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Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics

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Energy transmission in oscillator chains with disorder

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Energy transmission in oscillator chains with disorder

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Introduction: disorder and nonlinearity

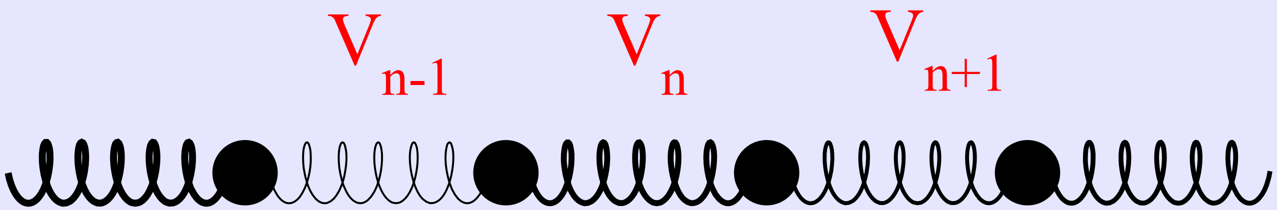
- Energy transport in coupled classical oscillators (mostly 1D)
- Linear disordered case (Anderson), discrete spectrum with exponentially localized eigenmodes: no diffusion!
- Nonlinear ordered case: generic localized periodic solutions (discrete breathers)
- Nonlinear *and* disordered, mode interactions: what effect on diffusion, transport etc.?
- Applications: BEC, photonic lattices etc.

Models

Chain of N coupled oscillators with n.n. coupling ($m = 1$):

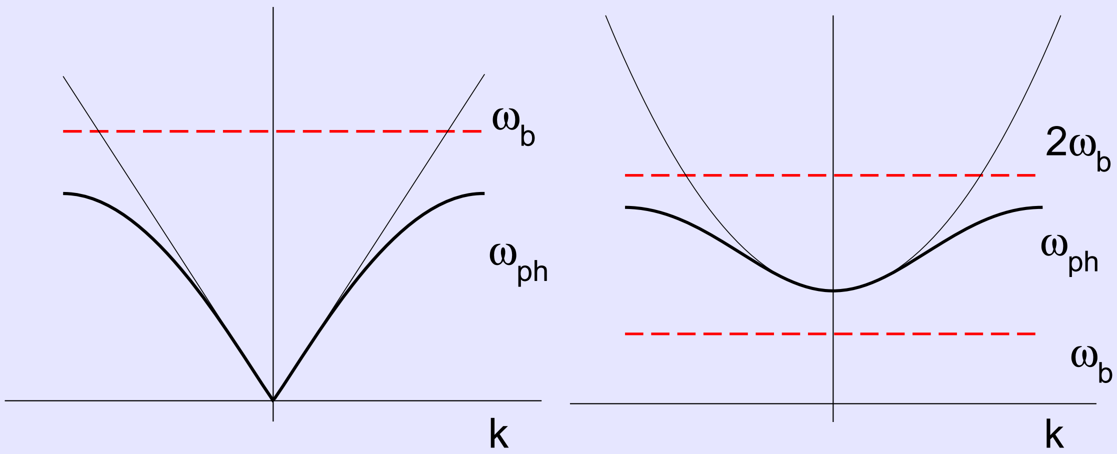
$$m\ddot{u}_n = -V'_n(u_n - u_{n-1}) + V'_{n+1}(u_{n+1} - u_n)$$

u_n displacement from eq. position, $L = Na$ chain length, $V_n(x)$ nonlinear potential



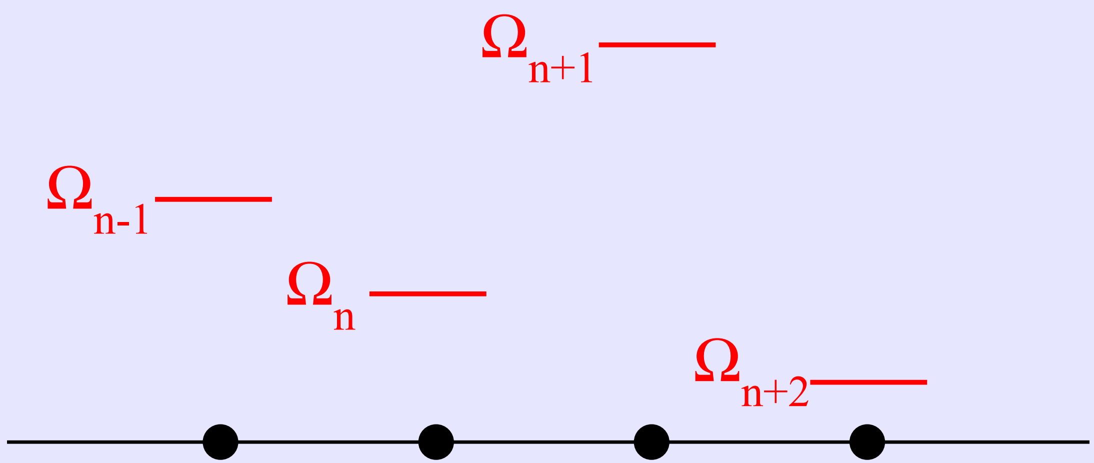
Nonlinear localization: discrete breathers

- Spatially localized, time-periodic
- Proved to exist under general condition
  [McKay and Aubry (1994)]
- Structural stability: one-parameter (e.g. ω_b) families



Linear localization: Anderson modes

- Quenched, uncorrelated disorder
- Spatially localized, time-periodic



Harmonic chain with bond disorder

Chain of N coupled oscillators with n.n. coupling:

$$\ddot{u}_n = K_n(u_{n+1} - u_n) - K_{n-1}(u_n - u_{n-1})$$

$K_0, K_1 \dots K_N$, i.i.d. positive random couplings, with given probability:

$$P(K) = \begin{cases} \frac{1}{k(R-1)} & \text{if } k \le K \le Rk, \\ 0 & \text{otherwise.} \end{cases}$$

($k = 1$ henceforth)

Anderson localization

- Integrated density of states: for $\omega \to 0$

$$I(\omega) = \frac{\sqrt{\langle K^{-1} \rangle}}{\pi}$$

- Localization length of eigenvectors $Q_n^{(\nu)}$:

$$\xi^{-1} = \frac{\langle K^{-2} \rangle - \langle K^{-1} \rangle^2}{8\langle K^{-1} \rangle}\,\omega^2$$

