Exact stationary state solution for one dimensional heat transport model with two conserved quantities

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Outline of the talk

- Introduction.
- Brief review of exactly known one dimensional heat transport model.
  - Purely harmonic chain.
  - Stochastic harmonic chain with three conserved quantities.
- Introduction of two conserved quantities model
- Results and conclusion

Introduction

- The transfer of heat from hot to cold temperature can be explained by Fourier's law (1810).
- Fourier's law follows diffusion equation for temperature as

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

  where κ is constant thermal conductivity and T is local temperature field.
- Interestingly, Fourier's law violated in lower dimension ($d \leq 2$).
- Many models with momentum conservation show anomalous transport.

Features of anomalous transport

- Conductivity κ, diverges with system size with an exponent α as
$$\kappa \sim N^{\alpha}, \quad 0 < \alpha < 1$$
- Models have nonlinear temperature profile in nonequilibrium steady state.
- Energy fluctuation has superdiffusive propagation.

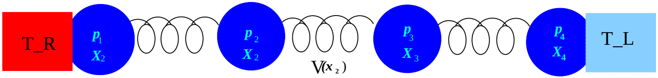
Studies on anomalous transport [1]

- Studied in many numerical simulations and in very few exactly solvable models.
  - 1d chain of particles with anharmonic interaction, disordered chain, coupled rotor chain, stochastic harmonic chain,etc.
- In experimental setup, like a rod of nanowire attached at two different temperature at its end
  - Breakdown of Fourier's law in nanotube thermal conductors, Chang *et al.*, 2008 .
  - Dimensional crossover of thermal transport in few-layer graphene, Suchismita Ghosh *et al.*, 2010, *etc*

[1] Lepri *et al.*, 2003 & *Dhar*, 2008

Purely harmonic chain

Rieder, Lebowitz, Lieb in 1967



$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i=1}^{N} k(X_{i+1} - X_i)^2,$$

where p_i momentum and $X_{i+1} - X_i = r_i$ is called stretch.

- One dimensional chain with two ends attached to Langevin bath with different temperature.
- Two neigboring particles have quadratic interaction.

Purely harmonic chain

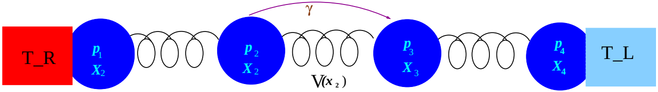
- Steady state distribution is Gaussian and exact correlation matrix is known.
- Conductivity diverges linearly (ballistic motion of phonons)

$$\kappa = \frac{C}{T_L - T_R} N$$

  where C is constant.
- In steady state, flat temperature profile with exponential deviation at its boundary is exactly known.

Stochastic harmonic chain

with three conserved quantities[2]



- Random exchange of momentum is allowed with rate γ.
- Exchange conserves total stretch, momentum and energy at all times.
- Interestingly, random exchange has same macroscopic behavior as due to nonlinearity in anharmonic chain.
- Current J, decay with exponent $N^{-1/2}$

$$J = \left(\frac{\pi^3}{\gamma N}\right)^{1/2} \frac{\Delta T}{8(\sqrt{8}-1)}$$

- As, $\kappa \sim JN \sim N^{1/2}$, divergence of conductivity with exponent $\alpha = 1/2$

[2] Basile *et al., 2006* & *Lepri et al., 2009*

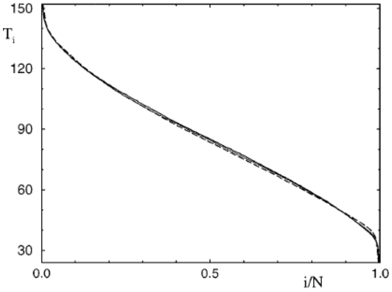


Figure: Temperature profile for three conserved quantities case (Lepri *et al., 2009)*

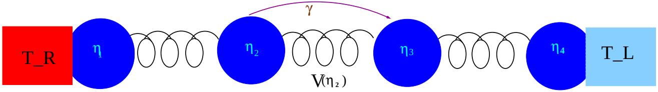
- Nonlinear temperature profile similar to the deterministic anharmonic oscillator
- Evolution of the temperature profile towards the steady state in infinite line is given as[3]

$$\partial_t T \sim |\Delta_y|^{3/4} T$$

[3]Basile *et al., 2016*

Stochastic harmonic chain

with two conserved quantities[4]



- η_i has only microscopic variable for particle i instead of momentum and stretch.
- Stochasticity is introduced with exchange of the variable η_i with η_{i+1} with rate γ
- Total volume $\sum_{i=1}^{N} \eta_i$ and energy $\sum_{i=1}^{N} \eta_i^2$ are conserved at all times.

