Nonintegrability and the Fourier Heat conduction Law

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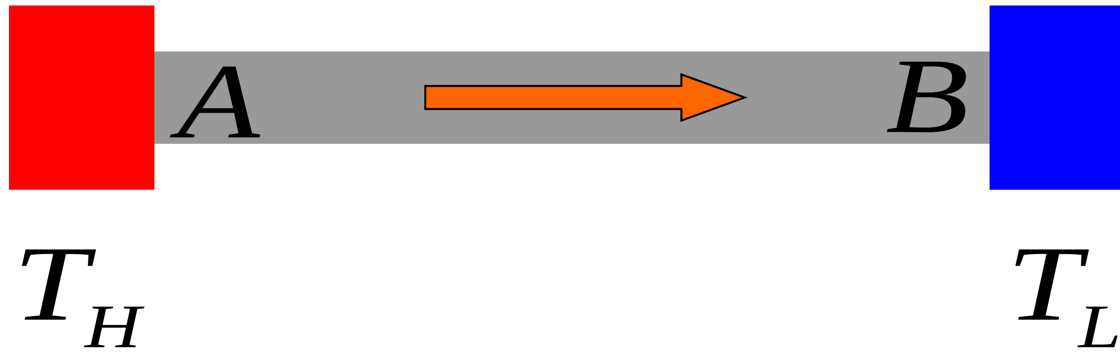
Outline

1. Introduction
2. Our recent progress
    - 2.1 Models and methods
    - 2.2 Results
3. Summary

Fourier Heat Conduation Law (1808)



$$\boxed{\boldsymbol{J} = -\kappa \nabla T}$$

$\boldsymbol{J}$: heat flux

∇: temperature gradient

κ: thermal conductivity

Jean Baptiste Joseph Fourier (1768-1830)

Fourier's Law: A Challenge to Theorists

(Review article)

F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet,

Mathematical Physics (Imperial College Press, London 2000)

What is the underlying mechanism?

How to relate the macroscopic heat conduction behavior with microscopic dynamics?

How do we know whether or not Fourier's law is valid in a given system with specified Hamiltonian dynamics?

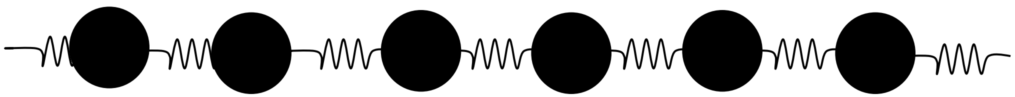
An old problem, and a long history

- 1808 - J.J. Fourier: study of the earth thermal gradient
- 19 century: Clausius, Maxwell, Boltzmann, kinetic theory
- 1914 - P . Debye: conjectured the role of nonlinearity for guaranteeing finite transport coefficients
- 1936 - R. Peierls: reconsider Debye's conjecture
- 1953 - E. Fermi, J. Pasta and S.Ulam: **(FPU) numerical experiment**: to verify Debye's conjecture

  (the first numerical experiment)

Klages R, Radons G, Sokolov I M.
Anomalous Transport: Foundations and Applications (2008).

- FPU model



$$H = \sum_i \frac{p_i^2}{2M} + V(x_i - x_{i-1} - 1)$$

$$\text{with } V(x) = \frac{1}{2}x^2 - \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4$$

E. Fermi, J. Pasta, and S. Ulam, Report No. LA-1940, 1955 (unpublished).
M.A. Porter, N.J. Zabusky, B. Hu and D.K. Campbell, "Fermi, Pasta, Ulam and the Birth of Experimental Mathematics", American Scientist, 97, 214-221 (2009),

(after FPU experiment)

- 1968 - Z. Rieder, J. Lebowitz and E. Lieb: harmonic chain $\kappa \sim L$
- 1984 - G. Casati et al.: ding–a–ling model $\kappa \sim L^0$
- 1997 - S. Lepri, R.L., A. Politi: FPU revisited $\kappa \sim L^{0.4}$
- 1998- B. Hu, B.Li, H. Zhao, FK model $\kappa \sim L^0$

……

For integrable system:

The heat conductivity is a linear function of the system size

$$\kappa \sim L$$

Fourier heat conduction Law is not obeyed, the heat conduction is anomalous.

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

For momentum non-conserving systems

$$\kappa \sim L^0$$

Fourier heat conduction Law is obeyed,
the heat conduction is normal

G. Casati, J. Ford, F. Vivaldi, and W.M. Visscher, PRL 52, 1861 (1984);
T. Prosen and M. Robnik, J. Phys. A 25, 3449 (1992).
B. Hu, B. Li, and H. Zhao, PRE 57, 2992 (1998);
B. Hu, B. Li, and H. Zhao, PRE 61,3828 (2000);
S. Lepri, et al, Phys. Rep. 377, 1 (2003);
A. Dhar, Adv. Phys. 57, 457 (2008)

For momentum conserving nonlinear system

3d $\kappa \sim L^0$ (**normal** heat conduction)

PRL 104, 040601 (2010); PRL 105, 160601 (2010).

$$\left\{\begin{array}{ll} \text{2d} & \kappa \sim \ln(L) \\ \text{1d} & \kappa \sim L^{\alpha} \end{array}\right.$$

2d: (**anomalous** heat conduction)

1d: (**anomalous** heat conduction) $\alpha > 0$

(For 1D integrable case, $\kappa \sim L$)

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

For **1D** momentum conserving non-integrable system

$$\kappa \sim L^{\alpha} \qquad \alpha > 0$$ (**anomalous** heat conduction)

Universality of the exponent α

Renormalization group analysis $\alpha = \frac{1}{3}$

PRL 89, 200601 (2002)

Kinetic theory $\alpha = \frac{2}{5}$

PRE 68, 056124 (2003), Commun. Pure Appl.Math. 61,1753 (2008)

Mode coupling theory

$$\begin{cases} \alpha = \frac{1}{3} & \text{(for asymmetric potential)} \\ \alpha = \frac{1}{2} & \text{(for symmetric potential)} \end{cases}$$

PRE 73, 060201(R) (2006); J.Stat. Mech. (2007) P02007.

Phys. Rep. 377, 1 (2003); Adv. Phys. 57, 457 (2008), PRL 108, 180601 (2012).

Recent numerical results in contradiction with the theories

Normal heat conduction is observed in
1D momentum conserving **lattice** models
with **asymmetric** interparticle interactions.

Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, Phys. Rev. E 85, 060102(R) (2012).

S. Chen, Y. Zhang, J. Wang, and H. Zhao, arXiv:1204.5933 (2012).

Y. Zhong, Y. Zhang, J. Wang, and H. Zhao,. *Chin. Phys. B* 22, 070505 (2013).

A. V. Savin and Y. A. Kosevich, Phys. Rev. E 89, 032102 (2014).

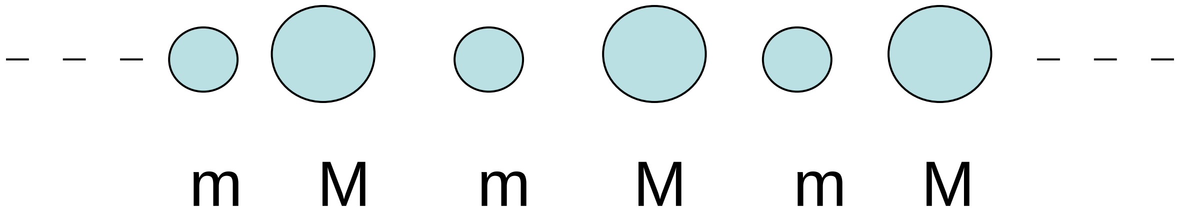
Our recent progress:

when a 1D momentum-conserving system
is **close to its integrable limit,**
Normal heat conduction could be observed ,
for a wide range of system size,
for both **gas** and **lattice** models.

S. Chen, J. Wang, G. Casati, and G. Benenti, *Phys. Rev. E* 90, 032134 (2014)

Models

(1) 1D diatomic hard-point gas (Particle number density is 1, L=N)



(m=1)

If M=m, the system is integrable.

If M>m, the system is non-integrable.

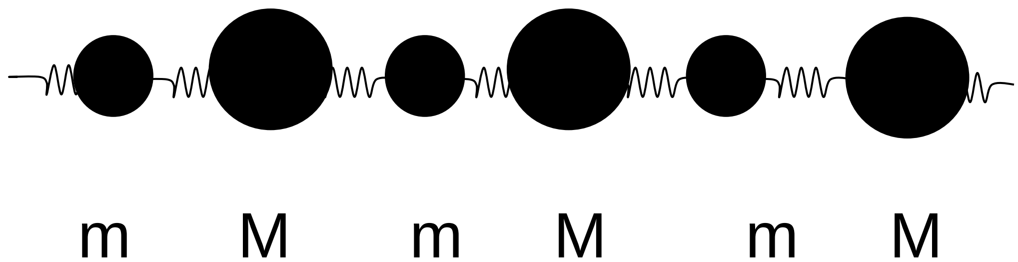
S. Chen, J. Wang, G. Casati, and G. Benenti, *Phys. Rev. E* 90, 032134 (2014).