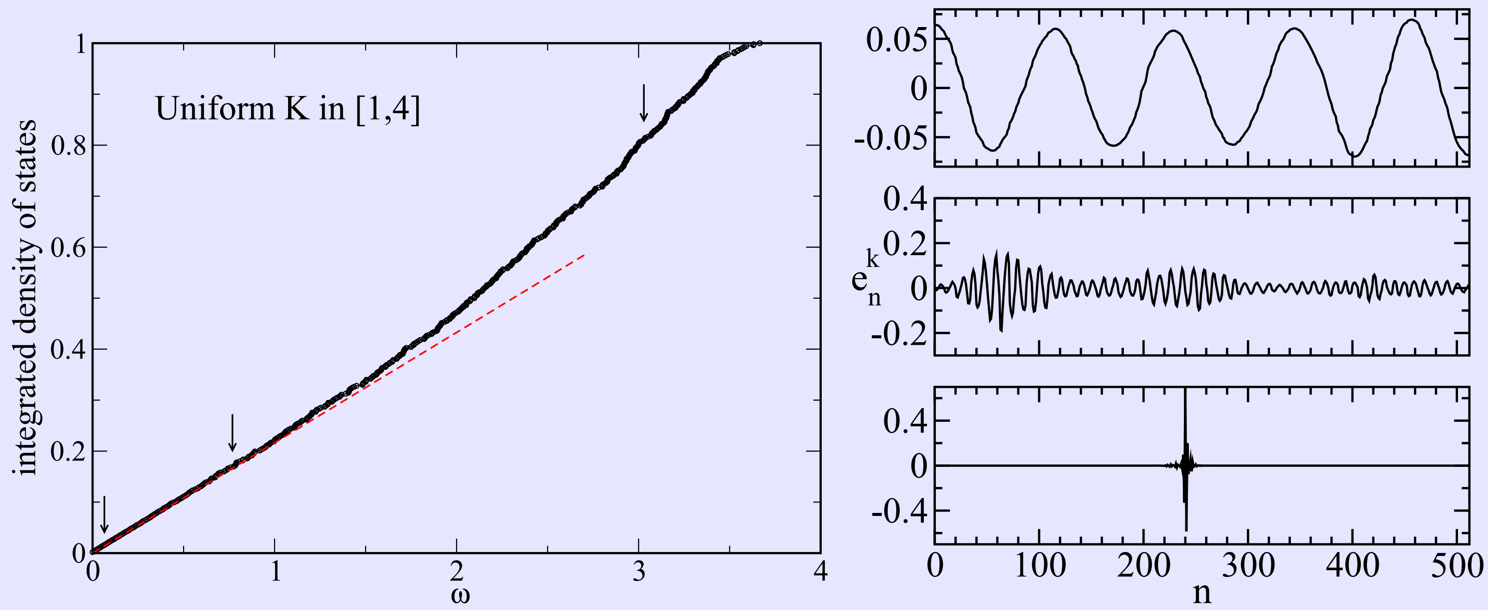
- Acoustic modes exist

$$c \; = \; \sqrt{\frac{\langle K^{-1} \rangle^{-1}}{m}}$$

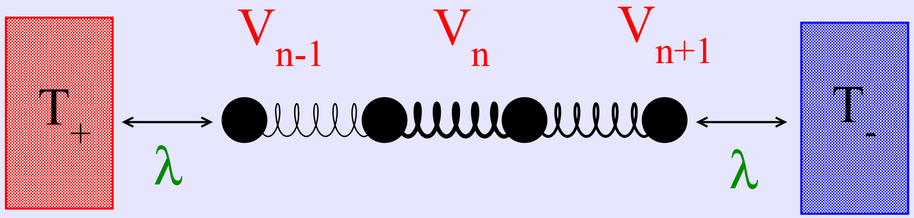
- In a finite chain: almost extended eigenvectors for

$$\omega \; < \; \omega_L \; \equiv \; \sqrt{\frac{8\langle K^{-1} \rangle}{N(\langle K^{-2} \rangle - \langle K^{-1} \rangle^2)}}$$

Anderson localization



Conseguences on thermal transport



Only the first $\mathcal{O}(\sqrt{N})$ modes such that $1/\xi > N$ contribute to the heat current, the conductivity depends on boundary conditions:

- Free boundaries: $|Q_1^k|^2 \sim |Q_N^k|^2 \sim 1/N$

$$\kappa_{free} \propto \lambda \frac{\langle K^{-1} \rangle}{\sigma_{K^{-1}}} \sqrt{N} \qquad .$$

- Fixed boundaries: $|Q_1^k|^2 \sim |Q_N^k|^2 \sim k^2/N^3$

$$\kappa_{fix} \propto \lambda \left(\frac{\langle K^{-1} \rangle}{\sigma_{K^{-1}}} \right)^3 \frac{1}{\sqrt{N}} \qquad .$$

Evolution of a wavepacket: analytics (1)

- Single site *displacement excitation*

$$u_n(t=0) \ = \ u_0\delta_{n,n_0}, \quad \dot{u}_n(t=0) \ = \ 0$$

- Time and disorder averaged kinetic energy profile

$$\overline{\langle e_n^{(\mathrm{kin})}(t)\rangle} = \frac{1}{4}\sum_{\nu=0}^{N-1}\langle\omega_\nu^2(Q_n^{(\nu)}Q_{n_0}^{(\nu)})^2\rangle =$$

$$\lim_{N\to\infty}\frac{N}{4}\int d\omega\,\omega^2 g(\omega)\langle(Q_nQ_{n_0})^2\rangle_\omega$$

g is the density of states

- Assume that $\omega \to 0$

$$\langle(Q_nQ_{n_0})^2\rangle_\omega \cong A(\omega)\exp[-|n-n_0|/\xi_2(\omega)], \qquad \xi_2(\omega) \cong c_2\omega^{-2}$$

(can be proven by TM approach)

- Then $A(\omega) \cong \omega^2/Nc_2$ (from normalization)

Evolution of a wavepacket: analytics (2)

- Altogether:

$$\langle \overline{e_n^{(\mathrm{kin})}(t)} \rangle \propto \int d\omega\, \omega^4 g(\omega) \exp[-\frac{\omega^2}{c_2}|n-n_0|]$$

- Since $g(\omega) \approx const.$, $\omega \to 0$

$$\langle \overline{e_n^{(\mathrm{kin})}(t)} \rangle \sim |n-n_0|^{-5/2}$$

- For the *momentum excitation* (ω^2 instead of ω^4):

$$u_n(t=0) \;=\; 0, \qquad \dot{u}_n(t=0) \;=\; p_0 \delta_{n,n_0}$$

one finds instead $|n-n_0|^{-3/2}$

Evolution of a wavepacket: analytics (3)

Local energy

$$e_n \;=\; \frac{\dot{u}_n^2}{2} + \frac{1}{2}\left[V_{n+1}(u_{n+1} - u_n) + V_n(u_n - u_{n-1})\right]$$

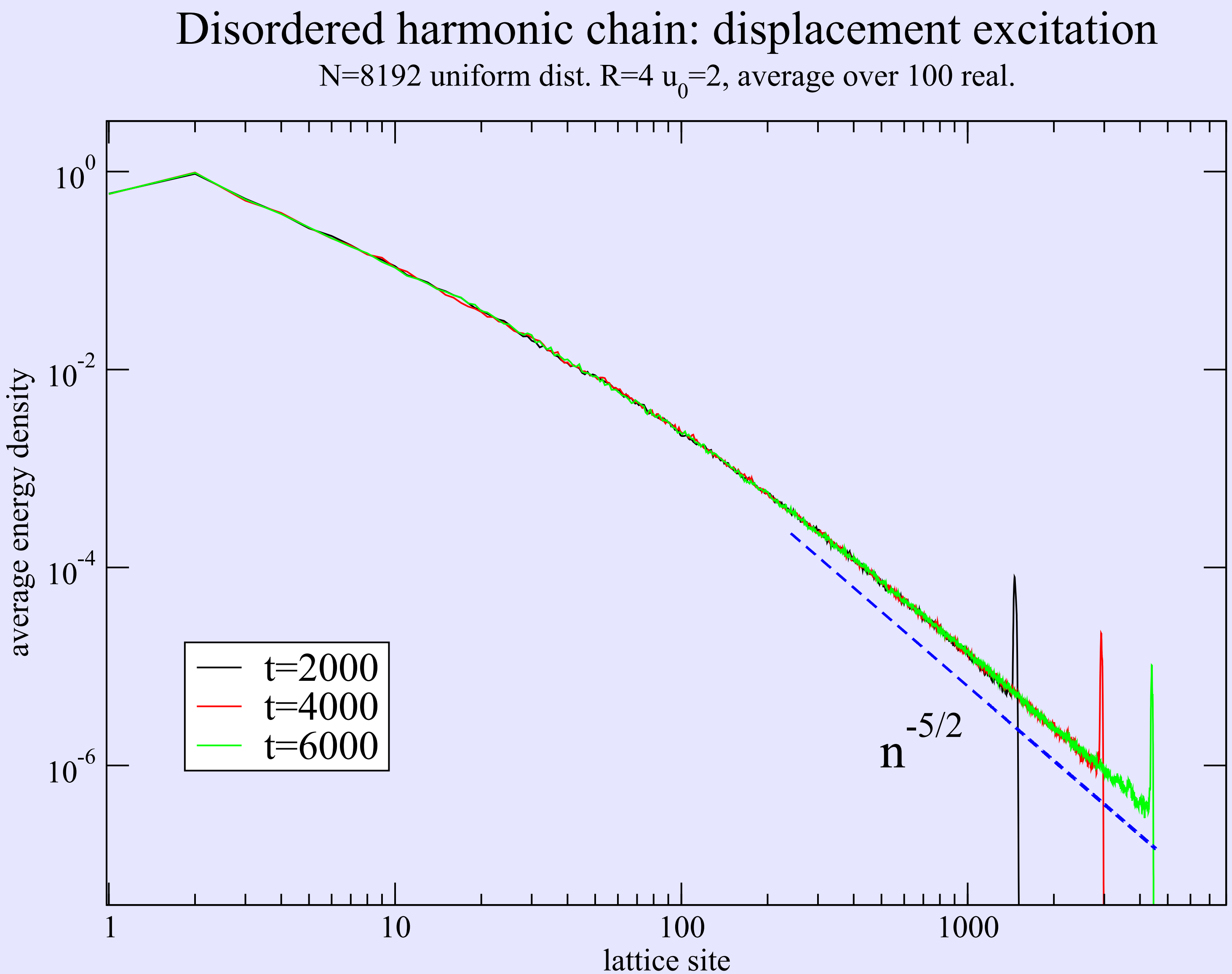
with $V_n(x) = K_n x^2/2$

Assuming the same behaviour for kinetic an potential terms:

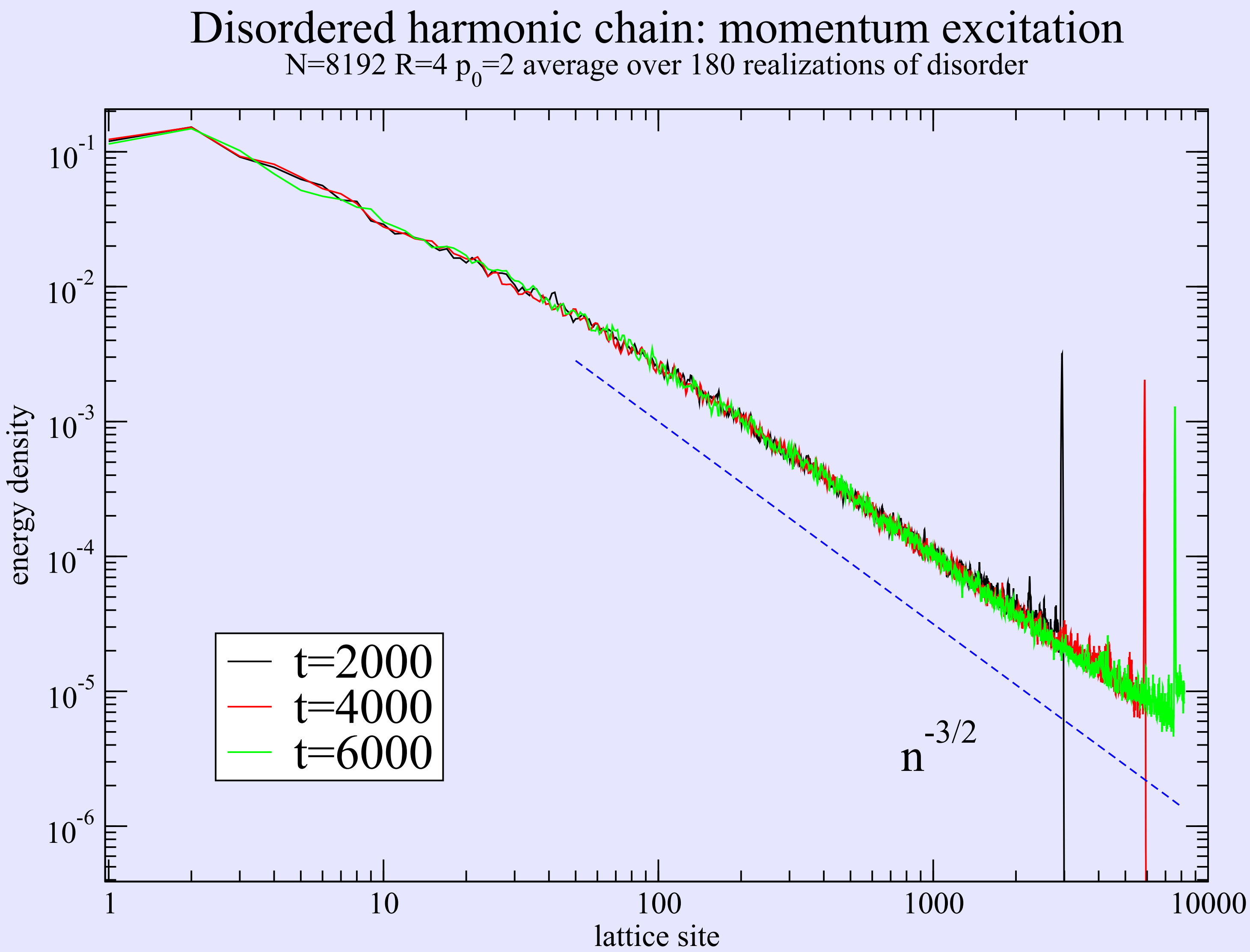
$$\langle e_n \rangle \;\propto\; |n - n_0|^{-\eta}$$

$$\eta = \begin{cases} \frac{5}{2} & \text{for displacement excitations} \\ \frac{3}{2} & \text{for momentum excitation} \end{cases}$$

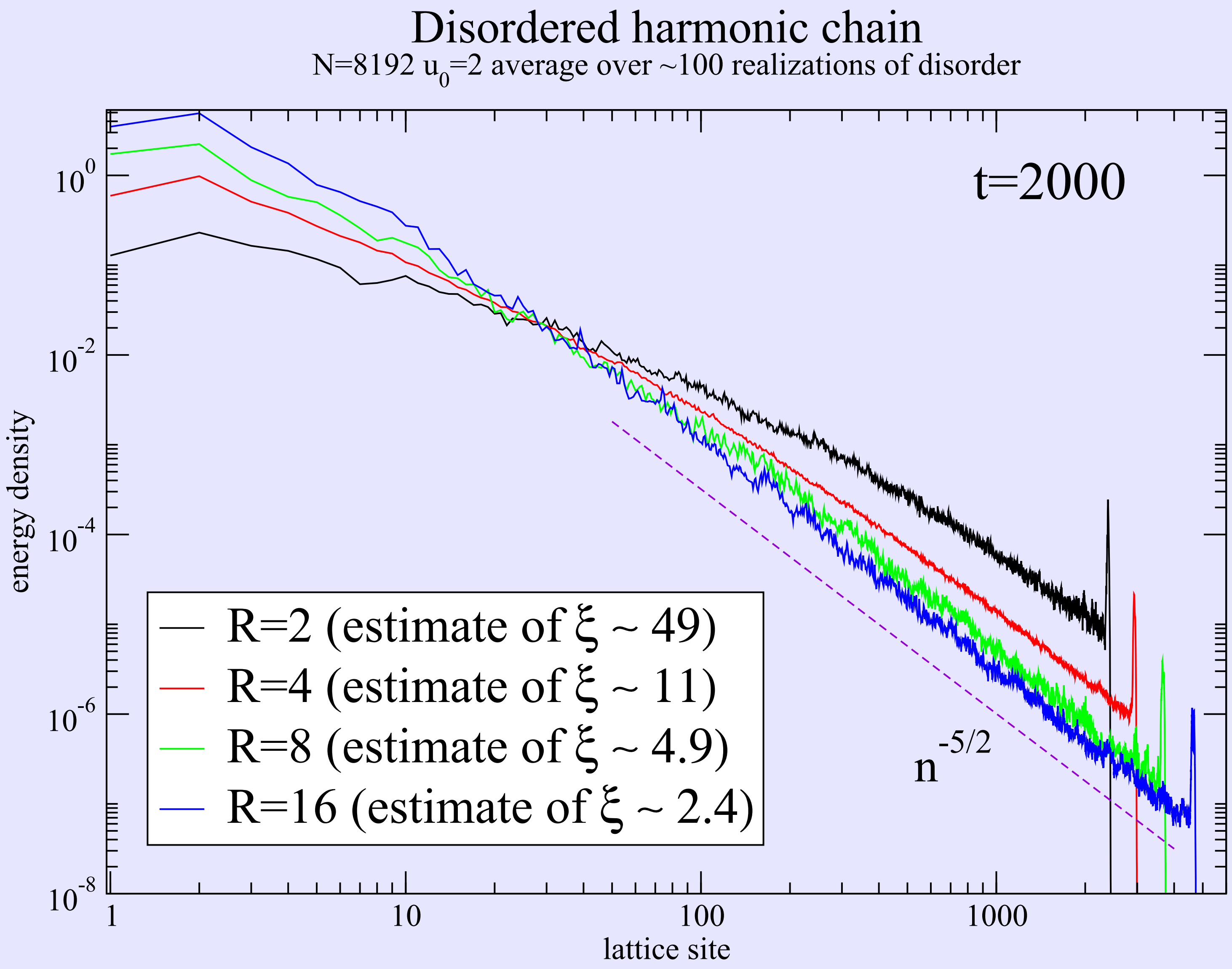
Harmonic chain: numerics



Harmonic chain: numerics



Dependence on disorder strength



Scaling of momenta

Let

$$m_\nu \;=\; \frac{\sum_n |n-n_0|^\nu e_n}{\sum_n e_n}$$

Introducing an upper cutoff at $|n-n_0| = ct$:

$$m_\nu \;\propto\; t^{\beta(\nu)} \qquad \beta(\nu) \;=\; \begin{cases} \nu+1-\eta & \nu > \eta - 1 \\ 0 & \text{otherwise} \end{cases}$$

E.g. $m_2 \sim t^{3/2}$ (displacement), $m_2 \sim t^{1/2}$ (momentum)