[4] Bernardin and Stoltz, 2012

Dynamics

- All particles have same mass and Hamiltonian dynamics is given as

$$\begin{aligned} \frac{d\eta_i(t)}{dt} &= V'(\eta_{i+1}) - V'(\eta_{i-1}) \\ \frac{d\eta_1(t)}{dt} &= V'(\eta_2) - \lambda_R V'(\eta_1) + \sqrt{2\lambda_R k_B T_R}\xi_R \\ \frac{d\eta_N(t)}{dt} &= -V'(\eta_{N-1}) - \lambda_L V'(\eta_N) + \sqrt{2\lambda_L k_B T_L}\xi_L \end{aligned}$$

where η_i is a variable assign to each particle and $V(\eta) = \eta^2/2$

Dynamical operators[5]

Consists of two parts

- The deterministic part of dynamics with bath is given as

$$\mathcal{D} = \sum_{i=1}^{N-1} \left(V'(\eta_{i+1}) - V'(\eta_{i-1})\right) \partial_{\eta_i} - V'(\eta_{N-1})\partial_{\eta_N} + V'(\eta_1)\partial_{\eta_1}$$
$$+\lambda_R(T_R\partial^2_{\eta_1} - V'(\eta_1)\partial_{\eta_1}) + \lambda_L(T_L\partial^2_{\eta_N} - V'(\eta_N)\partial_{\eta_N})$$

- The stochastic part $\mathcal{S}$, which shows the exchange of variable η_i at random with rate γ and given as

$$\mathcal{S}f(\eta) = \sum_{i=-N}^{N-1} \left(f(\eta^{i,i+1}) - f(\eta))\right)$$

[5]Bernardin and Stoltz, 2012

Harmonic model with two conserved qunatities

Known results[7]

- Divergence exponent of conductivity,α is known numerically, with value $\alpha = 1/2$ for finite exchange rate γ.
- Hydrodynamics predicts diffusive sound peak and $3/2-$Lévy a heat peak[6].
- The skew fractional Laplacian dynamics (Skewness due to presence of one sound mode)

[6] Stoltz and Sphon, 2015

[7] Bernardin and Stoltz *et al., 2012*

Question we address in this work

* How does temperature profile look in stationary state?
* Is it possible to have an exact solution in stationary state similar to purely harmonic and stochastic harmonic chain with three conserved quantities?

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Yes! If we calculate the covariance $\langle \eta_i \eta_j \rangle$ exactly.

$$\begin{aligned} T_i &= \langle \eta_i^2 \rangle, \\ J_{i \to i+1} &= -\langle \eta_{i+1} \eta_i \rangle + \gamma(\langle \eta_{i+1} \eta_{i+1} \rangle - \langle \eta_i \eta_i \rangle) \end{aligned} \quad (1)$$

Master equation

We can write the Fokker Planck equation as

$$\frac{\partial P}{\partial_t} = \sum_{i,j} \left(A_{ij} \frac{\partial \eta_j P}{\partial \eta_i} + \frac{D_{ij}}{2} \frac{\partial^2 P}{\partial \eta_i \partial \eta_j} \right) - \gamma \sum_{j=1}^{N-1} [P(..\eta_{j+1}, \eta_j, ..) - P(.., \eta_j, \eta_{j+1}, ..)] \quad (2)$$

where A and D is $N \times N$ matrices

- For two conserved quantities model

$$\boxed{A_{i,j} = \delta_{i,j}(\lambda_l \delta_{i,1} + \lambda_r \delta_{i,N}) + \delta_{i-1,j} - \delta_{i+1,j}}$$

and

$$\boxed{D_{ij} = \delta_{i,j}(2T_R \delta_{i,1} + 2T_L \delta_{i,N})}$$

- Dynamics for covariance, $C = \langle \eta_i \eta_j \rangle$ can be written as

$$\boxed{\dot{C} = D - AC - CA^\dagger - \gamma W} \quad (3)$$

Modelling

- The stochastic contribution W for the bulk is,

$$W_{ij} = \begin{cases} \langle \eta_{i+1}\eta_{j+1} \rangle - 2\langle \eta_i \eta_j \rangle + \langle \eta_{i-1}\eta_{j-1} \rangle, & \text{for } i = j \\ \langle \eta_{i-1}\eta_j \rangle - 2\langle \eta_i \eta_j \rangle + \langle \eta_i \eta_{j+1} \rangle, & \text{for } i - j = -1 \\ \langle \eta_i \eta_{j-1} \rangle - 2\langle \eta_i \eta_j \rangle + \langle \eta_{i+1}\eta_j \rangle, & \text{for } i - j = 1 \\ \langle \eta_i \eta_{j-1} \rangle + \langle \eta_i \eta_{j+1} \rangle + \langle \eta_{i+1}\eta_j \rangle + \langle \eta_{i-1}\eta_j \rangle - 4\langle \eta_i \eta_j \rangle, & \text{for } |i - j| > 1 \end{cases}$$