Models

(2) 1D diatomic Toda Lattice

(Particle number density is 1, L=N)

(m=1)



$$H = \sum_i \frac{p_i^2}{2m} + V(x_i - x_{i-1} - 1) \quad \text{with } V(x) = \exp(-x) + x$$

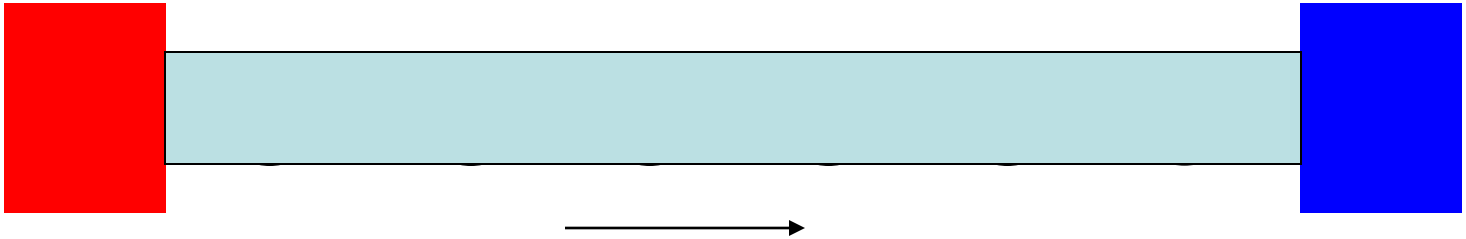
If M=m, the system is integrable.

If M>m, the system is non-integrable.

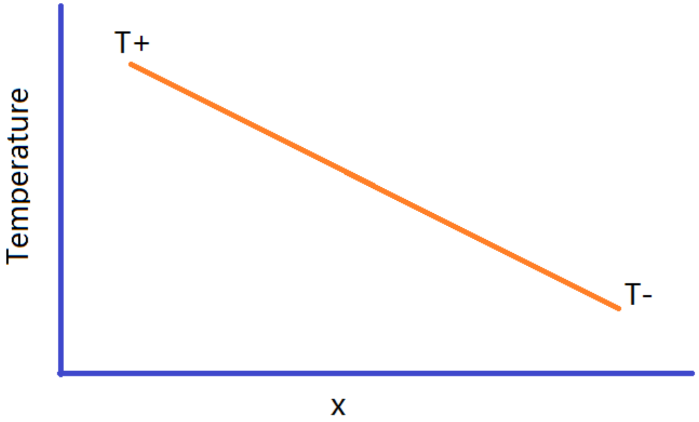
S. Chen, J. Wang, G. Casati, and G. Benenti, *Phys. Rev. E* 90, 032134 (2014).

Methods

(1) Nonequilibrium simulations



Heat bath T_H Heat flux J Heat bath T_L



Maxwellian heat baths for gas model

Langevin heat baths for lattice model

$$J = -\kappa \nabla T \rightarrow \kappa \approx -\frac{JL}{\Delta T}$$

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Methods

(2) Equilibrium simulations

Green-Kubo formula:

$$\kappa_{GK} = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{T^2 N}\int_0^{\tau} < J(t)J(0) > dt \ ,$$

$$J(t) = \sum_{i=1}^{N} J_i(t)$$

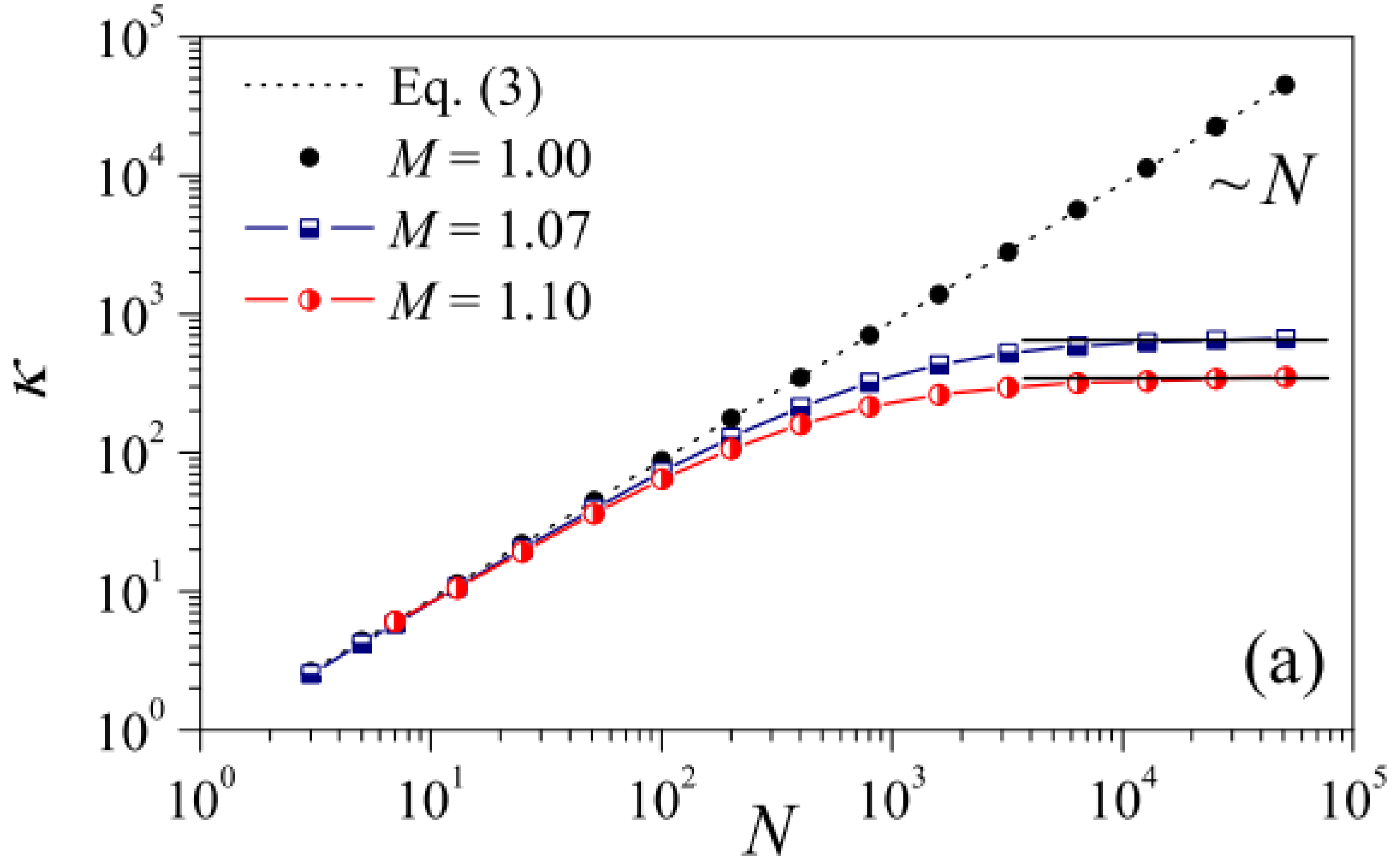
$$< J(t)J(0) > / N \sim t^{-\gamma} \quad \begin{cases} 0 \le \gamma \le 1 & \text{anomalous heat conduction} \\ \gamma > 1 & \text{normal heat conduction} \end{cases}$$

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Results

Results of Nonequilibrium simulations for Harf-point gas model

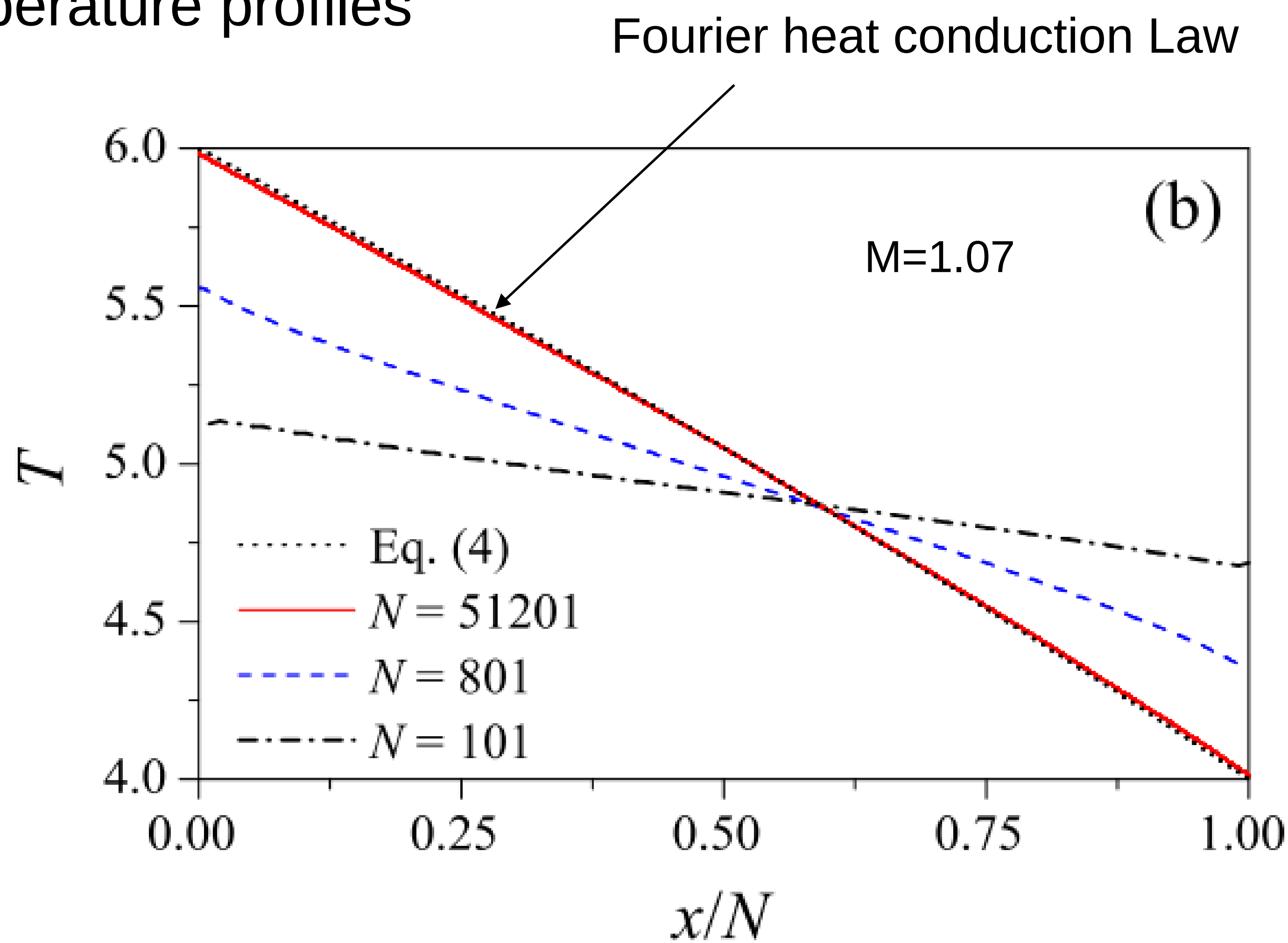
(m=1)



