

Transport in a non-acoustic anharmonic chain

Abhishek Dhar
International centre for theoretical sciences
TIFR, Bangalore
www.icts.res.in

Umesh Kumar (ICTS, Bangalore)

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- Anomalous heat transport in one dimensional momentum conserving anharmonic chains.
- Counter-example - non-acoustic harmonic chain with momentum conserving noise
- Question: what happens for non-acoustic Hamiltonian models?
- - 1 Simulation results for nonequilibrium state with different temperature heat baths at boundaries
 - 2 Simulation results for equilibrium space time correlation functions for the conserved fields
 - 3 Fluctuating hydrodynamics

Breakdown of Fourier's law — Anomalous heat transport

Fourier's law not valid in low-dimensional momentum-conserving systems.

Lecture notes in Phys. vol 921: Thermal transport in low dimensions (2016).

- Divergent conductivity: $\kappa \sim L^\alpha$.
- Anomalous spreading of heat pulses — Levy walk instead of random walk.
- Anomalous 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.

Understanding anomalous transport

Nonlinear fluctuating hydrodynamics - a general framework.

Narayan, Ramaswamy (2002), H. van Beijeren (2012)

Very detailed predictions: H. Spohn and C. Mendl (2013,2014)

- Look at decay of energy fluctuations in a system in thermal equilibrium. Thus one can look at spatio-temporal correlation functions such as

$$C(x, t) = \langle \delta\epsilon(x, t) \delta\epsilon(0, 0) \rangle,$$

where $\delta\epsilon(x, t)$ is fluctuation in local energy density.

Anomalous transport would imply super-diffusive spreading of such correlation functions.

Basics of fluctuating hydrodynamics

Fermi-Pasta-Ulam-Tsingou Hamiltonian:

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

- 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):

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

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 currents 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

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

$$\frac{\partial \phi_+}{\partial t} = -c \frac{\partial \phi_+}{\partial x} + D_s \frac{\partial^2 \phi_+}{\partial x^2} + \frac{\partial \eta_+}{\partial x}$$

$$\frac{\partial \phi_0}{\partial t} = D_h \frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x}$$

$$\frac{\partial \phi_-}{\partial t} = c \frac{\partial \phi_-}{\partial x} + D_s \frac{\partial^2 \phi_-}{\partial x^2} + \frac{\partial \eta_-}{\partial x}$$

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

Predictions of fluctuating hydrodynamics

- Including the nonlinear terms:

$$\frac{\partial \phi_+}{\partial t} = \frac{\partial}{\partial x}[-c\phi_+ + G^+ \phi^2] + D_s \frac{\partial^2 \phi_+}{\partial x^2} + \frac{\partial \eta_+}{\partial x}$$

$$\frac{\partial \phi_0}{\partial t} = \frac{\partial}{\partial x}[G^0 \phi^2] + D_h \frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x}$$

$$\frac{\partial \phi_-}{\partial t} = \frac{\partial}{\partial x}[c\phi_- + G^- \phi^2] + D_s \frac{\partial^2 \phi_-}{\partial x^2} + \frac{\partial \eta_-}{\partial x}$$

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 $C(x, t) = \langle \phi_\alpha(x, t) \phi_\beta(0, 0) \rangle$.

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

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

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 comparisons with theory.

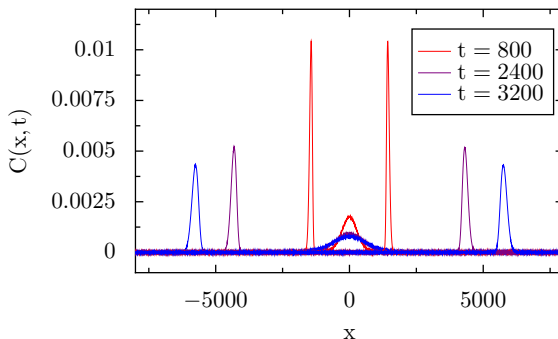
Equilibrium space-time correlation functions

Numerically compute heat mode and sound mode correlations in the $\alpha - \beta$ -Fermi-Pasta-Ulam chain with periodic boundary conditions.

