Equilibrium correlations and heat conduction in the Fermi-Pasta-Ulam chain.

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

Suman G. Das (Raman Research Institute, Bangalore)
Keiji Saito (Keio University)
Herbert Spohn (TU, Munich)
Christian Mendl (TU, Munich)
Onuttom Narayan (UC, Santa Cruz)

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Outline

- Anomalous heat conduction in one dimensional momentum conserving systems – a short introduction.
- New results
  1. Equilibrium space-time correlation functions of density, momentum and energy in the asymmetric $\alpha - \beta$ FPU model.
     [arXiv:1404.7081 (2014)]
  2. Nonequilibrium simulations of the asymmetric $\alpha - \beta$ Fermi-Pasta-Ulam model.
     [J. Stat. Phys (2013)]
- Discussion

Fourier's law

Fourier's law of heat conduction

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

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

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:

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

The problem of anomalous transport in low dimensional systems:

κ increases with system size and for large system sizes we have a divergence $\kappa \sim N^{\alpha}$.
Thus κ is not an intrinsic material property !

Anomalous heat transport

How do we know whether or not Fourier's law is valid in a given system with specified Hamiltonian dynamics?

1. Attach heat baths and measure heat current directly in the nonequilibrium steady state.
   Compute κ and study scaling with system size.
   Fourier's law implies $J = \frac{\kappa \Delta T}{N}$ (OR $\kappa = \frac{JN}{\Delta T} \sim N^0$).....otherwise anomalous.

2. 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.

3. Look at decay of energy fluctuations in a system in thermal equilibrium.
   Fourier's law implies diffusion equation and hence diffusive spreading of energy.
   Anomalous transport leads to super-diffusive spreading of energy.

Lepri, Livi, Poloti, Phys. Rep. (2003).
A.D, Advances in Physics, vol. 57 (2008).

Approach - I : Nonequilibrium linear response current

Nonequilibrium simulations of the Fermi-Pasta-Ulam chain.
Lepri, Livi, Politi (1997,1998)

Momentum conserving system with quartic anharmonic term —
the β-Fermi-Pasta-Ulam (FPU) model:

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

Nonequilibrium simulations of the FPU chain found that Fourier's law was not valid and $\kappa \sim N^\alpha$ with $\alpha \approx 0.5$.

This seems to be general: for many different momentum conserving anharmonic systems with/witouout disorder, κ diverges with system size N as:

$$\kappa \sim N^\alpha \quad \text{with } 0 < \alpha < 1 .$$

Approach-II: Green-Kubo relation to equilibrium current correlations

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

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

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

- Mode-coupling theory for anharmonic chains
  – Lepri,Livi,Politi (1998,2008).
- Fluctuating hydrodynamics for a one-dimensional gas
  – Narayan, Ramaswamy (2002), Beijeren (2012), Spohn, Mendl (2013).
- Exact solution of energy-momentum conserving stochastic model
  – Basile, Bernardin, Olla (2006).

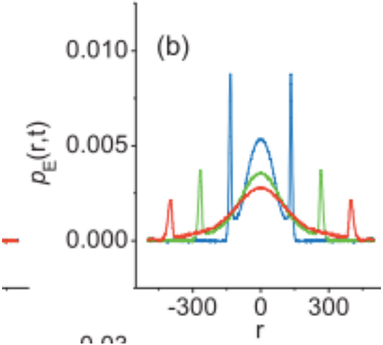
  These find $\langle J(t)J(0)\rangle \sim t^{-\delta}$ with $0 < \delta < 1$.

  This implies from Green-Kubo that $\kappa_{GK} \sim N^{1-\delta}$.

Approach – III: Energy spreading

Look at propagation of a heat pulse or equivalently at the decay of equilibrium fluctuations

Levy walk picture – Denisov, Klafter, Urbakh, Cipriani, Politi (2003,2005), Zhao (2006), Denisov,Hanggi (2012), Liu,Li (2014), Lepri, Politi (2011), Dhar, Saito, Derrida (2013).



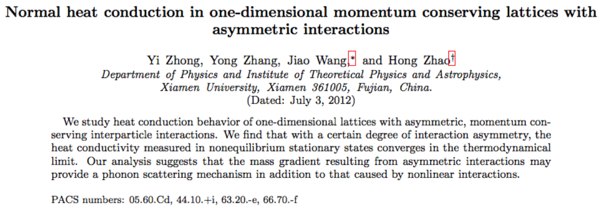
- The energy profile follows the Levy-stable distribution.
- Gaussian peak, power-law decay at large x.
- Finite speed of propagation.
- $\langle x^2 \rangle \sim t^{1+\alpha}$ (Super-diffusive).