$$\kappa_{\text{int}} = N\sqrt{\frac{2k_B^3}{m\pi}} \Bigg/ \left(\frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}}\right). \qquad (3)$$

Phys. Rev. E 90, 032134 (2014)

Temperature profiles



(m=1)

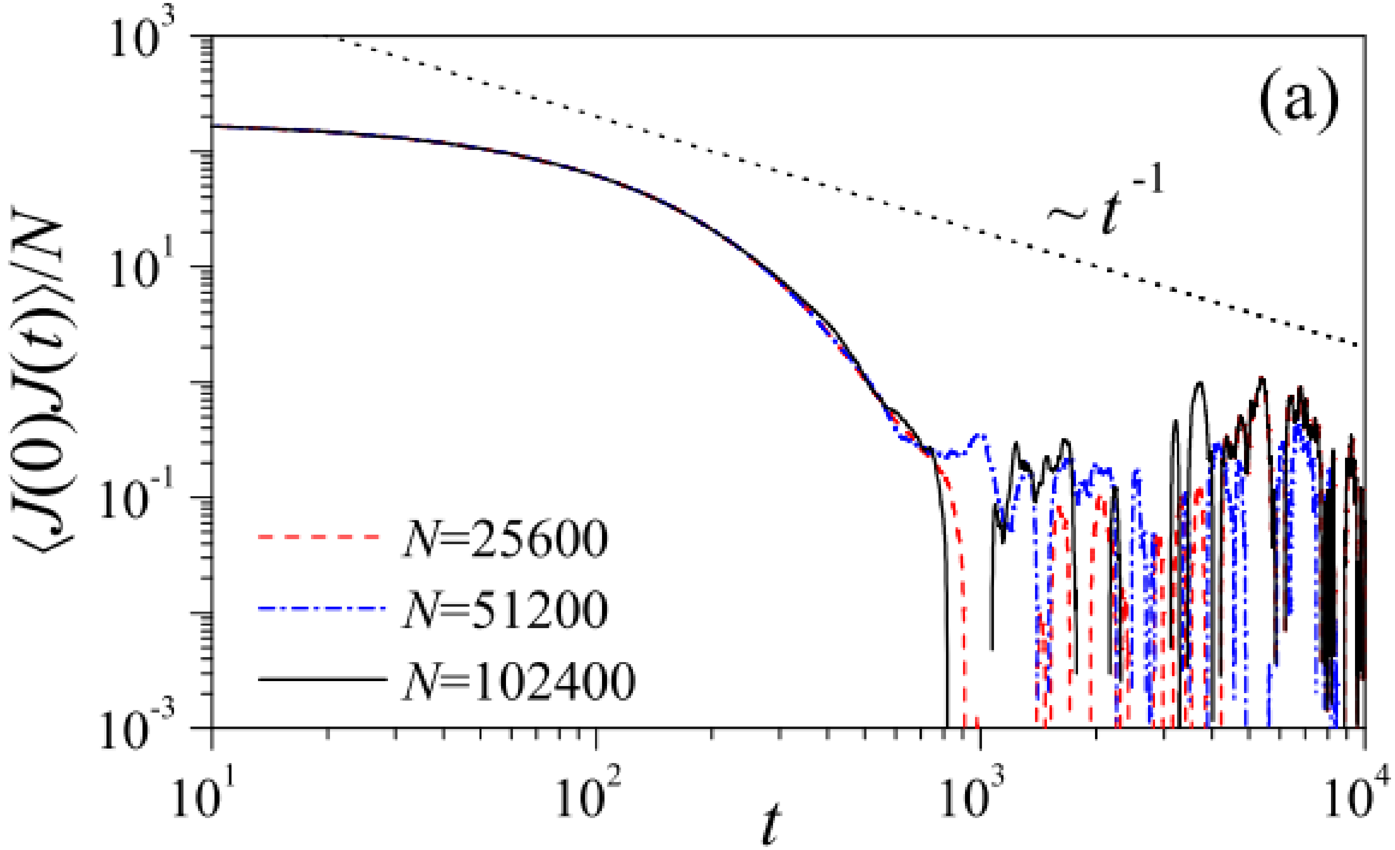
$$T(x) = \left[T_L^{3/2} \left(1 - \frac{x}{N} \right) + T_R^{3/2} \frac{x}{N} \right]^{2/3}. \qquad (4)$$

Phys. Rev. E 90, 032134 (2014)

Results of equilibrium simulations for Harf-point gas model

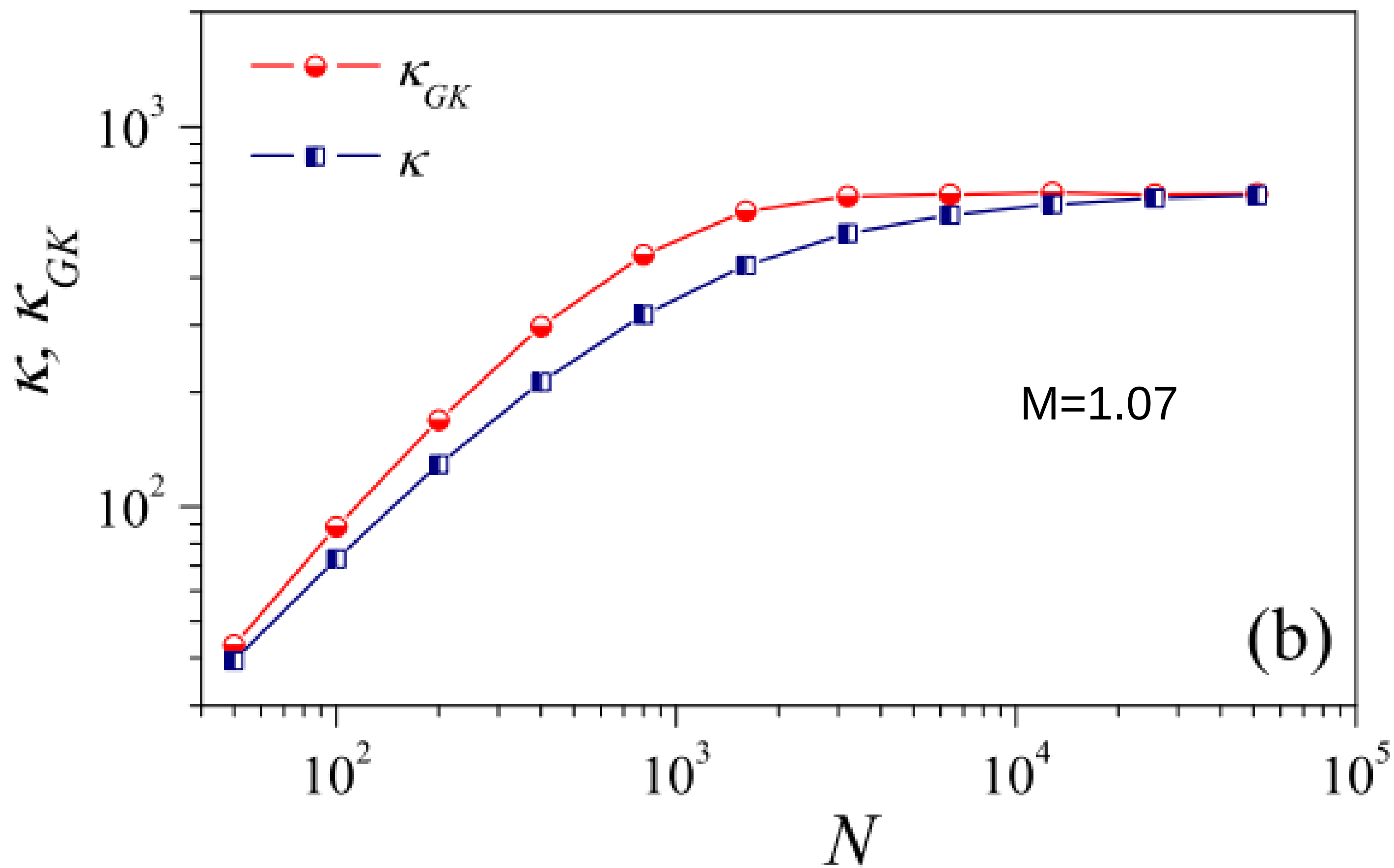
Current correlation functions M=1.07 (m=1)

Fast decay!

