Equilibrium spatio-temporal correlations of conserved quantities AND “OTOC” analogue in integrable Hamiltonian systems.

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A. Kundu and A. Dhar, PRE (2016).

Integrable systems in Mathematics and Physics,
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Outline

- Fluctuating hydrodynamics of non-integrable one-dimensional Hamiltonian systems with three conserved quantities (stretch, momentum, energy).
  Predictions for spatio-temporal correlation functions — Sound and heat modes with anomalous (non-diffusive) scaling.

- What happens in integrable Hamiltonian models such as the Toda lattice ?
  - Numerical results for correlation functions in Toda lattice.
  - Exact results in limiting cases (Harmonic chain and Hard particle gas).
  - Normal mode analysis.
- Behaviour of OTOC analogue in integrable systems [Preliminary results].
- Summary

Anomalous transport and decay of equilibrium fluctuations

1. Anomalous heat transport: Non-diffusive heat transport in one-dimensional energy-momentum conserving systems.

2. It is expected that the decay of energy fluctuations in a system in thermal equilibrium will tell us something about spread of a nonequilibrium heat pulse and hence about anomalous heat transport.

   [Zhao (2006), Zaburdaev, Denisov, Hanggi (2011)]

3. Our best understanding of anomalous heat transport thus comes from study of equilibrium correlation functions of conserved quantities
   [and also equilibrium current-current correlation functions].

4. Fluctuating hydrodynamic theory

   [Narayan, Ramaswamy (2002), van Beijeren (2012), Mendl,Spohn (2013-2016)]

Analytic approaches are mainly based on these.

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:

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

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

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

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

Predictions of fluctuating hydrodynamics

- Including the nonlinear terms:

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

$$\frac{\partial \phi_0}{\partial t} = \frac{\partial}{\partial x}[G^0(\phi_+^2 - \phi_-^2)] + D_h \frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x}$$

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

  Given $V(r)$, T, 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.

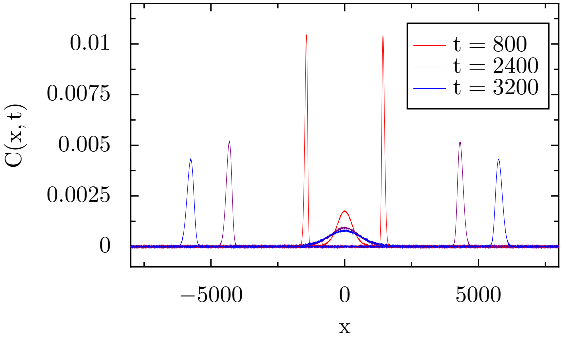
Equilibrium space-time correlation functions

S. Das, A. Dhar, K. Saito, C. Mendl, H. Spohn, PRE 90, 012124 (2014). Numerically compute heat mode and sound mode correlations in the Fermi-Pasta-Ulam chain with periodic boundary conditions.

Average over $\sim 10^7 - 10^8$ thermal initial conditions. Dynamics is Hamiltonian.

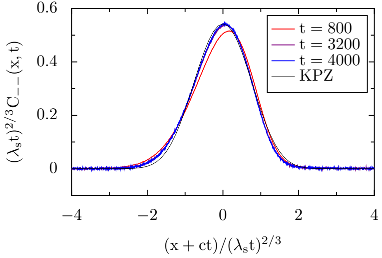
Parameters — $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 5.0,\ P = 1.0,\ N = 16384$.

Speed of sound $c = 1.803$.

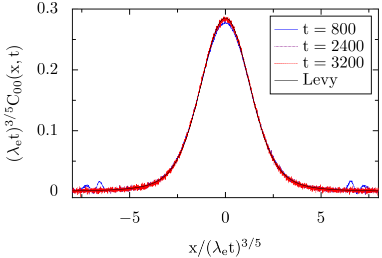


Equilibrium simulations of FPU

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



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



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-$3/2$.

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

Integrable models

- Classical integrable Hamitlonians are those which have N independent constants of motion - $\{I_1, I_2, \ldots, I_N\}$. [for N-particle one-dimensional system]

  These include the total momentum and energy.

