Equilibrium dynamical correlations in Toda chain

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joint work with

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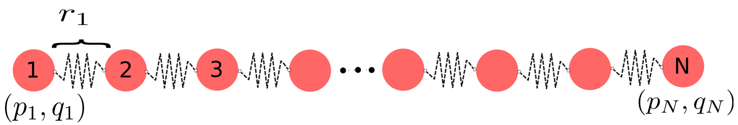
April 20, 2017

Overview

- Evolution of equilibrium space-time correlations of conserved quantities in Hamiltonian systems $\longrightarrow$ insight of non-equilibrium properties.
- Detailed prediction of the form of correlation function in case of non-integrable system was made in [Spohn2014] by non-linear fluctuating hydrodynamics.
- We study the form and scaling of correlation functions in integrable system. In some of the limits, we are able to compute analytic correlation functions.
- We compare the correlation functions of integrable and non-integrable models in normal modes.

The system



- The Nearest-neighbor 1-D Hamiltonian defined as :

$$H = \sum_{x=1}^{N} \frac{p_x^2}{2} + V(r_x) \ = \sum_{x=1}^{N} e_x, \quad r_x = q_{x+1} - q_i$$

- Periodic boundary conditions: $q_{N+1} = q_1 + L, \ q_0 = q_N - L.$
- Equation of Motions: $\dot{q}_x = p_x, \ \dot{p}_x = (V'(r_x) - V'(r_{x-1})),$

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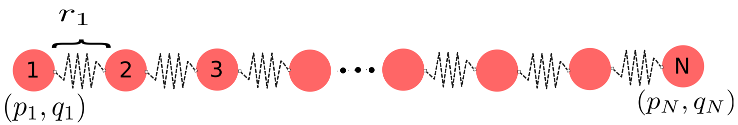

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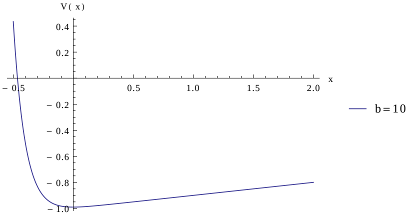
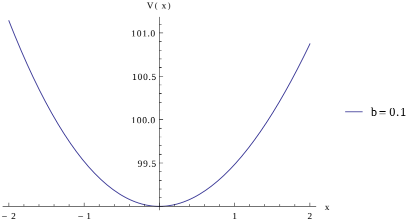
- Equation of Motions: $\dot{q}_x = p_x, \ \dot{p}_x = (V'(r_x) - V'(r_{x-1})),$
- The particles can cross each other. The nearest neighbor is determined by their original identity and not on actual position!

Potentials

(a) Integrable case (Toda potential):

$$V(r_x) = \frac{a}{b} e^{-br_x} \begin{cases} b \gg 1 \text{ Hard Particle Gas} \\ b \ll 1 \text{ Harmonic potential} \end{cases}$$





→ Conserved quantities:

$$I_0 = \sum_{x=1}^{N} r_x,\ \ I_1 = \sum_{x=1}^{N} p_x\ ,\ I_2 = \sum_{x=1}^{N} e_x,\ \ I_3 = \sum_{x=1}^{N} \left[\frac{p_x^3}{3} + (p_x + p_{x+1})\ V(r_x) \right].$$

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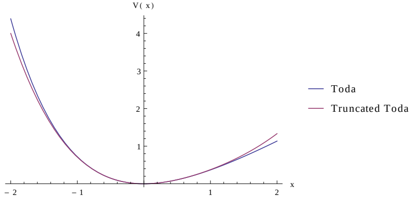
(b) Non-Integrable case

$$V_{tr}(r_x) = \frac{r_x^2}{2} - \frac{r_x^3}{6} + \frac{r_x^4}{24}$$



→ Conserved quantities: $I_0 = \sum_{x=1}^{N} r_x$, $I_1 = \sum_{x=1}^{N} p_x$, $I_2 = \sum_{x=1}^{N} e_x$.