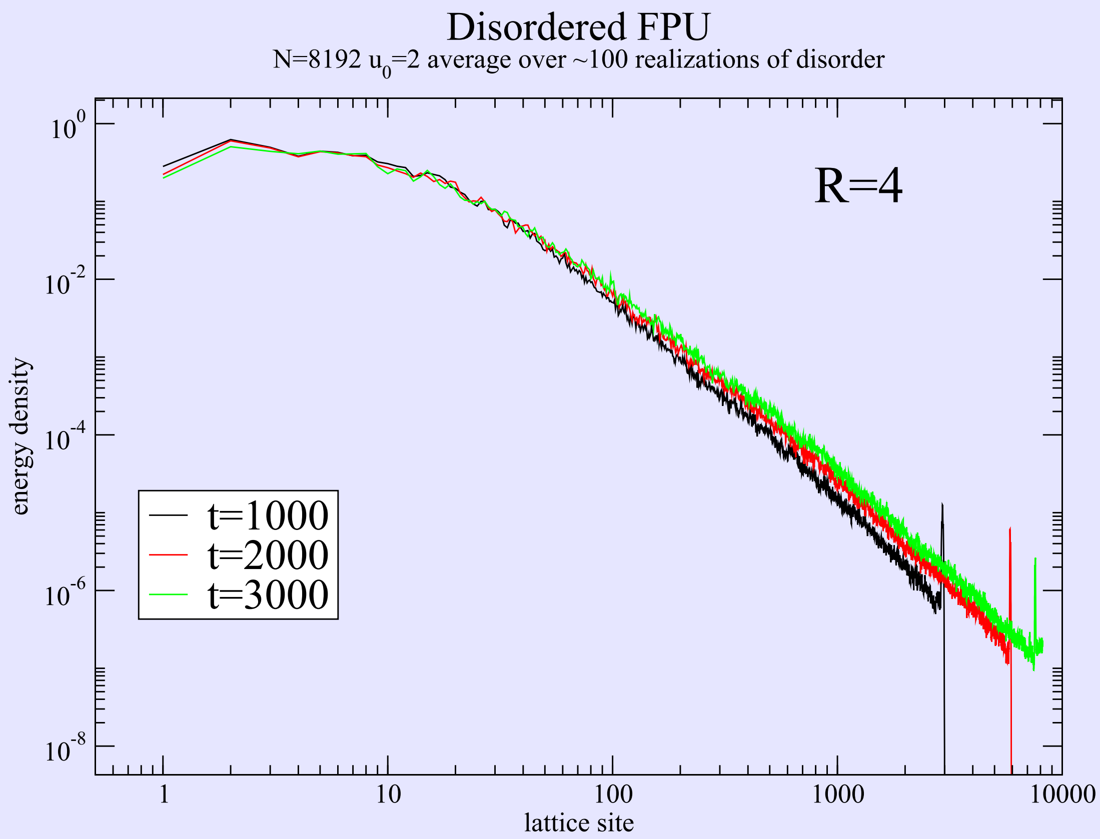
Fermi-Pasta-Ulam Model with disorder

$$\ddot{u}_n = K_n(u_{n+1} - u_n) - K_{n-1}(u_n - u_{n-1}) + (u_{n+1} - u_n)^3 - (u_{n-1} - u_n)^3$$

