Coupled rotors and classical spin chains: predictions from fluctuating hydrodynamics and numerical tests

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Outline

- Signatures of anomalous heat conduction in one dimensional momentum systems.
- Introduction to Fluctuating Hydrodynamic Theory and results for anharmonic chains.
- Other systems: Rotor models and Discrete NonLinear Schrodeinger equation (Gross-Pitaevski).
- Heisenberg spin-chains: hydrodynamic theory, numerical results.

References

1. Fermi-Pasta-Ulam chains: S. Das, AD, K. Saito, C. Mendl, H. Spohn, PRE 90, 012124 (2014).
2. Hydrodynamics of the rotor model: S. Das, AD, arXiv:1411.5247 (2014) / Spohn: arxiv:1411.3907 (2014)
3. Hydrodynamics and Correlations in the Toda lattice and other integrable models: Aritra Kundu and AD, PRE (2016). POSTER
4. Discrete nonlinear Schrodinger equation: Kulkarni, Huse, Spohn, PRA (2015), Mendl, Spohn, J. Stat. Mech. (2015).
5. Heisenberg spins: Damle, Spohn, AD, Kulkarni, Huse (Ongoing work).

Breakdown of Fourier's law — Anomalous heat transport

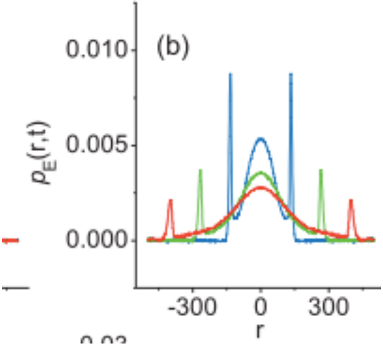
Fourier's law is probably not valid in low-dimensional momentum-conserving systems.

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

- Divergent conductivity: $\kappa \sim L^{\alpha}$.
- Nonlinear (and possibly singular) temperature profiles, EVEN for small temperature differences.
- Anomalous spreading of heat pulses — Levy walk instead of random walk.
- Anomlaous 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.

Look at propagation of a energy pulse



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

Understanding anomalous transport

Nonlinear fluctating hydrodynamics - a general framework.

Narayan, Ramaswamy (2002), H. vanBeijeren (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.

Systems studied so far in the framework of NIFHT

- Fermi-Pasta-Ulam chains: Zhao, Das-AD-Saito-Mendl-Spohn
- Hard particle gases: Mendl-Spohn
- Rotor chains: Das-AD, Spohn, Mendl-Spohn
- DNLS: Kulkarni-Huse-Spohn, Mendl-Spohn
- Stochastic models: Stoltz-Spohn, Lepri et al, Cividini-Kundu-Miron-Mukamel
- Coupled exclusion processes: Popkov-Schmidt-Schütz

What about spin-chains ?

Basics of fluctuating hydrodynamics

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:

$$
\begin{aligned}
\frac{\partial \phi_+}{\partial t} &= \frac{\partial}{\partial x}[-c\phi_+ + G^+\phi^2] + D_s\frac{\partial^2 \phi_+}{\partial x^2} + \frac{\partial \eta_+}{\partial x} \\
\frac{\partial \phi_0}{\partial t} &= \frac{\partial}{\partial x}[G^0\phi^2] + D_h\frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial \eta_0}{\partial x} \\
\frac{\partial \phi_-}{\partial t} &= \frac{\partial}{\partial x}[c\phi_- + G^-\phi^2] + D_s\frac{\partial^2 \phi_-}{\partial x^2} + \frac{\partial \eta_-}{\partial x}
\end{aligned}
$$

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

- $$\mathrm{Sound-mode:}\quad C_s(x,t) = \langle \phi_\pm(x,t)\phi_\pm(0,0)\rangle = \frac{1}{(\lambda_s t)^{2/3}}\, f_{KPZ}\left[\frac{(x\pm ct)}{(\lambda_s t)^{2/3}}\right]$$
  $$\mathrm{Heat-mode:}\quad C_h(x,t) = \langle \phi_0(x,t)\phi_0(0,0)\rangle = \frac{1}{(\lambda_e t)^{3/5}}\, f_{LW}\left[\frac{x}{(\lambda_e t)^{3/5}}\right]$$

  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.

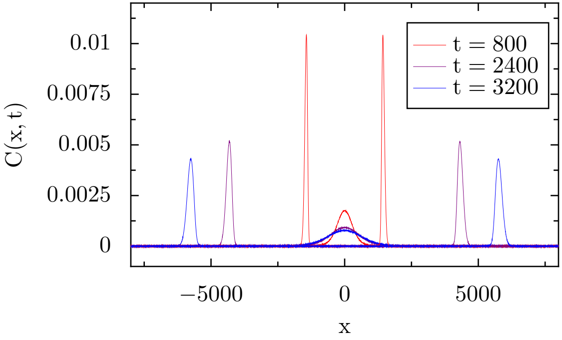
Equilibrium space-time correlation functions

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.

