Puzzles in the theory of heat conduction in low-dimensional systems

Abhishek Dhar
International centre for theoretical sciences
TIFR, Bangalore

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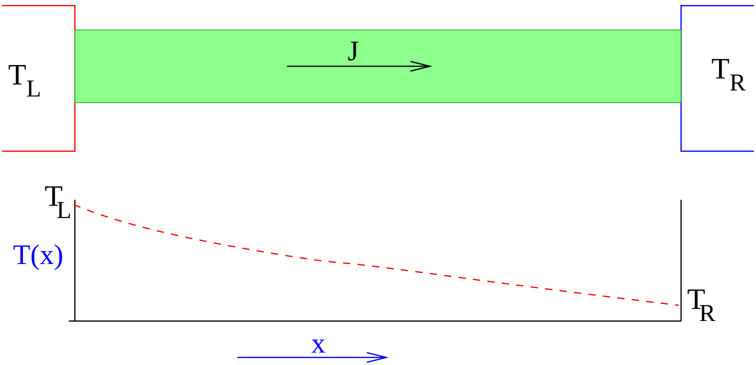
Outline

- Introduction
- Heat transport in one-dimensional systems
  - Heat transport in interacting (anharmonic) lattices
  - Description in terms of Levy walk model and fractional diffusion equation.
  - Fluctuating Hydrodynamics
  - Heat transport in disordered harmonic lattices
- Three-dimensional systems
- Discussion

Heat transfer through a body from HOT to COLD region.



Fourier's law

Fourier's law of heat conduction

$$J = -\kappa \nabla T(x)$$

κ – thermal conductivity of the material.

Using Fourier's law and the energy conservation equation

$$\frac{\partial \epsilon}{\partial t} + \nabla J = 0$$

and, writing $\partial \epsilon / \partial t = c \partial T / \partial t$ where $c = \partial \epsilon / \partial T$ is the specific heat capacity, gives the heat DIFFUSION equation:

$$\frac{\partial T}{\partial t} = \frac{\kappa}{c} \nabla^2 T \, .$$

Thus Fourier's law implies diffusive heat transfer.

Fourier's law

Joseph Fourier (∼ 1810).

- Use of PDEs' in formulating physical problems.
- Fourier Transforms.
- Fourier's transformational thinking - Nature 555, 413 (2018).

Important early application by Kelvin (1862)—- Quantitative theory of terrestrial temperatures.

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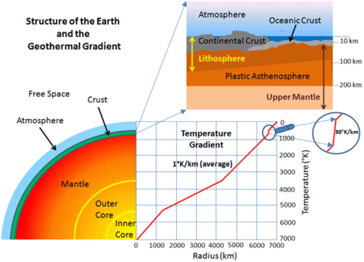


Kelvin' estimate of age of earth - 200 million years

Proving Fourier's law

Proving Fourier's law from first principles (Newton's equations of motion) is a difficult open problem in theoretical physics.

Review article:
Fourier's law: A challenge for theorists
Bonetto, Rey-Bellet, Lebowitz (2000).

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 nonconducting crystals.

R. Peierls in "Surproses in Theoretical Physics" (1961)

Big question: "Micro" $\rightarrow$ "Macro".
In this case: "Newton's equations of motion" $\rightarrow$ "Fourier's law"

Theory of heat conduction

Equilibrium Systems

As far as equilibrium properties of a system are concerned there is a well defined prescription to obtain macroscopic properties starting from the microscopic Hamiltonian – Statistical mechanics of Boltzmann and Gibbs. For a system in equilibrium at temperature T:

$$F = -k_B T \ln Z \qquad Z = Tr\,[\, e^{-\beta H}\,]$$

The free energy function or the entropy function contains all information about equiibrium properties of a system.

Nonequilibrium Systems

Heat conduction is a nonequilibrium process and there is no equivalent statistical mechanical theory for systems out of nonequilibrium.

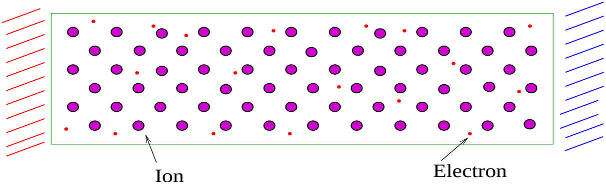
- We do not have a nonequilibrium free energy or a entropy function.
- Recent attempts based on Large Deviation Theory.

Theories of heat transport

- Kinetic theory
- Peierl's-Boltzmann theory
- Green-Kubo linear response theory
- Landauer theory – This is an open systems approach especially useful for mesoscopic systems.
    - Nonequilibrium Green's function formalism
    - Generalized Langevin equations formalism

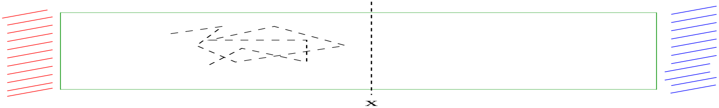
Kinetic theory

Heat conduction in a dilectric crystalline solid: Basic microscopic picture



Heat is carried by lattice vibrations *i*.e phonons.

Kinetic theory for phonon gas



Simplest "derivation" of Fourier's law.
Heat carried by phonons which undergo collisions at time intervals $\sim \tau$ - hence do random walks.
Let $\epsilon(x) =$ be energy density at x and $v =$ average velocity of particles. Then:

$$J = \frac{1}{2}\, v\, [\epsilon(x - v\tau) - \epsilon(x + v\tau)] = -v^2\tau \frac{\partial \epsilon}{\partial T}\frac{\partial T}{\partial x} = -v\ell_K c \frac{\partial T}{\partial x}$$

$$\text{Therefore } J = -\kappa \frac{\partial T}{\partial x} \text{ with } \kappa = v\ell_K c$$

$$\text{where } c = \text{ specific heat }, \ \ell_K = \text{ mean free path }.$$

Can calculate thermal conductivity κ if we know average velocity, mean free path and specific heat of the phonons.