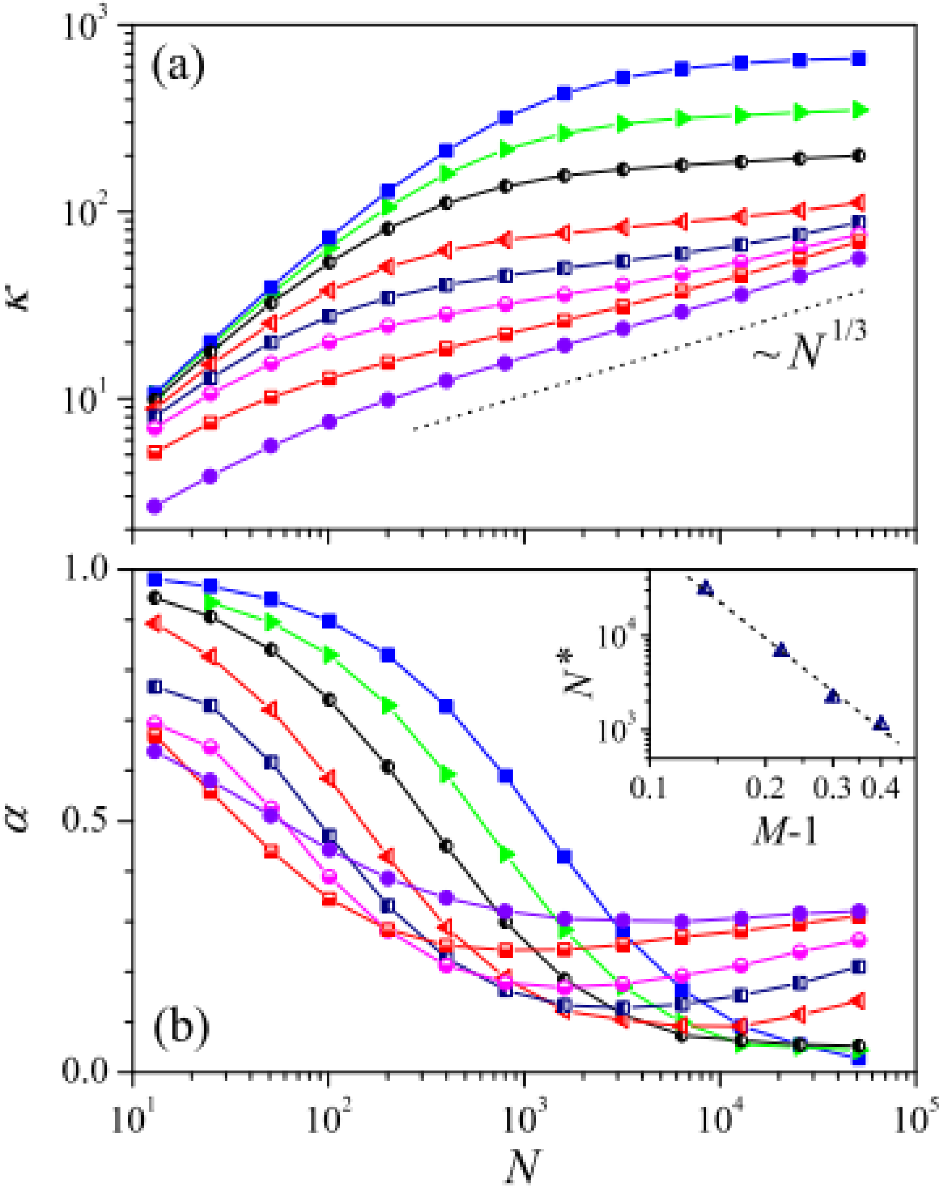


Phys. Rev. E 90, 032134 (2014)

Results for Harf-point gas model



Phys. Rev. E 90, 032134 (2014)



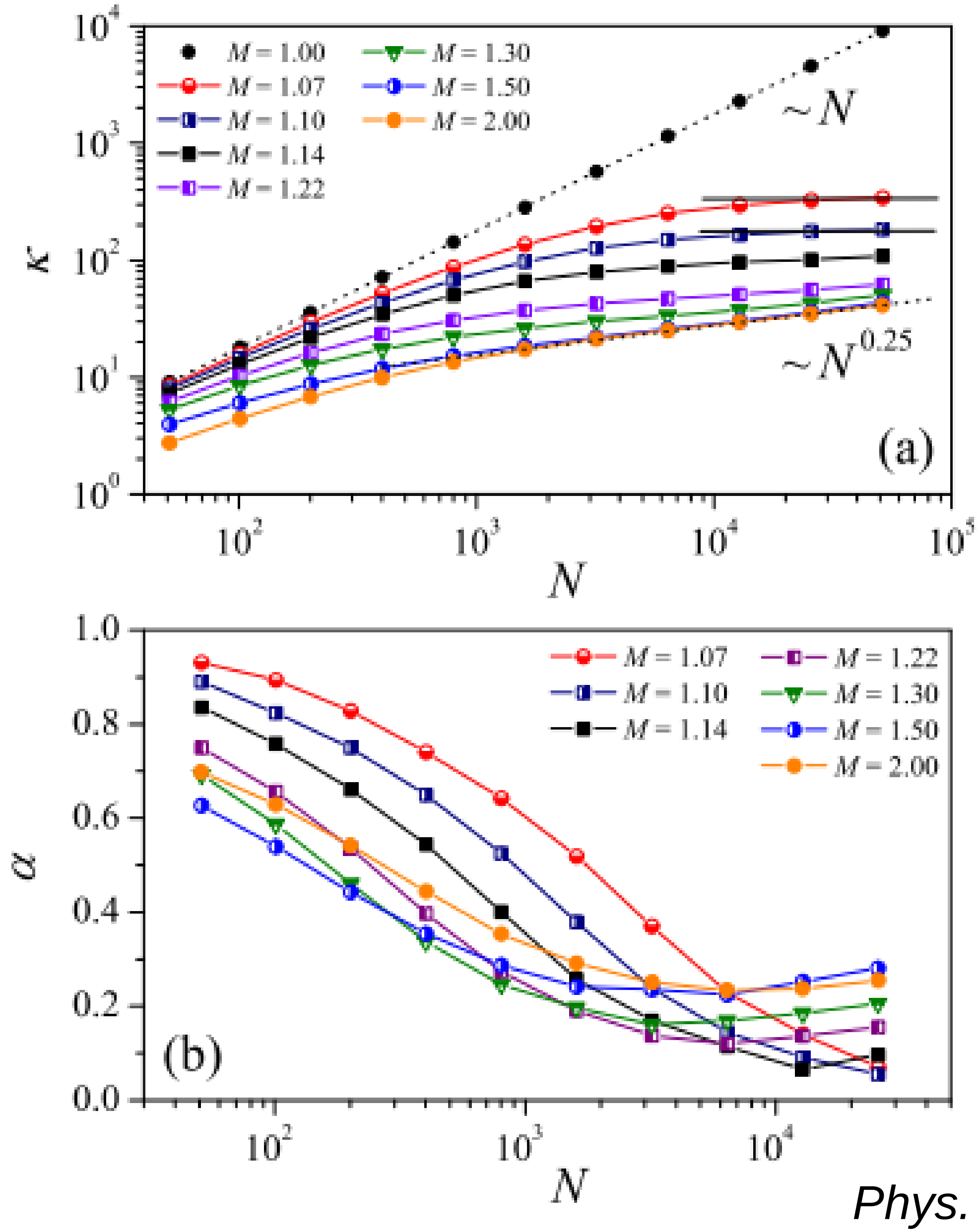
(m=1)

M is, respectively,
1.07, 1.10, 1.14, 1.22, 1.30, 1.40,
the golden mean (≈1.618), and 3.
(From top to bottom)

The corresponding tangent α
of the κ-N curve is given
in (b) with the same symbols.