Initial state and Equlibrium fluctuations

We consider initial system prepared in Gibbs ensemble with given Temperature $(1/\beta)$ and pressure P

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

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

Equilibrium fluctuations are defined as:
$u_1(x,t) = r_x(t) - \langle r \rangle,\ u_2(x,t) = p_x(t),\ u_3(x,t) = e_x(t) - \langle e \rangle.$

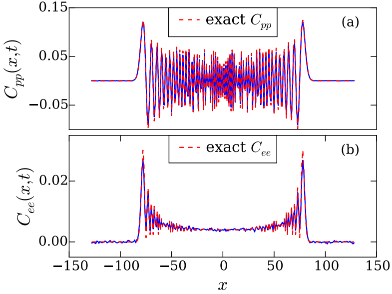
Spatio-temporal dynamic correlation functions are defined as
$C_{\alpha\nu}(x,t) = \langle u_\alpha(x,t) u_\nu(0,0) \rangle \ ,\ (\alpha,\nu) \in 1,2,3.$

Numerical Details

- The initial state is sampled using Inverse transform sampling.
- The Hamiltonian is evolved using velocity-Verlett algorithm with a small time-step $dt < 0.01$.
- Energy and few higher conservation laws are checked to be constant to good approximation.
- The spatio-temporal correlation functions are computed by averaging over $10^6 - 10^7$ initial conditions.

Exact correlation functions exactly in the two limiting cases.

(a) Harmonic



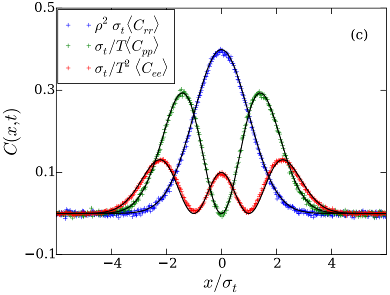
$$\omega^2 C_{rr}(x,t) = C_{pp}(x,t) = T\mathcal{J}_{2|x|}(2\omega t), \quad (\mathcal{J} \ : \text{Bessel functions of 1st kind})$$

$$C_{rp}(x,t) = C_{pr}(-x,-t) = T\left[-\frac{\mathcal{J}_{2|x|-1}(2\omega t)}{\omega}\theta(-x) + \frac{\mathcal{J}_{2|x|+1}(2\omega t)}{\omega}\theta(x)\right]$$

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

Exact correlation functions exactly in the two limiting cases.

(b) Hard Particle gas



$$C_{rr}(x,t) = \frac{1}{\rho^2\sigma_t}\frac{e^{-\frac{1}{2}(\frac{x}{\sigma_t})^2}}{\sqrt{2\pi}},\ C_{pp}(x,t) = \frac{\bar{v}^2}{\sigma_t}\left(\frac{x}{\sigma_t}\right)^2\frac{e^{-\frac{1}{2}(\frac{x}{\sigma_t})^2}}{\sqrt{2\pi}}$$

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

where $\rho = P/T$ is the average density and $\sigma_t = \rho\bar{v}t$, $\bar{v}^2 = T$.

Hydrodynamic description

Hydrodynamic equation to linear order: (Spohn, 2014)
$\partial_t u_\alpha(x,t) + \partial_x(A^{\alpha\beta} u_\beta(x,t)) = 0.$

Normal mode variables $\phi = Ru$, where $RAR^{-1} = diag(-c, 0, c)$, c is sound velocity of the system with two propagating sound modes ($\phi_\pm$) and one heat mode (ϕ_0).

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$r, s = +, 0, -$.

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Predictions from non-linear fluctuating hydrodynamics for non-integrable systems, $C_{++}(x,t) \sim \frac{1}{t^{2/3}} f_{KPZ}\left[\frac{(x \pm ct)}{t^{2/3}}\right]$, $C_{00}(x,t) \sim \frac{1}{t^{3/5}} f_{Levy}\left[\frac{(x)}{t^{3/5}}\right]$

Integrable systems ? $C_{rs}(x,t) \sim \frac{1}{t^1} f\left[\frac{(x \pm ct)}{t^1}\right]$,

Results in integrable case

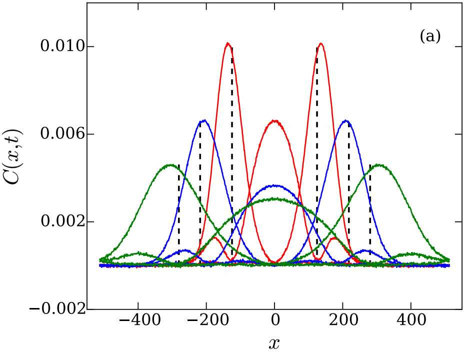

Figure : Normal mode correlations at different times in Toda chain ($V(r_x) = e^{-r_x}$) with $a = 1, b = 1, P = 1$ and $T = 5$ and system size of $N = 1024$. Black dots are sound velocity as predicted from theory.