Note that this is not a proof since it assumes diffusive motion.

Other approaches

- Peierls-Boltzmann theory - Phonon scattering is due to impurities or due ot interaction with other phonons (Umklapp processes). Some approximations lead to a kinetic theory like result

$$\kappa = \int d\omega \ v(\omega)\ell(\omega)\ C(\omega)\ \rho(\omega),$$

where $v(\omega)$ is the velocity, $\ell(\omega)$ the mean free path, $C(\omega)$ the specific heat and $\rho(\omega)$ the density of states for phonons at frequency ω.
Computation of $\ell(\omega)$ in a given system with specified Hamiltonian non-trivial. Usually from perturbation theory.

- Linear response theory – relates nonequilibrium transport coefficients to equilibrium time-dpendent correlation functions. For heat conduction:

$$\kappa = \lim_{\tau\to\infty} \lim_{L\to\infty} \frac{1}{k_B T^2 L^d} \int_0^\tau dt \langle J_x(t) J_x(0) \rangle \ .$$

Computation of current auto-correlation usually difficult.

Results so far

The computation of $\ell(\omega)$ or $\langle J(t)J(0)\rangle$ is usually quite difficult and requires further approximations.

In one and two dimensional system one finds that both these approaches lead to an infinite thermal conductivity.

- Boltzmann kinetic theory gives $\ell(\omega) \sim \omega^{-5/3}$ for an anharmonic chain.
- Linear response theory:

  Mode-coupling theory for anharmonic chains finds $\langle J(t)J(0)\rangle \sim t^{-\delta}$ with $\delta < 1$.

Thus both Kinetic theory and Linear response theory indicate a diverging thermal conductivity.

Direct computation of κ from nonequilibrium measurements.

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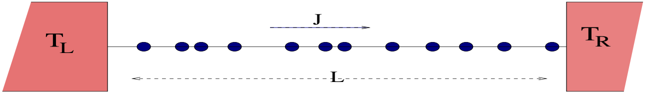


- Dynamics in bulk described by a Hamiltonian:

$$H = \sum_{\ell=1}^{N} \frac{p_\ell^2}{2m_\ell} + U(x_\ell - x_{\ell-1}) + V(x_\ell)$$

where $U(x)$ is the inter-particle interaction potential and $V(x)$ an external pinning potential.

- Boundary particles interact with heat baths. Example: Langevin baths.

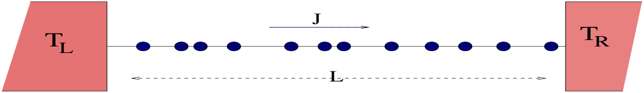
$$\begin{aligned} m_1 \ddot{x}_1 &= -\partial U/\partial x_1 - \gamma \dot{x}_1 + (2\gamma k_B T_L)^{1/2} \eta_L \\ m_\ell \ddot{x}_\ell &= -\partial U/\partial x_\ell \quad \ell = 2, \ldots, N-1 \\ m_N \ddot{x}_N &= -\partial U/\partial x_N - \gamma \dot{x}_N + (2\gamma k_B T_R)^{1/2} \eta_R \end{aligned}$$

- In nonequilibrium steady state compute temperature profile and current for different system sizes.

$$k_B T_\ell = m_\ell \langle \dot{x}_\ell^2 \rangle \ \text{and} \ J_\ell = \langle v_\ell f_{\ell-1,\ell} \rangle \,,$$

where $f_{\ell,\ell-1}$ is the force on l^{th} particle from $(l-1)^{\text{th}}$ particle.

Heat current and heat conductivity



- Connect system of length L to heat baths with small temperature difference $\Delta T = T_L - T_R$. We can measure the heat current J and this is always finite and it can be proven that $J = G \Delta T$, *i*.e that is the current response is linear.

- Fourier's law $J = -\kappa \nabla T$ implies

$$J = \kappa \frac{\Delta T}{L} \ .$$

The size-dependence is difficult to prove and probably not true.

CAN WE CHECK THIS NUMERICALLY ?

- We can compute the conductivity $\kappa_L = \frac{J \, L}{\Delta T}$.
Question: Does this converges to a finite constant value as $L \to \infty$.

Results so far

Direct studies (simulations and some exact results) in one and two dimensional systems find that Fourier's law is in fact not valid. The thermal conductivity is not an intrinsic material property.

For anharmonic systems without disorder , κ diverges with system size L as:

$$\begin{aligned} \kappa &\sim L^{\alpha} \quad 1D \\ &\sim L^{\alpha'}, \quad \log L \quad 2D \\ &\sim L^{0} \quad 3D \end{aligned}$$

– A.D, Advances in Physics, vol. 57 (2008).
– Lecture notes in physics, vol. 921, (2016).

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PRL **101,** 075903 (2008) PHYSICAL REVIEW LETTERS week ending 15 AUGUST 2008

Breakdown of Fourier's Law in Nanotube Thermal Conductors

C. W. Chang,[1,2,*] D. Okawa,[1] H. Garcia,[1] A. Majumdar,[2,3,4] and A. Zettl[1,2,4,+]

[1] *Department of Physics, University of California at Berkeley, California 94720, USA*

[2] *Center of Integrated Nanomechanical Systems, University of California at Berkeley, California 94720, USA*

[3] *Departments of Mechanical Engineering and Materials Science and Engineering, University of California at Berkeley, California 94720, USA*

[4] *Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

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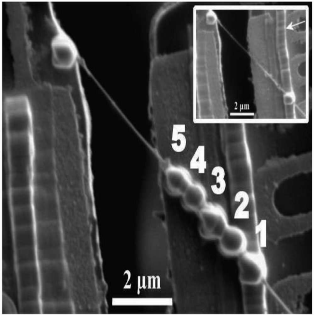
We present experimental evidence that the room temperature thermal conductivity (κ) of individual multiwalled carbon and boron-nitride nanotubes does not obey Fourier's empirical law of thermal conduction. Because of isotopic disorder, κ's of carbon nanotubes and boron-nitride nanotubes show different length dependence behavior. Moreover, for these systems we find that Fourier's law is violated even when the phonon mean free path is much shorter than the sample length.

