Understanding anomalous energy transport in one-dimensional systems through fluctuating hydrodynamics.

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Phonons and PTES 2018 at Nanjing
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Outline

- Characteristics of anomalous heat transport
- Levy walk: a phenomenological model for anomalous heat transport.
- Fractional diffusion equation for an exactly solvable model of heat transport.
- A microscopic basis: Nonlinear Fluctuating hydrodynamics.
- Summary

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

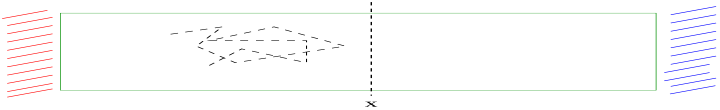
$$\frac{\partial \epsilon}{\partial t} + \nabla J = 0$$

gives the heat DIFFUSION equation (assuming κ independent of T):

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

Fourier's law implies diffusive heat transfer.

Kinetic theory description



Simplest "derivation" of Fourier's law.

Heat carried by quasi-particles 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:

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

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

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

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

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We try to first understand Fourier's law in the simplest possible situation:
—- a one-dimensional system of interacting particles following Newton's equations of motion [one-dimensional phonon gas].

This talk — Only discuss the strictly one-dimensional case (linear chain with no transverse degrees of motion).

Direct test of Fourier's law from nonequilibrium simulations.

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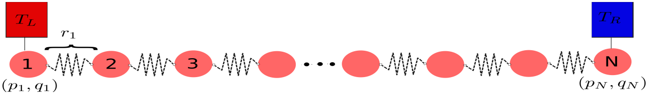


- Dynamics in bulk described by a Hamiltonian:

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

where $U(x)$ is the inter-particle interaction potential.

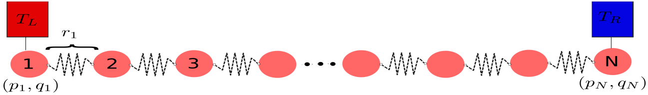
- Boundary particles interact with heat baths. Example: Langevin baths.

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

- 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.



- 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 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 ?

- The thermal conductivity is given by $\kappa_L = \frac{J\,L}{\Delta T}$.

For a few atoms, this will depend on L but in the thermodynamic limit ($L \to \infty$), this should converge to a constant value. Is this true?

Results so far

Direct studies (simulations and some exact results) in one dimensional systems find that Fourier's law is in fact not valid. —- this is referred to as **anomalous transport**.

For anharmonic momentum-conserving systems, κ diverges with system size L as:

$$\kappa \sim L^{\alpha}$$

The divergence exponent $\alpha = 1/3$, except for special cases.

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

Signatures of anomalous energy transport

OPEN SYSTEM STUDIES — systems connected to heat baths at different temperatures.

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

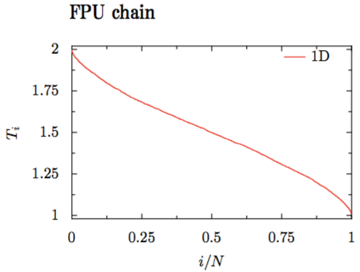
Studies of ISOLATED SYSTEM in equilibrium

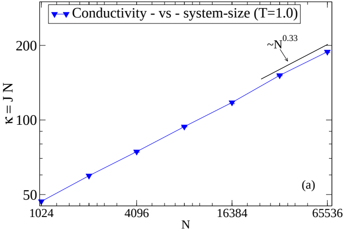
- Anomalous spreading of heat pulses — Levy walk instead of random walk.
  $$\langle x^2 \rangle \sim t^{\gamma}, \quad \gamma > 1$$
  $$\alpha = \gamma - 1.$$
- Anomlaous behaviour of equilibrium space-time correlations of conserved quantities.

  Predictions of fluctuating hydrodynamics — Levy heat peak and KPZ sound peaks.
- Slow temporal decay of total energy-current correlations. The Green-Kubo formula relates
- Large Current fluctuations - e.g: look at system-size scaling of $\mathcal{Q} = \int_0^{\tau} dt\, J(t)$.

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

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



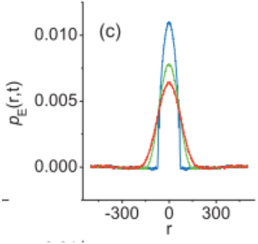


Conductivity diverges with system size (For FPU chain $\kappa \sim N^{0.33}$).
S.Das, AD, O. Narayan (2014).