- and for boundaries

$$W_{ij} = \begin{cases} \delta_{i,-N}\langle \eta_{i+1}\eta_{j+1} \rangle - \langle \eta_i \eta_j \rangle + \delta_{i,N}\langle \eta_{i-1}\eta_{j-1} \rangle, & \text{for } i = j \\ \delta_{i,-N}\langle \eta_i \eta_{j+1} \rangle - \langle \eta_i \eta_j \rangle + \delta_{j,N}\langle \eta_{i-1}\eta_j \rangle, & \text{for } i - j = -1 \\ \delta_{j,-N}\langle \eta_{i+1}\eta_j \rangle - \langle \eta_i \eta_j \rangle + \delta_{j,N}\langle \eta_{i-1}\eta_j \rangle, & \text{for } i - j = 1 \\ \langle \eta_i \eta_{j-1} \rangle + \delta_{i,-N}\langle \eta_i \eta_{j+1} \rangle + \langle \eta_{i+1}\eta_j \rangle + & \\ \delta_{j,N}\langle \eta_{i-1}\eta_j \rangle + \delta_{i,-N}\delta_{j,N}\langle \eta_i \eta_j \rangle - 3\langle \eta_i \eta_j \rangle, & \text{for } |i - j| > 1 \end{cases}$$

Exact and numerical stationary state results

Temperature profile

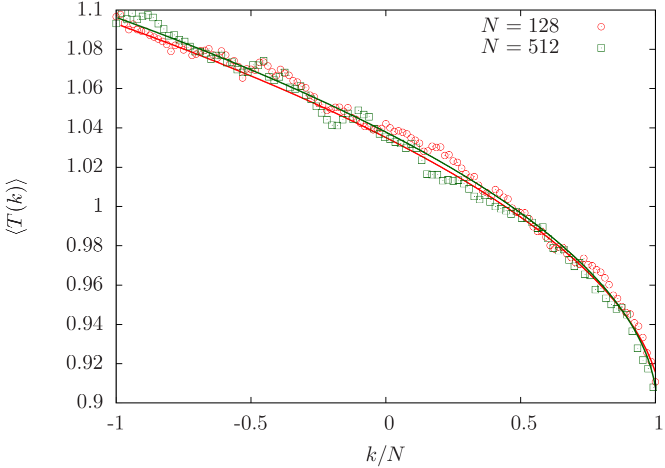


Figure: Points are molecular dynamics simulation using Störmer-Verlet scheme and solid line is solving covariance matrix

Current scaling with system size

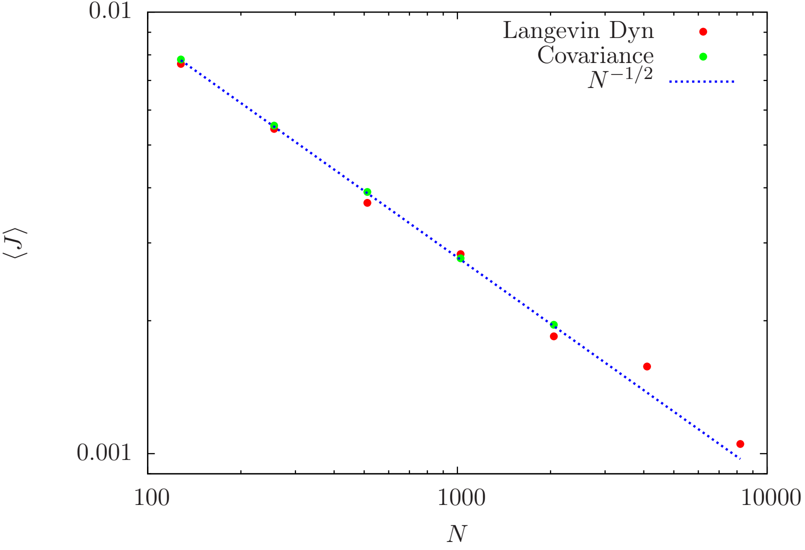
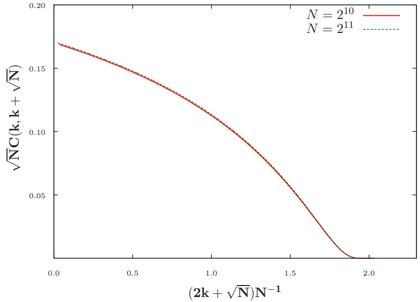
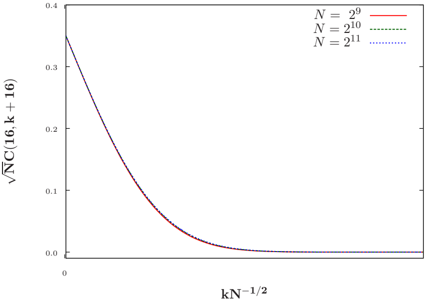