DOI: 10.1103/PhysRevLett.101.075903 PACS numbers: 65.80.+n, 63.22.Gh, 73.63.Fg, 74.25.Kc



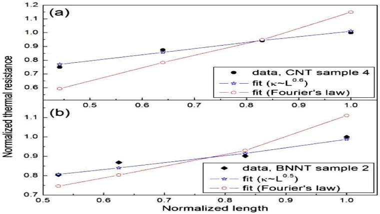


FIG. 3 (color online). (a) Normalized thermal resistance vs normalized sample length for CNT sample 4 (solid black circles), best fit assuming $\beta = 0.6$ (open blue stars), and best fit assuming Fourier's law (open red circles). (b) Normalized thermal resistance vs normalized sample length for BNNT sample 2 (solid black diamonds), best fit assuming $\beta = 0.4$ (open blue stars), and best fit assuming Fourier's law (open red circles).

Experiments: graphene

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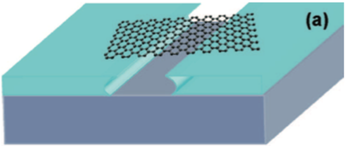

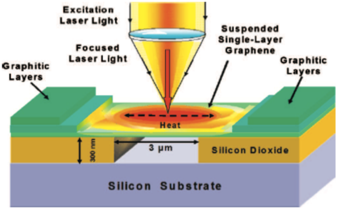

Figure 3. Schematic of the experiment showing the excitation laser light focused on a graphene layer suspended across a trench. The focused laser light creates a local hot spot and generates a heat wave inside SLG propagating toward heat sinks.

Very large thermal conductivity.
$\kappa \sim \log(L)$ has been reported. [Balandin etal, Nat. Phys. (2011), Li etal (2012)]

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C. W. Chang etal, Phys. Rev. Lett. (2017)

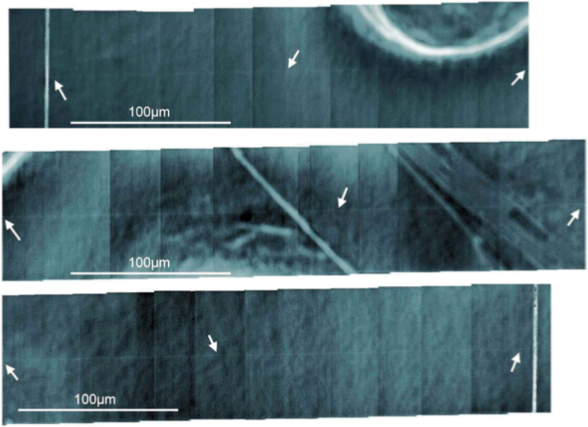

FIG. 2. SEM panorama of sample 9 (divided into three parts), where a CNT is suspended across a heater and a sensor (the horizontal beams in the top right and the bottom left images). The total suspended length of sample 9 is 1.039 mm. The arrows in the figures denote the the CNT.

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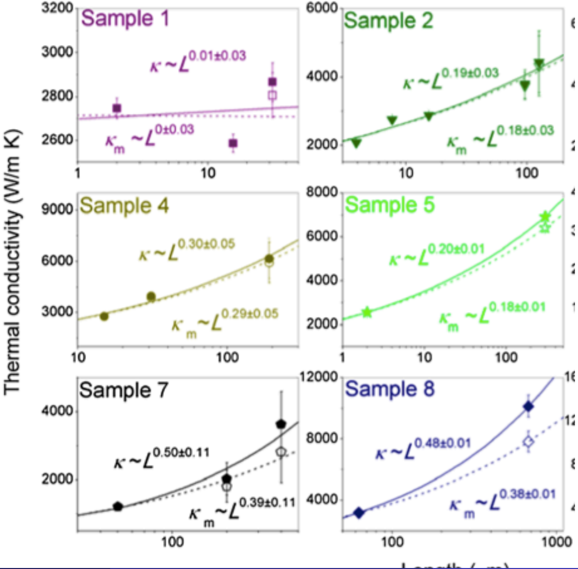
Phys. Rev. Lett. (2017)



Experiments: Graphene

nature COMMUNICATIONS

ARTICLE

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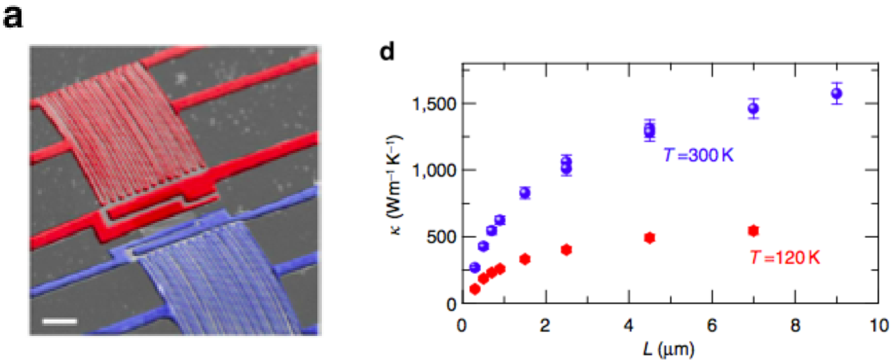
Length-dependent thermal conductivity in suspended single-layer graphene

