# Nonequilibrium processes in disordered nonlinear lattices:
# From nonlinear diffusion to second sound

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Nonlinear Waves, 2020

# Fermi-Pasta-Ulam-Tsingou lattice: an example of computational nonlinear physics

Los Alamos report (1955): Study of a relaxation from an initially non-equilibrium state to a thermodynamic equilibrium – check for equipartition and ergodicity

982 266. – *Studies of non Linear Problems*

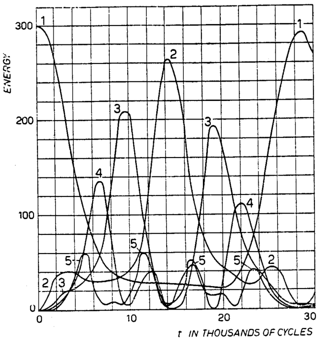



Fig. 1. – The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. N = 32 ; $\alpha = 1/4$ ; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

# Weakly nonlinear lattices

$$H = \sum \frac{p_l^2}{2} + \omega^2 \frac{q_l^2}{2} + \kappa \frac{(q_{l+1} - q_l)^2}{2} + U_{\mathrm{nl}}(q_l) + V_{\mathrm{nl}}(q_{l+1} - q_l)$$

- Examples: Fermi-Pasta-Ulam lattice, nonlinear Klein-Gordon lattice, etc
- Small perturbations: sound waves / phonons
- Large perturbations: nonlinearly interacting sound waves / interacting gas of phonons

# Nonequilibrium settings

- FPUT problem: equilibration in Fourier space: from one several modes to equipartition
- Equilibration in real space: from a localized perturbations on top of vacuum: dominated by spreading with sound velocity
- Slightly non-equilibrium state at constant density: Thermal conductivity paradox [see Lepri, Livi, and Politi, Thermal conduction in classical low-dimensional lattices, Physics Reports, v. 377 (2003)]
- Perturbations on top of finite phonon density: concepts of first and second sound on top of an underground turbulent/chaotic state as density and temperature modes in the “phonon gas”

# Disordered weakly nonlinear lattices

A way to prohibit linear waves: introduce disorder

$$H = \sum \frac{p_l^2}{2} + \omega_l^2 \frac{q_l^2}{2} + \kappa_l \frac{(q_{l+1} - q_l)^2}{2} + U_{\text{nl}}(q_l) + V_{\text{nl}}(q_{l+1} - q_l)$$

$\omega_l, \kappa_l$: random quenched disorder

- Anderson localization: exponentially localized linear modes instead of propagating phonons
- Large perturbation: interacting localized modes
- Localized perturbations on top of vacuum: weak sub-diffusive spreading due to nonlinear interaction of localized modes

# Strongly nonlinear lattices - sonic vacuum

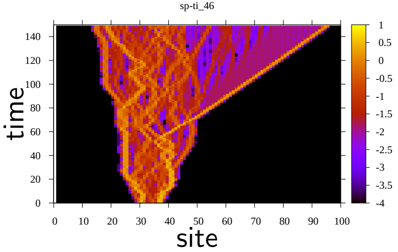
Strongly nonlinear lattice: no linear coupling terms

$$H = \sum \frac{p_l^2}{2} + \omega^2 \frac{q_l^2}{2} + U_{\mathrm{nl}}(q_l) + V_{\mathrm{nl}}(q_{l+1} - q_l)$$

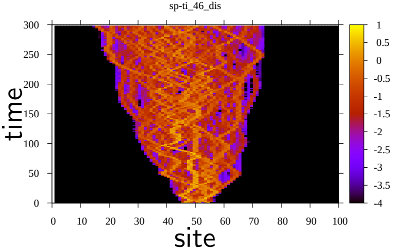
- No phonons, no linear propagating waves and modes (like in Anderson localization, localization length $= 1$)
- The only propagating waves are nonlinear ones – typically compactons (exist in homogeneous lattices only)
- At finite energy density: typically strongly chaotic/turbulent states (no chaoticity threshold like e.g. in the FPU lattice)

# Initially localized perturbation in a strongly nonlinear lattice

Regular lattice




Disordered lattice




Disordered strongly nonlinear lattices: similar to nonlinear Anderson localization, but

- extremely localized modes – sharp profiles of the field
- if power of all nonlinear terms the same - no essential dependence of energy (energy can be rescaled, it influences the characteristic time only)

# Two setups for disordered strongly nonlinear lattices

We consider below two setups:

- localized initial spot (zero density) on top of vacuum:
  how it spreads?
- periodic in space modulation on top of finte energy density:
  do we see the first and the second sound?

