Energy current fluctuations for one-dimensional equilibrium systems in ring geometries

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New approaches to non-equilibrium and random systems:KPZ...
KITP

Outline

- Anomalous heat conduction in one dimensional systems – a brief introduction.
- Basics of fluctuating hydrodynamics for anharmonic chains.
  Numerical tests of predictions of equilibrium space-time correlation functions of density, momentum and energy in the $\alpha - \beta$ Fermi-Pasta-Ulam model.
  S. Das, AD, K. Saito, C. Mendl, H. Spohn, PRE 90, 012124 (2014).
- Results on energy current fluctuations (large deviations) on the ring geometry—

  Numerical results for two $1D$ systems:
  (I) Alternating mass hard particle gas
  (II) Harmonic chain with conservative noise

  Heuristic predictions from fluctuating hydrodynamic theory and Levy walk model.

  A. Dhar, K. Saito, A. Roy (arXiv:1512.00561)

Anomalous energy transport

Fourier's law of heat conduction

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

κ – thermal conductivity of the material (expected to be an intrinsic property).

Fourier's law implies diffusive spreading of heat.

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

Fourier's law: A challenge for theorist's (Bonetto, Lebowitz, Rey-Bellet, 2000)

The problem of anomalous heat transport:

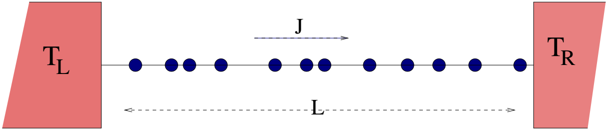
In one dimensional systems with momentum conservation, κ increases with system size, L (N), and for large system sizes diverges as $\kappa \sim N^{\alpha}$.

Thus κ is not an intrinsic material property ! Fourier's law not valid!!

Anomalous heat transport - Approach I: Non-equilibrium steady state

Checking the validity of Fourier's law in a system with specified Hamiltonian dynamics?

Attach heat baths and measure heat current directly in the nonequilibrium steady state. Compute κ and study scaling with system size.



Measure heat current —Fourier's law implies $J = \frac{\kappa \Delta T}{L}$

Conductivity $\rightarrow \quad \kappa = \frac{JL}{\Delta T}$

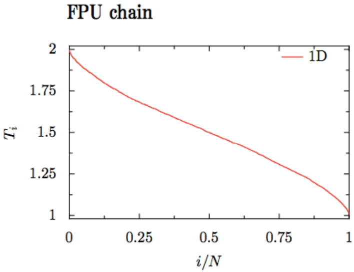
Fourier law requires κ to be independent of L (for large enough L).

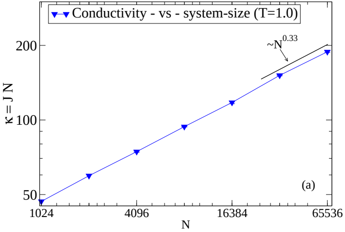
Otherwise — Anomalous $\rightarrow \quad \kappa \sim L^{\alpha}$

Anomalous transport -steady state study

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

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



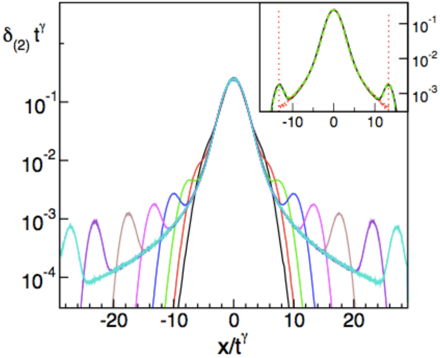


Conductivity diverges with system size (For FPU chain $\kappa \sim N^{0.33}$).
S.Das, AD, O. Narayan (JSP, 2014).

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

Anomalous transport - transient experimental signatures

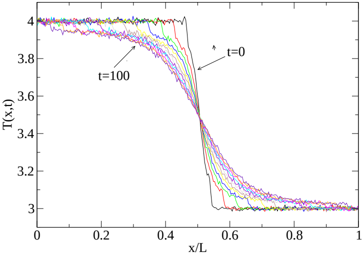
Speading of a heat pulse in alternate mass HPG [Cipriani,Denisov,Politi (2005)].