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

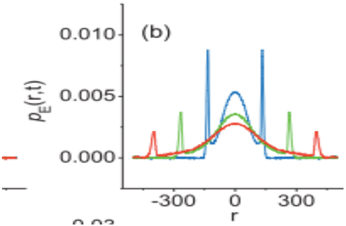
Propagation of pulses OR $\langle \delta\epsilon(x,t)\delta\epsilon(0,0)\rangle$

- 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.
- $\langle x^2 \rangle \sim t^\gamma$, $\gamma > 1$.

Experiments

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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

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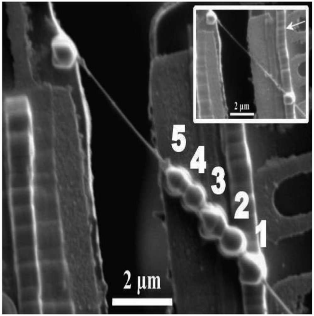
(Received 11 March 2008; revised manuscript received 9 July 2008; published 15 August 2008)

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



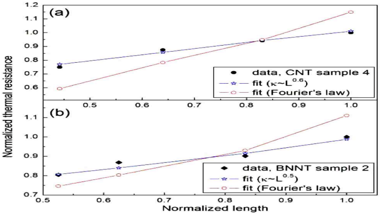


FIG. 3 (color online). (a) Normalized thermal resistance vs normalized sample length for CNT sample 4 (solid black circles), best fit assuming $\beta = 0.6$ (open blue stars), and best fit assuming Fourier's law (open red circles). (b) Normalized thermal resistance vs normalized sample length for BNNT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

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C. W. Chang et al, Phys. Rev. Lett. (2017)

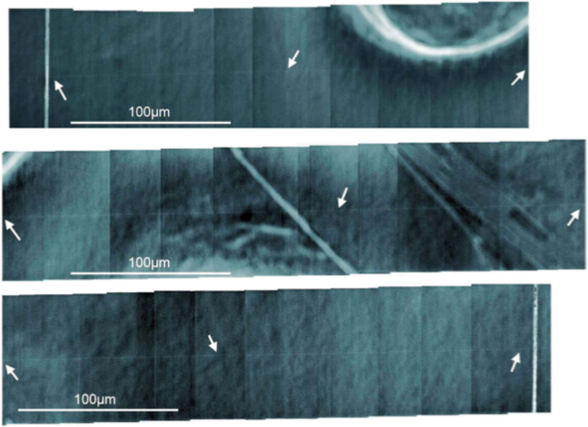

FIG. 2. SEM panorama of sample 9 (divided into three parts), where a CNT is suspended across a heater and a sensor (the horizontal beams in the top right and the bottom left images). The total suspended length of sample 9 is 1.039 mm. The arrows in the figures denote the CNT.

Experiments: Nanotubes

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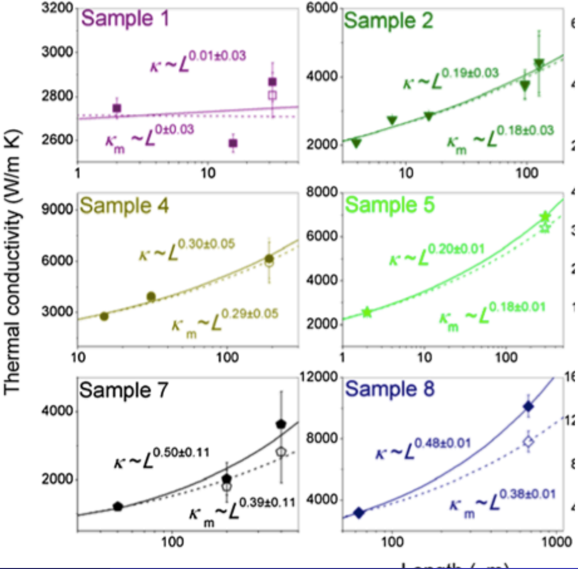
Phys. Rev. Lett. (2017)



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, $\langle x^2 \rangle \sim t^\gamma$.
- Current fluctuations.

- It is clear that the heat carriers are not doing a simple random walk.
- Possible description — heat carriers are Levy walkers.
  S. Denisov, J. Klafter, and M. Urbakh (2003), B. Li and J. S. Wang (2003).
  $\alpha = \gamma - 1$.

