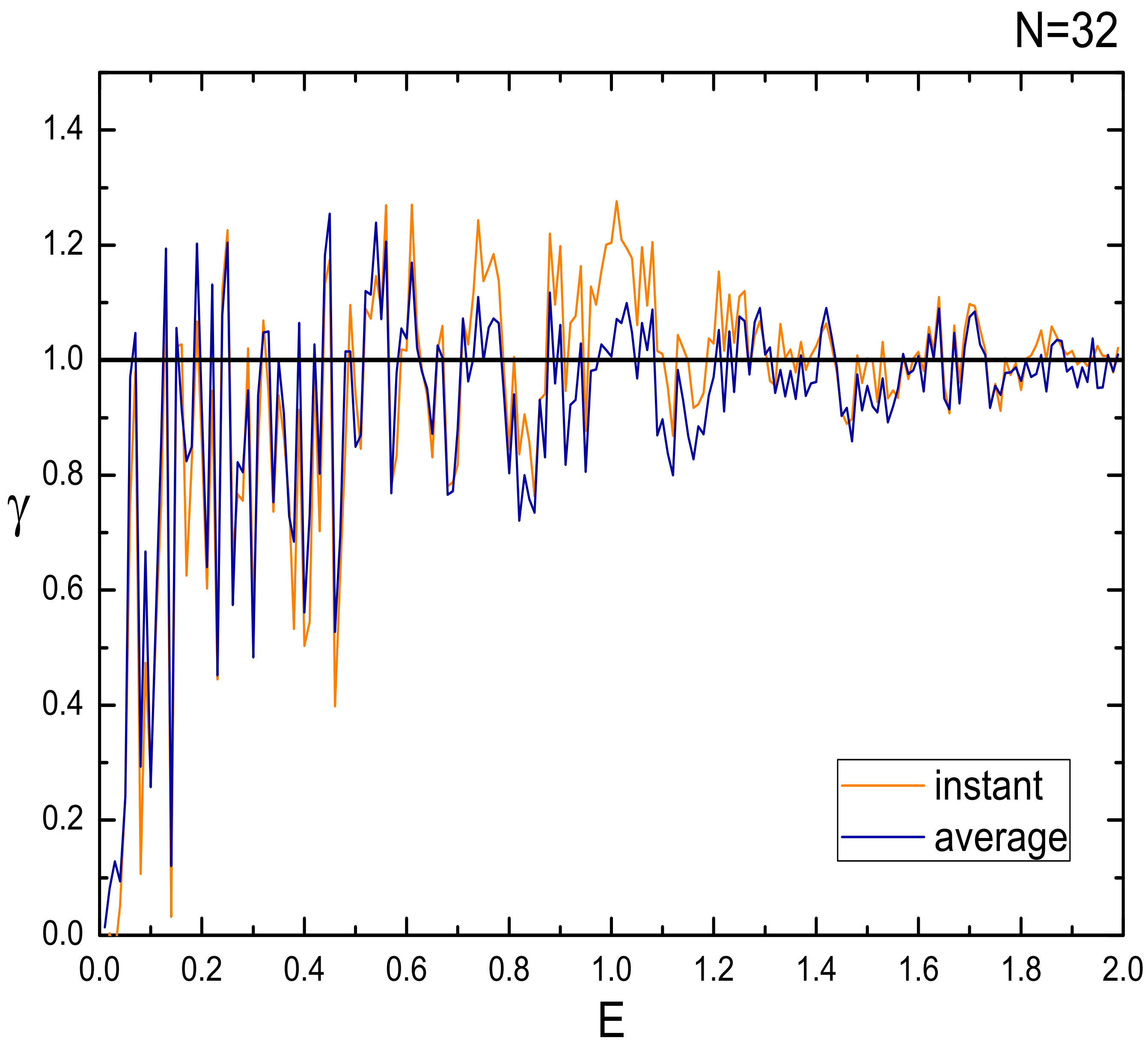