- Examples - Harmonic chain, ideal gas of elastically colliding equal mass particles, Toda lattice, Calogero-Moser-Sutherland model.

- Some interesting questions:

  (i) Clearly, hydrodynamics (with three conservations) will not work. What is the scaling-form of correlation functions ?

  (ii) Nonequilibrium heat transport: what is the size-dependence of heat current, what do temperature profiles look like ?

Can one make any general statement ?

Earlier work

The Toda potential: $V(r) = ae^{-br}$.

- Theodorakopoulos and Peyrard (1999)— Look at dynamical structure functions $S(q, \omega)$ for energy and density.
- Zhao (2006) — Ballistic spreading of energy correlations in Toda lattice.
- Xotos (2002) — Non-decay of energy current correlations and relation to Mazur relations.
- Shastry and Young (2010)
  — Numerical study of energy current correlations, modification of Mazur.
  — Exact periodic wave like "CNOIDAL" solutions, which look like waves or solitons in two limiting cases.
- Xiong and Barkai (2016)— Levy walk treatment.
- Recent progress on hydrodynamics of integrable models—discuss later.

Present study

- Toda potential $V(r) = ae^{-br}$.
- Prepare system in canonical equilibrium with specified temperature T and pressure P.

$$Prob(\{r_x, p_x\}) = \frac{e^{-\beta \sum_{x=1}^{N} [p_x^2/2 + V(r_x) + Pr_x]}}{Z},$$

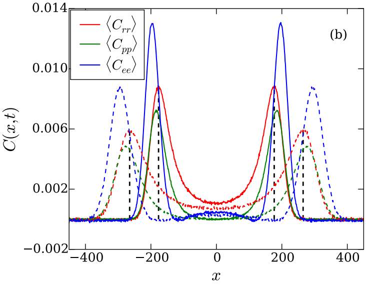
  where $Z = \left[\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dr e^{-\beta(p^2/2 + V(r) + Pr)}\right]^N$.

- Let (u_1, u_2, u_3) be fluctuations of conserved fields about equilibrium values:
  $r_x(t) = \langle r_x \rangle + u_1(x,t), \quad p_x(t) = u_2(x,t), \quad e_x(t) = e + u_3(x,t).$

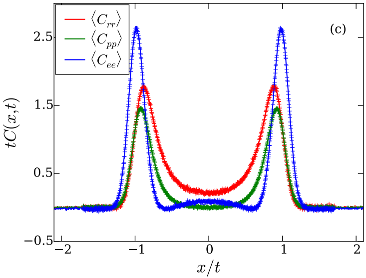
  Measure $C_{\alpha\nu} = \langle u_\alpha(x,t) u_\nu(0,0) \rangle$, where average is over equilibrium initial conditions.

- Important parameters a, b and also T, P.

Simulation results for correlation functions



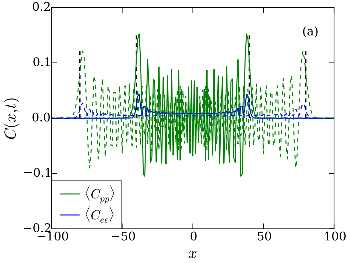
Plots of C_{rr}, C_{pp}, C_{ee}.
$N = 1024$, $P = 1$, $T = 1$, $a = b = 1$.
Correlations of stretch, momentum and energy at times $t = 100$ and $t = 200$.

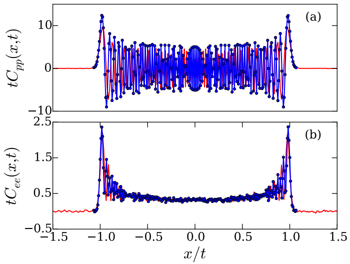


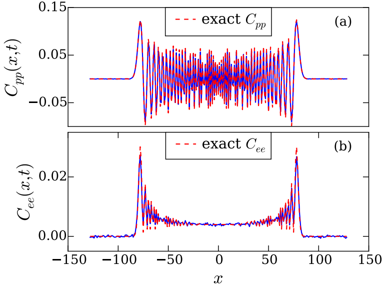
$t \times [C_{rr},\ C_{pp},\ C_{ee}]$ plotted against $\frac{x}{t}$ for above data.
Collapse of data — Ballistic scaling of the correlations.