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

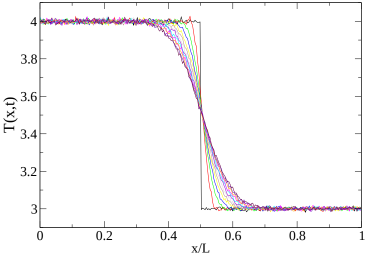
Evolution of a shock profile (AD):

Anomalous system



$x/t^{2/3}$ scaling

Diffusive system



$x/t^{1/2}$ scaling

Anomalous transport - Approach II: Equilibrium correlations

1. Look at heat current auto-correlation function in thermal equilibrium and use Green-Kubo formula to calculate thremal conductivity.

$$\kappa_{GK} = \lim_{\tau \to \infty} \lim_{N \to \infty} \frac{1}{k_B T^2 N} \int_0^{\tau} dt \langle J(t) J(0) \rangle \ .$$

   Fourier's law requires finite κ_{GK}, hence fast decay of $\langle J(0)J(t)\rangle$.
   Anomalous transport implies slow decay of $\langle J(0)J(t)\rangle$, hence diverging conductivity.

2. 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.

Analytic approaches are mainly based on these.

Some open questions and theoretical approaches

- Is it always so ? Are all momentum conserving Hamiltonian systems ?
- Establishing universality classes and computing the exponent α ($\kappa \sim N^{\alpha}$).
- What replaces the diffusion equation for systems with anomalous transport ?

  Levy walk description — Lepri, Politi (2013), Dhar, Saito, Derrida (2014).

  Fractional diffusion equation — Olla, Bernardin, Jara, Goncalves, Komorowski, Simon, Sasada (2014).
- Fluctuating hydrodynamic theory —
  Narayan, Ramaswamy (2002), H. vanBeijeren(2012)
  Very detailed predictions: H. Spohn and C. Mendl (2013-)

Basics of fluctuating hydrodynamics

Spohn (JSP,2014)

- Identify the conserved quantities. For the FPU chain they are the extension (or particle density) $r_i = q_{i+1} - q_i$, momentum: p_i and energy: e_i. They satisfy the exact conservation laws:

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

 where P is the pressure.

- Consider fluctuations about the equilibrium values: $r_i = \ell + u_1(i), \quad v_i = u_2(i), \quad e_i = e + u_3(i)$. Expand the curents about their equilibrium value (to second order in nonlinearity) and write hydrodynamic equations for these fluctuations.

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

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}\left[Au + uGu - \frac{\partial}{\partial x}Cu + B\xi\right]. \quad \text{1D noisy Navier} - \text{Stokes equation}$$

 A, G known explicitly in terms of microscopic model.

- Consider normal modes of linear equations and the normal mode variables $\phi = Ru$. One finds that there are two propagating sound modes ($\phi_\pm$) and one diffusive heat mode (ϕ_0).

Predictions of fluctuating hydrodynamics

- 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 sound modes.
- Solving the nonlinear hydrodynamic equations within mode-coupling approximation, one can make predictions for the equilibrium space-time correlation functions $C(x,t) = \langle \phi_\alpha(x,t)\phi_\beta(0,0)\rangle$.
-
$$\text{Sound} - \text{mode}: \quad C_s(x,t) = \langle \phi_\pm(x,t)\phi_\pm(0,0)\rangle = \frac{1}{(\lambda_s t)^{2/3}}\, f_{KPZ}\left[\frac{(x \pm ct)}{(\lambda_s t)^{2/3}}\right]$$
$$\text{Heat} - \text{mode}: \quad C_e(x,t) = \langle \phi_0(x,t)\phi_0(0,0)\rangle = \frac{1}{(\lambda_e t)^{3/5}}\, f_{LW}\left[\frac{x}{(\lambda_e t)^{3/5}}\right]$$

  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 $x = ct$.

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

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

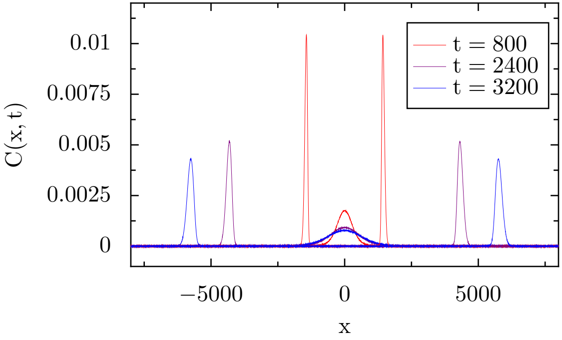
Equilibrium space-time correlation functions

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

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

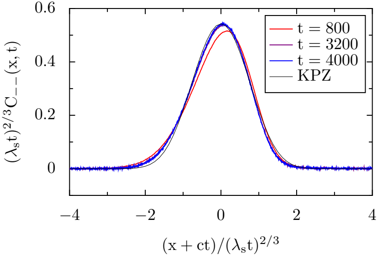
Parameters — $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 5.0,\ P = 1.0,\ N = 16384.$

Speed of sound $c = 1.803$.