Phys. Rev. E 90, 032134 (2014)

Results of Nonequilibrium simulations for diatomic Toda lattice



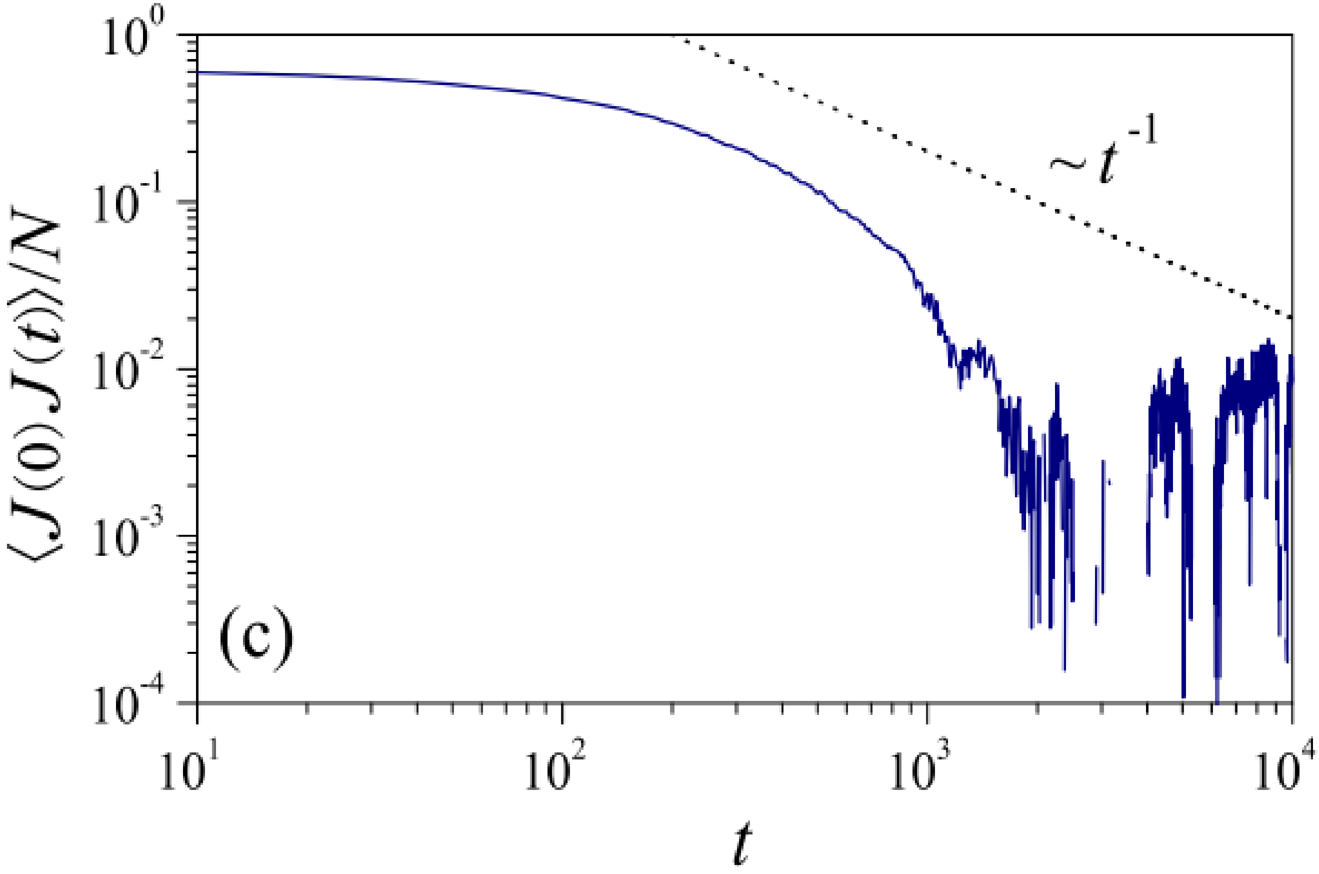
Phys. Rev. E 90, 032134 (2014)

Results of equilibrium simulations for diatomic Toda lattice

Current correlation functions

M=1.07

Fast decay!



Phys. Rev. E 90, 032134 (2014)

Summary

Heat conduction problem is a very **old problem**.

The microscopic ingredients for Fourier heat conduction law are still not clear.

Fourier heat conduction law is obeyed in 1D momentum-conserving systems, for a wide range of system size, when the system is **close to integrable limit**.

This is a new connection between the macroscopic thermal transport properties and the underlying nonlinear dynamics. (More efforts are needed to reveal the deeper underlying mechanisms.)

Thanks！

All the standard theories of transport involve uncontrolled approximations and do not provide a “proof” of Fourier’s law.

Mode-coupling theory---1

$$\kappa \propto \lim_{t\to\infty} \int_0^t \langle J(\tau)J(0)\rangle \,\mathrm{d}\tau \tag{36}$$

where $J(t)$ is the total heat current, and $\langle\cdots\rangle$ brackets denote the equilibrium average. A general expression for the heat current has been derived in [11]. For the determination of the scaling behaviour it is sufficient to consider only the harmonic part, which can be expressed as a sum over wavevectors:

$$J = \sum_q b(q)Q(q,t)P^*(q,t) \tag{37}$$

where $Q(q,t)$, and $P(q,t) = \dot{Q}(q,t)$ are the canonical variables in Fourier space and

$$b(q) = \mathrm{i}\omega(q)\frac{\partial\omega(q)}{\partial q}. \tag{38}$$

This amounts to disregarding higher-order terms which are believed not to modify the leading behaviour. Under the same approximations as allow deriving the mode-coupling equations, i.e. by neglecting correlations of order higher than two, one obtains

$$\langle J(t)J(0)\rangle = \sum_q |b(q)|^2\{\langle Q(q,t)Q(q,0)\rangle\langle P(q,t)P^*(q,0)\rangle + \langle Q(q,t)P^*(q,0)\rangle^2\}. \tag{39}$$

Mode-coupling theory- ---2

This expression can be further simplified under the assumption $P(q) \approx \omega(q)Q(q)$, which is certainly valid in the small-q limit. Altogether, this leads to the expression proposed in [17],

$$\langle J(t)J(0)\rangle \propto \sum_q \left(\frac{\mathrm{d}\omega(q)}{\mathrm{d}q}\right)^2 G^2(q,t). \tag{40}$$

The main observable we are interested in is the normalized correlator $G(q,t) = \langle Q^*(q,t)Q(q,0)\rangle / \langle |Q(q)|^2\rangle$, where $Q(q,t)$ is the Fourier transform of the displacement field $u_i(t)$. Assuming periodic boundary conditions for a chain made of N sites, the wavenumber is given by $q = 2\pi k/N$, with $-N/2+1 \leq k \leq N/2$. Notice also that $G(q,t) = G(-q,t)$. We simplify the notation by setting to unity the particle mass, the lattice spacing and the bare sound velocity. The equations for the correlator $G(q,t)$ then read [25, 15]

$$\ddot{G}(q,t) + \varepsilon \int_0^t \Gamma(q,t-s)\dot{G}(q,s)\,\mathrm{d}s + \omega^2(q)G(q,t) = 0 \tag{2}$$

where the memory kernel $\Gamma(q,t)$ is proportional to $\langle \mathcal{F}(q,t)\mathcal{F}(q,0)\rangle$ with $\mathcal{F}(q)$ being the non-linear part of the fluctuating force between particles. Equations (2) must be solved with the initial conditions $G(q,0) = 1$ and $\dot{G}(q,0) = 0$. Equations (2) are exact and they are derived within the well-known Mori–Zwanzig projection approach [24].

The mode-coupling approach basically amounts to replacing the exact memory function Γ with an approximate one, where higher-order correlators are written in terms of $G(q,t)$. This yields a closed system of non-linear integro-differential equations. For potentials like (1) this has been worked out in detail in references [25, 15]. Both the

“Heat, like gravity, penetrates every substance of the universe, its ray occupy all parts of space. “

The theory of of heat will hereafter form one of **the most important branches of general physics** …

“But whatever may be the range of **mechanical theories**, they **do not apply to the effects of heat**. These make up a special order of phenomena, which cannot be explained by the principles of motion and equilibria”

Jean Baptiste Joseph Fourier (1768-1830)

“Theorie analytique de la chaleur”
（ “The Analytical Theory of Heat”）

“It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of (electrically) nonconducting crystals.”

R. E. Peierls (1961),
Theoretical Physics in the Twentieth Century.

Los Alamos, Summers 1953-4 Enrico Fermi, John Pasta, and Stan Ulam decided to use the world's then most powerful computer, the

MANIAC-1

(Mathematical Analyzer Numerical Integrator And Computer)

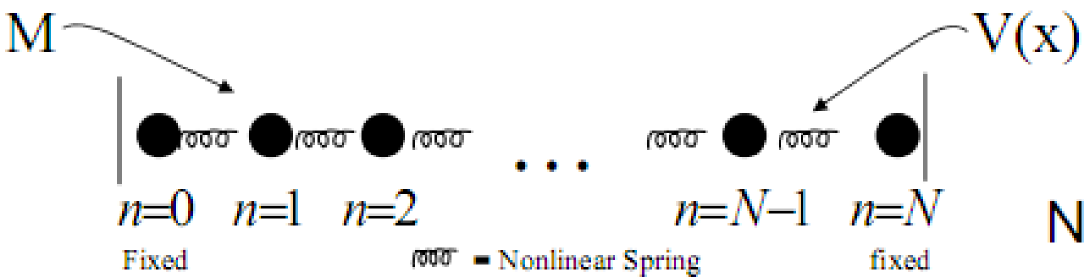
to study the equipartition of energy expected from statistical mechanics in the simplest classical model of a solid: a ID chain of equal mass particles coupled by *nonlinear** springs. Fermi expected "these were to be studied preliminary to setting up ultimate models …where "mixing" and "turbulence" could be observed. The motivation then was to observe the *rates* of the mixing and thermalization with the hope that the calculational results would provide hints for a future theory." [S. Ulam].