Xiangfan Xu[1,2,3,†], Luiz F.C. Pereira[4,†], Yu Wang[5], Jing Wu[1,2], Kaiwen Zhang[1,2,6], Xiangming Zhao[1,2,6], Sukang Bae[7], Cong Tinh Bui[8], Rongguo Xie[1,6,9], John T.L. Thong[9,8], Byung Hee Hong[10], Kian Ping Loh[2,8,11], Davide Donadio[4], Baowen Li[1,2,6,8] & Barbaros Özyilmaz[1,2,3,8]

Graphene exhibits extraordinary electronic and mechanical properties, and extremely high thermal conductivity. Being a very stable atomically thick membrane that can be suspended between two leads, graphene provides a perfect test platform for studying thermal conductivity in two-dimensional systems, which is of primary importance for phonon transport in low-dimensional materials. Here we report experimental measurements and non-equilibrium molecular dynamics simulations of thermal conduction in suspended single-layer graphene as a function of both temperature and sample length. Interestingly and in contrast to bulk materials, at 300 K, thermal conductivity keeps increasing and remains logarithmically divergent with sample length even for sample lengths much larger than the average phonon mean free path. This result is a consequence of the two-dimensional nature of phonons in graphene, and provides fundamental understanding of thermal transport in two-dimensional materials.

Experiments: Graphene



Signatures of anomalous energy transport

OPEN SYSTEM STUDIES — systems connected to heat baths.

- Divergent conductivity: $\kappa \sim L^{\alpha}$.
- Nonlinear (and possibly singular) temperature profiles, EVEN for small temperature differences.

CLOSED SYSTEM STUDIES — equilibrium systems

- Anomalous spreading of heat pulses — Levy walk instead of random walk.

  $\langle x^2 \rangle \sim t^{\gamma}, \quad \gamma > 1$

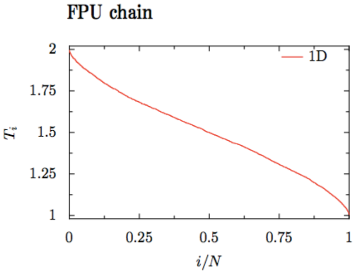
  $\alpha = \gamma - 1.$
- Anomlaous behaviour of equilibrium space-time correlations of conserved quantities.

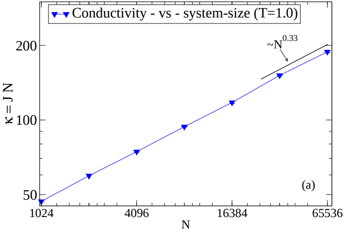
  Predictions of fluctuating hydrodynamics — Levy heat peak and KPZ sound peaks.
- Slow temporal decay of total energy-current correlations and conclusions from Green-Kubo formula.

Anomalous transport -steady state study

Nonequilibrium simulations of the Fermi-Pasta-Ulam chain — Lepri, Livi, Politi(1997).

$$H = \sum_{\ell=1}^{N} \frac{p_\ell^2}{2m} + \sum_{\ell=1}^{N+1} \left[k_2 \frac{(q_\ell - q_{\ell-1})^2}{2} + k_3 \frac{(q_\ell - q_{\ell-1})^3}{3} + k_4 \frac{(q_\ell - q_{\ell-1})^4}{4} \right] .$$

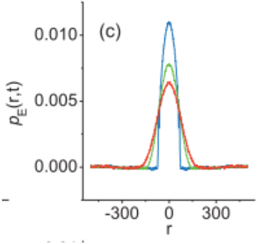




Conductivity diverges with system size (For FPU chain $\kappa \sim N^{0.33}$).
S.Das, AD, O. Narayan (2014).

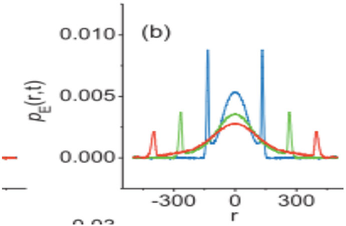
Seems to be a generic feature of momentum conserving systems in one dimension.

- Diffusive system.



$$P(x,t) = \frac{e^{-x^2/4Dt}}{(4\pi Dt)^{1/2}} ,$$
$$\langle x^2 \rangle = 2Dt .$$

- FPU chain or hard particle gas (Cipriani, Denisov, Politi, 2005; Zhao, 2006).



- Gaussian peak.
- Power-law decay at large x.
- Finite speed of propagation.
- $\langle x^2 \rangle \sim t^\gamma$, $\gamma > 1$.

Levy walkers — a phenomenological description of anomalous heat transport

Anomalous heat conduction: main features.

- Thermal conductivity $\kappa \sim L^{\alpha}$, $\alpha > 0$.
- Non-linear temperature profiles.
- Super-diffusive progagation of heat pulses, $\langle x^2 \rangle \sim t^{\gamma}$.

- It is clear that the heat carriers are not doing a simple random walk.
- Possible description — heat carriers are Levy walkers.
  $\alpha = \gamma - 1$.

  Numerical results supporting Levy walk picture:

  Energy pulse propagation can be accurately understood.

  Temperature profile and current scaling in nonequilibrium steady state.

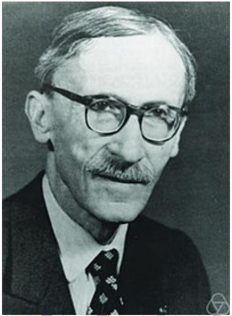
Precise model

Think of system as a gas of non-interacting Levy-walkers. The energy and the temperature at any point in the system is assumed to be proportional to the local density of Levy walkers.

Each step of a walker consists of:

- choosing a time of flight τ from the distribution $\phi(\tau)$.
- choosing a random direction of motion with equal probability.
- move in chosen direction with unit speed for time τ.