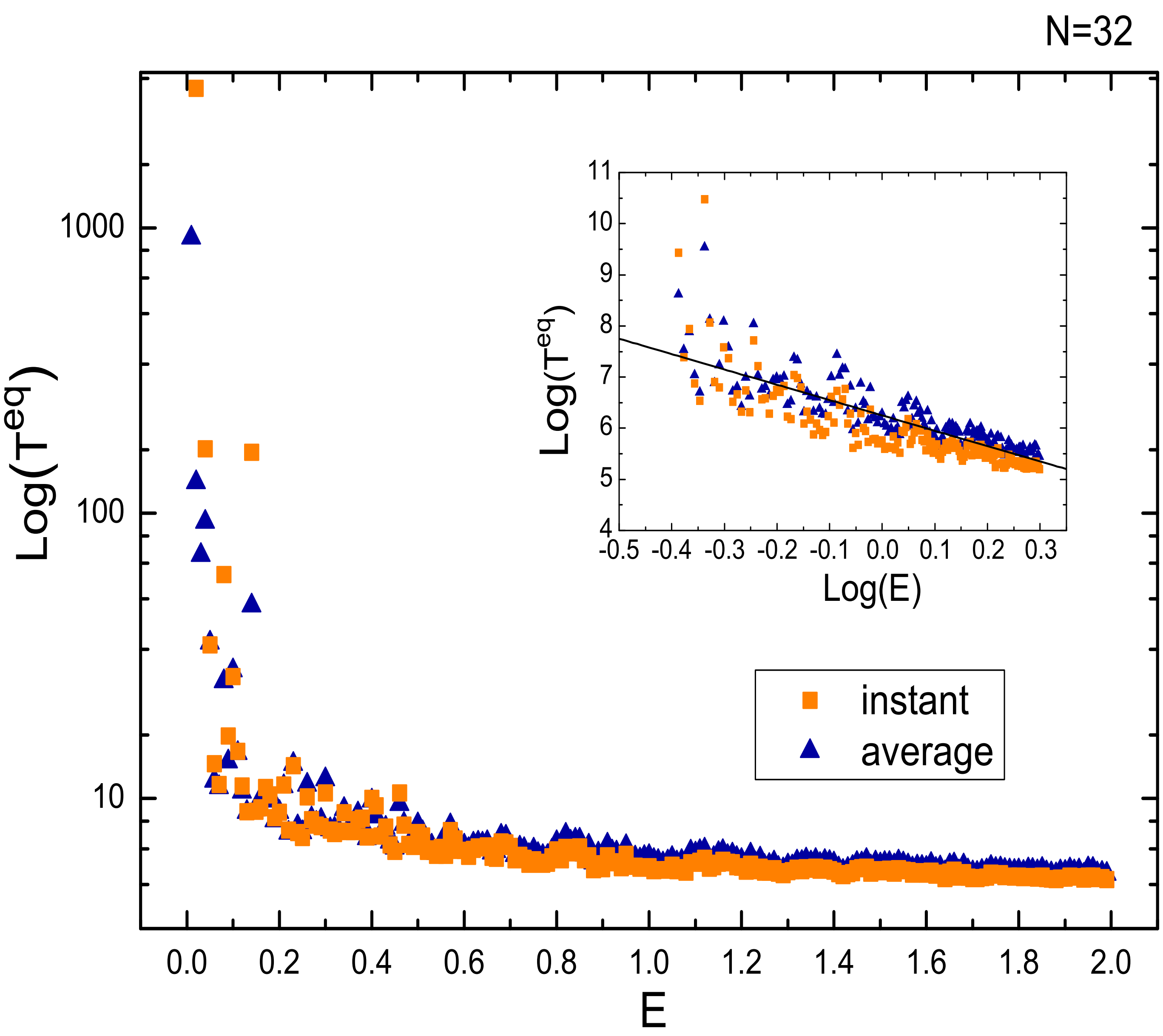
10^3
10^4
10^5
10^6
10^7
10^8