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

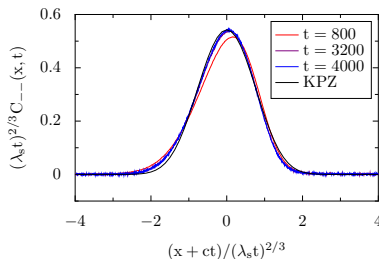
Parameters — $k_2 = 1$, $k_3 = 2$, $k_4 = 1$, $T = 5.0$, $\mathcal{P} = 1.0$, $N = 16384$.

Speed of sound $c = 1.803$.

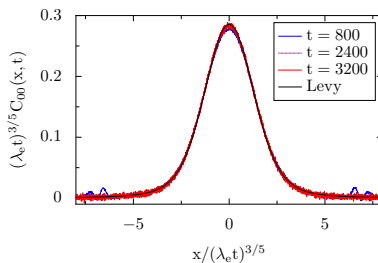


Equilibrium simulations of FPU

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



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



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Diffusive Propagation of Energy in a Non-acoustic Chain

TOMASZ KOMOROWSKI & STEFANO OLLA

Communicated by C. LE BRIS

Model: a harmonic chain of N unit-mass particles with displacements q_ℓ and momenta p_ℓ .
Hamiltonian is

$$H = \sum_{\ell=1}^N \varepsilon_\ell, \quad \varepsilon_\ell = \frac{p_\ell^2}{2} + V(\mathfrak{K}_\ell), \quad V(\mathfrak{K}) = \frac{K_2}{2} \mathfrak{K}^2,$$

where $\mathfrak{K}_\ell = \Delta q_\ell = q_{\ell+1} - 2q_\ell + q_{\ell-1}$.

Equations of motion:

$$\begin{aligned} \frac{dq_\ell}{dt} &= p_\ell \quad [\text{OR} \quad \frac{d\mathfrak{K}_\ell}{dt} = \Delta p_\ell], \\ \frac{dp_\ell}{dt} &= -\Delta \mathfrak{K}_\ell + \text{momentum conserving noise.} \end{aligned}$$

Spectrum: $\omega(k) = 4\sqrt{K_2} \sin^2\left(\frac{k}{2}\right)$ or $\omega \sim k^2$: hence non-acoustic.

Main result: diffusive scale hydrodynamics given by:

$$\partial_t \mathfrak{K}(x, t) = \Delta p(x, t), \quad \partial_t p(x, t) = -\Delta \mathfrak{K}(x, t) + 3\gamma \Delta p(x, t),$$

$$\partial_t T(x, t) = \left(\frac{(\sqrt{3}-1)K_2}{2\sqrt{3}\gamma} + 3\gamma \right) \Delta T + 3\gamma (\partial_x p(x, t))^2.$$

Hamiltonian model

N unit-mass particles with displacements q_ℓ and momenta p_ℓ . The Hamiltonian is:

$$H = \sum_{\ell=1}^N \varepsilon_\ell, \quad \varepsilon_\ell = \frac{p_\ell^2}{2} + V(\mathfrak{K}_\ell), \quad V(\mathfrak{K}) = \frac{K_2}{2} \mathfrak{K}^2 + \frac{K_4}{4} \mathfrak{K}^4,$$

where $\mathfrak{K}_\ell = \Delta q_\ell = q_{\ell+1} + q_{\ell-1} - 2q_\ell$

Equations of motion:

$$\frac{d\mathfrak{K}_\ell}{dt} = \Delta p_\ell, \quad \frac{dp_\ell}{dt} = -\Delta V'(\mathfrak{K}_\ell).$$

Conservation laws: curvature $\mathfrak{K}_\ell$, momentum p_ℓ , and energy ε_ℓ ,

$$\mathfrak{K}_\ell = q_{\ell+1} - 2q_\ell + q_{\ell-1}, \quad p_\ell = \dot{q}_\ell, \quad \varepsilon_\ell = \frac{p_\ell^2}{2} + V(\mathfrak{K}_\ell).$$