Paul Levy (1886-1971)

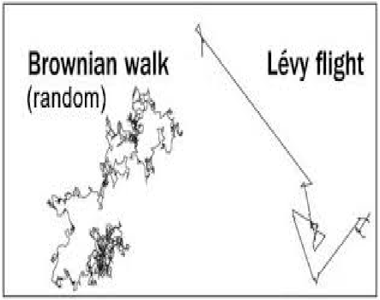


Form of distribution:

$$\phi(\tau) \sim \frac{1}{\tau^{\beta+1}} \ , \quad 1 < \beta < 2 \ ,$$

The mean flight time $\langle \tau \rangle$ is finite but $\langle \tau^2 \rangle = \infty$.

Levy walk versus Random walk



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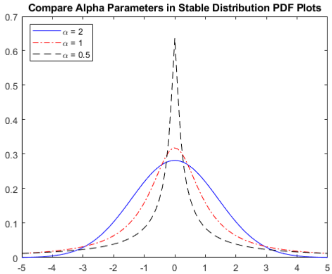


Compare the motion of a two-dimensional Levy walker with an ordinary random walker.

Growth of Mean square deviation with time is different from diffusion —

$$\langle x^2 \rangle_c \quad \sim \quad t^\gamma , \quad \gamma = 3 - \alpha \, .$$

An exactly solvable stochastic model of anomalous transport

Consider harmonic chain with nearest-neighbour interactions. The dynamics has two components:

- Deterministic Hamiltonian part

$$\dot{q}_\ell = p_\ell, \quad \dot{p}_\ell = (q_{\ell+1} - 2q_\ell + q_{\ell-1}), \quad \ell = 1, \ldots, N \, .$$

- At a rate γ, exchange momenta of neighbors $p_\ell \leftrightarrow p_{\ell+1}$.
- Same conservation laws as FPU chain.

Exact results for equilibrium infinite system

- Slow decay of current-correlations: $\langle J(t)J(0)\rangle \sim \frac{1}{t^{1/2}}$.
- Energy density, under appropriate space-time rescaling, satisfies a fractional diffusion equation:

$$\partial_t e(x,t) = -\kappa(-\Delta)^{3/4} e(x,t) \, ,$$

where the fractional derivative is defined through the relation

$$(-\Delta)^{3/4} \int_{-\infty}^{\infty} dk e^{ikx} f(k) = \int_{-\infty}^{\infty} dk |k|^{3/2} e^{ikx} f(k)$$

General Microscopic theory

We now ask if one can understand anomalous transport and the Levy-walk features from some general theory for a one-dimensional interacting system.

Presently, the best general microscopic theory to explain anomalous transport is that of "Non-Linear Fluctuating Hydrodynamics".

- Write equations for the three conserved fields — mass, momentum and energy.
- Make predictions for equilibrium spatio-temporal correlation functions (dynamical structure factor).

O. Narayan and S. Ramaswamy (2006)
H. van Beijeren (2012)

H. Spohn (2013-)

Basics of fluctuating hydrodynamics

- Identify the conserved fields. For the Fermi-Pasta-Ulam chain they are
  - Extension: $r_x = q_{x+1} - q_x$
  - Momentum: p_x
  - Energy: e_x

Let (u_1, u_2, u_3) be fluctuations of conserved fields about equilibrium values:
$r_x = \langle r_x \rangle + u_1(x), \quad p_x = u_2(x), \quad e_x = \langle e_x \rangle + u_3(x)$.
Write hydrodynamic equations for these fluctuations.

Fluctuating hydrodynamics basics

- Let $u = (u_1, u_2, u_3)$. Equations have the form:

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}\left[Au + uHu\right] + \left[\tilde{D}\frac{\partial^2 u}{\partial x^2} + \tilde{B}\frac{\partial \xi}{\partial x}\right].$$

1D noisy Navier-Stokes equation

A, H known explicitly in terms of microscopic model.
$\tilde{D}$, $\tilde{B}$ unknown but satisfy fluctuation dissipation.

Normal modes: Take linear combinations of u_1, u_2, u_3 .
New fields $\phi_+(x,t), \phi_0(x,t), \phi_-(x,t)$.

Two propagating sound modes ($\phi_\pm$)
One diffusive heat mode (ϕ_0).

Universal predictions for form of correlation functions.

Predictions of fluctuating hydrodynamics

- Predictions for equilibrium space-time correlation functions

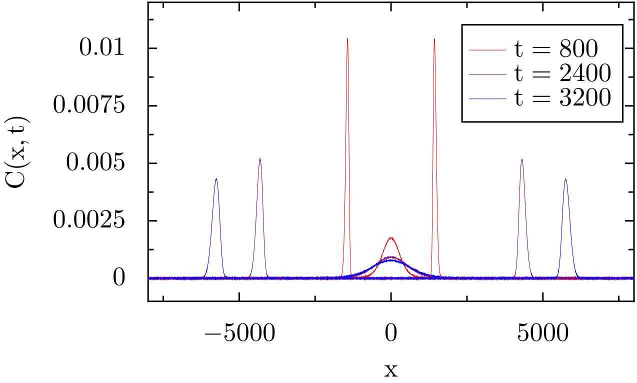
$$\text{Sound}-\text{mode}: \quad C_s(x,t) = \langle \phi_{\pm}(x,t)\phi_{\pm}(0,0)\rangle = \frac{1}{(\lambda_s t)^{2/3}} f_{KPZ}\left[\frac{(x \pm ct)}{(\lambda_s t)^{2/3}}\right]$$

$$\text{Heat}-\text{mode}: \quad C_h(x,t) = \langle \phi_0(x,t)\phi_0(0,0)\rangle = \frac{1}{(\lambda_e t)^{3/5}} f_{LW}\left[\frac{x}{(\lambda_e t)^{3/5}}\right]$$

c, the sound speed and λ are given by the theory.
f_{KPZ} - universal scaling function that appears in the solution of the Kardar-Parisi-Zhang equation.
f_{LW} – Levy-stable distribution with a cut-off at $|x| = ct$.