Correlation functions in harmonic limit

$a = 20.0, b = 0.05, P = 20, N = 256$ times $t = 80, 120$.



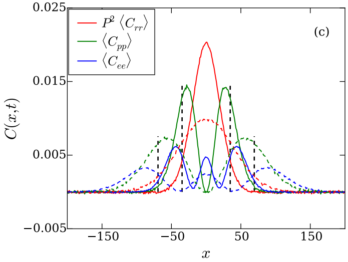


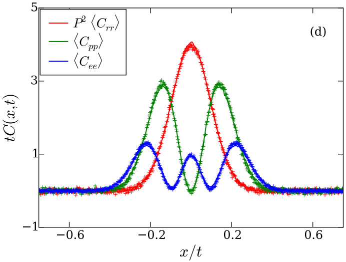


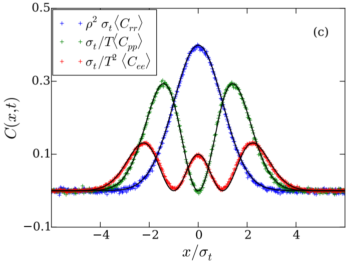
← Comparision between TODA simulations and exact harmonic results.

Correlation functions in hard particle gas limit

$a = 0.1, b = 10, P = 0.1, N = 1024$ times $t = 200, 400.$







←Comparision between TODA simulations and exact hard particle gas results.

Exact results for harmonic chain

Since the dynamics is linear it is easy to find the following correlations [Montroll and Mazur (1960)]

$$
\begin{aligned}
C_{rr}(x,t) &= T\mathcal{J}_{2|x|}(2\omega t)/\omega^2 \\
C_{rp}(x,t) &= T\left[-\frac{\mathcal{J}_{2|x|-1}(2\omega t)}{\omega}\theta(-x)+\frac{\mathcal{J}_{2|x|+1}(2\omega t)}{\omega}\theta(x)\right] \\
C_{pr}(x,t) &= T\left[-\frac{\mathcal{J}_{2|x|+1}(2\omega t)}{\omega}\theta(-x)+\frac{\mathcal{J}_{2|x|-1}(2\omega t)}{\omega}\theta(x)\right] \\
C_{pp}(x,t) &= T\mathcal{J}_{2|x|}(2\omega t)
\end{aligned}
$$

$\mathcal{J}_n(z)$ — Bessel function of first kind

Since the process is Gaussian, the energy correlation is got using Wicks theorem,

$$
C_{ee}(x,t)=\frac{1}{2}\left[C_{rr}^2(x,t)+C_{rp}^2(x,t)+C_{pr}^2(x,t)+C_{pp}^2(x,t)\right] \ .
$$

Exact results for equal mass hard particle gas

- First studied by Jepsen (1965) - exact computation of $\langle p_x(t)p_0(0)\rangle$ — mapping to non-interacting gas.
- Much simpler computation scheme proposed by Sabhapandit and Dhar in the context of tagged particle correlations (JSP 2014, PRL 2015,JSM 2016).
- This scheme can be extended to compute all correlations [paper in preparation (Kundu,Sabhapandit,Dhar)].

  Results:

$$
\begin{aligned}
C_{rr}(x,t) &= \frac{1}{\rho^2\sigma_t}\,\frac{e^{-(\frac{x}{\sigma_t})^2}}{\sqrt{2\pi}} \\
C_{pp}(x,t) &= \frac{\bar{v}^2}{\sigma_t}\left(\frac{x}{\sigma_t}\right)^2\frac{e^{-(\frac{x}{\sigma_t})^2}}{\sqrt{2\pi}} \\
C_{ee}(x,t) &= \frac{\bar{v}^4}{4\sigma_t}\left[\left(\frac{x}{\sigma_t}\right)^4-2\left(\frac{x}{\sigma_t}\right)^2+1\right]\frac{e^{-(\frac{x}{\sigma_t})^2}}{\sqrt{2\pi}}
\end{aligned}
$$