N=32
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
γ
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
E
instant
average


N=32
Log(T^eq)
1000
100
10
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
E
instant
average
Log(T^eq)
11
10
9
8
7
6
5
4
-0.5
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
Log(E)

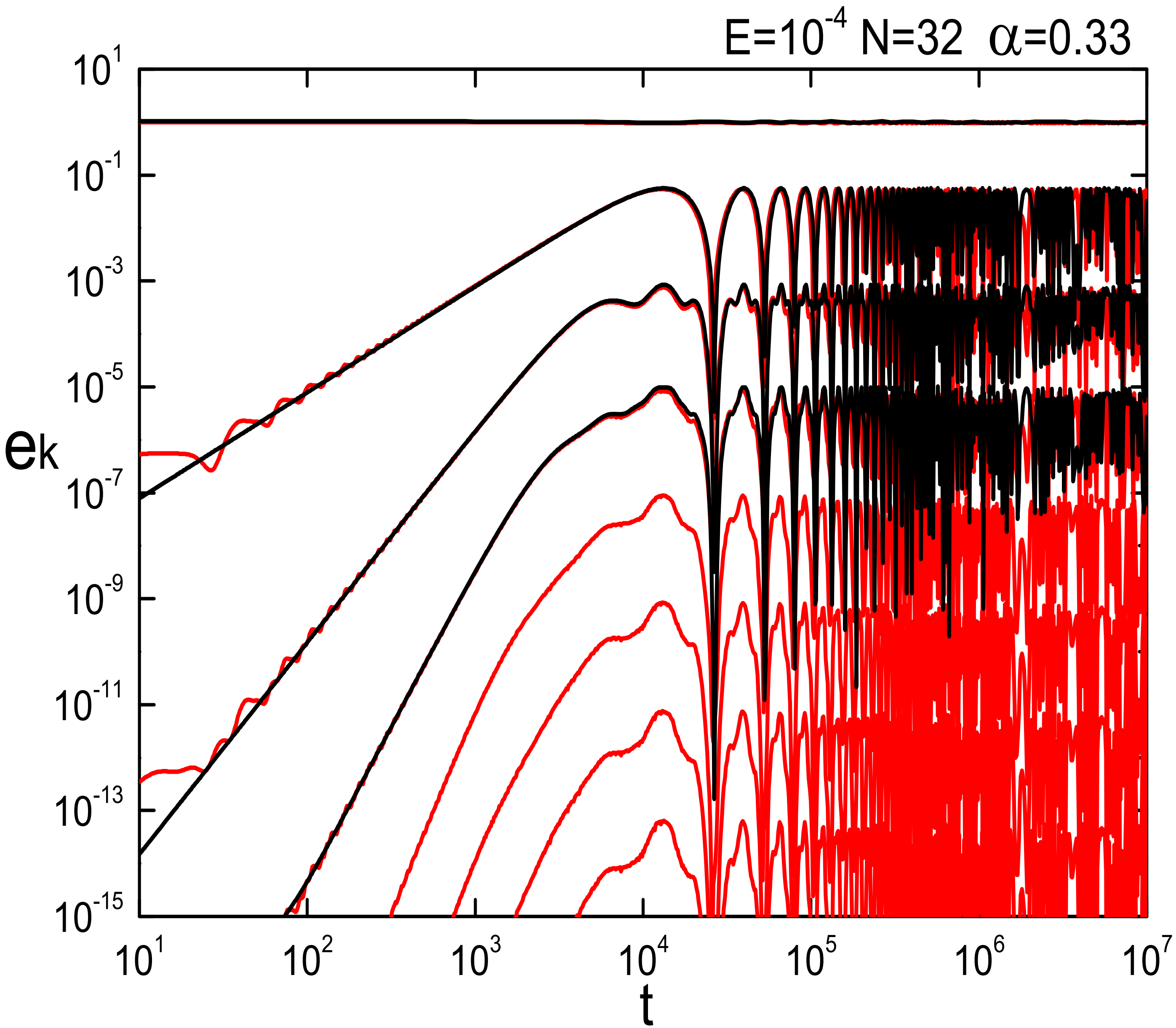
Another list of conclusions

- $T^{eq} \sim E^{-3}$ in the high energy range $0.4 < E < 2$
- Maybe one enters a Nekhoroshev-like stability regime at low energy ($E < 0.1$?)
- N-dependence of T^{eq} is a nontrivial problem
- The anomalously diffusive growth of tail modes has, at present, no analytic explanation

On the analytic side

Tool: resonant normal form Hamiltonian

- Approximate explicit solution of the Cauchy problem valid for very low energy: $E < 10^{-3}$