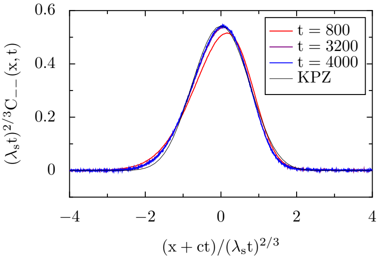
- Universality classes can be identified.

Spread of an energy pulse — $C(x,t) = \langle \delta\epsilon(x,t)\delta\epsilon(0,0)\rangle$— emergence of three peaks

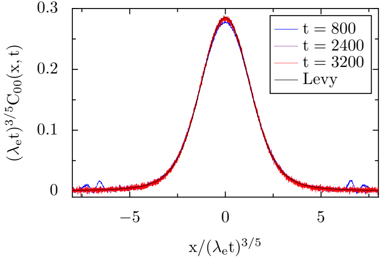


Scaling of heat and sound modes

Sound mode — described by Kardar-Parisi-Zhang scaling function



Heat mode spreads super-diffusively — Levy distribution



Systems studied so far in the framework of NIFHT

- Fermi-Pasta-Ulam chains
- Hard particle gases
- Rotor chains
- Discrete nonlinear Schrodinger equation
- Multi-component exclusion processes
- Heisenberg spin chains

Fluctuating Hydrodynamics reveals an amazing Universality !!
— Herbert Spohn (2019 Boltzmann Medal)

One-dimensional systems satisfying Fourier's law

Hamiltonian systems with nonintegrable interactions—

Momentum conserving system: Fermi-Pasta-Ulam (FPU) - model

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m} + \sum_{l=1}^{N+1} \left[k_2 \frac{(q_l - q_{l-1})^2}{2} + k_3 \frac{(q_l - q_{l-1})^3}{3} + k_4 \frac{(q_l - q_{l-1})^4}{4} \right] .$$

Momentum non-conserving system: ϕ^4 - model

$$H = \sum_{l=1}^{N} \left[\frac{p_l^2}{2m} + k_o \frac{q_l^2}{2} \right] + \sum_{l=1,N+1} k_2 \frac{(q_l - q_{l-1})^2}{2} + \sum_{l=1}^{N} \lambda \frac{q_l^4}{4} .$$

- Momentum conserving: $\kappa \sim L^{1/3}$.
- Momentum non-conserving (pinned case): $\kappa \sim L^0$
  — Finite thermal conductivity, Fourier's law valid.

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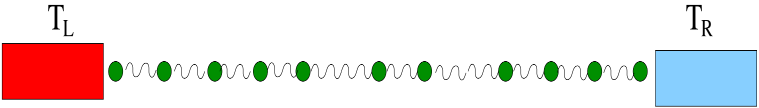
- Anharmonic chains with momentum conservation: Anomlaous transport — Simulation results, effective description using Levy-walkers model, hydrodynamic theory.
- Pinned anharmonic systems (no momentum conservation): Diffusive transport.
- Disordered Harmonic chains - Exact results using Landauer-type formulation.

Ordered harmonic Chain [Rieder, Lebowitz, Lieb (1967)].



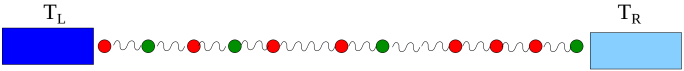
This case can be solved exactly and the nonequilibrium steady state distribution function computed. One finds
$J \sim (T_L - T_R)$ unlike expected $(T_L - T_R)/N$ from Fourier law.
Flat Temperature profiles.

No local thermal equilibrium. Fourier's law is not valid.

This can be understood since there are no mechanism for scattering of phons and heat transport is purely ballistic. In real systems we expect scattering in various ways:

- Phonon-phonon interactions: In oscillator chain take anharmonic springs (*e*.g Fermi-Pasta-Ulam chain).
- Disorder: In harmonic systems make masses random.

Landauer formula for heat current



$$J = \frac{k_B(T_L - T_R)}{4\pi} \int_0^\infty d\omega \mathcal{T}(\omega) ,$$

where $\mathcal{T}(\omega) = 4\gamma^2\omega^2|G_{1N}|^2$, (Phonon transmission)

with the matrix $G = [-\omega^2 M + \Phi - \Sigma]^{-1}$

$M =$ mass matrix , $\Phi =$ force matrix

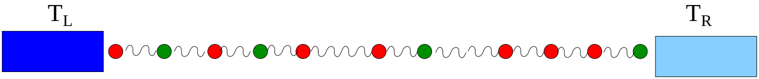
Σ is a "self-energy" correction from baths.

Quantum mechanical case:

$$J = \frac{1}{2\pi} \int_0^\infty d\omega \, \hbar \, \omega \, \mathcal{T}(\omega) \, [\, f_b(T_L) - f_b(T_R) \,]$$

where $f_b(\omega) = (e^{\beta\hbar\omega} - 1)^{-1}$.

Disordered Harmonic systems: Results in $1D$



The exact formula for current is given by

$$J = \frac{k_B \Delta T}{2\pi} \int_0^\infty d\omega \mathcal{T}(\omega) ,$$

where $\mathcal{T}(\omega)$ is the phonon transmission function.

Similar closed form expressions for the temperature profile can also be obtained in terms of the Green's function $G = [-\omega^2 M + \Phi - \Sigma]^{-1}$.

To understand the N-dependence of J we thus need to understand the N-dependence of the transmission coefficient $\mathcal{T}(\omega)$ – Anderson localization is important.