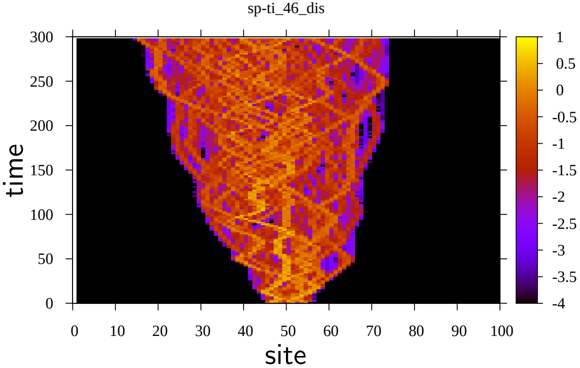
# Part I: Zero density: Spreading of a localized wave packet

[with Mario Mulansky, New J. Phys. (2013)]

Strong compactness of the spreading field:

Here "Anderson modes" are one site oscillators ⇒ no exponential tails, the excitation width $L$ is well-defined at each moment of time

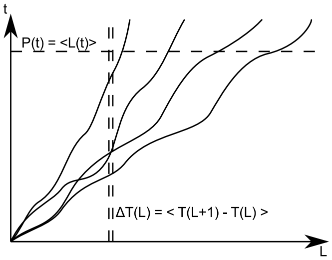
Disorder prevents ballistic quasi-compactons



# How to average

Traditionally width is measured at a fixed time :
$\log P(t) = \langle \log L(t) \rangle$, but due to large fluctuations one averages the propagation speed at different densities

Here the averaging of propagation/waiting time at fixed width, i.e. at fixed density, is possible (because the field has sharp edges):
$\log \Delta T = \langle \log(T(L+1) - T(L)) \rangle$




Goal: to describe $\Delta T(L, E)$ for different total energies $E$

# Guiding phenomenology

Use Nonlinear Diffusion Equation (NDE) as a heuristic model

$$\frac{\partial \rho}{\partial t} = D\frac{\partial}{\partial x}\left(\rho^a \frac{\partial \rho}{\partial x}\right), \qquad \text{with} \qquad \int \rho \, dx = E$$

Self-similar solution (Zeldovich and Kompaneyets, 1950; Barenblatt, 1952)

$$\rho(x,t) = \frac{1}{[D(t-t_0)]^{1/(2+a)}}\left(E - \frac{ax^2}{2(a+2)[D(t-t_0)]^{2/(a+2)}}\right)^{1/a}$$

yields subdiffusion

$$L = \sqrt{2\frac{2+a}{a}} E^{a/(2+a)}[D(t-t_0)]^{1/(2+a)}$$

# One parameter scaling

Reformulate

$$L = \sqrt{2\frac{2+a}{a}} E^{a/(2+a)} (D(t-t_0))^{1/(2+a)}$$

as scaling relaions:

$$\frac{L}{E} \sim \left(\frac{t-t_0}{E^2}\right)^{1/(2+a)} \qquad \boxed{\frac{1}{E}\frac{\mathrm{d}t}{\mathrm{d}L} \sim \left(\frac{E}{L}\right)^{-(a+1)}} \qquad a(w)+1 = -\frac{\mathrm{d}\log\frac{1}{E}\frac{\mathrm{d}t}{\mathrm{d}L}}{\mathrm{d}\log w}$$

where $w = E/L$ is the characteristic density, $\frac{\mathrm{d}t}{\mathrm{d}L} \approx \Delta T$

# Spreading in a homogeneously nonlinear lattice

Fully self-similar lattice:
rescaling energy $\Leftrightarrow$ rescaling time

$$H = \sum_k \frac{p_k^2}{2} + W\omega_k^2 \frac{q_k^\kappa}{\kappa} + \beta \frac{(q_{k+1} - q_k)^\kappa}{\kappa}$$

