Nonintegrability and the Fourier Heat conduction Law

Shunda Chen
Center for Nonlinear and Complex systems
University of Insubria, Como, Italy
Shunda.chen@uninsubria.it
Collaborators

Center for Nonlinear and Complex systems
University of Insubria, Como, Italy

Prof. Giuliano Benenti
Prof. Giulio Casati

Complex Systems Group
Xiamen University, Xiamen, China

Prof. Hong Zhao
Prof. Jiao Wang
Prof. Yong Zhang
Prof. Dahai He
Outline

1. Introduction
2. Our recent progress
   2.1 Models and methods
   2.2 Results
3. Summary
Fourier Heat Conduction Law (1808)

\[ J = -\kappa \nabla T \]

- **\( J \)**: heat flux
- **\( \nabla \)**: temperature gradient
- **\( \kappa \)**: 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.
• FPU model

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

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

(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.

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);
B. Hu, B. Li, and H. Zhao, PRE 57, 2992 (1998);
B. Hu, B. Li, and H. Zhao, PRE 61, 3828 (2000);
For momentum conserving nonlinear system

$$3d \quad \kappa \sim L^0 \quad \text{(normal heat conduction)}$$

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

$$\begin{cases} 
2d \quad \kappa \sim \ln(L) \quad \text{(anomalous heat conduction)} \\
1d \quad \kappa \sim L^\alpha \quad \text{(anomalous heat conduction)} \quad \alpha > 0 
\end{cases}$$

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

For 1D momentum conserving non-integrable system

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

**Universality of the exponent $\alpha$**

- **Renormalization group analysis**
  - $\alpha = \frac{1}{3}$
  - PRL 89, 200601 (2002)

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

- **Mode coupling theory**
  - $\alpha = \frac{1}{3}$ (for asymmetric potential)
  - $\alpha = \frac{1}{2}$ (for symmetric potential)
Recent numerical results in contradiction with the theories

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


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.

Models

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

If $M=m$, the system is integrable.

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

Models

(2) 1D diatomic Toda Lattice  

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

If M=m, the system is integrable.

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

Methods

(1) Nonequilibrium simulations

\[ J = -\kappa \nabla T \rightarrow \kappa \approx -\frac{J_L}{\Delta T} \]

Maxwellian heat baths for gas model

Langevin heat baths for lattice model

Methods

(2) Equilibrium simulations

**Green-Kubo formula:**

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

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

\[
< J(t)J(0) > / N \sim t^{-\gamma}
\]

\[
\begin{cases} 
0 \leq \gamma \leq 1 & \text{anomalous heat conduction} \\
\gamma > 1 & \text{normal heat conduction}
\end{cases}
\]

Results

Results of Nonequilibrium simulations for Harf-point gas model

\[ \kappa = N \sqrt{\frac{2k_B^3}{m\pi}} \left( \frac{1}{\sqrt{T_L}} + \frac{1}{\sqrt{T_R}} \right). \]  

\((m=1)\)

Temperature profiles

Fourier heat conduction Law

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

Eq. (4)

\[ M = 1.07 \]

\[ (m=1) \]
Results of equilibrium simulations for Harf-point gas model

Current correlation functions \( M = 1.07 \)  \( (m=1) \)

Fast decay!

\[ \langle J(0)J(t) \rangle/N \]

\[ 10^{-3} \]

\[ 10^{-1} \]

\[ 10^{1} \]

\[ 10^{3} \]

\[ 10^{5} \]

\[ 10^{7} \]

\[ t \]

\[ 10^{1} \]

\[ 10^{2} \]

\[ 10^{3} \]

\[ 10^{4} \]

\( N = 25600 \)

\( N = 51200 \)

\( N = 102400 \)

\( \sim t^{-1} \)

\( \text{Phys. Rev. E 90, 032134 (2014)} \)
Results for Harf-point gas model

\[ M = 1.07 \]

\[ K, K_{\text{GK}} \]

\[ N \]

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*Phys. Rev. E 90, 032134 (2014)*
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 $\alpha$ of the $\kappa$-N curve is given in (b) with the same symbols.
Results of Nonequilibrium simulations for diatomic Toda lattice

Results of equilibrium simulations for diatomic Toda lattice

Current correlation functions

M = 1.07

Fast decay!

\[ \left\langle J(0)J(t) \right\rangle / N \]

(c)

\( t \)

\( t^{-1} \)

\( t \)

\( 10^0 \)

\( 10^{-1} \)

\( 10^{-2} \)

\( 10^{-3} \)

\( 10^{-4} \)

\( 10^1 \)

\( 10^2 \)

\( 10^3 \)

\( 10^4 \)

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

\[ \kappa \propto \lim_{t \to \infty} \int_0^t \langle J(\tau)J(0) \rangle \, d\tau \]

where \( J(t) \) is the total heat current, and \( \langle \cdot \cdot \cdot \rangle \) 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:

\[ J = \sum_q b(q) Q(q, t) P^*(q, t) \]

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

\[ b(q) = i\omega(q) \frac{\partial \omega(q)}{\partial q}. \]

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

\[ \langle J(t)J(0) \rangle = \sum_q |b(q)|^2 \left\{ \langle Q(q, t)Q(q, 0) \rangle \langle P(q, t)P^*(q, 0) \rangle + \langle Q(q, t)P^*(q, 0) \rangle^2 \right\}. \]
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],

$$\langle J(t)J(0) \rangle \propto \sum_q \left( \frac{d \omega(q)}{dq} \right)^2 G^2(q, t).$$  \hspace{1cm} (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]

$$\ddot{G}(q, t) + \varepsilon \int_0^t \Gamma(q, t - s) \dot{G}(q, s) \, ds + \omega^2(q)G(q, t) = 0$$  \hspace{1cm} (2)

where the memory kernel $\Gamma(q, t)$ is proportional to $\langle F(q, t)F(q, 0) \rangle$ with $F(q)$ 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 $\Gamma$ 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 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”

“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 1D 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

\[ V(x) = \frac{1}{2} kx^2 + \frac{\alpha}{3} x^3 + \frac{\beta}{4} x^4 \]

“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.)

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.

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

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

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

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

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


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.
Methods
Equilibrium simulations
(with periodic boundary condition)

Green-Kubo formula:

\[ \kappa_{\text{GK}} = \lim_{N \to \infty} \lim_{\tau \to \infty} \frac{1}{T^2 N} \int_0^\tau \langle J(t) J(0) \rangle \, dt, \]

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


\[ \tau \sim \frac{N}{2 v_s}, \quad v_s \text{ is sound velocity} \]

\[ \langle J(t) J(0) \rangle / N \sim t^{-\gamma} \]

\[ \gamma \begin{cases} 0 \leq \gamma \leq 1, & \text{anomalous heat conduction} \\ \gamma > 1, & \text{normal heat conduction} \end{cases} \]
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 $\alpha$ 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 $\alpha$ of the $\kappa$-$N$ curve is given in (b) with the same symbols.
INTEGRABLE SYSTEMS

Maciej Dunajski

Department of Applied Mathematics and Theoretical Physics
University of Cambridge
Wilberforce Road, Cambridge CB3 0WA, UK
Integrable systems are nonlinear differential equations which ‘in principle’ can be solved analyti-
cally. 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 con-
cept (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 analyti-
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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.

Maciej Dunajski (2009) Solitons, Instantons and Twistors, Oxford Graduate
Texts in Mathematics 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.