  Numerical results supporting Levy walk picture:

  Energy pulse propagation can be accurately understood.
  Cipriani, Denisov, Politi (2005), Zaburdaev, Denisov, Hanggi (2011)

  Temperature profile
  Lepri and Politi (2011) .
- Exact results for steady state properties including large deviation function for current.
  AD, Saito, Derrida (2013).

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.

NOTE: Levy flights and Levy walks are different — Infinite/Finite second moment

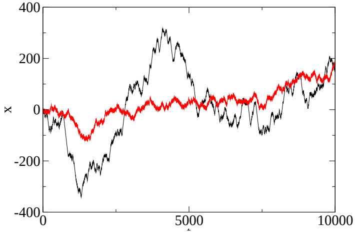
Form of distribution:

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

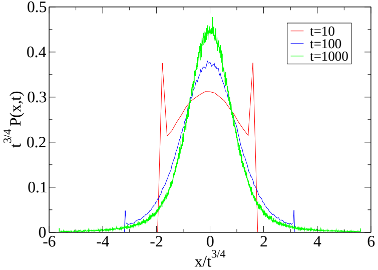
The mean flight time $\langle \tau \rangle$ is finite but $\langle \tau^2 \rangle = \infty$.

Definition: $\psi(\tau) = \int_\tau^\infty dt \phi(t)$ is the probability of choosing a flight time larger than τ.

Levy walk



The time evolution of a one-dimensional Levy walker and an odinary random walker.



For large t one finds:

$$\langle x^2 \rangle_c \quad \sim \quad t^{\gamma}, \quad \gamma = 3 - \beta \; .$$

$$\widetilde{P}(k,s) = \frac{1}{s - c(s - ikv)^{\beta} - c(s + ikv)^{\beta}} \; .$$

For normal diffusion:

$$\widetilde{P}(k,s) = \frac{1}{s + Dk^2} \; .$$

Steady state current

In non-equilibrium case we find

- $\partial P(x,t)/\partial t + \partial J(x,t)/\partial x = 0$

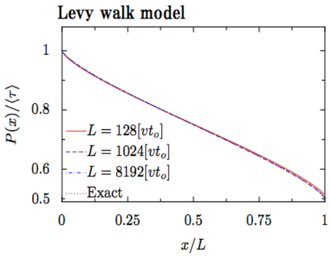
$$J = -\frac{1}{2\langle\tau\rangle}\int_0^L dx' \chi(|x-x'|)\frac{dP(x')}{dx'} \quad \text{instead of} \quad J = -D\frac{dP(x)}{dx} .$$

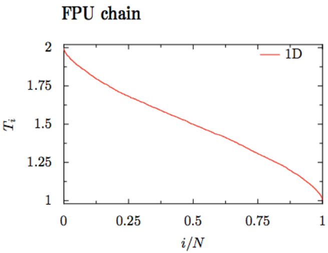
Non-local generalization of Fourier's law.

- Exact solution for $P(x)$ gives

$$\kappa \sim L^\alpha, \quad \alpha = 2-\beta = \gamma - 1 .$$

- Density (temperature) profile shows the expected singular structure.





An exactly solvable stochastic model of anomalous transport

Basile,Bernardin,Olla,Jara,Komorowski (2006,2015)

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

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

An exactly solvable stochastic model of anomalous transport

Lepri,Politi,Mejia-Monasterio,Livi,Delfini (2009,2010).

Analytic results for open system with Langevin type heat baths:

- $$j \sim \frac{1}{N^{1/2}}$$
- Exact form of steady-state temperature profile.
- What about transient dynamics, e.g time evolution of temperature?

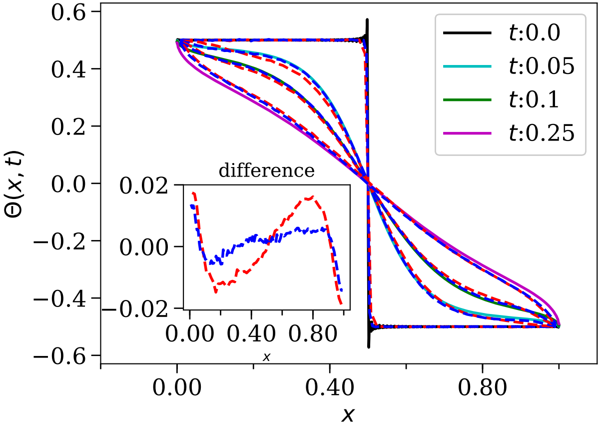
  For regular diffusion equation case one needs to solve the diffusion equation $\partial_t T(x,t) = \partial_x^2 T(x,t)$, with boundary conditions $T(0,t) = T_L$ and $T(1,t) = T_R$ and initial condition $T(x,0)$
  —This fails.
  Instead we need to solve the fractional Laplacian

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

  Non-trivial to define in the finite domain.