From the rescaling of energy and time it follows

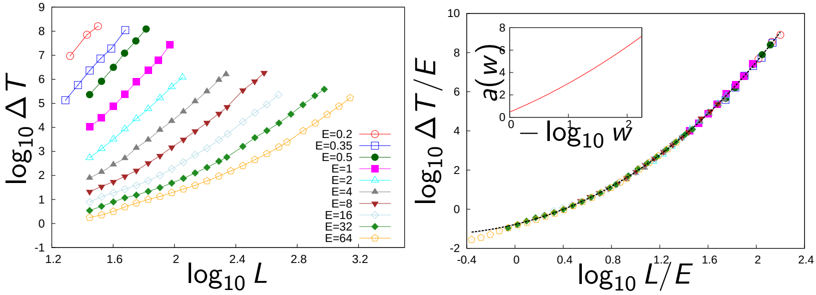
$$t \sim E^{\frac{2\kappa}{2-\kappa}} \quad \Rightarrow \quad a = \frac{\kappa - 2}{2\kappa} \quad \Rightarrow \quad L \sim (t - t_0)^{\frac{2\kappa}{5\kappa - 2}}$$

For the case $\kappa = 4$ we have

$$L \sim (t - t_0)^{4/9} \qquad \Delta T \sim L^{5/4}$$

# Spreading in a lattice of nonlinearly coupled linear oscillators

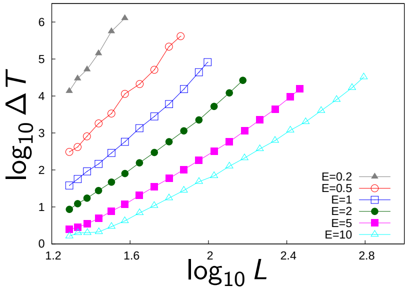
$$H = \sum_k \frac{p_k^2 + \omega_k^2 q_k^2}{2} + \frac{(q_{k+1} - q_k)^4}{4}$$

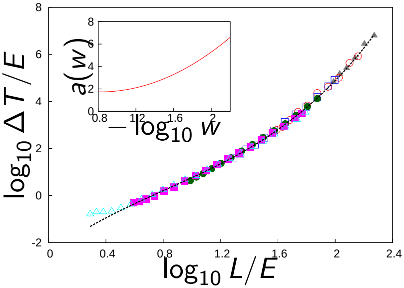



- Good news: Scaling of NonlDiffEq works
- Bad news: nonlinearity index $a$ is not a constant, but increases in course of spreading

# Spreading in a lattice of nonlinearly coupled linear oscillators

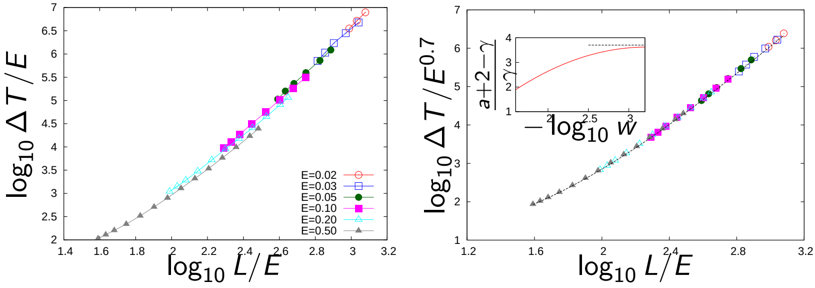
$$H = \sum_k \frac{p_k^2 + \omega_k^2 q_k^2}{2} + \frac{(q_{k+1} - q_k)^6}{6}$$



# Nonlinearly coupled nonlinear oscillators

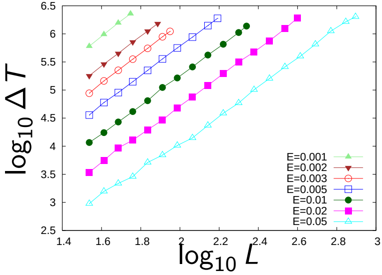
$$H = \sum_k \frac{p_k^2}{2} + \omega_k^2 \frac{q_k^4}{4} + \frac{(q_{k+1} - q_k)^8}{8}$$