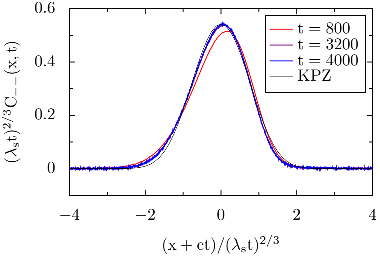
Parameters — $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 5.0,\ \mathcal{P} = 1.0,\ N = 16384.$

Speed of sound $c = 1.803$.

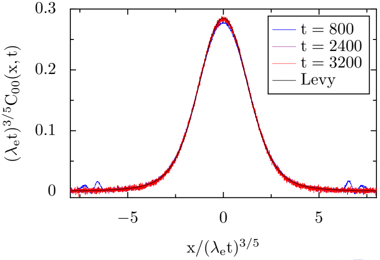


Equilibrium simulations of FPU

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



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



Equilibrium simulations of FPU

Other results:

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

- Second universality class: even potential and zero pressure.

  Sound modes diffusive, heat mode Levy with different exponent [$\tilde{f}(k,t) = \exp(-|k|^{3/2} t)$].

  Other possible special points — See "Fibonacci family of dynamical universality classes", V. Popkova, A. Schadschneidera, J. Schmidta, and G. M. Schütz [PNAS **112**, 12645 (2015)].

Rotor model

- Hamiltonian of the Rotor model —

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m} - \sum_{l=1}^{N-1} V_0 \cos(q_{l+1} - q_l)$$

- Non-equilibrium simulations show that this model satisfies Fourier's law and does not show anomalous transport, even though it is momentum conserving.
Giardina, Livi, Politi, Vassali (2000), Gendelman, Savin (2000).

- This can be understood in the framework of the hydrodynamics theory.

Hydrodynamic theory for the Rotor model

Spohn: arxiv:1411.3907
S. Das and AD, arXiv:1411.5247 (2014)

1. (a) The coordinate variables are now angles, defined modulo 2π. Hence stretch not conserved.

   (b) Since $V(r)$ is bounded, the pressure is identically zero.

2. Recall the conservation laws —

$$\frac{\partial r}{\partial t} = -\frac{\partial p}{\partial x}, \quad \frac{\partial p}{\partial t} = -\frac{\partial \mathcal{P}}{\partial x}, \quad \frac{\partial e}{\partial t} = -\frac{\partial p\mathcal{P}}{\partial x} \qquad + [\mathit{Dissipation} \ + \ \mathit{Noise}] \ ,$$

   Since $\mathcal{P}$ is zero, in the final description, only the dissipative and fluctuation terms survive.

   Thus the hydrodynamic equations for $\vec{u} = (r, p, e)$ are

$$\partial_t u_\alpha = -\partial_x \left[-\partial_x D_{\alpha\beta} u_\beta + B_{\alpha\beta} \xi_\beta \right] \ .$$

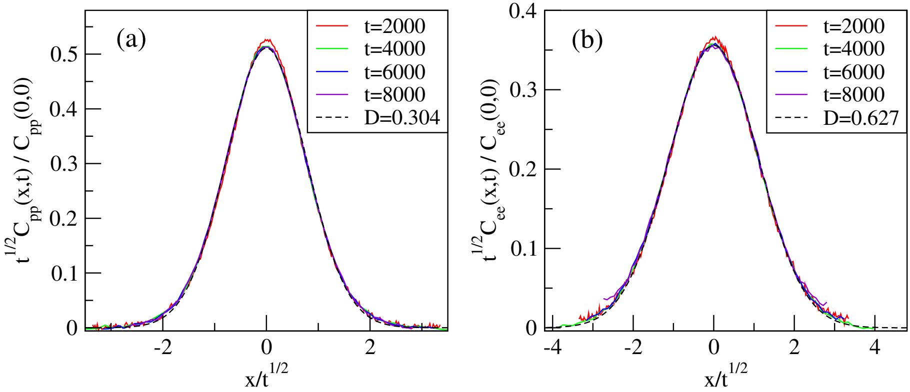
   [Chaikin and Lubensky!]

Rotor model

- Numerical observation: Cross elements $D_{\alpha \neq \beta}$ vanish.