Time evolution of non-equilibrium profile: Comparison of theory with simulations of the microscopic dynamics

However in this case, some progress is possible
[Kundu, Bernardin, Saito, Kundu, AD — work in progress].



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.

Presetly, 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

Fermi-Pasta-Ulam Hamiltonian:

$$H = \sum_{x=1}^{N} \frac{p_x^2}{2} + V(q_{x+1} - q_x) \,, \qquad V(r) = k_2 \frac{r^2}{2} + k_3 \frac{r^3}{3} + k_4 \frac{r^4}{4} \,.$$

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

  Using equations of motion one can directly arrive at the following conservation laws (Euler equations):

  $$\frac{\partial r}{\partial t} = \frac{\partial p}{\partial x}, \qquad \frac{\partial p}{\partial t} = -\frac{\partial \mathcal{P}}{\partial x}, \qquad \frac{\partial e}{\partial t} = -\frac{\partial p\mathcal{P}}{\partial x} \,,$$

  where $\mathcal{P}_x = \langle -V'(r_x) \rangle$ is the pressure.

- Consider constant $T, \mathcal{P}$ and zero momentum ensemble.
  Let (u_1, u_2, u_3) be fluctuations of conserved fields about equilibrium values:
  $r_x = \langle r_x \rangle + u_1(x), \quad p_x = u_2(x), \quad e_x = \langle e_x \rangle + u_3(x).$
  Expand the curents about their equilibrium value (to second order in nonlinearity) and write hydrodynamic equations for these fluctuations.

Fluctuating hydrodynamics basics

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

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

  1D noisy Navier-Stokes equation
  [Spohn,Mendl (2013), Narayan,Ramaswamy (2006), Beijeren (2012)].

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

- Neglecting nonlinear terms, one can construct normal mode variables (ϕ_+, ϕ_0, ϕ_-), as linear combinations of the original fields $\phi = Ru$. These satisfy equations of the form

$$\begin{aligned}
\frac{\partial \phi_+}{\partial t} &= -c\frac{\partial \phi_+}{\partial x} + D_s\frac{\partial^2 \phi_+}{\partial x^2} + \frac{\partial \eta_+}{\partial x} \\
\frac{\partial \phi_0}{\partial t} &= D_h\frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x} \\
\frac{\partial \phi_-}{\partial t} &= c\frac{\partial \phi_-}{\partial x} + D_s\frac{\partial^2 \phi_-}{\partial x^2} + \frac{\partial \eta_-}{\partial x}
\end{aligned}$$

NOTE: two propagating sound modes ($\phi_\pm$) and one diffusive heat mode (ϕ_0).

Predictions of fluctuating hydrodynamics

- Including the nonlinear terms:

$$\begin{aligned}
\frac{\partial \phi_+}{\partial t} &= \frac{\partial}{\partial x}[-c\phi_+ + G^+\phi^2] + D_s\frac{\partial^2 \phi_+}{\partial x^2} + \frac{\partial \eta_+}{\partial x} \\
\frac{\partial \phi_0}{\partial t} &= \frac{\partial}{\partial x}[G^0\phi^2] + D_h\frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x} \\
\frac{\partial \phi_-}{\partial t} &= \frac{\partial}{\partial x}[c\phi_- + G^-\phi^2] + D_s\frac{\partial^2 \phi_-}{\partial x^2} + \frac{\partial \eta_-}{\partial x}
\end{aligned}$$

  Given $V(r), T, \mathcal{P}$, the form of the G-matrices is completely determined.

- Generic case: To leading order, the oppositely moving sound modes are decoupled from the heat mode and satisfy noisy Burgers equations. For the heat mode, the leading nonlinear correction is from the two sound modes.

- Solving the nonlinear hydrodynamic equations within mode-coupling approximation, one can make predictions for the equilibrium space-time correlation functions $C(x,t) = \langle \phi_\alpha(x,t)\phi_\beta(0,0)\rangle$.