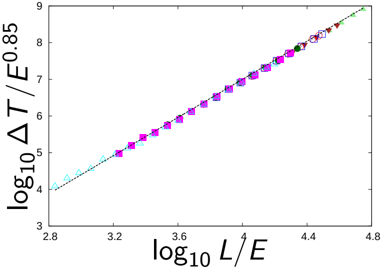



- Bad news: Different scaling: $\Delta T/E^{0.7} = F(L/E)$
- Good news: nonlinearity index appears to approach to a constant

# Nonlinearly coupled nonlinear oscillators

$$H = \sum_k \frac{p_k^2}{2} + \omega_k^2 \frac{q_k^4}{4} + \frac{(q_{k+1} - q_k)^6}{6}$$




Yet another power but nearly a straight line in rescaled coordinates

# Another strongly nonlinear lattice: Ding-Dong model

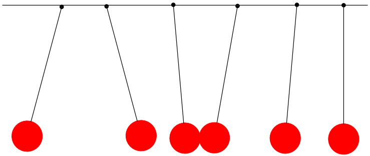
Newton's cradle:

The elastic force between two spheres is, according to H. Hertz (1881), $\sim x^{3/2}$. A chain of spheres is strongly nonlinear

$$\frac{d^2 x_l}{dt^2} = (x_{l-1} - x_l)^{3/2} - (x_l - x_{l+1})^{3/2}$$

# Toy strongly nonlinear lattice model: Ding-Dong lattice

This is a strongly nonlinear lattice that is easy to model numerically



Ding-Dong model (Prosen, Robnik, 92) is a chain of linear oscillators with elastic collisions

# Ding-Dong dynamics

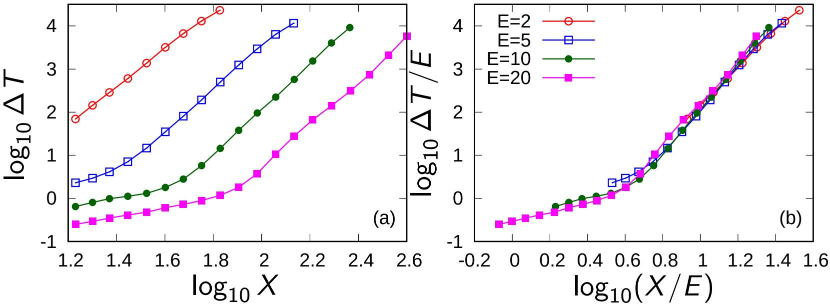
Hamiltonian and collision condition

$$H = \sum_k \frac{p_k^2 + q_k^2}{2} \qquad \text{when } q_k - q_{k+1} = 1 \text{ then } p_k \to p_{k+1},\ p_{k+1} \to p_k$$

Effective calculation of the collision times – simulation on very long times pissible

Strongly nonlinear lattice: no linear waves, no phonons, all propagating perturbations are nonlinear

# Check for Nonlinear Diffusion Equation scaling [JSTAT, to appear]




Slow subdiffusion:

$$\frac{\Delta T}{E} \sim \left(\frac{X}{E}\right)^5 \qquad X \sim T^{1/6}$$

# Conclusions for wavepacket spreading

- Nonlinearly coupled linear oscillators:
  Nonlinear Diffusion Equation scaling works, slowing down of spreading
- Nonlinearly coupled nonlinear oscillators:
  Nonlinear Diffusion Equation scaling does not work, but some scaling works , good power-law
- How to extend to weakly (exponentially) localized modes in the Anderson localization problems?

Conclusions for Ding-Dong model

- simple but singular strongly nonlinear lattice
- NDE scaling works without slowing down
- holds for distance and mass disorder

# Part II: Finite energy density: "sound" modes on top of turbulence [JSTAT, 2015]

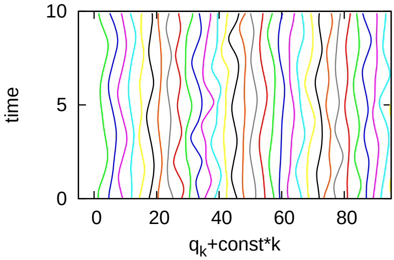
Basic model for numerics:

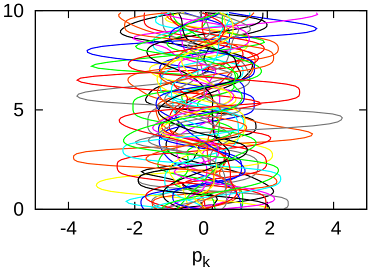
Strongly nonlinear lattice with local and coupling nonlinearities

$$H = \sum_l \frac{p_l^2}{2} + \beta_l \frac{q_l^4}{4} + \kappa_l \frac{(q_{l+1} - q_l)^4}{4}$$

Homogeneous lattices: $\beta, \kappa =$ const, Disorder: random $\beta_l, \kappa_l$
Energy can be rescaled: $E \to \alpha E'$, $t \to \alpha^{-1/2} t'$, below we set energy density to one
Energy level determines time scale only, there is no transition order-chaos

# Chaotic state



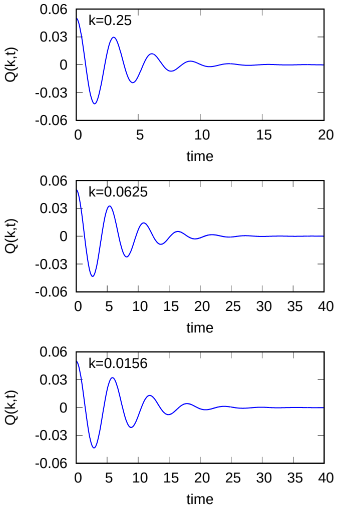
# First sound on top of chaos in disordered lattices

Protocol of numerical simulations:

- fix energy density, evolve to equilibrium chaos
- add a perturbation having wave number $k$:
  $q_l \to q_l + \varepsilon \cos 2\pi kl$
- follow amplitude of this mode $Q(k,t) = \langle \sum_l q_l \cos 2\pi kl \rangle$

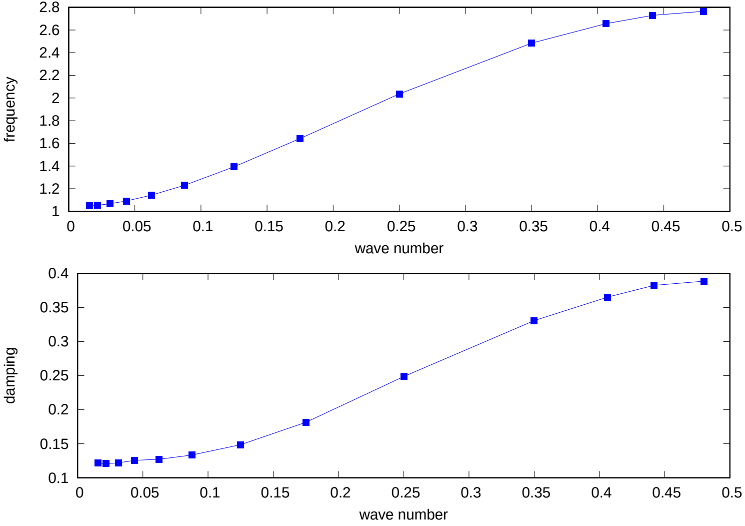
[cf. Lepri, Livi, Politi, Chaos, 15, 015118 (2005), Zhirov, Pikovsky, Shepelyansky, PRE 83, 016202 (2011)]

# First sound results




The data are nicely reproduced by a fit $Q(t) = A \exp(-\gamma t) \cos \Omega t$

# First sound results: dispersion and damping



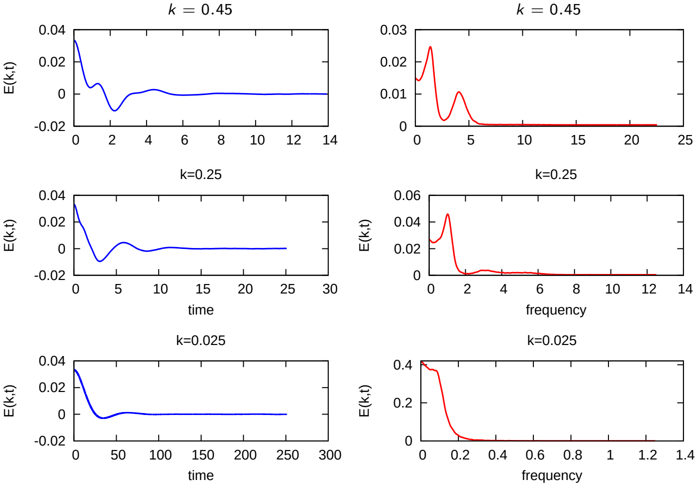
# Second sound on top of chaos in disordered lattices