Figure: $T_L = 0.9$ and $T_R = 1.1$ for $\gamma = 1$

Exact stationary state results

scaling





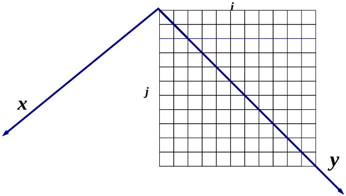
$$C(i,j) = L^{-a} S\left((i-j)L^{-b}, (i+j)L^{-c})\right)$$

J fixes $a = 1/2$, thus the scaling of other covariance for different system sizes gives $b = 1/2$ and $c = 1$ (exponents are same as that for the three conserved quantities model)

Calculation

Mapping to new domain

$$x = (i - j)\epsilon, \qquad y = (i + j)\epsilon^2,$$



where $\epsilon = 1/\sqrt{L}$, $x \in [0, \infty]$, and $y \in [0, 2]$.

- Defining new scaled field variable as

$$C(i, j) = \epsilon S(x, y), \quad \text{for } i \neq j$$

$$C(i, i) = T(y)$$

Continuum equation

- Using the discrete set of covariance equation for bulk, diagonal, and nearest to diagonal separately ,we get following continuum equations

$$\begin{aligned} \frac{\gamma}{2}\partial_x^2 S(x,y) &= -\partial_y S(x,y), \\ \partial_y T(y) &= -\gamma \partial_x S(0,y), \\ S(0,y) &= \mathcal{J}, \end{aligned}$$

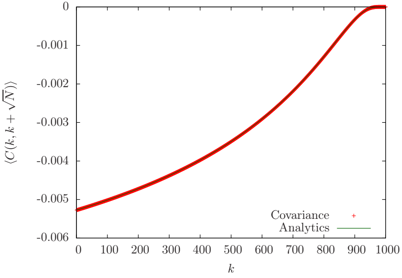
  where $\mathcal{J}$ is size independent constant current present in the system.

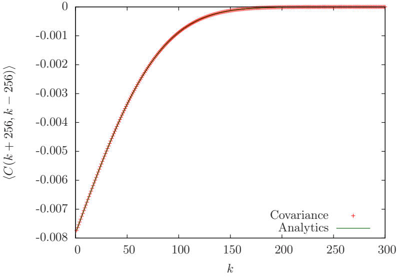
- The boundary term suggest $S(x,2) = 0$

Solution of continuum equation

The exact expression for the stationary state two point covariance $C(i,j) = \epsilon S(x,y)$ is

$$C(i,j) = \epsilon S(x,y) = \frac{\Delta T}{4}\sqrt{\pi\gamma}\,\mathrm{Erfc}\left(\frac{x}{\sqrt{2\gamma(2-y)}}\right)$$





Solution of continuum equation

$$J = \frac{\Delta T}{4}\sqrt{\frac{\pi\gamma}{N}}$$

$$T(y) = T(2) + \frac{\Delta T}{\sqrt{2}}\sqrt{2-y}$$

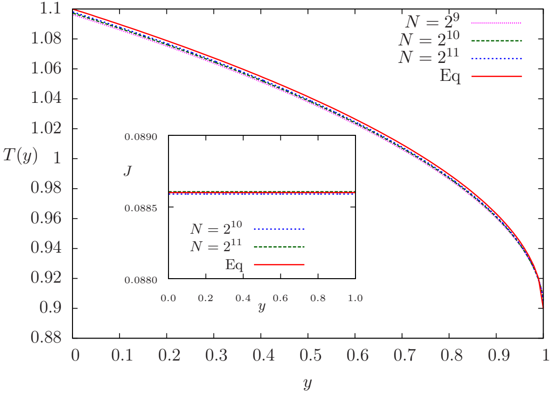


Figure: Broken line is from solving discrete equations. Solid line is above mention solution for J and T.

Conclusion

- We have the exact expression for two point covariance for full system.
- We have also calculated exact current expression which support earlier numerical prediction.
- The temperature profile is not anti symmetric about the mean as shown in three conserved quantities case.
- We also have continuum equation for relaxation dynamics for which work is going on.

Dynamics towards Steady state

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