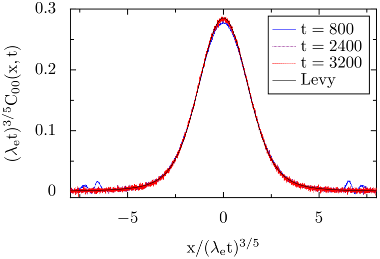


Equilibrium simulations of FPU

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



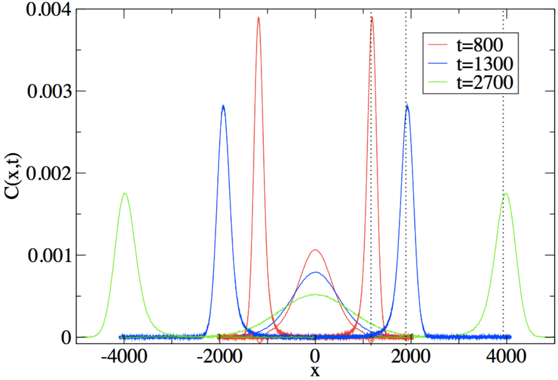
Heat mode scaling: $\lambda_{\text{theory}} = 5.89$, $\lambda_{\text{sim}} = 5.86$.



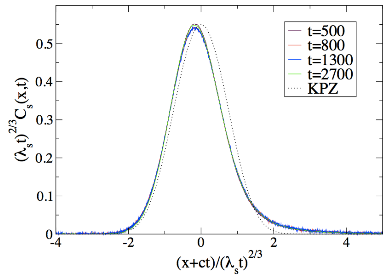
Low temperature data

Parameters — $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 0.5,\ p = 1.0,\ N = 8192.$

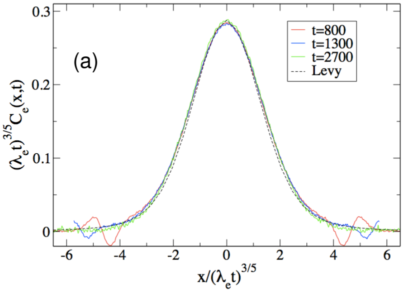
Speed of sound $c = 1.455$.



Scaling of sound and heat modes



Very good scaling obtained. The scaling function is not yet symmetric and deviates from the expected KPZ form.
$\lambda_{\text{theory}} = 0.675, \ \lambda_{\text{sim}} = 2.05.$



Good fit to Levy distribution
$\tilde{f}_{LW} = exp(-|k|^{5/3} t)$
with cut-off at $x = ct$.
$\lambda_{\text{theory}} = 1.97, \ \lambda_{\text{sim}} = 13.8.$

This scaling corresponds to the thermal conductivity exponent $\alpha = 1/3$.

Equilibrium simulations of FPU

Summary of results:

- Two universality classes based on interparticle potential $V(r)$ and equilibrium parameters (T, P) [structure of non-linearity -G-matrix)].

  Class (I): Sound modes show KPZ scaling. Heat mode is Levy-$5/3$.

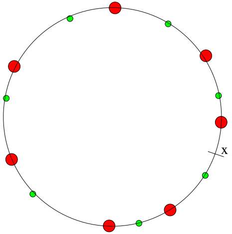
  Class (II): Sound modes are diffusive. Heat mode is Levy-$3/2$.

  ?? Class (III): Both sound and heat modes are Levy-"golden mean"

- Numerics: KPZ and Levy scaling are always very good. Values of scaling parameters sometimes far from theory. Fit to KPZ scaling function not always good.

- Provides some understanding of anomalous energy transport in $1D$ systems with three conserved variables.

Fluctuations of the heat flux of a one-dimensional hard particle gas with alternating masses:
E. Brunet, B. Derrida and A. Gerschenfeld



Measure the total energy crossing a given point x in time τ.

$$q(x) = \int_0^\tau dt\, j(x,t) \text{or} \;\; Q = \frac{1}{L}\int_0^L q_\tau(x) dx.$$

What are the statistics of q, Q for large τ and finite systems (fix length L) ?