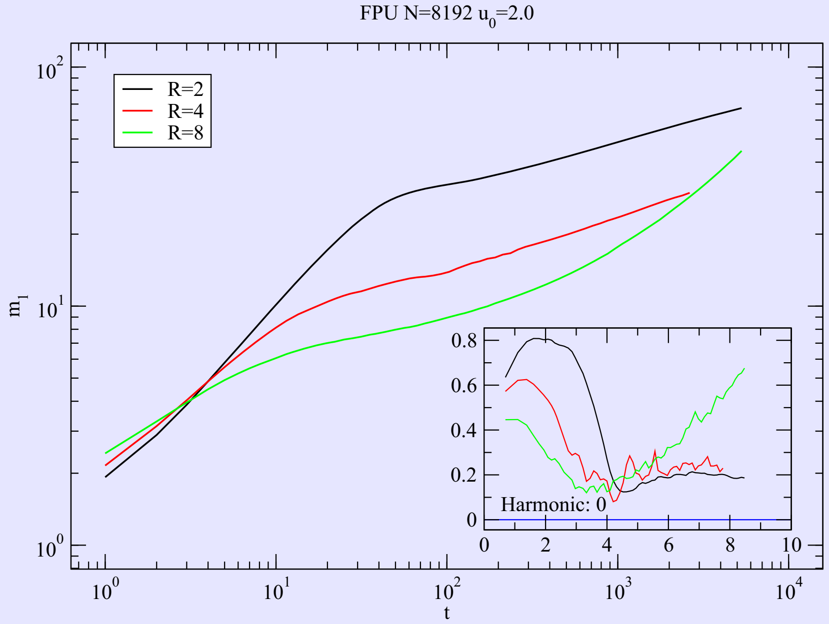
Evolution of a wavepacket

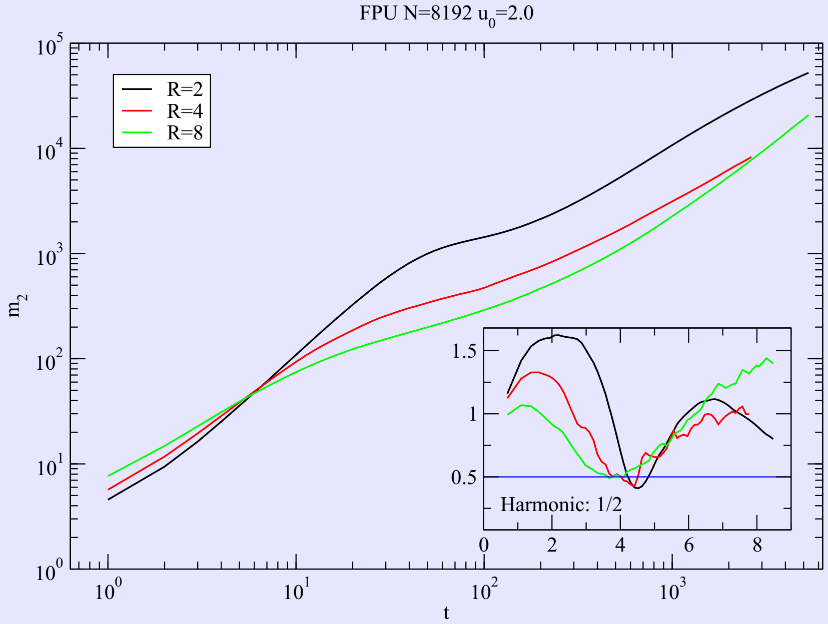
Single site displacement excitation

$$u_n(t=0) \ = \ u_0\delta_{n,n_0}, \quad \dot{u}_n(t=0) \ = \ 0$$



Evolution of momenta

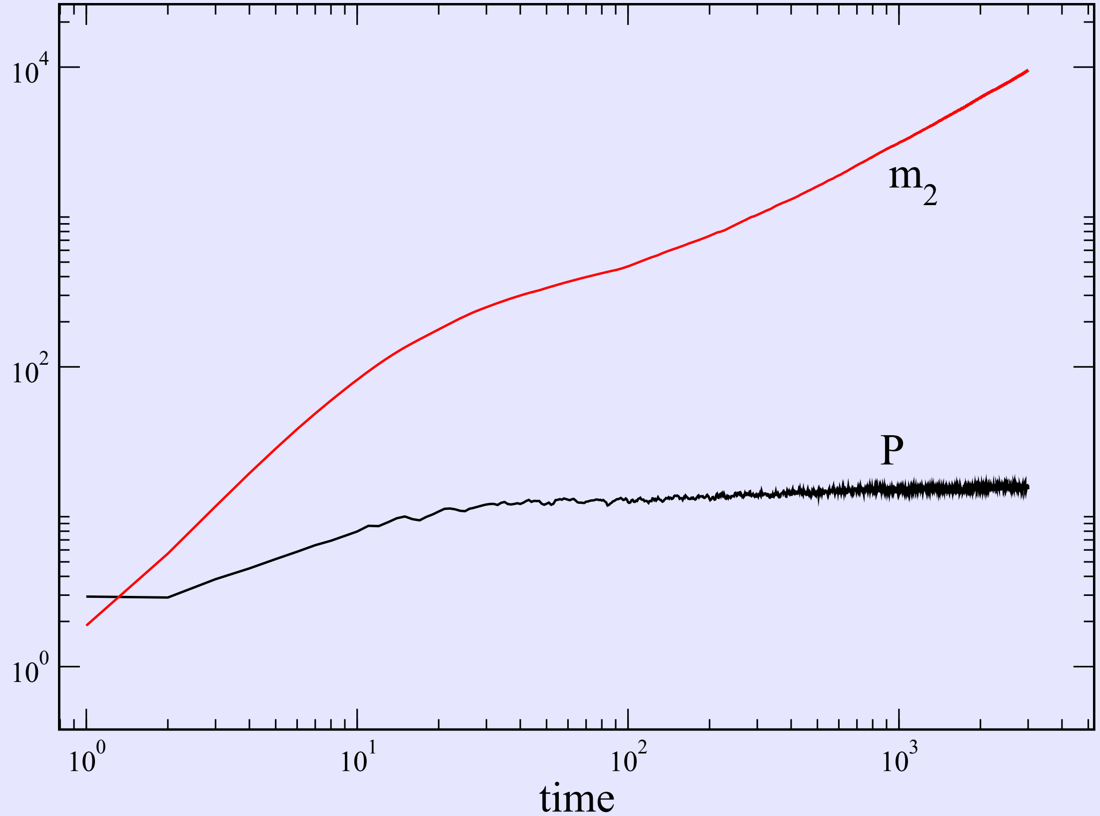




$$\beta_{eff}(\nu, t) \; = \; \frac{d \log m_\nu}{d \log t}$$

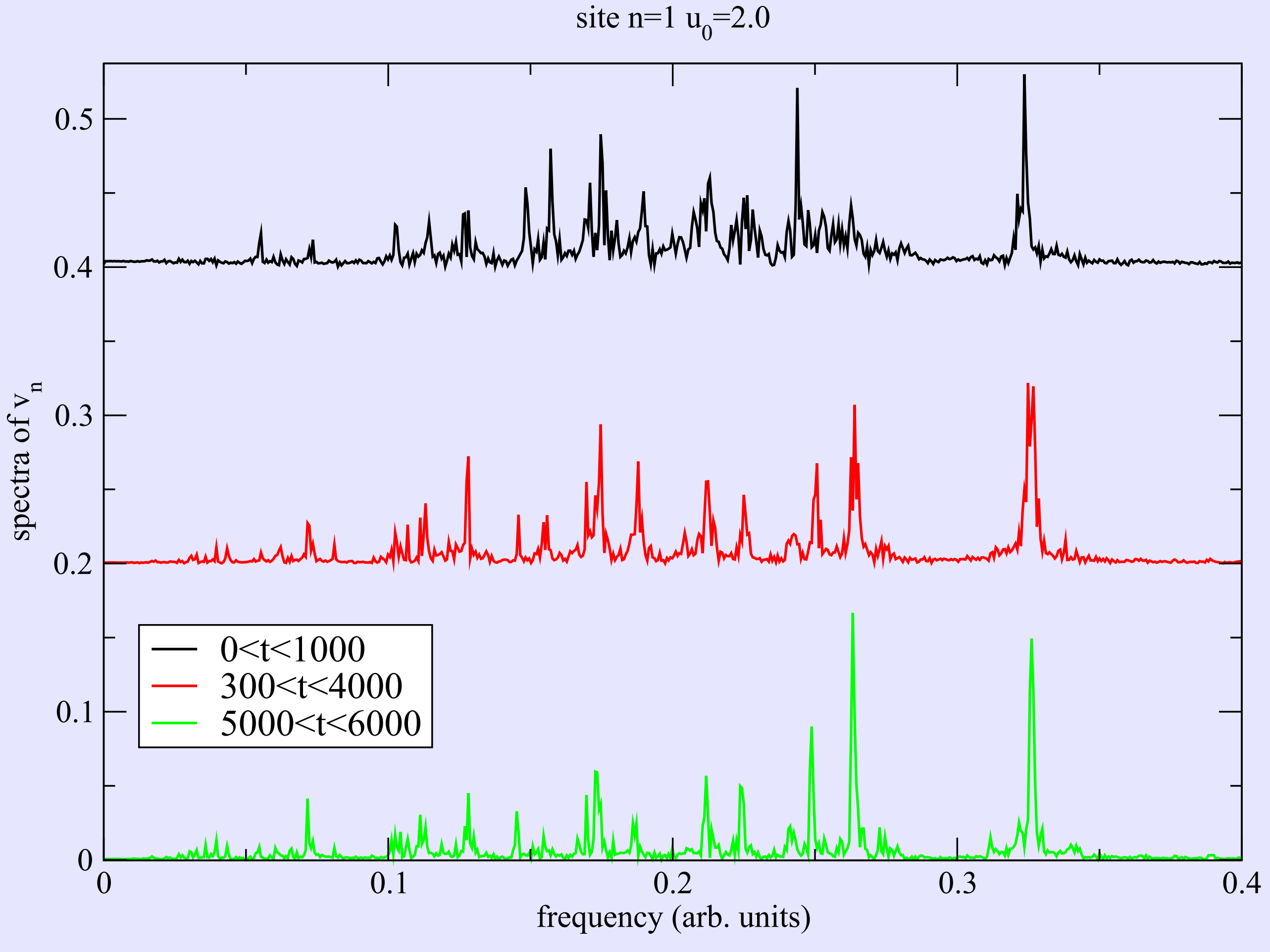
Evolution of a wavepacket

$$P = \frac{(\sum_n e_n)^2}{\sum_n e_n^2}, \qquad m_2 = \frac{\sum_n |n-n_0|^2 e_n}{\sum_n e_n}$$

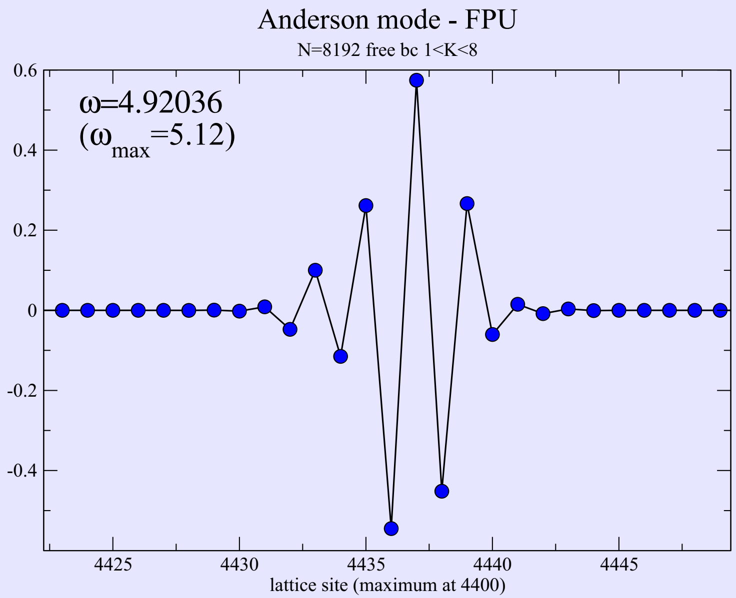


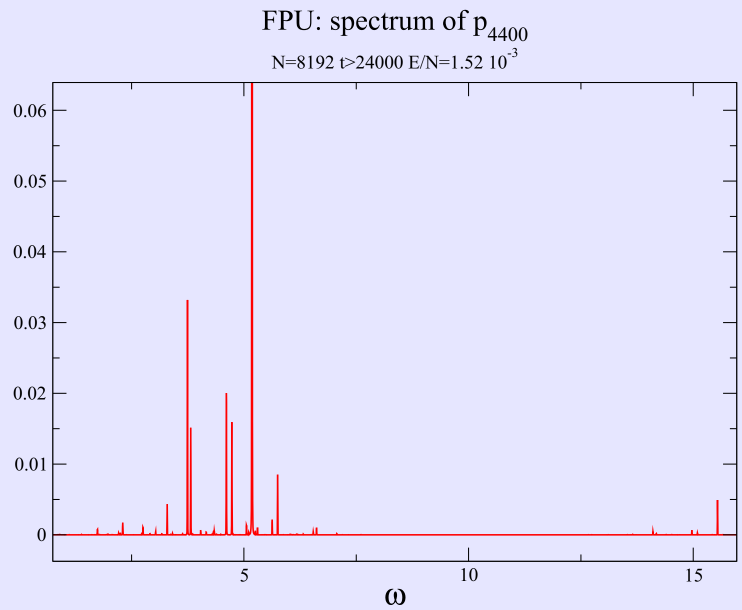
Evolution of a wavepacket

(Almost) quasiperiodic spectrum



Starting from an Anderson mode





Packet stays localized (simulation: t 2 10^4 periods).

Remarks

- Participation number is almost constant
- Spectra have many discrete components
- The Lyapunov exponent decreases slowly to zero
- Higher-order momenta grow (e.g. $m_2(t) \sim t^{\beta}(2)$) due to power-law tail !

Energy mostly does not spread: slow diffusion in phase space around a quasiperiodic breather solution?
Existence proofs (with "large probability"): Fröhlich, Spencer and Wayne (1986): (KAM theory)
More detailed investigation needed ...