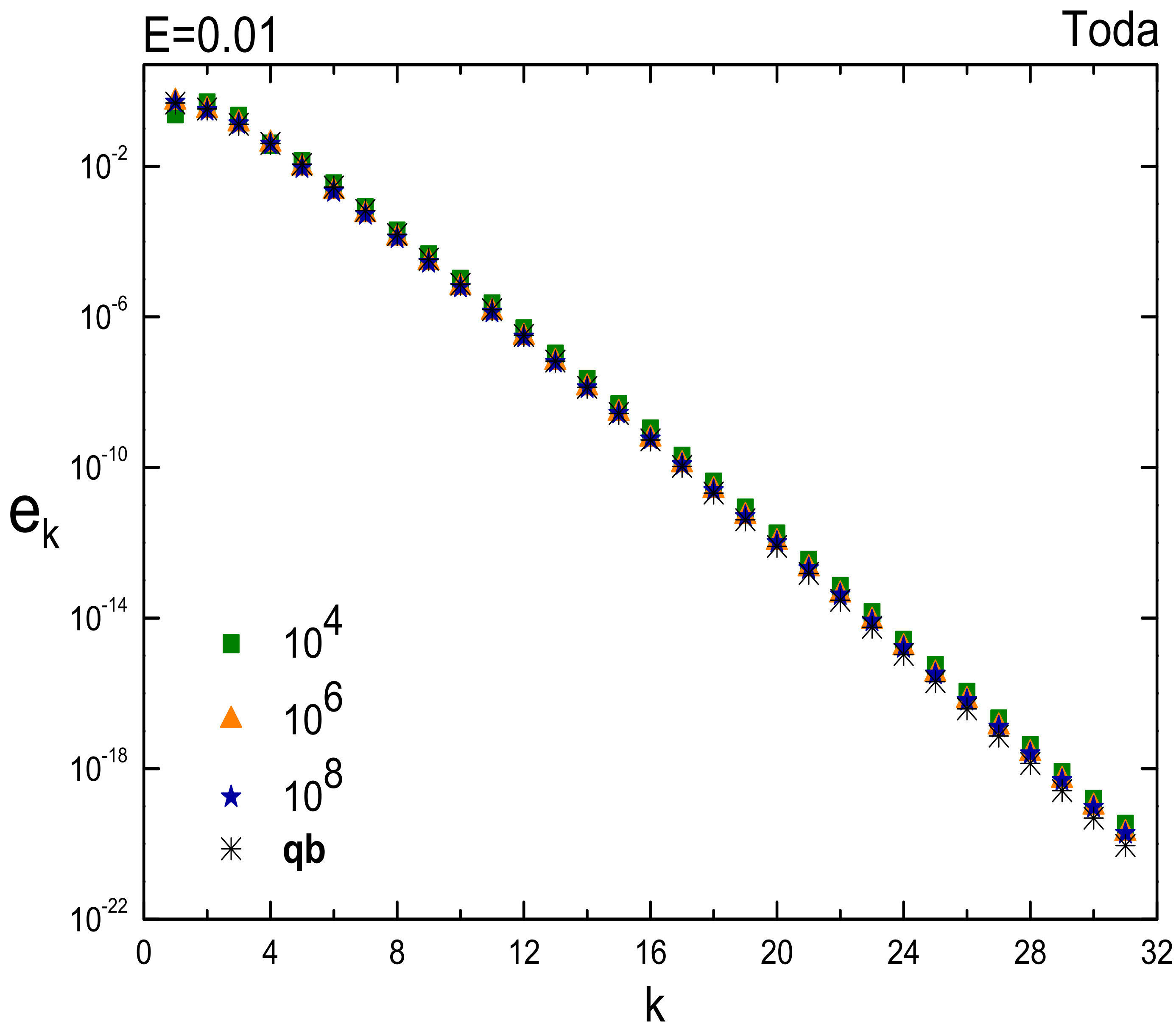


E=10^-4 N=32 α=0.33
e_k
t
10^1
10^-1
10^-3
10^-5
10^-7
10^-9
10^-11
10^-13
10^-15
10^1
10^2
10^3
10^4
10^5
10^6
10^7

On the analytic side

Tool: resonant normal form Hamiltonian

- Approximate explicit solution of the Cauchy problem valid for very low energy: $E < 10^{-3}$
- The fixed point of the normal form equations is a q-breather (Lyapunov continuation of mode 1): very good description of the quasi state up to $E = 0.1$



E=0.01
Toda
e_k
k
10^{-2}
10^{-6}
10^{-10}
10^{-14}
10^{-18}
10^{-22}
0
4
8
12
16
20
24
28
32
10^4
10^6
10^8
qb