Some open questions

- Establishing universality classes and computing the exponent α ($\kappa \sim N^\alpha$).
- What is the correct hydrodynamic description of systems with anomalous transport ?

  What replaces the heat diffusion equation ? Perhaps Levy walk description ($\approx$ fractional diffusion equation): But there has been no microscopic derivation of the Levy-walk picture so far.
- No rigorous proof that the thermal conductivity does diverge !
  Recent simulations of some models indicate finite conductivity at low temperatures (e.g asymmetric FPU).

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

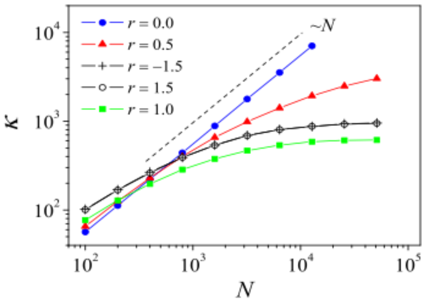


Normal heat conduction in one-dimensional momentum conserving lattices with asymmetric interactions

Yi Zhong, Yong Zhang, Jiao Wang,* and Hong Zhao†
Department of Physics and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen 361005, Fujian, China.
(Dated: July 3, 2012)

We study heat conduction behavior of one-dimensional lattices with asymmetric, momentum conserving interparticle interactions. We find that with a certain degree of interaction asymmetry, the heat conductivity measured in nonequilibrium stationary states converges in the thermodynamical limit. Our analysis suggests that the mass gradient resulting from asymmetric interactions may provide a phonon scattering mechanism in addition to that caused by nonlinear interactions.

PACS numbers: 05.60.Cd, 44.10.+i, 63.20.-e, 66.70.-f



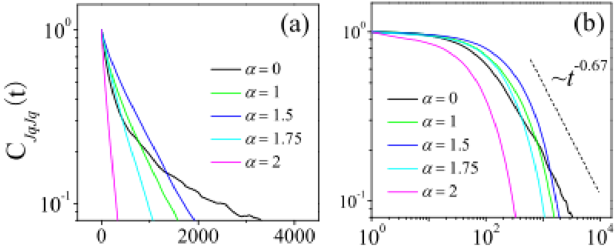
$$
\begin{aligned}
V(x) &= \frac{1}{2}(x+r)^2 + e^{-rx} \, . \\
T &= 2.5
\end{aligned}
$$

Recent results on systems with asymmetric potentials

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*
Department of Physics and Institute of Theoretical Physics and Astrophysics, Xiamen University, Xiamen 361005, Fujian, China

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 $T \approx 0.1$.

New results in this talk

1. A recent theory of fluctuating hydrodynamics of momentum conserving anharmonic chains makes detailed predictions for the form of equilibrium correlation functions of conserved quantities in these systems [Spohn, Mendl (2013,2014)].

   We perform equilibrium molecular dynamics simulations to test these predictions for the asymmetric FPU chain. Main results:

   (i) Most of the predictions of the theory seem to hold quite accurately, though some discrepancies are found.

   (ii) Transport IS anomalous.

   (iii) We do not see signatures of normal transport in any parameter regime.

2. Nonequilibrium simulations of the asymmetric FPU chain.

   Main result: The claims of finite thermal conductivity is a result of strong finite size effects that appear in nonequilibrium simulations in some parameter regimes.

Predictions 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: v_i and energy: e_i.
  They satisfy the exact conservation laws:
  $$\frac{\partial r}{\partial t} = \frac{\partial v}{\partial x}, \quad \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x}, \quad \frac{\partial e}{\partial t} = -\frac{\partial vp}{\partial x},$$
  where p is the pressure.

- Consider fluctuations about the equilibrium values:
  $r_i = \ell + u_1(i)$, $v_i = u_2(i)$ and $e_i = e + u_3(i)$.
  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 $\langle J(0)J(t)\rangle \sim 1/t^{2/3}$.

We check these detailed predictions from direct simulations of FPU chains.

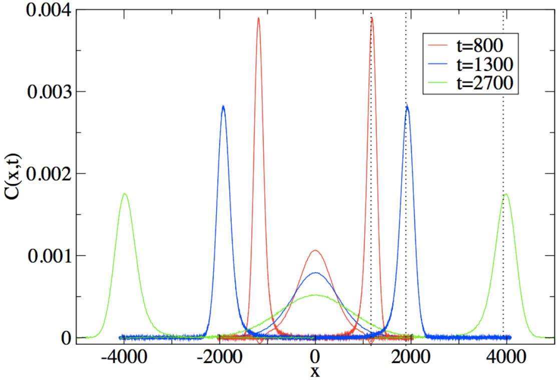
Equilibrium space-time correlation functions — Finite pressure case

Numerically compute heat mode and sound mode correlations in the asymmetric-FPU chain with periodic boundary conditions.