*They knew linear springs could not produce equipartition

Aside: Birth of computational physics ("experimental mathematics")

(D.K. Campbell's slide)

- FPU model



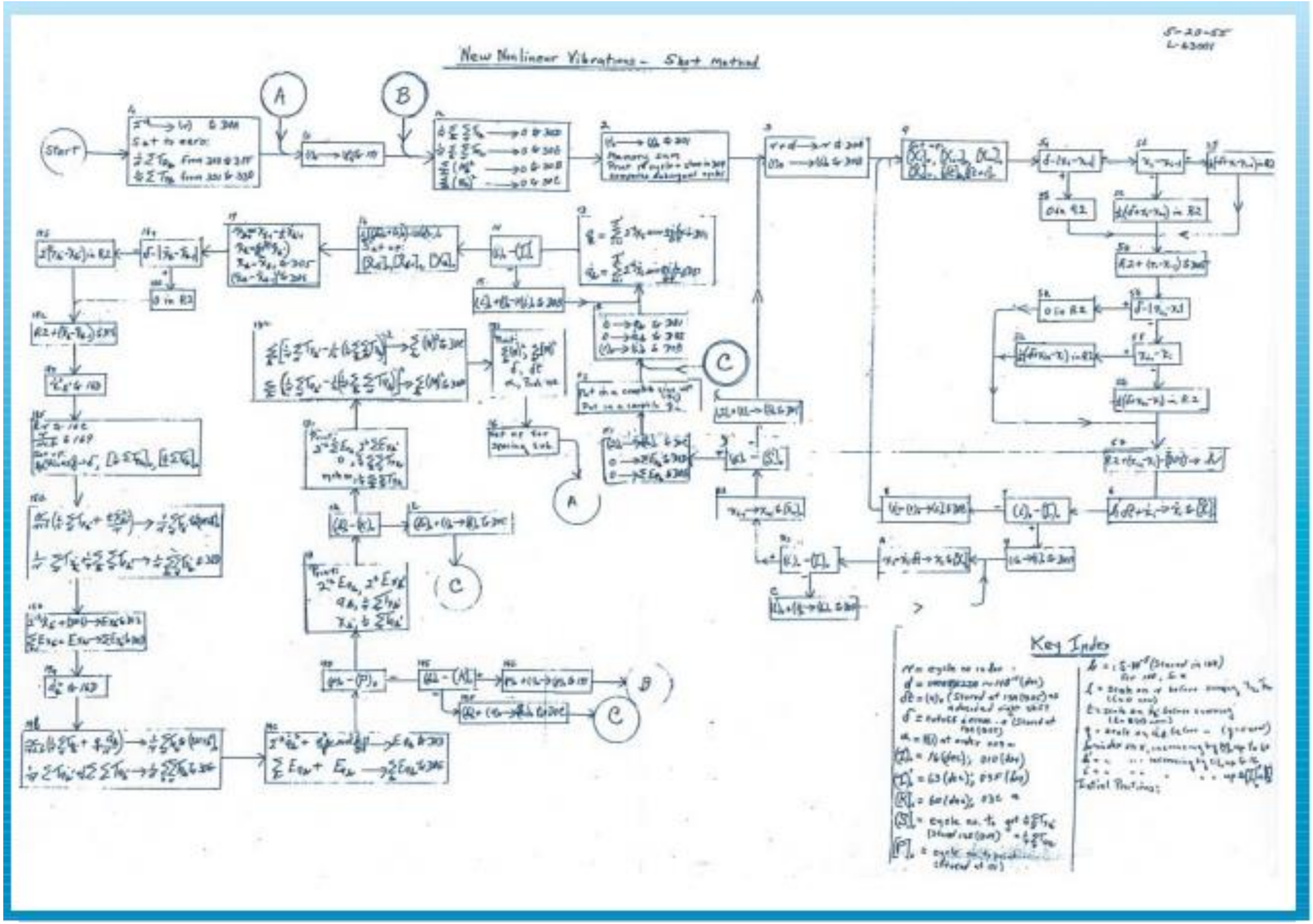
N=32, 64

$$V(x) = \frac{1}{2} kx^2 + \alpha/3\, x^3 + \beta/4\, x^4$$

"The results of the calculations (performed on the old MANIAC machine) were interesting and quite surprising to Fermi. He expressed to me the opinion that they really constituted a little discovery in providing limitations that the prevalent beliefs in the universality of "mixing and thermalization in *non-linear* systems may not always be justified."

[S. Ulam]

(D.K. Campbell's slide)



(The algorithm used to code the first numerical experiment.)

T. Dauxois, [Phys. Today, **61**, 1, 55 (2008)].

For integrable system:

The heat conductivity is a linear function of the system size

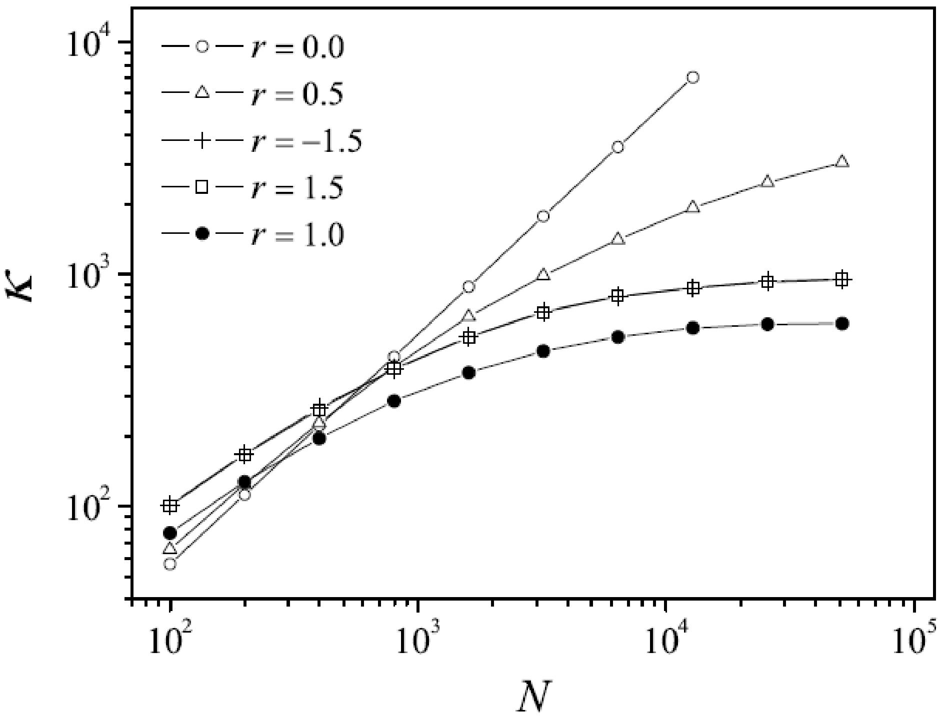
$$\kappa \sim L$$

Fourier heat conduction Law is not obeyed, the heat conduction is anomalous.

S. Lepri, et al, Phys. Rep. 377, 1 (2003); A. Dhar, Adv. Phys. 57, 457 (2008)

Recent numerical results in contradiction with the theories

$$H = \sum_i \frac{p_i^2}{2m} + V(x_i - x_{i-1} - 1) \text{ with } V(x) = \frac{1}{2}(x+r)^2 + e^{-rx}$$



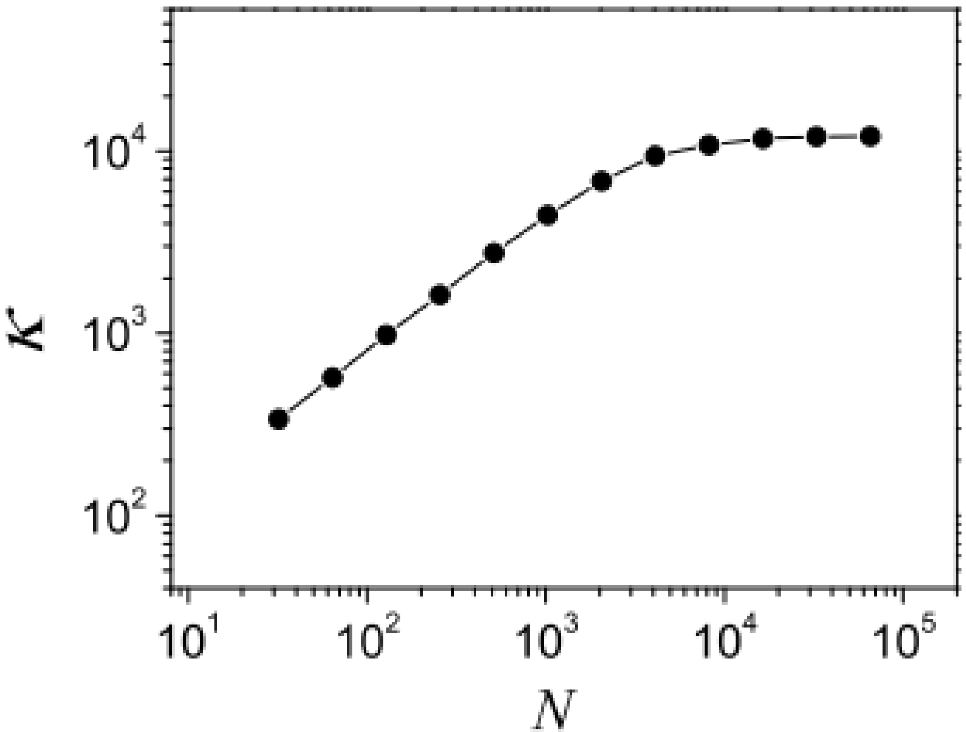
Normal heat conduction is observed in an 1D momentum conserving **lattice** model with **proper asymmetric interparticle interaction**

Y. Zhong *et al*, PRE **85**, 060102(R) (2012)

Recent numerical results in contradiction with the theories

$$H = \sum_i \frac{p_i^2}{2m} + V(x_i - x_{i-1} - 1)$$

$$\text{with } V(x) = [(\frac{x_c}{x+x_c})^m - 2(\frac{x_c}{x+x_c})^n + 1]$$



Normal heat conduction is observed in 1d momentum conserving Lennard-Jones lattice

S. Chen *et.al.*, arXiv:1204.5933V2 (2012)

Recent numerical results in contradiction with the theories

Normal heat conduction is observed in
1D momentum conserving **lattice** models
with **asymmetric** interparticle interactions.

Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, Phys. Rev. E 85, 060102(R) (2012).

S. Chen, Y. Zhang, J. Wang, and H. Zhao, arXiv:1204.5933 (2012).

Y. Zhong, Y. Zhang, J. Wang, and H. Zhao,. *Chin. Phys. B* 22, 070505 (2013).

A. V. Savin and Y. A. Kosevich, Phys. Rev. E 89, 032102 (2014).

Our more recent progress:

The heat conductivity may keep significantly unchanged over a certain range of the system size in 1D momentum-conserving systems, for a wide range of system size, when the system is close to integrability.

The range for observing Fourier heat conduction behavior may expand rapidly, as the system tends to integrability

S. Chen, J. Wang, G. Casati, and G. Benenti, *Phys. Rev. E* 90, 032134 (2014).

Methods

Equilibrium simulations

(with periodic boundary condition)

Green-Kubo formula:

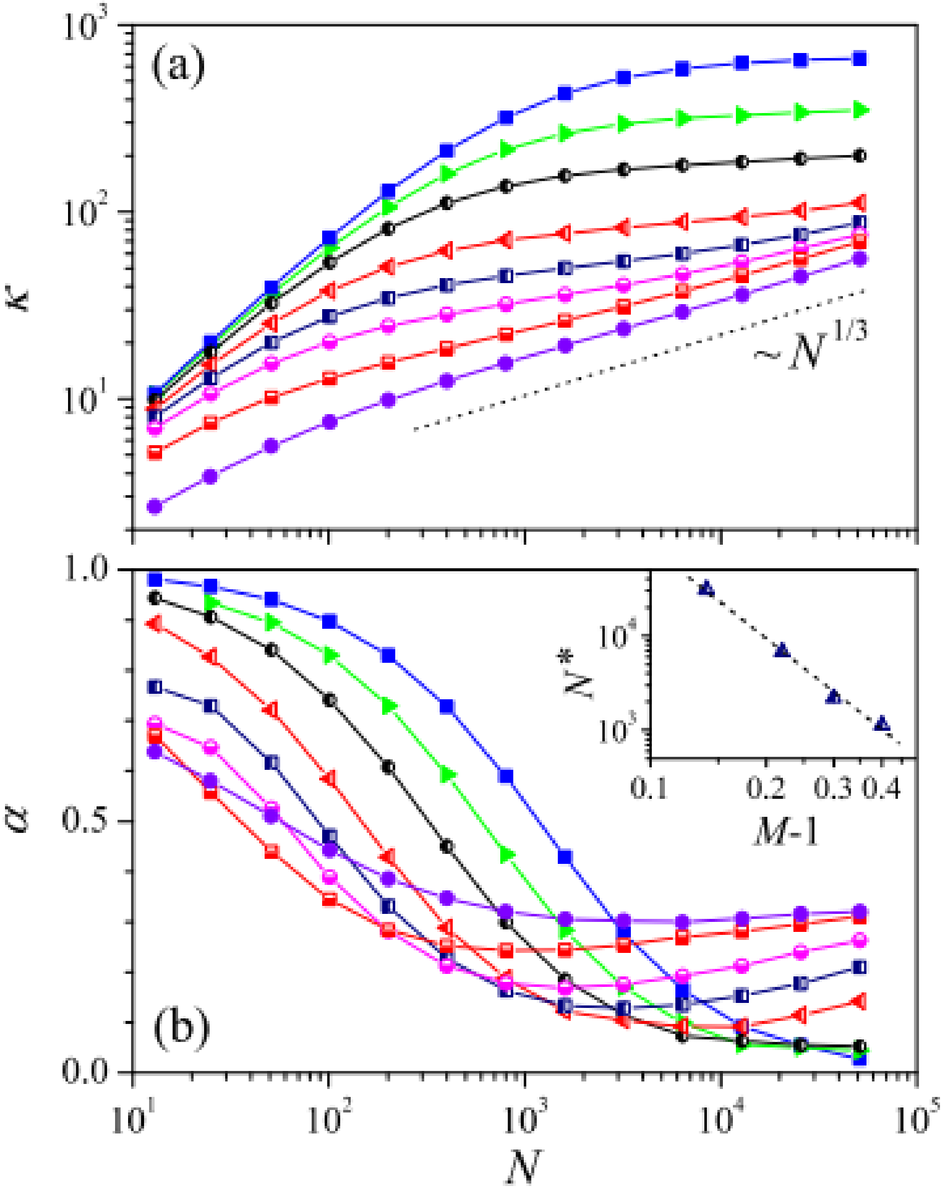
$$\kappa_{GK} = \lim_{\tau\to\infty}\lim_{N\to\infty}\frac{1}{T^2 N}\int_0^{\tau} < J(t)J(0) > dt \ ,$$

$$J(t) = \sum_{i=1}^{N} J_i(t)$$

S. Chen et.al, *PRE* **89**, 022111 (2014).

$\tau \sim \dfrac{N}{2v_s}$, v_s is sound velocity

$$< J(t)J(0) > / N \sim t^{-\gamma} \quad \begin{cases} 0 \le \gamma \le 1 & \text{anomalous heat conduction} \\ \gamma > 1 & \text{normal heat conduction} \end{cases}$$



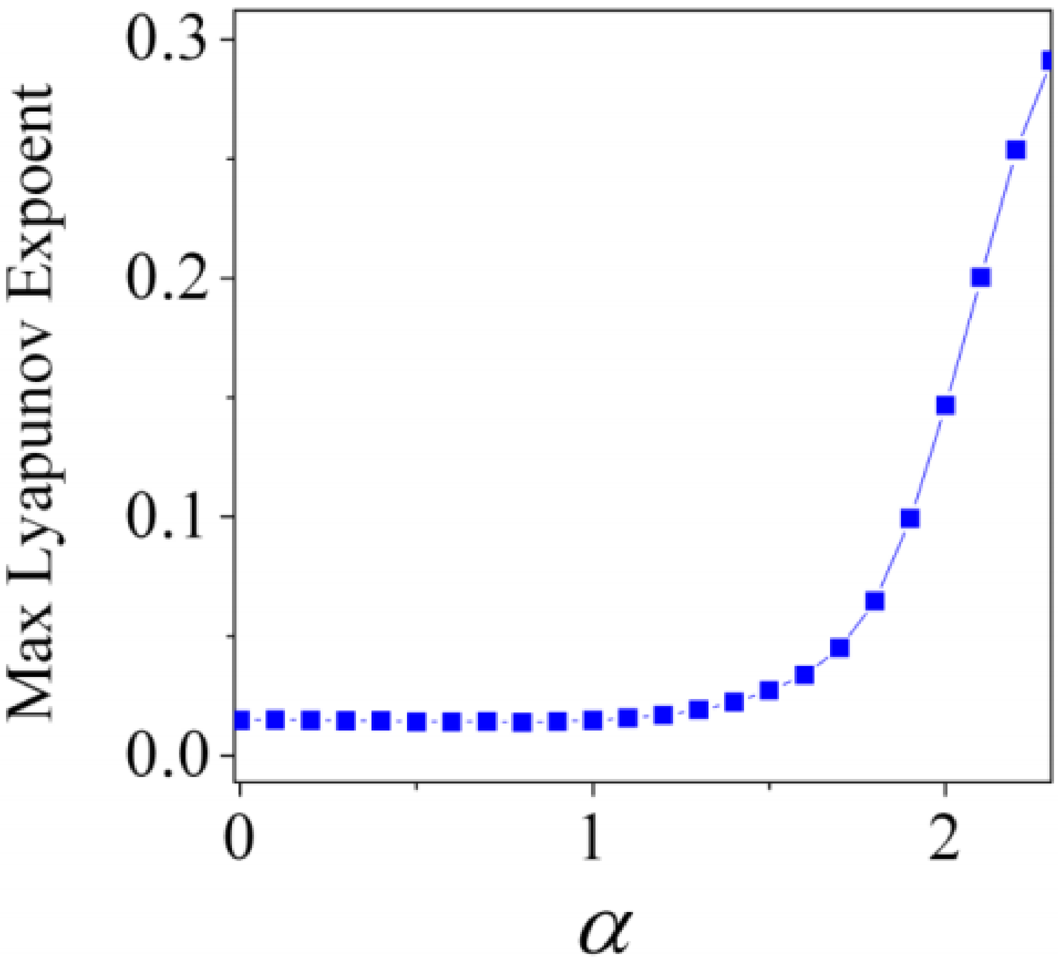
(m=1)

M is, respectively,
1.07, 1.10, 1.14, 1.22, 1.30, 1.40,
the golden mean (≈1.618), and 3.
(From top to bottom)

The turning point N_*, after which
α starts growing with N,
as a function of M − 1.
The best fitting (the dotted line)
Suggests $N_* = 54/(M - 1)^{3.2}$
.