These quantities obey the discrete continuity equations

$$\dot{\mathfrak{K}}_\ell = \Delta p_\ell = J_\ell^{\mathfrak{K}} - J_{\ell+1}^{\mathfrak{K}},$$

$$\dot{p}_\ell = -\Delta V'(\mathfrak{K}_\ell) = J_\ell^p - J_{\ell+1}^p,$$

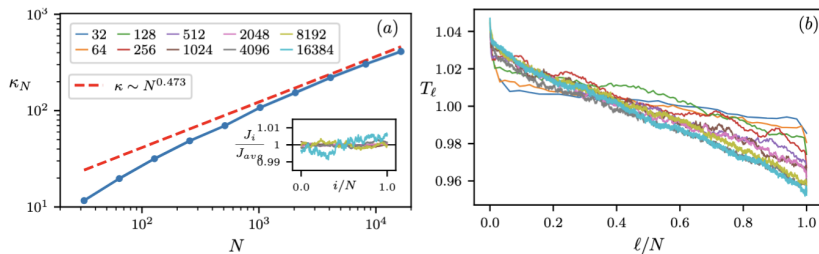
$$\dot{\varepsilon}_\ell = V'(\mathfrak{K}_\ell) \Delta p_\ell - p_\ell \Delta V'(\mathfrak{K}_\ell) = J_\ell^e - J_{\ell+1}^e.$$

$$J_\ell^{\mathfrak{K}} = p_{\ell-1} - p_\ell, \quad J_\ell^p = V'(\mathfrak{K}_\ell) - V'(\mathfrak{K}_{\ell-1}), \quad J_\ell^e = p_{\ell-1} V'(\mathfrak{K}_\ell) - p_\ell V'(\mathfrak{K}_{\ell-1}).$$

Results from Nonequilibrium Simulations

Chain with fixed ends $q_0 = q_{N+1} = 0$ and Langevin thermostats for q_1 and q_N at temperatures T_L on the left end and T_R on the right end.

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Anomalous transport: $\kappa \sim N^{1/2}$

Equilibrium space-time correlations

Equilibrium distribution:

$$\text{Prob}(\{q_\ell, p_\ell\}) = \prod_\ell \mathcal{P}_{\beta, \varphi, \nu}(\mathfrak{K}_\ell, p_\ell)$$

$$\mathcal{P}_{\beta, \varphi, \nu}(\mathfrak{K}, p) = \frac{1}{\mathcal{Z}(\beta, \varphi, \nu)} \exp \left[-\beta \left(\frac{(p - \nu)^2}{2} + V(\mathfrak{K}) - \varphi \mathfrak{K} \right) \right].$$

β, ν, ϕ are the conjugate fields corresponding to $e, p, \mathfrak{K}$.

The fluctuation fields are

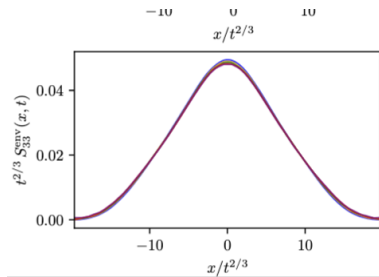
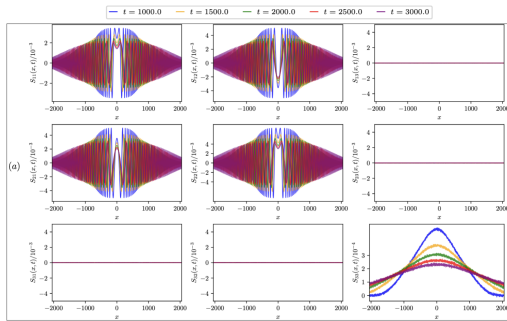
$$u_1(x, t) = \mathfrak{K}(x, t) - \langle \mathfrak{K} \rangle, \quad u_2(x, t) = p(x, t) - \langle p \rangle, \quad u_3(x, t) = e(x, t) - \langle e \rangle.$$

Equilibrium space-time correlations:

$$S_{ij}(x, t) = \langle u_i(x, t) u_j(0, 0) \rangle.$$

Simulation results: equilibrium space-time correlations

$\phi = 0$ case:



Energy decoupled (follows from symmetry of invariant measure under $(p_x, \mathfrak{R}_x) \rightarrow (-p_x, -\mathfrak{R}_x)$).

Energy exponent is KPZ ($z = 3/2$), scaling function (?).

Other fields: Oscillations, scaling difficult to observe, need to go to NORMAL modes.