Protocol of numerical simulations:

- fix energy density, evolve to equilibrium chaos
- add a perturbation (wave number $k$) to kinetic energy $p_l^2 \to p_l^2[1 + \varepsilon \cos(2\pi k l)]$
- follow amplitude of this mode $E(k, t) = \langle \sum_l \mathcal{E}_l \cos 2\pi k l \rangle$, where $\mathcal{E}_l$ is the local energy

[cf. Gendelman et al, PRE, 2010,2012]

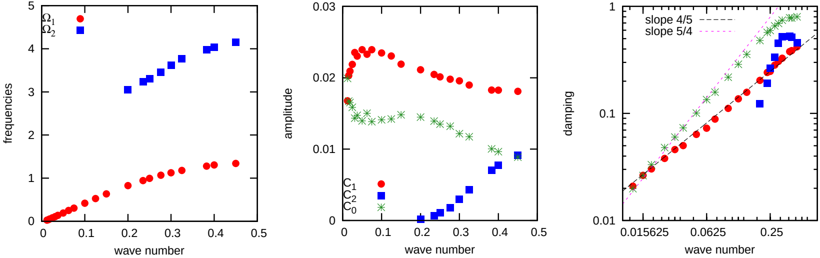
# Second sound results




Fourier transform of $E(k,t)$ suggests fit

$$E(t) \sim C_0 \exp(-\gamma_0 t) + C_1 \exp(-\gamma_1 t)\cos(\Omega_1 t) + C_2 \exp(-\gamma_2 t)\cos(\Omega_2 t)$$

# Second sound results: dispersion

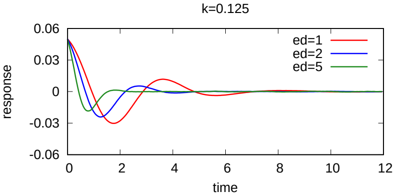


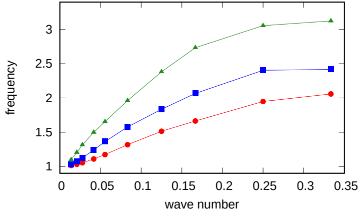

Two frequencies observed for large $k$, no one coincides with that of first sound

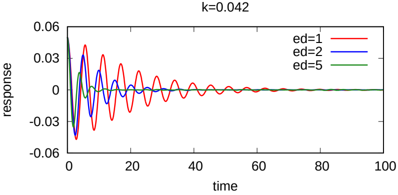
Damping constants $\gamma_0 \sim k^{5/4}$, $\gamma_1 \sim k^{4/5}$

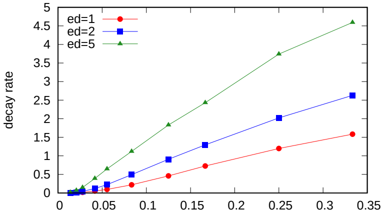
# First sound in the Ding-Dong lattice

Properties of perturbations depend on the basic energy density, we study $\mathcal{E} = 1, 2, 5$