$\rho = P/T,\ \sigma = \rho\bar{v}t,\ \ \bar{v} = \sqrt{T}.$

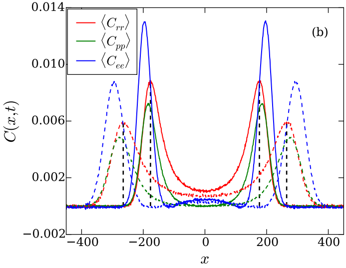
Normal mode transformation

- Recall that the linearized Euler equations for the first three modes has the form
$$\frac{\partial u_\alpha(x,t)}{\partial t} = -A_{\alpha\beta}\frac{\partial u_\beta(x,t)}{\partial x} \ .$$
Suppose R diagonalizes A, i.e $R\ A\ R^{-1} = \Lambda$.
The "normal modes" are described by the variables
$$\phi_s(x,t) = \sum_\alpha R_{s\alpha} u_\alpha(x,t) \ \ , \ \ s = \pm, 0$$
In usual hydrodynamics, this transformation separates the heat and sound modes, and the correlation between these modes dies down very fast.
- How do correlations look in these transformed variables in the Toda chain ?

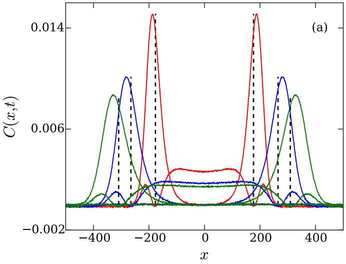
ANSWER:
(i) The heat and sound modes still separate.
(ii) The cross-correlations between the heat and sound modes does not decay.

Normal mode correlations

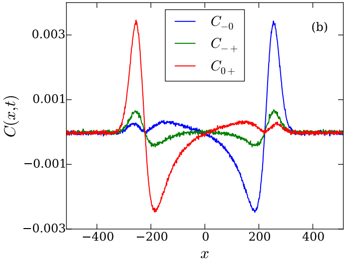
Original variables $\delta r, \delta p, \delta\epsilon$



Normal modes ϕ_+, ϕ_-, ϕ_0

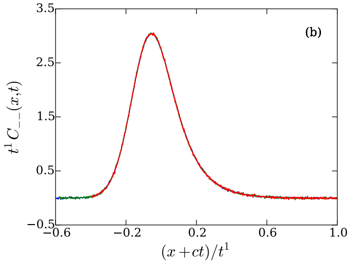


Parameters: $a = b = 1$, $N = 1024$,
$T = P = 1$.
times: $t = 200, 300, 350$.
Cross correlations between modes

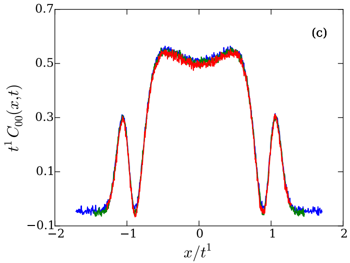


Ballistic scaling again as expected

Sound mode – translated by *ct* and scaled by *t*



Heat mode scaled b *t*



Other interesting developments

- Integrable diffusive models: Classical Faddeev-Takhtajan spin chain (Prosen) and quantum Heisenberg XXZ chain (Prosen) —- These models show diffusive transport in the gapped phase (easy axis) and ballistic transport in the gap-less phase (easy plane).
- Interacting and noninteracting integrable systems— Spohn (2018).
  Let $j_i^{(n)}$ be local current corresponding to $n-$th consevered quantity. Define
  $$\Gamma_{mn}(t) = \sum_i \left\langle j_i^{(m)}(t) j_0^{(n)}(0) \right\rangle , \qquad D_{mn} = \lim_{t\to\infty} \Gamma_{mn}(t) .$$
  $$L_{mn} = \int_0^\infty dt \; [\Gamma_{mn}(t) - D_{mn}] .$$
  Proposed classification:
  Interacting integrable system: Some $L_{mn} \neq 0$. [Toda, integrable XXZ, hard rods, Lieb-Liniger gas]
  Non-interacting integrable system: All $L_{mn} = 0$. [Harmonic chain, free fermions, XX chain, TFIM]
- Hydrodynamic Diffusion in Integrable Systems— Nardis, Bernard, Doyon (2018).
- Emergent hydrodynamics in integrable quantum systems out of equilibrium — Castro-Alvaredo, Doyon, Yoshimura (2018).