Anderson localization

Oscillator chain with random masses.

$$H = \sum_{l=1,N} [\frac{p_l^2}{2m_l} + k_o \frac{x_l^2}{2}] + \sum_{l=1,N+1} k \frac{(x_l - x_{l-1})^2}{2}$$

$k_o, k > 0$, $\{m_l\} = [m - \Delta, m + \Delta]$.

Finding normal modes in this system is closely related to the problem of finding electronic eigenstates in a disordered potential as described by the following Hamiltonian:

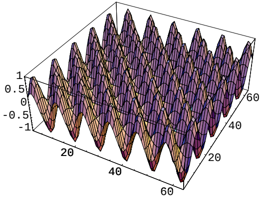
Electrons on a $1D$ lattice with onsite disorder.

$$H = \sum_{l=1}^{N-1} -t[c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l] + \sum_{l=1}^{N} \epsilon_l c_l^\dagger c_l$$

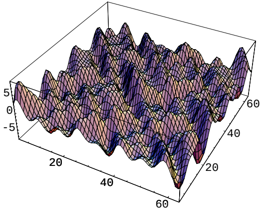
$\{\epsilon_l\} = [-\Delta, \Delta]$.

In both cases: all states are exponentially localized.

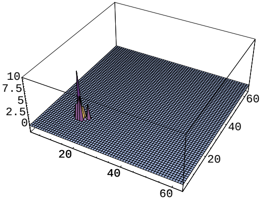
Character of normal modes of a disordered crystal



Extended periodic mode
(Ballistic)



Extended random mode
(Diffusive)



Localized mode
(Non-conducting)

Anderson localization implies: $T(\omega) \sim e^{-L/\ell(\omega)}$ with $\ell(\omega) \sim 1/\omega^2$ for $\omega \to 0$.

For pinned systems, no low-frequency modes hence

- Almost all normal modes of the chain are localized and their amplitude at the boundaries is exponentially small (in L) leading to transmission decaying exponentially.
- Hence $J \sim e^{-L/\ell}$. — Anderson heat insulator.

For unpinned systems, frequencies $\omega \lesssim L^{-1/2}$ “do not see” the randomness and can carry current. These are the ballistic modes.

$$J \sim 1/L^{3/2}$$

[Ford and Allen (1966), Matsuda, Ishi (1968), Rubin, Greer, Casher, Lebowitz (1972), Dhar (2001), Huveneers (2012)]

Effect of interaction on localization

Suppose we take an anharmonic system with a finite thermal conductivity e.g the ϕ^4 chain and add some sort of disorder. What happens ?

Disorder $\rightarrow$ Localization and so heat insulator.

Anharmonicity or interactions $\rightarrow$ Chaos and heat Conductor

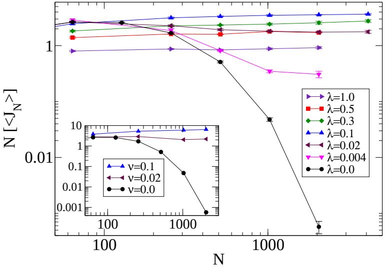
Interesting question: What wins, disorder or interactions ?

Effect of interaction on localization

Disordered ϕ^4 model [Dhar and Lebowitz (2008)]

$$H = \sum_{l=1,N} \left[\frac{p_l^2}{2m_l} + k_o \frac{q_l^2}{2} \right] + \sum_{l=1,N+1} k \frac{(q_l - q_{l-1})^2}{2} + \sum_{l=1,N} \lambda \frac{q_l^4}{4} .$$

$\{m_l\} = [m - \Delta, m + \Delta]$. Disorder $\rightarrow \Delta$, Anharmonicity $\rightarrow \lambda$.



Dramatic transition: $e^{-cN/\ell} \rightarrow \frac{1}{N}$
for small amount of interaction.

Big new area in statistical physics/condensed matter physics —- Many-Body-Localization (MBL).

Key ideas - (breaking of KAM tori, Arnold diffusion,ergodicity and thermalization)

Conclusions and questions

- Deriving Fourier's law rigorously is a surprisingly hard problem. Fourier's law seems to be not valid in low-dimensional systems - anomalous heat transport.
- The thermal conductivity κ is expected to be an intrinsic material property.
  e.g at room temperature $\kappa = 2000$ W/mK (Diamond) But the conductivity of nanotubes, nanowires and graphene sheets presumably depends on the size of the sample!!
- It follows that the diffusion equation $\partial T/\partial t = D\, \partial^2 T/\partial x^2$ is not valid in such systems.
  — A good decription seems to be obtained by assuming that the heat carriers are performing Levy walks instead of simple random walks [$\equiv$ fractional diffusion equation].
- Microscopic derivation of Levy diffusion - big progress using theory of nonlinear fluctuating hydrodynamics. Connection to KPZ equation.

Open questions

- Effect of interactions on localization. Is it true that the smallest amount of anharmonicity destroys localization ?
- Quantum transport
- Understanding more realistic models.

– Lecture notes in physics, vol. 921, (2016).

Collaborators

STUDENTS: Anupam Kundu, Dibyendu Roy, Suman Das, Anjan Roy, Aritra Kundu, Archak Purkayastha, Rahul Marathe, Debasish Chaudhuri, Chaitra Hegde, Avijit Das, Santhosh Ganappa

OTHERS: Deepak Dhar, Joel Lebowitz, Herbert Spohn, Keiji Saito, Cedric Bernardin, Christian Mendl, Onuttom Narayan, David Huse, Francois Huveneers, Chandan Dasgupta, Pinaki Chaudhuri, Wojciech De Roeck, Pranab Jyoti Bhuyan, Rituparno Mandal, Abhishek Chaudhuri, Kshitij Wagh, Trieu Mai, Venky Kannan, Sanjib Sabhapandit, Kedar Damle, Manas Kulkarni, Manoj Kumar, Diptiman Sen, Bernard Derrida.