Predictions of fluctuating hydrodynamics

Predictions for equilibrium space-time correlation functions $C(x,t) = \langle \phi_\alpha(x,t)\phi_\beta(0,0)\rangle$.

- $$\text{Sound} - \text{mode}: \quad C_s(x,t) = \langle \phi_\pm(x,t)\phi_\pm(0,0)\rangle = \frac{1}{(\lambda_s t)^{2/3}}\, f_{KPZ}\left[\frac{(x \pm ct)}{(\lambda_s t)^{2/3}}\right]$$
  $$\text{Heat} - \text{mode}: \quad C_h(x,t) = \langle \phi_0(x,t)\phi_0(0,0)\rangle = \frac{1}{(\lambda_e t)^{3/5}}\, f_{LW}\left[\frac{x}{(\lambda_e t)^{3/5}}\right]$$

  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 $|x| = ct$.

  Cross correlations negligible at long times.

- Also find $\langle J(0)J(t)\rangle \sim 1/t^{2/3}$.

Correlations from direct simulations of FPU chains and comparisions with theory.

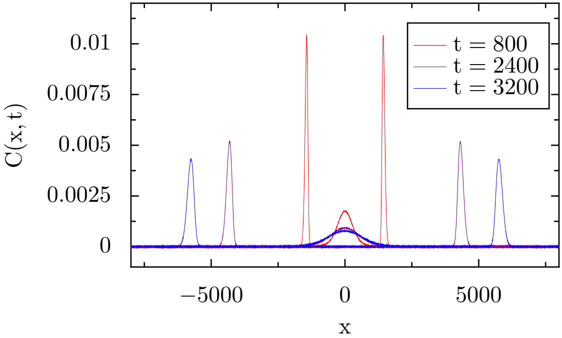
Equilibrium space-time correlation functions

Numerically compute heat mode and sound mode correlations in the $\alpha-\beta$-Fermi-Pasta-Ulam chain with periodic boundary conditions.
[S. Das, AD, K. Saito, C. Mendl, H. Spohn, PRE 90, 012124 (2014)]

Average over $\sim 10^7$ thermal initial conditions. Dynamics is Hamiltonian.

Parameters — $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 5.0,\ \mathcal{P} = 1.0,\ N = 16384.$

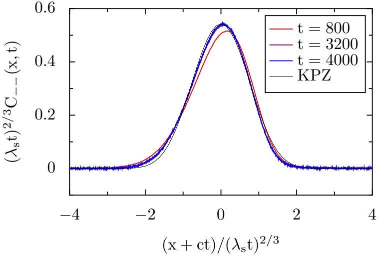
Speed of sound $c = 1.803$.



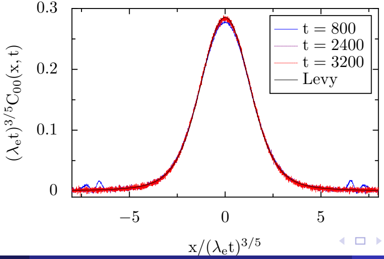
Equilibrium simulations of FPU

Das,AD,Saito,Mendl,Spohn (2013)

Sound mode scaling: $\lambda_{\text{theory}} = 0.396$, $\lambda_{\text{sim}} = 0.46$.



Heat mode scaling: $\lambda_{\text{theory}} = 5.89$, $\lambda_{\text{sim}} = 5.86$.



Hydrodynamic theory for other one-dimensional interacting systems

- Rotor model (josephson junction circuit array)
  H. Spohn (2014), S. Das and AD (2014), Y. Li, S. Liu, N. Li, P. Hänggi, B. Li (2015)

- Non-linear Schrodinger equation
  M. Kulkarni, D. Huse, H. Spohn (2015)

- *XXZ*-spin chain
  A. Das, K. Damle, D. Huse, M. Kulkarni, AD, H. Spohn (work in progress)

In all these systems, Hydrodynamics predicts diffusive energy transport at high temperatures and anomalous transport at low temperatures.