On the analytic side

Tool: resonant normal form Hamiltonian

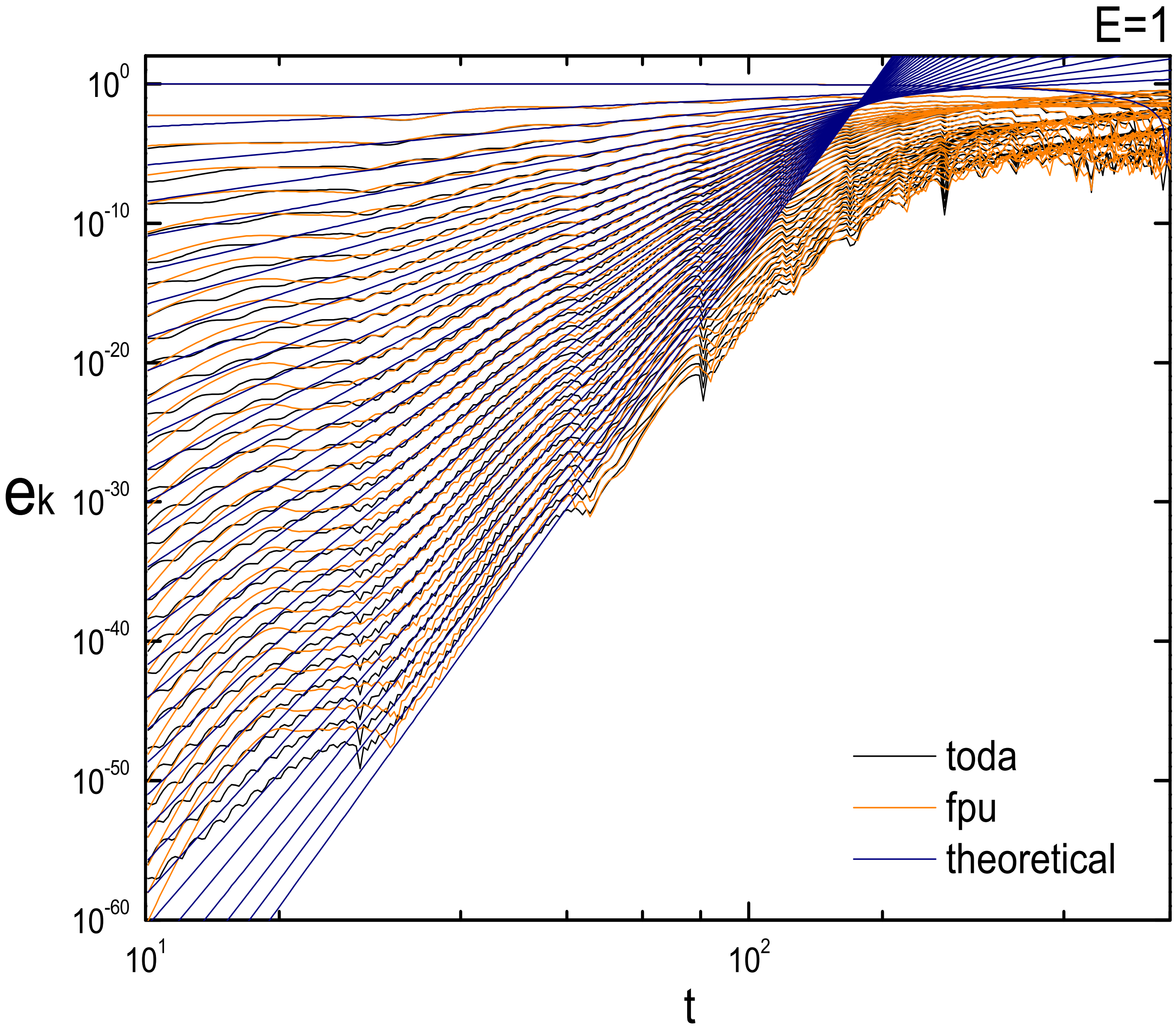
- Approximate explicit solution of the Cauchy problem valid for very low energy: $E < 10^{-3}$
- The fixed point of the normal form equations is a q-breather (Lyapunov continuation of mode 1): very good description of the quasi state up to $E = 0.1$
- Secular avalanche ruling the energy cascade on very short times, valid all over the energy range explored

The very short term growth of modes follows the law:

$$\boxed{\frac{E_1(t)}{E} = 1 - c_1^2\ t^2} \qquad \boxed{\frac{E_k(t)}{E} = c_k^2\ t^{2(k-1)} \quad k \geq 2}$$

The law is one and the same for FPU and Toda

Physical mechanism: RESONANCE $\boxed{\omega_k \simeq k\omega_1}$


E=1
e_k
10^{0}
10^{-10}
10^{-20}
10^{-30}
10^{-40}
10^{-50}
10^{-60}
10^{1}
10^{2}
t
toda
fpu
theoretical

Conclusions

1. The Toda and FPU short and intermediate term dynamics coincide and are rather well understood (possibility of improvement unbounded!)
2. In particular, the saturation to the quasi-state (Toda equilibrium) is integrable in character
3. The long term dynamics of the FPU system, on the road to equipartition, is nontrivial, essentially chaotic
4. Understanding the diffusive growth of tail modes is the next mandatory challenge