Driven chain

- Response to a sinusoidal force on the extrema:

$$u_0(t) \; = \; A\cos\omega t \quad .$$

- Ordered case: nonlinear supratransmission for $\omega > \omega_{max}$ [Khomeriki, Lepri and Ruffo, 2004]
- Numerical experiment: initial condition $u_n = 0, \dot{u}_n = 0$, switch on the driving at time $t = 0$ as

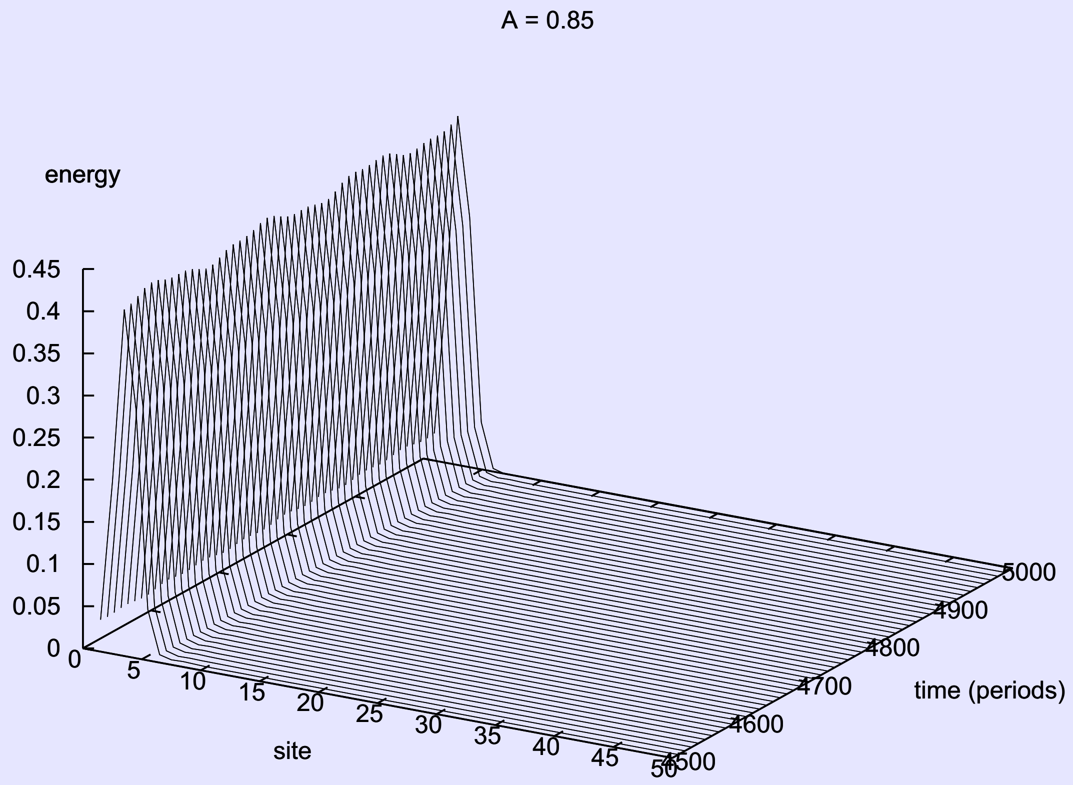
$$u_0(t) \; = \; A\cos\omega t \left[1 - e^{-t/\tau}\right]$$

Adiabatic case: τ large enough ($\tau\omega_{max} \gg 1$)

Simulation: subthreshold case $A < A_c$

Periodic solution at the driving frequency ($\omega < \omega_{max}$)

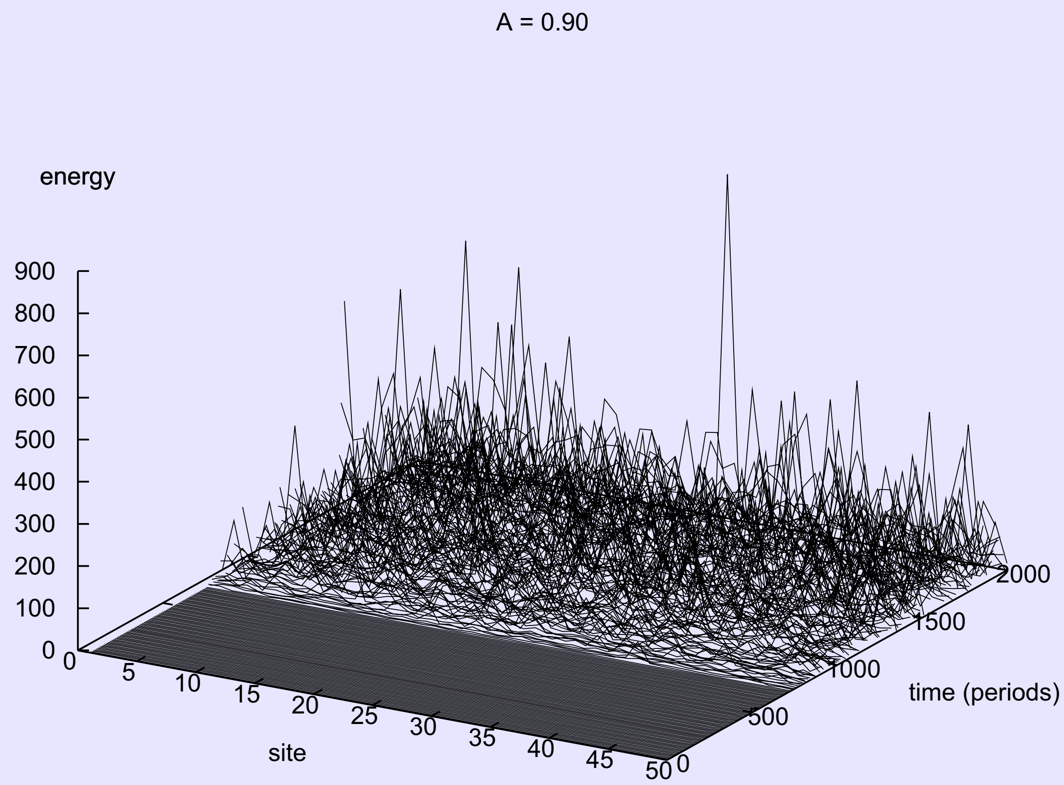
$\omega = 3.02$, $\tau = 400$, $N = 512$, K uniform in $[1, 4]$



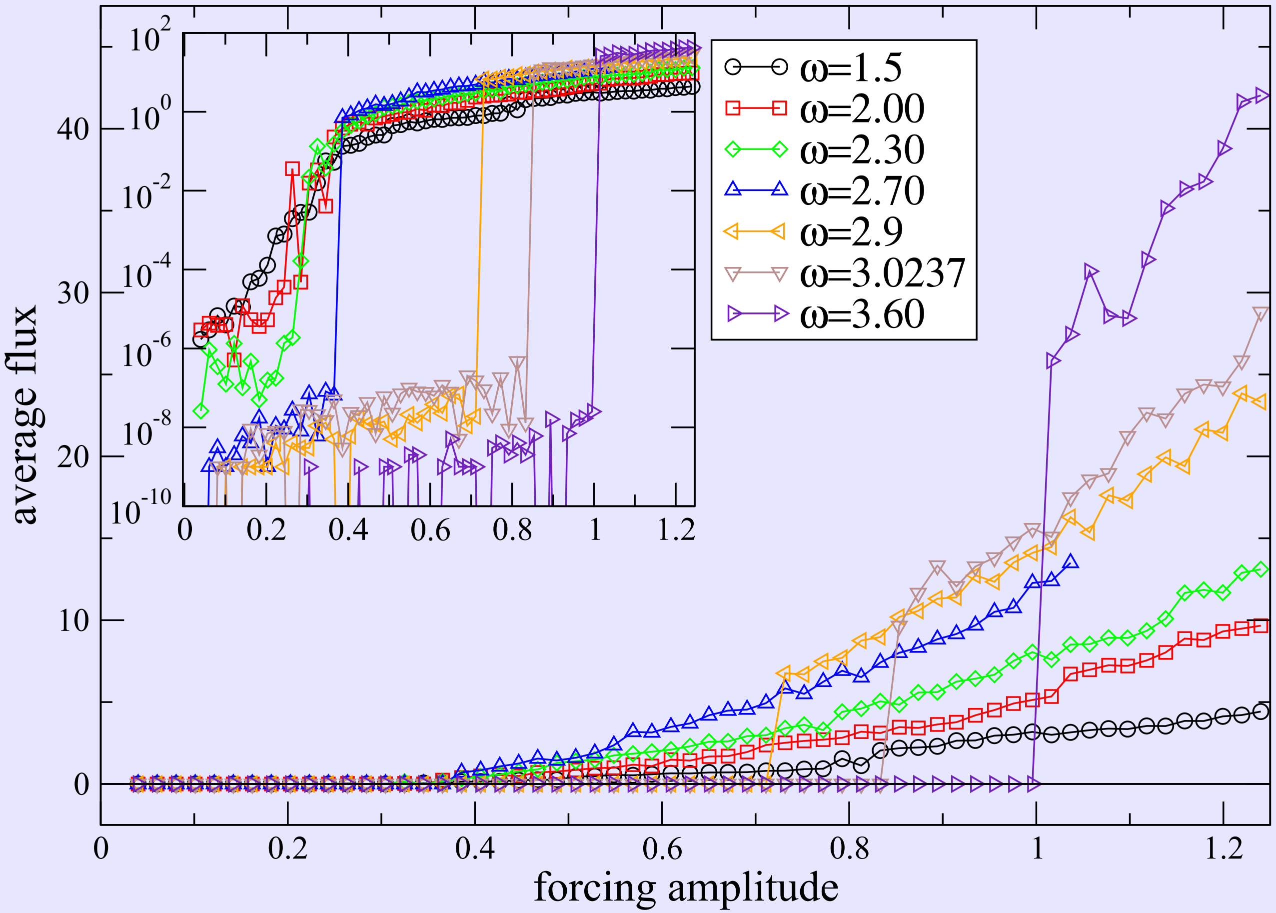
Simulation: suprathreshold case $A > A_c$