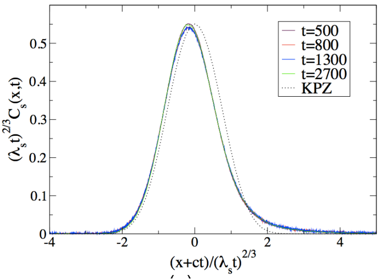
Average over $\sim 10^7$ thermal initial conditions. Dynamics is Hamiltonian.

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

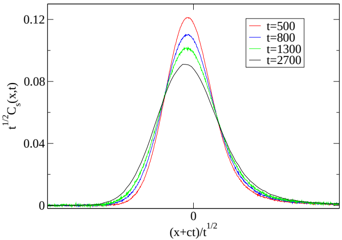
Speed of sound $c = 1.455$.



Scaling of sound modes - asymmetric FPU



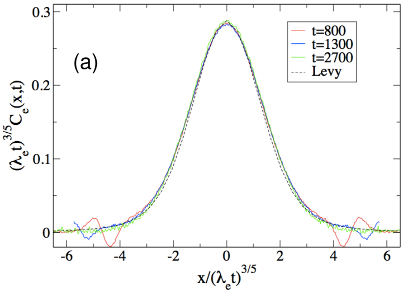
(a) Very good scaling obtained. The scaling function is not yet symmetric and deviates from the expected KPZ form.
$\lambda_{\text{theory}} = 0.675, \ \lambda_{\text{sim}} = 2.05.$



(b)

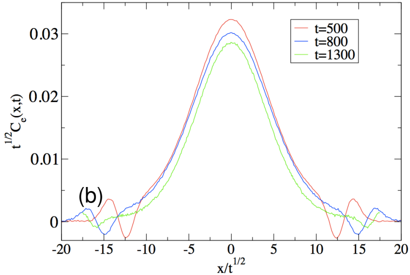
(b) This corresponds to diffusive scaling and is clearly not good.

Scaling of heat mode - asymmetric FPU



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

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



(b) This corresponds to diffusive scaling and is not good.

Equilibrium simulations of FPU

Thus we see that:

(i) Very good scaling of data is obtained, in accordance to the theoretical predictions.
The expected fit to the KPZ scaling function is not too good.
Fit to Levy distribution is good.

(ii) The scaling parameters seem to be far from the theoretically predicted values.

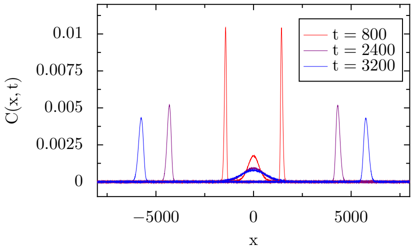
(iii) It is possible that the approach to the expected behaviour is slow. We might expect a faster convergence if the separation of heat and sound modes is stronger.

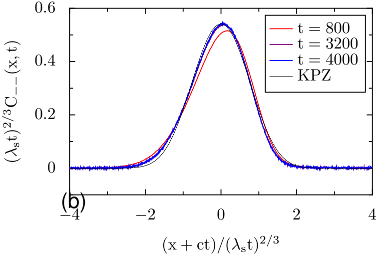
We now check this.

Equilibrium simulations of FPU - second parameter set

(a)

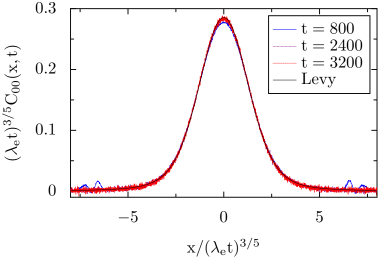
We try a different parameter set for which the separation of heat and sound modes is stronger ($T = 5.0$). System size $N = 16384$.





(b)

$\lambda_{\text{theory}} = 0.396, \ \lambda_{\text{sim}} = 0.46.$



$\lambda_{\text{theory}} = 5.89, \ \lambda_{\text{sim}} = 5.86.$

Conclusions

- Equilibrium space-time correlations of conserved variables —
  Very detailed theoretical predictions (Spohn, 2013) which allow direct comparision with microscopic simulations.

- Our simulations for FPU chain verify the scaling predictions quite well.