Outline

- Chaos in classical systems.
- Propagation of chaos in many-body systems.
- The out-of-time-ordered-correlator (OTOC) as a probe of quantum chaos and of ballistic propagation of information.
- Numerical results for behaviour of OTOC in integrable and non-integrable models.

A butterfly fluttering its wings in Beijing causes a tornado in Kansas!!

Classical Chaos - Sensitivity to initial conditions

Consider a dynamical system with deterministic time-evolution

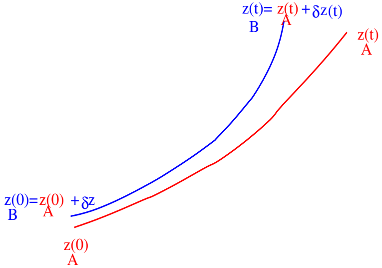
$$\frac{dz_x}{dt} = f_x(\mathbf{z}) \ , \quad x = 1, 2, \ldots, N \ .$$

Consider two different initial conditions

$$z^A(0) \ \text{ and } \ z^B(0) = z^A(0) + \delta z(0) \ .$$

After time t let

$$\delta z(t) = z^B(t) - z^A(t)$$



Definition of chaos — at large t

$$\lim_{\delta z(0) \to 0} \frac{|\delta z(t)|}{|\delta z(0)|} \sim e^{\lambda(\mathbf{z}) t}$$

with $\lambda > 0$ — LYAPUNOV EXPONENT

Propagation of chaos

Suppose that the initial perturbation is localized in space

$$\delta z_x(0) = \epsilon \delta_{x,0} \ .$$

We expect that the differences in phase-space variables at any point in space should eventually diverge with time. Thus

$$\lim_{\delta z_0(0) \to 0} \frac{|\delta z_x(t)|}{|\delta z_0(0)|} \sim \phi(x,t) e^{\lambda(\mathbf{z})t} \ .$$

Some questions:

- How long does it take before the perturbation is felt at point x ?
- How does the spatio-temporal evolution of the perturbation take place?

Spread of perturbations in a Hamiltonian system

Consider a chain of coupled oscillators (e.g coupled pendula).

$z_x = (q_x,\ p_x)$ — (position, momentum) of $x^{\rm th}$ particle. $[x = -N/2, \ldots, N/2]$.

- Disturb system locally.
- The spread of the perturbation can be expressed as a Poisson bracket:

$$\frac{\partial p_x(t)}{\partial p_0(0)} = -\{p_x(t), q_0(0)\} \qquad \{A, B\} = \sum_x \frac{\partial A}{\partial q_x}\frac{\partial B}{\partial p_x} - \frac{\partial A}{\partial p_x}\frac{\partial B}{\partial q_x}$$

- Linear response $\langle \partial p_x(t)/\partial p_0(0)\rangle_{eq} = -\langle\{p_x(t), q_0(0)\}\rangle = \beta\langle p_x(t)p_0(0)\rangle$
  —- Equilibrium correlation functions
- Chaos and non-linear response — $\left\langle \left(\frac{\partial p_x(t)}{\partial p_0(0)}\right)^2 \right\rangle$

Chaos in quantum systems

- $z \to \psi$ — No chaos since linear dynamics.
- Usual characterization of quantum chaos: level-spacing statistics
- Maldacena,Shenker,Stanford — replace Poisson bracket by commutator. Hence look at

$$-\langle [q_x(t), p_0(0)]^2 \rangle / \hbar^2 \ ,$$

  $< ... >$ represents expectation over pure or thermal state.
- No long time divergence but perhaps the short-time growth shows a exponential growth regime and one can extract a Lyapunov exponent.
- Ehrenfest time and scrambling time.
- Ballistic spread characterized by butterfly velocity, light-cone velocity, Lieb-Robinson velocity.