"Chaotic" solution with broadband spectrum

$\omega = 3.02$, $\tau = 400$, $N = 512$, K uniform in $[1, 4]$



Dependence on driving frequency



Nonlinear response manifold

- Define a family of periodic solutions $\{u_n(A)\}$ (for given ω).
- Linear response: $\{u_n(A)\}$ proportional to amplitude A
- Nonlinear case: compute $\{u_n(A)\}$ (e.g. by Newton method)
- Projection of the manifold $(A, u_1(A))$ is an involved function with many "turning points" [Kopidakis and Aubry, 2006]

Approximated nonlinear response manifold for FPU

1. Periodic solutions of the form $u_n = U_n \cos \omega t$
2. Rotating Wave Approximation: $\cos^3 \omega t \approx \frac{3}{4} \cos \omega t$

$$\begin{aligned} -\omega^2 U_n &= K_n(U_{n+1} - U_n) - K_{n-1}(U_n - U_{n-1}) + \\ &+ \frac{3}{4}(U_{n+1} - U_n)^3 - \frac{3}{4}(U_{n-1} - U_n)^3. \end{aligned}$$

3. Solve with respect to $U_n - U_{n-1}$: 2D (backward) map

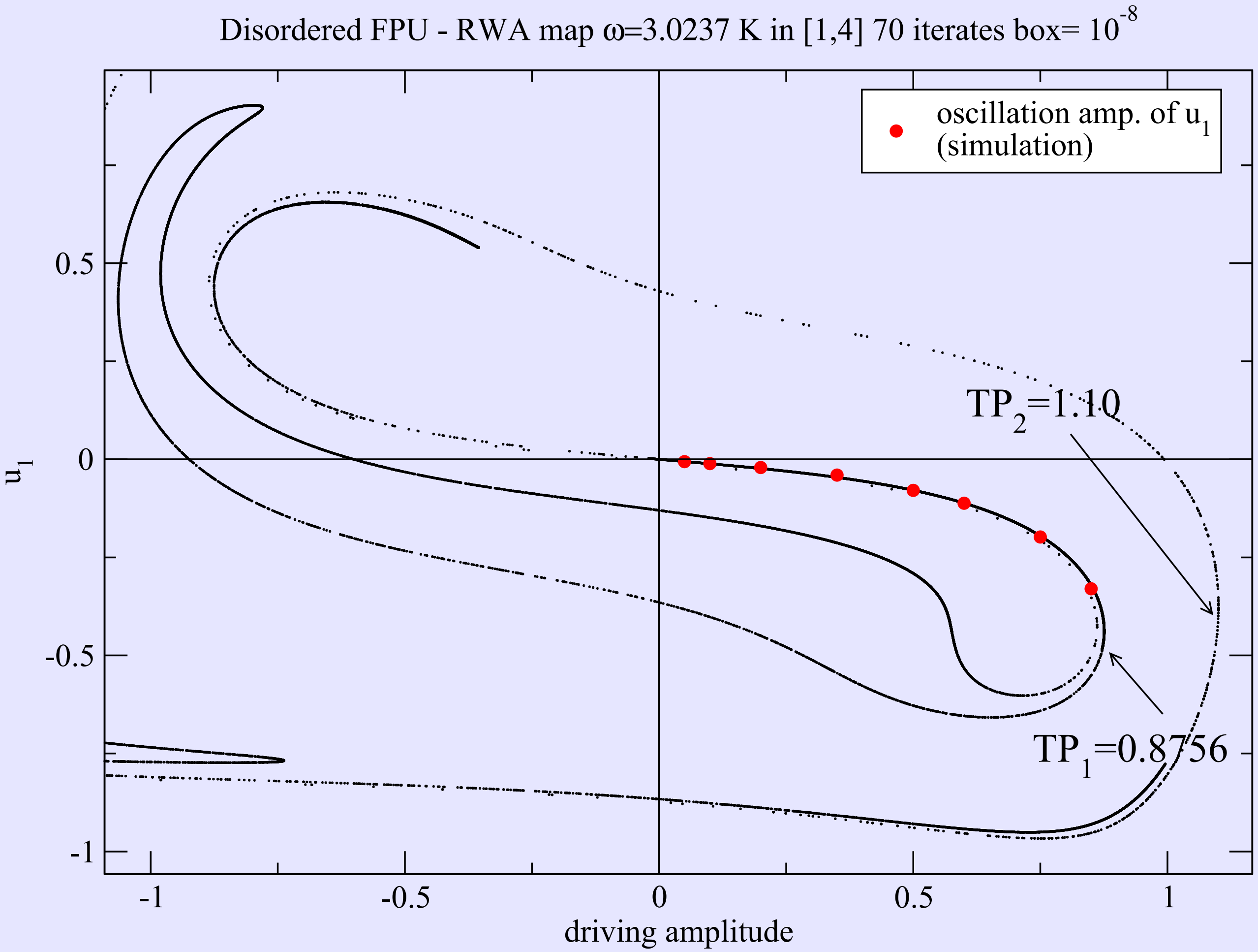
$$U_{n-1} = U_n - F(V_n, U_n), \qquad V_{n-1} = U_n$$

   F from the solution of the cubic equation

4. Iterate a set of initial conditions close to the origin, plot (A, U_1)

Threshold prediction

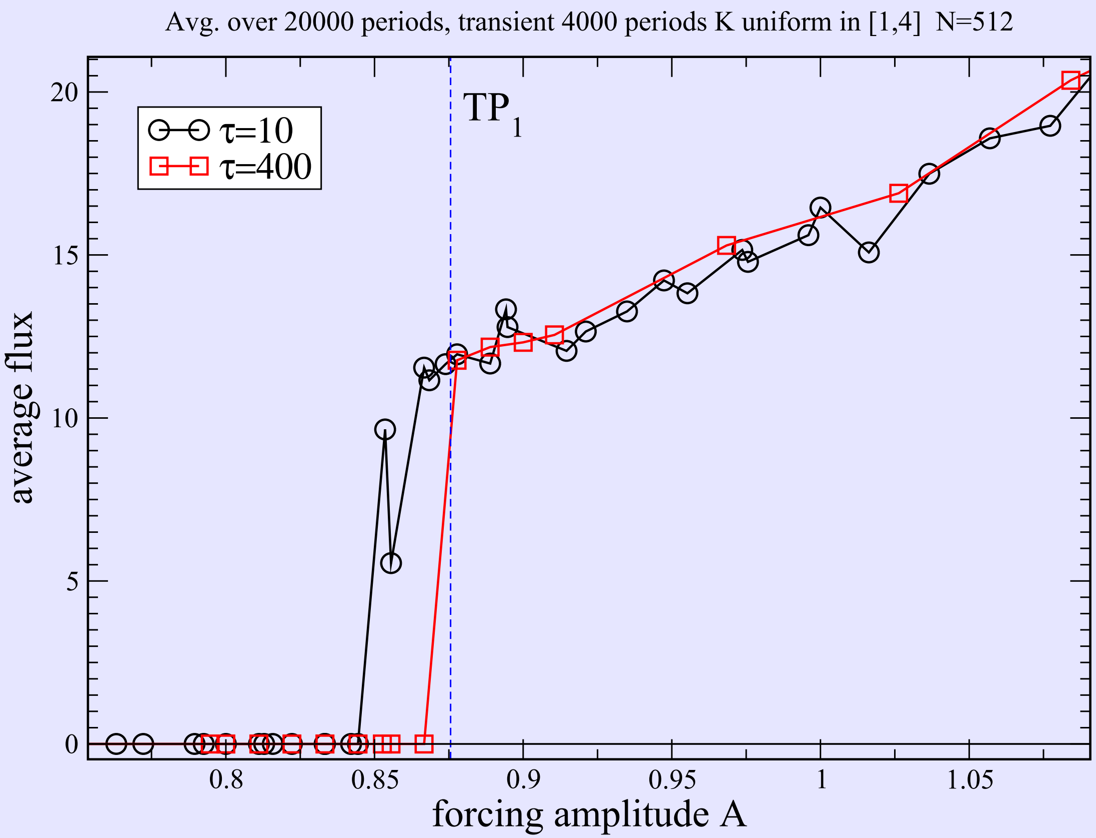
$$A_c^{(TP_1)} = 0.8756, \qquad A_c^{num} = 0.878$$