Expect $Prob_L(Q) \sim e^{h(Q/\tau)\tau}$. Results for current cumulants $\langle Q^n \rangle_c / \tau$.

Current Cumulants on ring geometry

Results of Brunet,Derrida,Gerschenfeld (2010).

- Equilibrium simulations of Alternate mass hard particle gas (HPG). This is a system with anomalous transport and in same class as FPU ($\kappa \sim L^{1/3}$).
- Even cumulants of the current grow linearly with τ. Look at $C_{2n} = \frac{\langle Q^{2n} \rangle_c}{\tau}$.
- Numerical results: $C_2 \sim L^{-1/2}, \quad C_4 \sim L^{1/2}$
  In contrast,
  for diffusive systems, $C_2 \sim L^{-1}$, all higher cumulants $\sim L^{-2}$.

Results of Mendl, Spohn on a related question (2014).

- Look at integrated energy current fluctuations for an infinite system and compute *Prob*(q). Comparision with Baik-Rains distribution.
- Important point: Mendl/Spohn measure current across two particles and not across a fixed spatial location.

Current Cumulants on ring geometry

Present work:
1) Simulations for equilibrium current cumulants for two models belonging to the two universality classes — (a) HPG, (b) harmonic chain with energy-momentum-conserving noise.
2) A theory, based on fluctuating hydrodynamics, leading to connections with current fluctuations in ASEP (Derrida, Lebowitz).

Theory.

- Recall, system is described by two sound modes $\phi_\pm(x,t)$ and a heat mode $\phi_0(x,t)$.
- It turns out that the heat current depends only on the sound mode and is given by

$$j_3 = \frac{c}{\sqrt{6}\beta}(\phi_+ - \phi_-) + \frac{c}{2\beta}(\phi_+^2 - \phi_-^2) \, .$$

Hence the integrated energy current is the sum of two counter-propagating Burgers currents

$$q = \frac{P}{c\sqrt{2\beta}}\,(q_+ + q_-).$$

- Thus the generating function of the energy current is

$$Z(\lambda) = Z_{\mathrm{BG}}\left(\frac{P}{c\sqrt{2\beta}}\lambda\right)\, Z_{\mathrm{BG}}\left(-\frac{P}{c\sqrt{2\beta}}\lambda\right) \, .$$

Cumulant generating function for Alternate mass model

Thus $Z(\lambda) \sim e^{\mu(\lambda)\tau}$ with

$$\mu(\lambda) = \mu_{\rm BG}(\lambda) + \mu_{\rm BG}(-\lambda)\ .$$

Using Derrida-Lebowitz ASEP results for $\mu_{BG}(\lambda)$ we get:

- The the odd cumulants of the heat flux vanish.
- Even cumulants are given by

$$C_2 = \frac{a^3}{4\pi 2^{1/2} N^{1/2}}\ ,$$

$$C_4 = \left[\frac{9}{4} + \frac{15}{4\ 2^{1/2}} - 2\ 6^{1/2}\right] \frac{a^5 N^{1/2}}{2\pi},$$

$$C_6 = \left[\frac{1575}{8} + \frac{8435}{24\ 2^{1/2}} - 50\ 3^{1/2} - 100\ 6^{1/2} - 36\ 10^{1/2}\right] \frac{a^7 N^{3/2}}{2\pi}\ .$$

- The ratios are universal parameter-independent constants.

$$r_C = C_2\ C_6/C_4^2 = 2.99248...$$

Cumulant generating function for momentum exchange model

- Linear equations of motion + exchange momenta of randomly chosen nearest neighbor pairs at a fixed rate — exactly solved model (Basile,Bernardin, Olla), in universality class (II).
- $j_3 = k(\phi_+^2 - \phi_-^2)$. Hence
  $q = k(q_+ + q_-)$ where $q_= \int_0^\tau \; dt \; \phi_+^2(x, t.)$
- The equations for the sound modes are linear, hence it is possible to obtain exactly the statistics of the energy current. A simple computation involving Gaussian integrations gives

$$\mu_\phi(\lambda) = -\frac{1}{2\pi} \sum_{q \neq 0} \int_{-\infty}^{\infty} d\omega \log \left[1 + \frac{\lambda}{N} \frac{2Dq^2}{\omega^2 + D^2 q^4} \right] ,$$

where $q = 2s\pi/N$ and $s = 1, 2, \ldots$.