Breakdown of the power-law decay prediction of the heat current correlation in one-dimensional momentum conserving lattices

Shunda Chen, Yong Zhang, Jiao Wang, and Hong Zhao*
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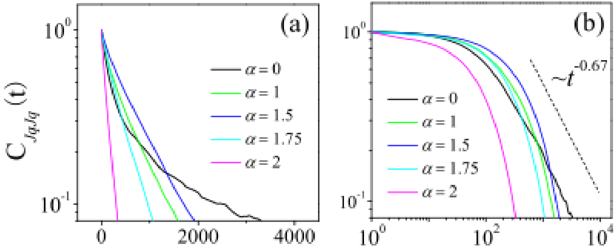
We show that the asymmetric inter-particle interactions can induce rapid decay of the heat current correlation in one-dimensional momentum conserving lattices. When the asymmetry degree is appropriate, even exponential decay may arise. This fact suggests that the power-law decay predicted by the hydrodynamics may not be applied to the lattices with asymmetric inter-particle interactions, and as a result, the Green-Kubo formula may instead lead to a convergent heat conductivity in the thermodynamic limit. The mechanism of the rapid decay is traced back to the fact that the heat current has to drive a mass current additionally in the presence of the asymmetric inter-particle interactions.



$\alpha - \beta$-FPU model at $T \approx 0.1$.

Longer time simulations

Larger sizes studied by L. Wang, B. Hu, B. Li (2013) ($N = 16384$, $k_3 = 2$, $T = 0.1, 1$, pressure ?)
See a cross-over to $1/t^{2/3}$ decay at larger times.

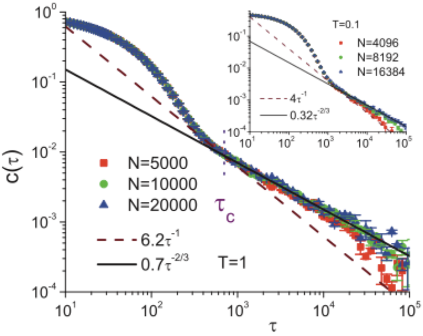


FIG. 2. (Color online) The rescaled heat current autocorrelation function $c(\tau)$ of the FPU $\alpha\beta$ lattice, for $T = 1$ and various particle numbers N. Lines with slope -1 and $-2/3$ are drawn for reference. Inset: The same lattices but for temperature $T = 0.1$. This lower value of T enlarges the threshold time lag τ_c, but it does not change the asymptotic decay of $c(\tau)$, which remains slower than τ^{-1}.

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Nonintegrability and the Fourier heat conduction law

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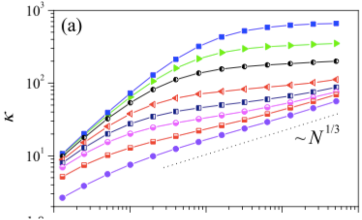
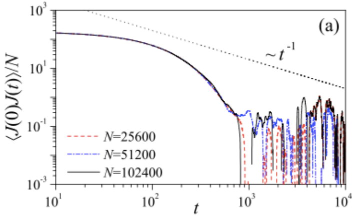
We study in momentum-conserving systems, how nonintegrable dynamics may affect thermal transport properties. As illustrating examples, two one-dimensional (1D) diatomic chains, representing 1D fluids and lattices, respectively, are numerically investigated. In both models, the two species of atoms are assigned two different masses and are arranged alternatively. The systems are nonintegrable unless the mass ratio is one. We find that when the mass ratio is slightly different from one, the heat conductivity may keep significantly unchanged over a certain range of the system size and as the mass ratio tends to one, this range may expand rapidly. These results establish a new connection between the macroscopic thermal transport properties and the underlying dynamics.

System shows diffusive transport in “integrable” limit.





Summary

- Fourier's law of heat conduction and the heat difusion equation not valid in one-dimensional systems with energy, momentum and particle conservation — Anomalous transport.
- Discussed signatures of anomalous energy transport — open and closed system studies.
- Levy walk and fractional diffusion equation description seem appropriate.
- A microscopic theory — Nonlinear fluctuating hydrodynamics.
- Apparent finite conductivity at low temperatures. Finite size effect? — the hydrodynamic theory does not explain this.

Other things:

- Large current fluctations in anomalous systems —Brunet, Derrida Gerschenfeld (2011). Explanation from fluctuating hydrodynamics — AD, Saito, Roy (PRL, 2018).
- Relevance for real systems ? [See D. Donadio in " Lecture notes in physics: Thermal transport in low-dimensional systems, and discussions on experiments.]
  — need to develop fluctuating hydrodynamics theory for:
  (a) systems with transverse modes, (b) quantum systems.