Classical version of the OTOC

Let $\{Q_x, P_x\} = \{\delta q_x, \delta p_x\}$ be the perturbation of an initial condition $(\mathbf{q}, \mathbf{p})$.
Time evolution is given by:

$$\dot{q}_x = p_x \ , \quad \dot{p}_x = f_x$$
$$\dot{Q}_x = P_x, \quad \dot{P}_x = \frac{\partial f_x}{\partial q_y} Q_y = M_{xy}(\mathbf{q}) Q_y \ .$$

Solve with initial condition $(\mathbf{q}, \mathbf{p})$ chosen from an equilibrium distribution and $Q_x = 0, \ P_x = \delta_{x,0} \ , x = 0, 1, \ldots, N-1$.
Compute

$$C(x,t) = -\langle \{p_x(t), q_0\} \rangle = \langle P_x(t) \rangle, - - - - \text{Correlations}$$
$$D(x,t) = \langle \{p_x(t), q_0\}^2 \rangle = \langle P_x^2(t) \rangle - - - - \text{OTOC}$$

Spread of OTOC

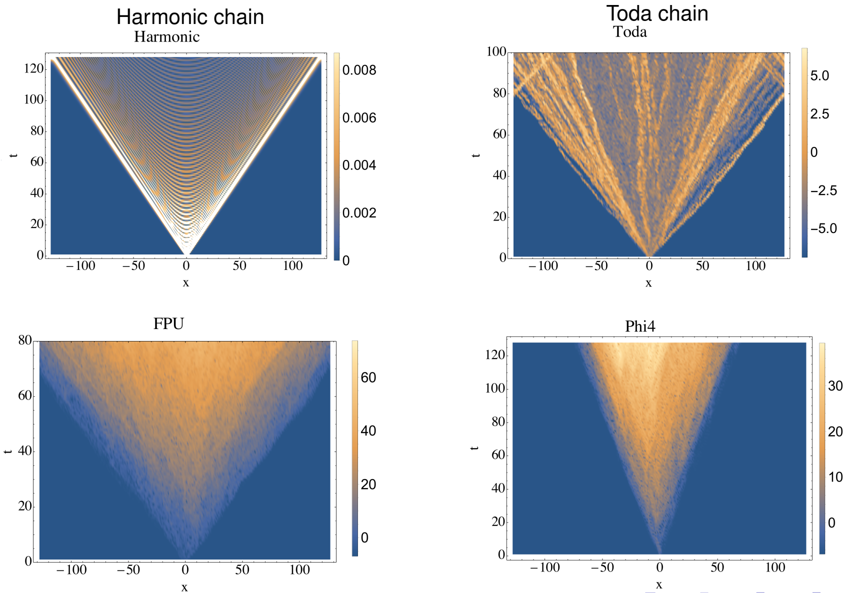
- Non-integrable systems- classical Heisenberg spin chain [Das,Chakrabarty,AD,Huse,Kundu,Moessner,Ray, Bhattacharjee, PRL (2018)]

$$D(x,t) \sim e^{-t\lambda(x/t)}, \quad \lambda(v) \approx 2\mu[(v/v_c)^2 - 1] \ .$$

  Linear near v_c.

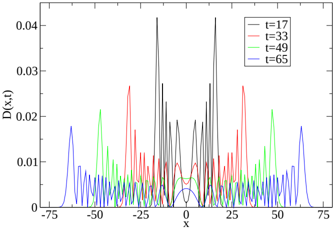
- Integrable systems:
  $\lambda(v_c) = 0$ determines the light-cone velocity.
  $\lambda(v < v_c) = 0$
  $v \gtrsim v_c; \lambda(v) \sim (v - v_c)^{3/2}$
  – Harmonic chains, non-interacting lattice fermions or bosons, TFIM, XX-chain. – OTOC can essentially be expressed in terms of the two-point correlator.
- Behaviour in interacting integrable models ? —Numerical results for quantum XXZ chain (Xu,Swingle).