Results in integrable case

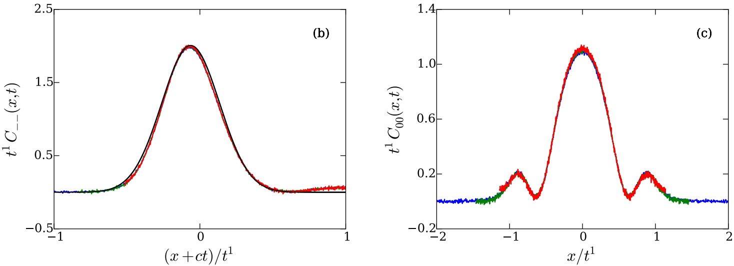

Figure : Sound (Left) and Heat (Right) modes for $T = 5$

Results in integrable case

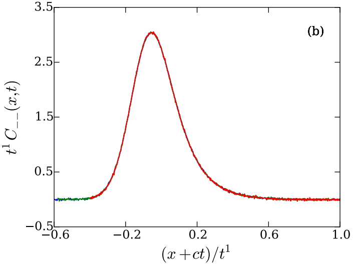

Figure : Sound (Left) and Heat (Right) modes for $T = 1$

Results in non-integrable case

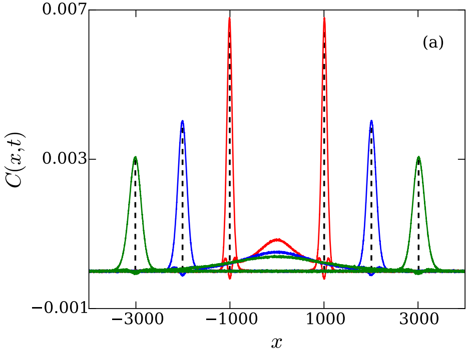

Figure : Normal mode correlations at different times in truncated Toda chain $V_{tr}(r_x) = \frac{r_x^2}{2} - \frac{r_x^3}{6} + \frac{r_x^4}{24}$ with $P = 0$ and $T = 0.5$ and system size of $N = 8192$.

Results in non-integrable case

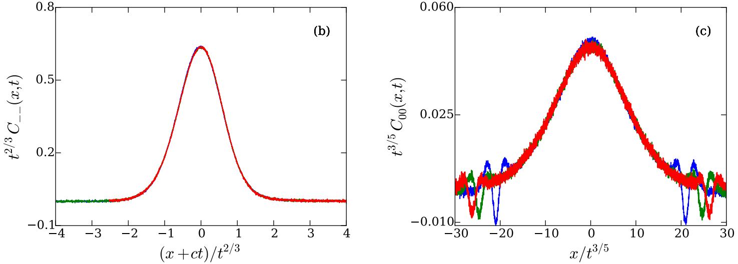

Figure : Sound (Left) and Heat (Right) modes for $T = 5$

Conclusions

- Integrable case has excellent ballistic scaling and the form of correlation function is non-universal.
- The speed of sound can be derived from hydrodynamic theory.
- Unlike non-integrable systems, the normal modes have peaks with large width and overlap.

Conclusions

- Integrable case has excellent ballistic scaling and the form of correlation function is non-universal.
- The speed of sound can be derived from hydrodynamic theory.
- Unlike non-integrable systems, the normal modes have peaks with large width and overlap.
- Open questions: Can the correlation functions for Toda chain be computed exactly in all parameter regime?
- Proving rigorously integrable systems have ballistic scaling.

References

H. Spohn (2014)
Nonlinear fluctuating hydrodynamics for an- harmonic chains
J. Stat. Phys. 154.5 (2014): 1191-1227

A. Kundu, A. Dhar (2016)
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Phys. Rev. E 94, 062130

Thank you!

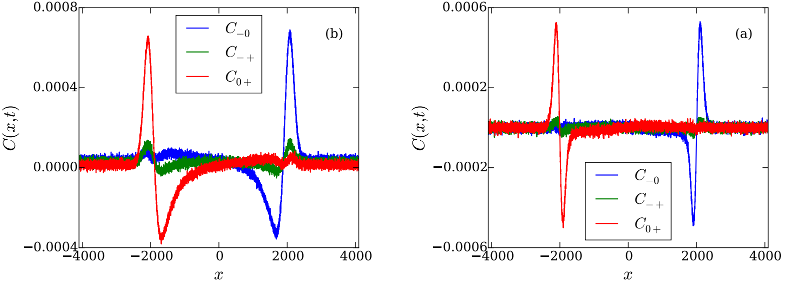

Figure : Left: Cross correlations in Toda chain. Right: Cross correlations in Truncated Toda chain in normal modes.