Higher dimensional systems

- What about systems in three dimensions ? Is Fourier's law valid ?

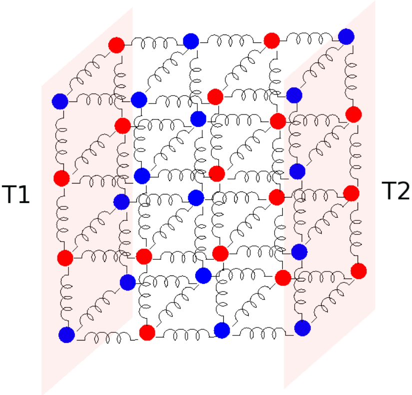
- Consider isotopically disordered dielectric crystals.
  - Heat conduction is through lattice vibrations .
  - Harmonic approximation: solid can be thought of as a gas of phonons with frequencies corresponding to the vibrational spectrum of ordered crystal.
  - Phonons get scattered by:
    (i) Impurities
    (ii) Other phonons (anharmonicity).

It is usually expected that these scattering mechanisms should lead to a finite conductivity. - NO PROOF EXISTS.

$$H = \sum_{\mathbf{x}} \frac{m_{\mathbf{x}}}{2} \dot{q}_{\mathbf{x}}^2 + \sum_{\mathbf{x},\hat{\mathbf{e}}} \frac{k}{2} (q_{\mathbf{x}} - q_{\mathbf{x}+\hat{\mathbf{e}}})^2 + \sum_{\mathbf{x}} \frac{k_o}{2} q_{\mathbf{x}}^2$$

$q_{\mathbf{x}}$: scalar displacement, masses $m_{\mathbf{x}}$ random.

$k_o = 0$: Unpinned. (Free and Fixed BC) $k_o > 0$: Pinned.



Heuristic theory

- Nonequilibrium heat current is given by the Landauer formula:

$$J = \frac{\Delta T}{2\pi} \int_0^\infty d\omega\, \mathcal{T}(\omega) ,$$

  where $\mathcal{T}(\omega)$ is the transmission coefficient of phonons.

- Phonons can be classified as:

  Ballistic: Plane wave like states with $\mathcal{T}(\omega)$ independent of system size.

  Diffusive: Extended disordered states with $\mathcal{T}(\omega)$ decaying as $1/N$.

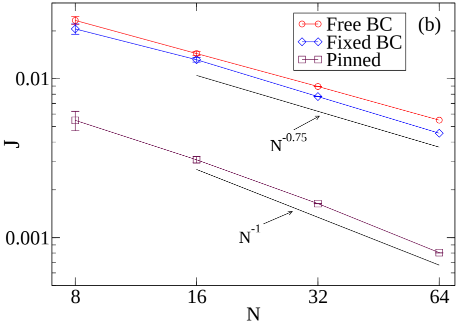
  Localized states: $\mathcal{T}(\omega) \sim e^{-N/\ell_L}$.

- Find contribution to J of the different types of modes and estimate the asymptotic size dependence.

- Effect of localization is much weaker then in $1D$.

J-versus-N plots: 3D

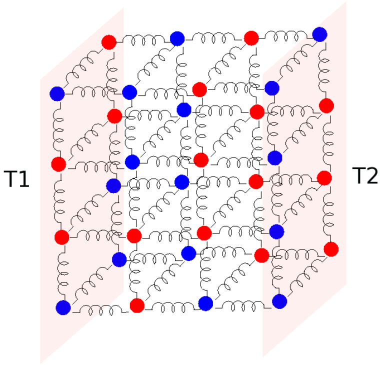
Simulations and Numerics on $N \times N \times N$ samples.
Kundu, Chaudhuri, Roy, Dhar, Lebowitz, Spohn (2010).



FOURIER'S LAW NOT VALID FOR DISORDERED HARMONIC CRYSTAL (except with pinning)

Kinetic theory: Mean free path $\ell(\omega) \sim 1/\omega^{d+1}$ explains the size dependence.

Heat conduction in ordered anharmonic (FPU potential) crystal

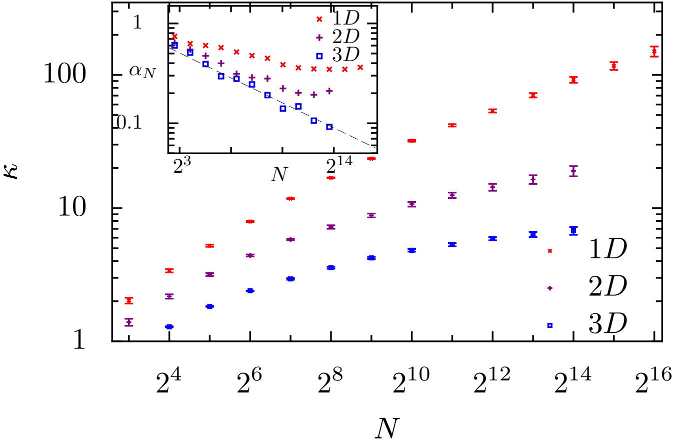


$$H = \sum_{\mathbf{x}} \frac{m}{2} \dot{q}_{\mathbf{x}}^2 + \sum_{\mathbf{x},\hat{\mathbf{e}}} \frac{k}{2} (q_{\mathbf{x}} - q_{\mathbf{x}+\hat{\mathbf{e}}})^2 + \sum_{\mathbf{x}} \frac{\nu}{4} (q_{\mathbf{x}} - q_{\mathbf{x}+\hat{\mathbf{e}}})^4$$

Simulations of three dimensional crystals with Langevin heat baths.

Heat conduction in an ordered anharmonic 3D crystal

Results from nonequilibrium molecular dynamics simulations on $N \times W \times W$ slabs.
AD and K. Saito, PRL **104**, 040601 (2010).



FOURIER's LAW VALID IN 3D.