Cumulant generating function for momentum exchange model

- Expanding $\mu_\phi(\lambda)$ in a series about $\lambda = 0$ we get

$$\langle q_+^n \rangle_c / \tau = N^{n-2} \frac{(-1)^n B_{2(n-1)}}{(n-1)!(2D)^n} ,$$

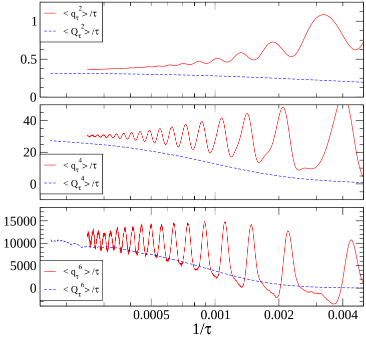
where B_{2n} are the Bernoulli numbers.

- The even current cumulants are given by

$$C_2 = 2k^2 \frac{1/6}{(2D)^2} ,$$
$$C_4 = 2k^4 N^2 \frac{1/42}{3!(2D)^4} ,$$
$$C_6 = 2k^6 N^4 \frac{5/66}{5!(2D)^6} .$$

- Ratio of cumulants

$$r_C = C_2 C_6 / C_4^2 = 147/22.$$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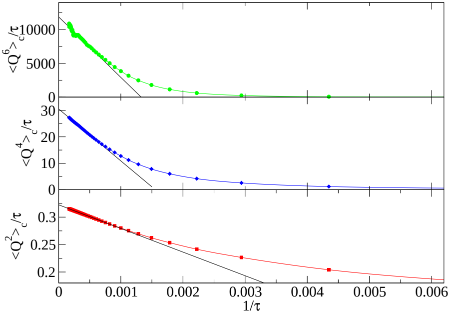
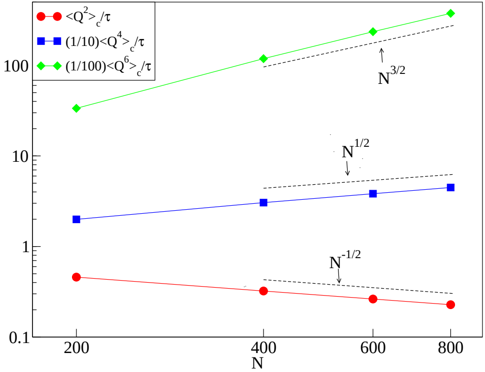

$<Q^6>_c/\tau$
$<Q^4>_c/\tau$
$<Q^2>_c/\tau$
$1/\tau$

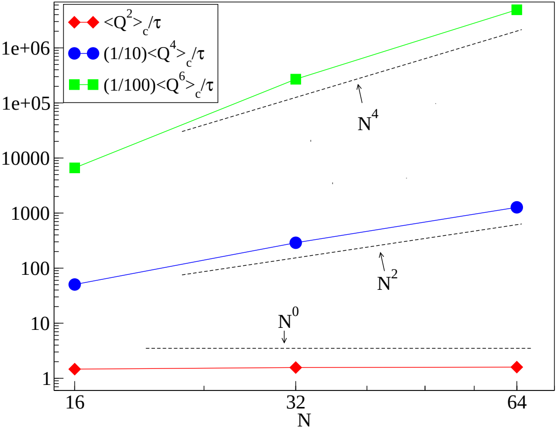
Numerical results: Current Cumulants for Alternate mass gas

- 2^{nd}, 4^{rd} and 6^{th} cumulants of current for alternate mass hard particle gas



Numerical results: Current Cumulants for momentum exchange model

- 2^{nd}, 4^{rd} and 6^{th} cumulants of current for momentum exchange model.



Conclusions

- Theory for understanding large deviations in equilibrium energy current fluctuations.
- Connections to current fluctuations in KPZ (or Burgers).
- Exact solution for momentum exchange model.
- Main results:

  Current fluctuations are large in systems with anomalous transport!

  Scaling with system size:

  Model I: $C_2 \sim L^{-1/2},\ C_4 \sim L^{1/2}, C_6 \sim L^{3/2}$
  Model II: $C_2 \sim L^0,\ C_4 \sim L^2, C_6 \sim L^4$

  Compare with diffusive case: $C_2 \sim L^{-1},\ C_4 \sim L^{-2}, C_6 \sim L^{-2}$
- Universal ratio of cumulants.
- Assumptions: Heat and sound modes interact weakly. This is required since the sound modes are allowed to go around the circle many times.
- Understanding in terms of Levy walk picture.