Fluctuating hydrodynamics

The conserved fields obey the discrete continuity equations

$$\dot{\mathfrak{K}}_\ell = \Delta p_\ell = J_\ell^{\mathfrak{K}} - J_{\ell+1}^{\mathfrak{K}},$$

$$\dot{p}_\ell = -\Delta V'(\mathfrak{K}_\ell) = J_\ell^p - J_{\ell+1}^p,$$

$$\dot{\epsilon}_\ell = V'(\mathfrak{K}_\ell)\Delta p_\ell - p_\ell\Delta V'(\mathfrak{K}_\ell) = J_\ell^e - J_{\ell+1}^e.$$

$$J_\ell^{\mathfrak{K}} = p_{\ell-1} - p_\ell, \quad J_\ell^p = V'(\mathfrak{K}_\ell) - V'(\mathfrak{K}_{\ell-1}), \quad J_\ell^e = p_{\ell-1} V'(\mathfrak{K}_\ell) - p_\ell V'(\mathfrak{K}_{\ell-1}).$$

We obtain the “Euler” equations by taking averages over slowly varying local equilibrium measures.
“Euler” currents:

$$J^{\mathfrak{K}}(x, t) = -\partial_x v(x, t), \quad J^p(x, t) = \partial_x \varphi(x, t), \quad J^e(x, t) = -\varphi(x, t) \partial_x v(x, t) + v(x, t) \partial_x \varphi(x, t),$$

where $\varphi = \langle V'(\mathfrak{K}) \rangle$.

“Euler” equations:

$$\partial_t \chi = \partial_x^2 v, \quad \partial_t v = -\partial_x^2 \varphi, \quad \partial_t \epsilon = \varphi \partial_x^2 v - v \partial_x^2 \varphi.$$

$$\varphi(x, t) = \varphi(\chi, e), \quad e(x, t) = \epsilon(x, t) - \frac{v(x, t)^2}{2}.$$

Fluctuating hydrodynamics

The fluctuations (u_1, u_2, u_3 around the equilibrium values satisfy the following equations:

$$\partial_t \mathbf{u}(x, t) = -\partial_x^2 (\mathbf{A} \mathbf{u}) - \partial_x^2 H \mathbf{u} \mathbf{u} + \mathcal{D} \partial_x^4 \mathbf{u} - \mathcal{B} \partial_x^2 \boldsymbol{\xi}(x, t),$$

Fluctuation-Dissipation: $BB^T = DC + CD^T$.

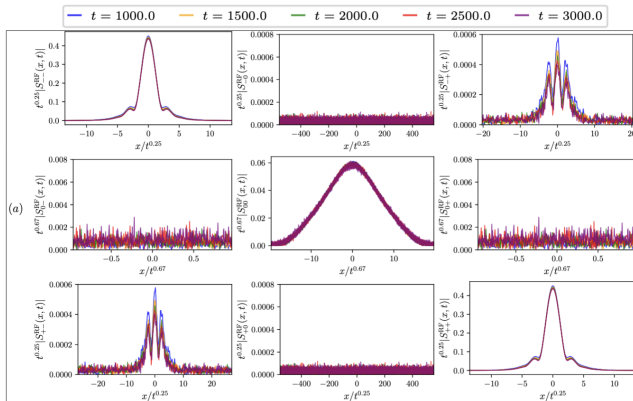
- The flux-Jacobian matrix A has one zero and two imaginary eigenvalues.
- No sound peaks, as expected.
- First go to normal modes and then to a rotating frame (to remove the oscillations).

$$S_{\sigma\rho}^{\sharp}(x, t) = \langle \phi_{\sigma}(x, t) \phi_{\rho}(0, 0)^* \rangle, \quad \sigma, \rho \in \{-, 0, +\}.$$

$$\hat{S}_{\sigma\rho}^{\sharp}(k, t) = e^{i\Omega_{\sigma}(k)t} \hat{S}_{\sigma\rho}^{\text{RF}}(k, t), \quad \Omega_{\sigma}(k) = \sigma \alpha_b k^2,$$

- We add fourth-order dissipation since this seems to explain our simulational observations — phenomenological.

Simulation results for normal-mode correlations



Two sub-diffusive modes and one KPZ-mode.

- Hamiltonian non-acoustic anharmonic chain still seems to show anomalous transport.
- $\kappa \sim N^{1/2}$ from nonequilibrium simulations.
- Heat mode shows KPZ exponent $C_{ee}(x, t) = t^{-2/3} f(xt^{-2/3})$.
- Not clear how to reconcile equilibrium and nonequilibrium studies.
[See also Tamaki, Sasada, Saito (2017)—stochastic non-acoustic model]

Some questions:

- Obtaining predictions from nonlinear fluctuating hydrodynamics.
- Change noise from Δp to $\Delta^2 p$ form. Does this lead to superdiffusion in the noisy beam model?