Nonadiabatic case (1)

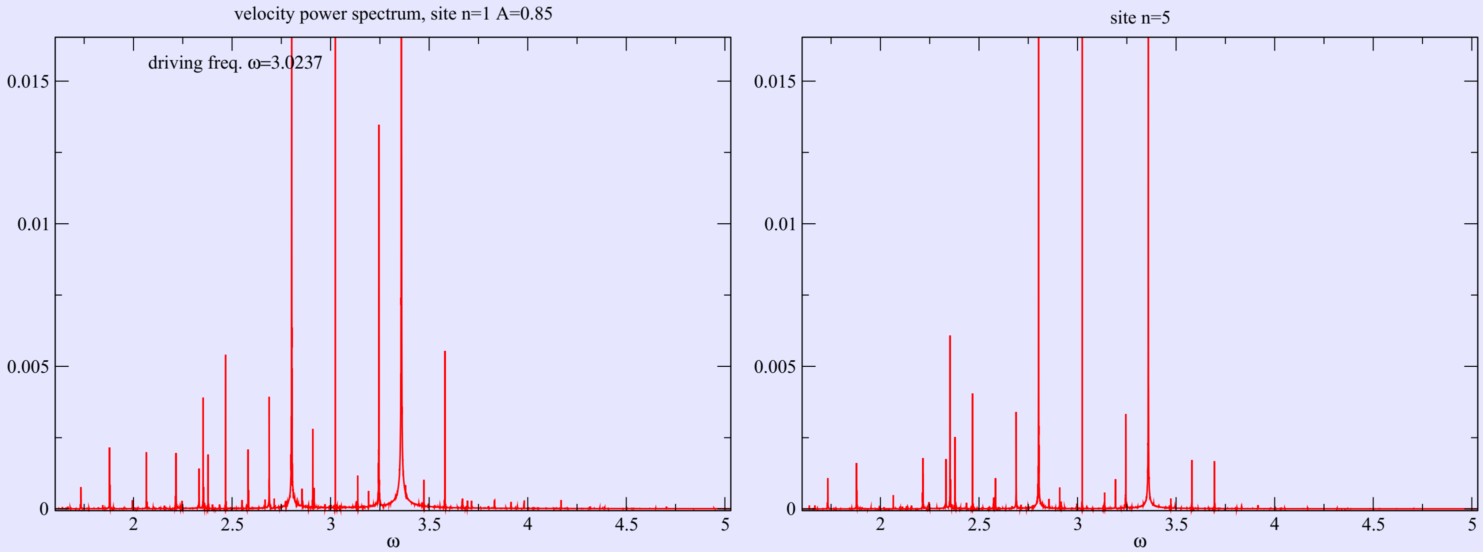
Dependence of threshold on the switching time τ

$$j_n = \frac{1}{2}(\dot{u}_n + \dot{u}_{n+1})\left[K_n(u_{n+1} - u_n) + (u_{n+1} - u_n)^3\right].$$

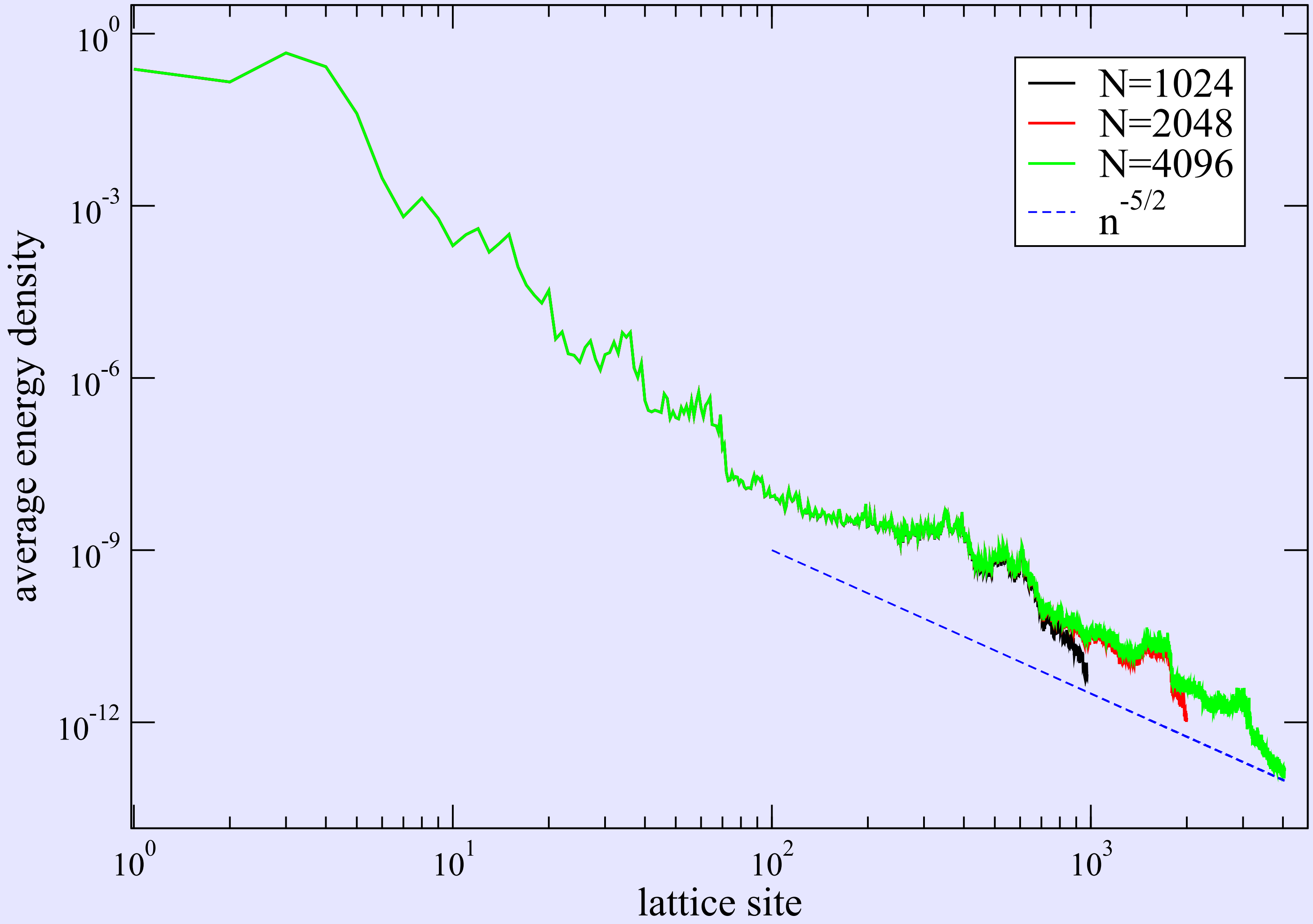


Nonadiabatic case (2)

Spontaneous creation of quasiperiodic solutions



Subthreshold profile



Outlook

1. **Evolution of a wavepacket:**
   - Harmonic case
     - Absence of diffusion: power-law localized packet
     - Momenta grow!
     - Scaling depends on type of i.c.
   - FPU:
     - Large localized component + weak diffusion
     - Numerics not conclusive on scaling exponents
     - Convergence towards a quasiperiodic localized solution (?)
     - Quasiperiodic breathers as continuation of Anderson modes
2. **Driven FPU chain:**
   - Existence of transmission threshold $A_c(\omega)$
   - Adiabatic case: nonlinear response manifold
   - Nonadiabatic case: spontaneous generation of quasiperiodic localized states