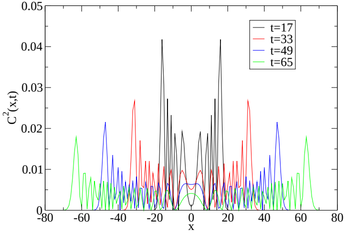
Numerical results: evolution of $D(x,t)$ and $C^2(x,t)$



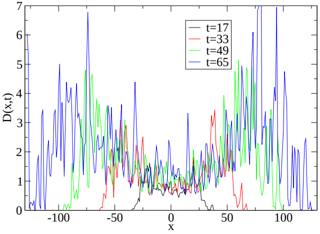
Numerical results: evolution of $D(x,t)$ and $C^2(x,t)$

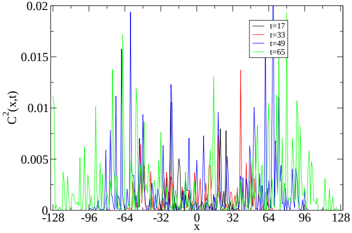
Harmonic chain



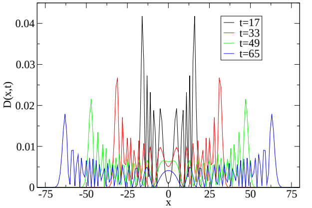


Toda chain

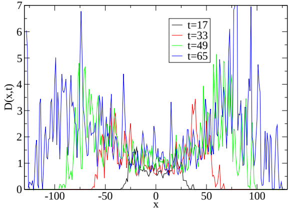




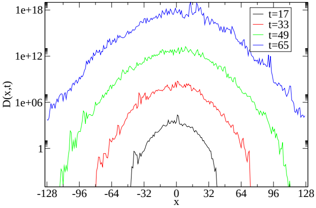
Harmonic chain



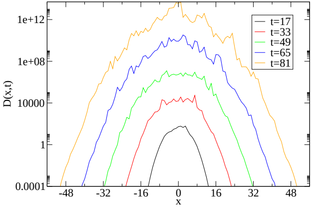
Toda chain



FPU-chain

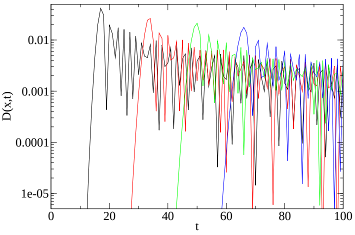


phi-4 chain

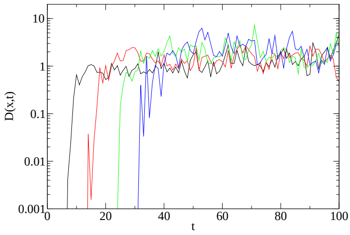


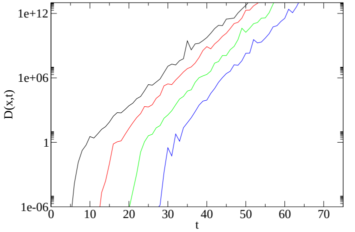
Numerical results: evolution of $D(x,t)$

Harmonic chain



Toda chain





Exponential growth is seen in FPU case.

Summary

- Equilibrium state of Toda chain, with specified Temperature, Pressure and zero average momentum, was studied.
- Decay of equilibrium correlation functions of energy, stretch and momenta was studied — BALLISTIC scaling observed in all parameter regimes.
- Exact solution for correlation functions in two limiting cases —

  (i) harmonic chain limit [PHONONS],
  (ii) hard particle gas limit [SOLITONS].
- Normal modes lead to separation of peaks, however strong cross-correlations.
- Other results: Nonequilbrium heat transport also shows some typical features — heat current INDEPENDENT of system size, FLAT bulk temperature profile.
- Is OTOC an interesting object for integrable systems?
- OTOC for toda chain shows $D(x,t) \sim e^{-t\lambda(v)}$, with $\lambda(v) \sim (v - v_c)^{3/2}$, same as for non-interacting systems.