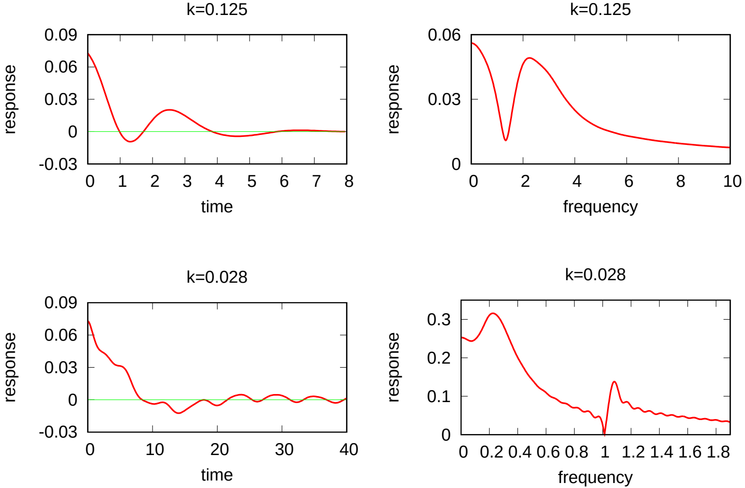




The data are nicely reproduced by a fit $Q(t) = A \exp(-\gamma t) \cos \Omega t$

# Second sound in the Ding-Dong lattice

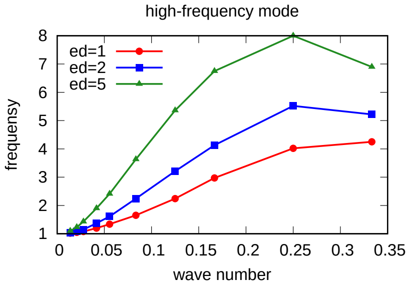
Results for small energy density $\mathcal{E} = 1$

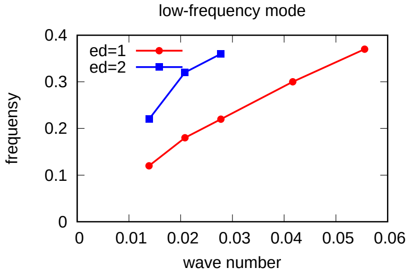



Fourier transform suggests a two-frequency fit

$$E(t) \sim C_0 \exp(-\gamma_0 t) + C_1 \exp(-\gamma_1 t)\cos(\Omega_1 t) + C_2 \exp(-\gamma_2 t)\cos(\Omega_2 t)$$

# Second sound in the Ding-Dong lattice: dispersion



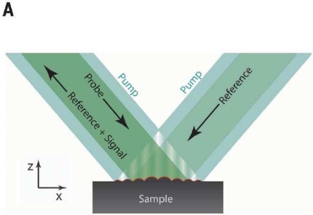

Two frequencies observed for small wave numbers $k$ for low energy densities

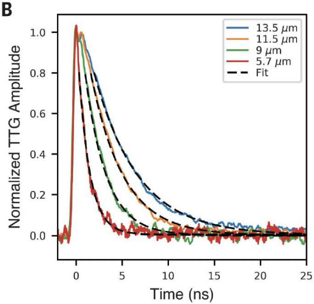
# Second sound in experiments

**Observation of second sound in graphite at temperatures above 100 K**

S. Huberman[1]*, R. A. Duncan[2]*, K. Chen[1], B. Song[1], V. Chiloyan[1], Z. Ding[1], A. A. Maznev[2], G. Chen[1]†, K. A. Nelson[2]†

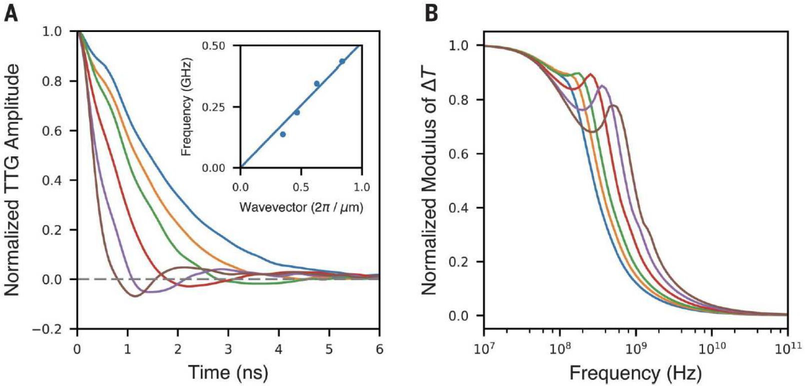
*Science* **364**, 375–379 (2019) 26 April 2019




At room temperature no second sound is observed

# Second sound in experiments




Second sound at $T = 85K$

# Conclusions for the 1st and the 2nd sound calculations

- In strongly nonlinear lattices, with a smooth potential and in the Ding-Dong model, on top of a "turbulent state" one can excite first sound (density variations) and second sound (energy variations)
- Two second sound modes
- The same protocol can be realized experimentally
- Any link to the nonlinear diffusion equation ?