  — Levy form for heat mode is verified.

  — KPZ scaling for sound-mode is also verified.

- The fit to the KPZ scaling function and agreement with the scaling parameters requires study of large system sizes and longer times. Presumably this is required for the effective decoupling of the heat and sound modes which happens at long times.

- Other results:

  — Results are universal [Hard point gas: Mendl, Spohn (2014)]

  — Special case: Zero pressure, even potential: different universality class.

  — At low temperatures we do not see any signatures of diffusive transport (in contrast to findings of Zhao et al).

Nonequilibrium simulations of asymmetric FPU

- Zhao *et al* find normal transport at low temperatures and anomalous transport at high temperatures. Is there a nonequilibrium phase-transition in this system as a function of temperature ?

- Are these finite size effects ? These are stronger at low temperatures, and perhaps the true asymptotic (anomalous) behavior is seen at much larger system sizes?

In this study —

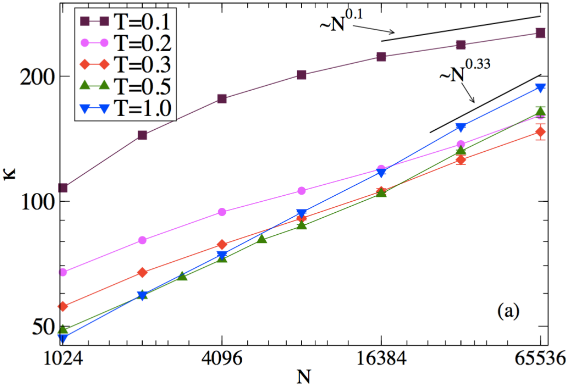
- We change the temperature of the system and see if we can differentiate between the above two possibilities.

(i) Size-dependence of κ.

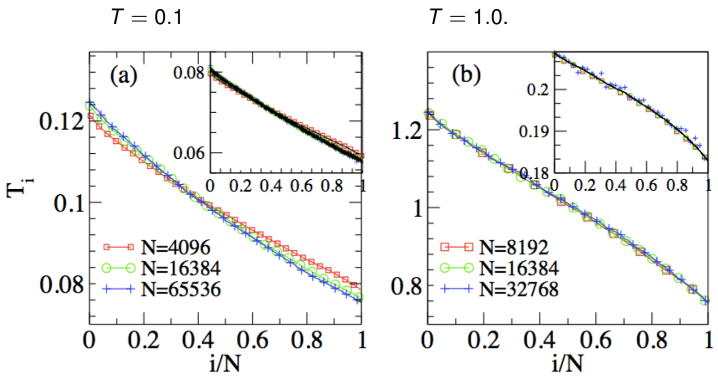
(ii) Temperature profiles (especially check if boundary-jumps remain)

Length-dependence of conductivity

- Nonequilibrium simulations with heat baths at temperatures $T + \Delta T/2$ and $T - \Delta T/2$.
- The system Hamiltonian is the asymmetric FPU chain ($k_2 = k_4 = 1$, $k_3 = -1$).
- Heat bath dynamics — Langevin equations for boundary particles, Newton's equations for bulk particles.
- Measure steady state current $J = \langle v_l f_{l,l-1} \rangle$, temperature $T_l = \langle v_l^2 \rangle$.



Temperature profiles



Insets show expansion ($\langle x_{\ell+1} - x_{\ell} \rangle$) profiles. Can be obtained from temperature profile by assuming local equilibrium.

Note that convergence of temperature profiles better at high temperature.

Summary and questions

- Nonequilibrium studies of asymmetric FPU

  Heat transport is anomalous with $\alpha = 1/3$.

  — However it seems that at low temperatures, finite size effects are strong. At small system sizes conductivity appears to converge.

  — one has to go to very large system sizes to again see a divergence. Why? Not clear !

  Two other papers:
  Savin, Kosevich (2014) — FPU is anomalous, Lennard-Jones is diffusive!!
  Wang, Hu Li (2014) — FPU is anomalous.

- Equilibrium results on FPU correlation functions
  — very good agreement with predictions from fluctuating hydrodynamics.

  — Anomalous scaling is always observed.

  — Strong finite-size effects as seen in the nonequilibrium studies not observed here.

- Some open questions:
  — What is the origin of the strong finite size effects seen (leading to apparent diffusive transport) in nonequilibrium studies?

  — Current fluctuations computed in open and closed geometries have different behaviour ? [Deutsch, Narayan (2003), Brunet, Derrida, Gerschenfeld (2010), Dhar, Saito, Derrida (2013)].