The corresponding tangent α
of the κ-N curve is given
in (b) with the same symbols.

Phys. Rev. E 90, 032134 (2014)



0.3
0.2
0.1
0.0
Max Lyapunov Expoent
0
1
2
α

INTEGRABLE SYSTEMS

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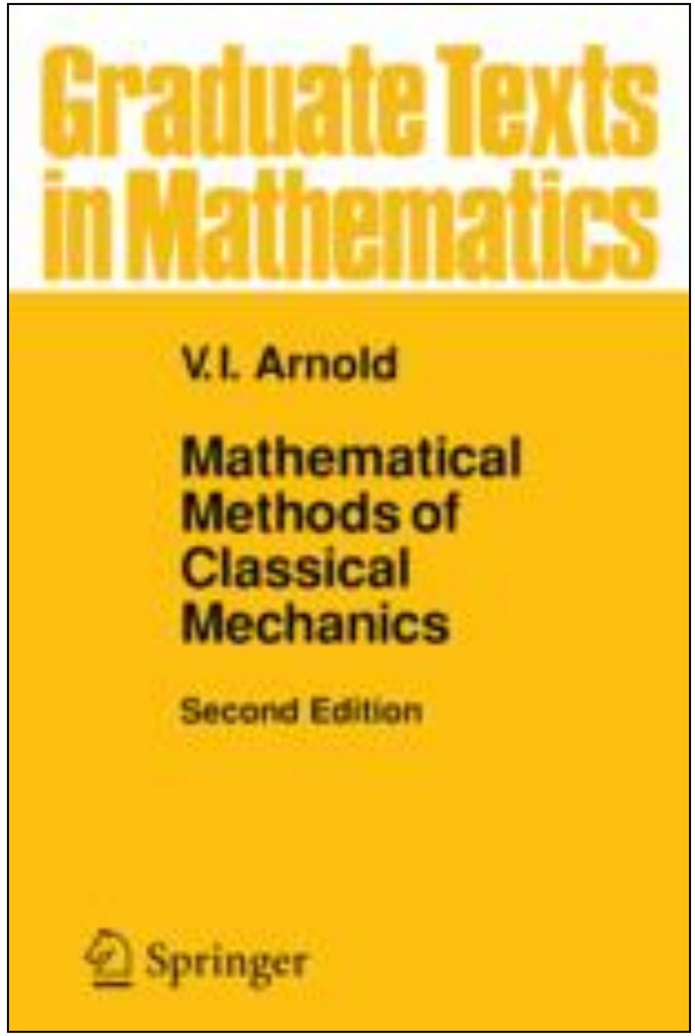
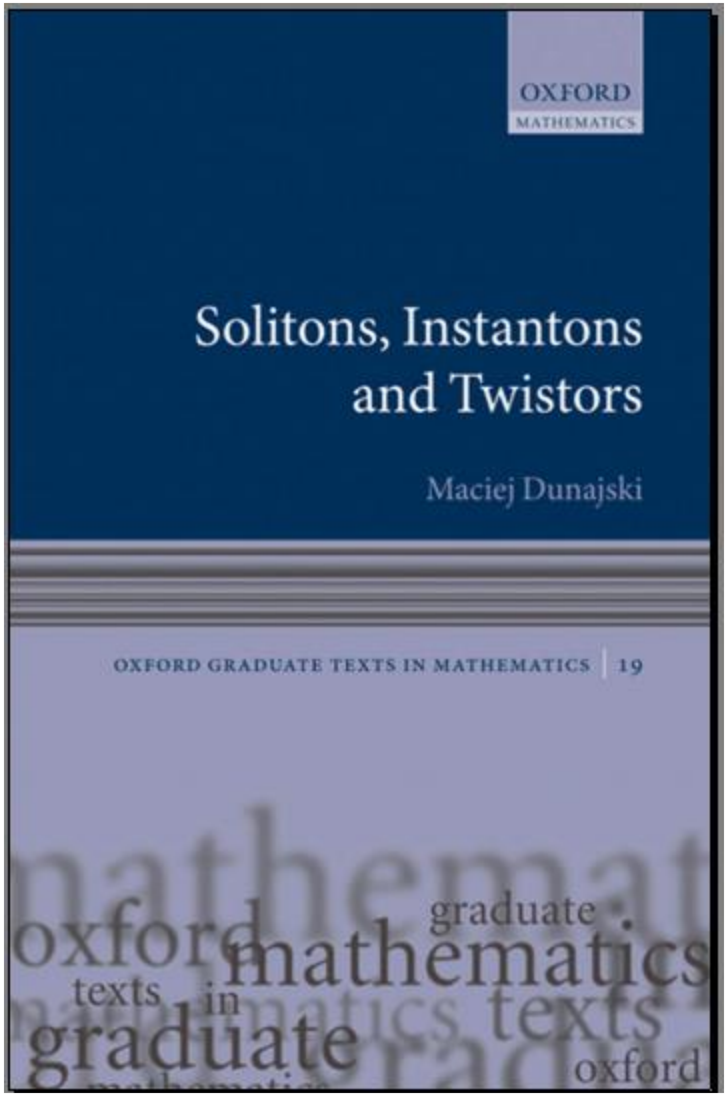


V. I. Arnold, (1989) Mathematical Methods of Classical Mechanics., second edition. Graduate Texts in Mathematics, 60, Springer.



Maciej Dunajski (2009) Solitons, Instantons and Twistors, Oxford Graduate Texts inMathematics 19, OUP, Oxford.

Integrable systems are nonlinear differential equations which 'in principle' can be solved analytically. This means that the solution can be reduced to a finite number of algebraic operations and integrations. Such systems are very rare - most nonlinear differential equations admit chaotic behaviour and no explicit solutions can be written down. Integrable systems nevertheless lead to a very interesting mathematics ranging from differential geometry and complex analysis to quantum field theory and fluid dynamics. The main reference for the course is [6]. There are other books which cover particular topics treated in the course:

- **Integrability of ODEs** [4] (Hamiltonian formalism, Arnold–Liouville theorem, action–angle variables). The integrability of ordinary differential equations is a fairly clear concept (i.e. it can be defined) based on existence of sufficiently many well behaved first integrals, or (as a physicist would put it) constant of motions.

- **Integrability of PDEs** [15], [5](Solitons, Inverse Scattering Transform). The universally accepted definition of integrability does not exist in this case. The phase space is infinite dimensional but having 'infinitely many' first integrals may not be enough - we could have missed every second one. Here one focuses on properties of solutions and solutions generation techniques. We shall study solitons - solitary non-linear waves which preserve their shape (and other characteristics) in the evolution. These soliton solutions will be constructed by means of an inverse problem: recovering a potential from the scattering data.

- **Lie symmetries** [9], [16] (Group invariant solutions, vector fields, symmetry reduction, Painlevé equations). The powerful symmetry methods can be applied to ODEs and PDEs alike. In case of ODEs a knowledge of sufficiently large symmetry group allows a construction of the most general solution. For PDEs the knowledge of symmetries is not sufficient to construct the most general solution, but it can be used to find new solutions from given ones and to reduce PDEs to more tractable ODEs. The PDEs integrable by inverse problems reduce to equations with Painlevé property.

Integrable systems are nonlinear differential equations which 'in principle' can be solved analytically. This means that the solution can be reduced to a finite number of algebraic operations and integrations. Such systems are very rare - most nonlinear differential equations admit chaotic behaviour and no explicit solutions can be written down. Integrable systems nevertheless lead to a very interesting mathematics ranging from differential geometry and complex analysis to quantum field theory and fluid dynamics. The main reference for the course is [6]. There are other books which cover particular topics treated in the course:

- **Integrability of ODEs** [4] (Hamiltonian formalism, Arnold–Liouville theorem, action–angle variables). The integrability of ordinary differential equations is a fairly clear concept (i.e. it can be defined) based on existence of sufficiently many well behaved first integrals, or (as a physicist would put it) constant of motions.

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Maciej Dunajski (2009) Solitons, Instantons and Twistors, Oxford Graduate Texts inMathematics 19, OUP, Oxford.

Integrability in classical mechanics

Integrable systems are non-linear differential equations (DEs) which 'in principle' can be solved analytically. This means that the solution can be reduced to a finite number of algebraic operations and integrations. Such systems are very rare – most non-linear DEs admit chaotic behaviour and no explicit solutions can be written down. Integrable systems nevertheless lead to very interesting mathematics ranging from differential geometry and complex analysis to quantum field theory and fluid dynamics. In this chapter we shall introduce the integrability of ordinary differential equations (ODEs). This is a fairly clear concept based on existence of sufficiently many well-behaved first integrals, or, as a physicist would put it, constants of the motion.