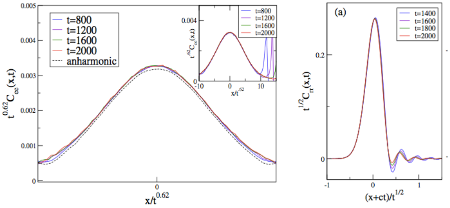
$V(r) = -\cos(r)$, $T = 1$.

- Momentum and Energy correlations decay diffusively — completely different from FPU chain.



Rotor model at low temperatures

- At low temperatures the angles q_l make small fluctuations around some fixed value (Broken symmetry phase!) — replace $-\cos(r)$ by $-1 + r^2/2 - r^4/24 + r^6/720$.
- Hence the restriction $q_l \in (0, 2\pi)$ is NOT relevant.
- In this case one finds two diffiusive sound modes (Zero pressure and even potential) and a Levy heat mode.



- The hydrodynamic equations for both the high temperature “disordered phase” and the “broken symmetry phase” have been discussed earlier (Chaikin and Lubensky, Principles of condensed matter physics).

  However it was not realized that the heat mode is actually non-diffusive and with Levy characteristics.

XXZ classical Heisenberg spin chains

Heisenberg spins $\mathbf{S} = (S^x, S^y, S^z)$ on a ring with nearest neighbor interactions. Hamiltonian given by

$$H = \sum_{\ell=1}^{N} -J\left[S^x_\ell S^x_{\ell+1} + S^y_\ell S^y_{\ell+1}\right] - J_z S^z_\ell S^z_{\ell+1} \ .$$

Consider $J > J_z$ — easy-plane magnetization.

Equations of motion $- >$

$$\dot{S}^\alpha_\ell = -e^{\alpha\beta\gamma} S^\beta_\ell \frac{\partial H}{\partial S^\gamma_\ell}. \qquad \text{OR} \ \ [\dot{\mathbf{S}}_\ell = \mathbf{S}_\ell \times \mathbf{B}_{eff}(\ell)] \quad - - - - \ \text{Symplectic dynamics}$$

Explicitly

$$\dot{S}^x_\ell = -J\left[S^y_{\ell+1} + S^y_{\ell-1}\right] S^z_\ell + J_z\left[S^z_{\ell+1} + S^z_{\ell-1}\right] S^y_\ell$$
$$\dot{S}^y_\ell = -J_z\left[S^z_{\ell+1} + S^z_{\ell-1}\right] S^x_\ell + J\left[S^x_{\ell+1} + S^x_{\ell-1}\right] S^z_\ell$$
$$\dot{S}^z_\ell = -J\left[S^x_{\ell+1} + S^x_{\ell-1}\right] S^y_\ell + J\left[S^y_{\ell+1} + S^y_{\ell-1}\right] S^x_\ell \ .$$

Regular Hamiltonian form

Define new variables $\{s_\ell, \theta_\ell\}$

$$S^z_\ell = s_\ell, \quad S^x_\ell = (1 - s^2_\ell)^{1/2} \cos \theta_\ell, \quad S^y_\ell = (1 - s^2_\ell)^{1/2} \sin \theta_\ell.$$

This defines a canonical transformation leading to equations of motion

$$\dot{\theta}_\ell = \frac{\partial H}{\partial s_\ell}\,, \quad \dot{s}_\ell = -\frac{\partial H}{\partial \theta_\ell}\,,$$

with

$$H = -J \sum_{\ell=1}^{N} (1 - s^2_\ell)^{1/2} (1 - s^2_{\ell+1})^{1/2} \cos(\theta_{\ell+1} - \theta_\ell) - J_z s_\ell s_{\ell+1} \;= \sum_{\ell=1}^{N} \epsilon_\ell.$$

Conservation laws

Two Exact conservation laws: Energy and z-magnetization-> continuity equations:

$$\dot{s}_\ell = -(j^s_{\ell+1} - j^s_\ell)\ , \quad \dot{\epsilon}_\ell = -(j^\epsilon_{\ell+1} - j^\epsilon_\ell)\ ,$$

with currents

$$j^s_\ell = -J(1-s_\ell^2)^{1/2}(1-s_{\ell+1}^2)^{1/2}\sin(r_\ell)\quad ,$$

$$\begin{aligned} j^\epsilon_{\ell+1} = & -J^2 s_{\ell+1}(1-s_\ell^2)^{1/2}(1-s_{\ell+2}^2)^{1/2}\sin(r_{\ell+1}-r_\ell) \\ & + JJ_z s_\ell(1-s_{\ell+1}^2)^{1/2}(1-s_{\ell+2}^2)^{1/2}\sin r_{\ell+1} \\ & - JJ_z s_{\ell+2}(1-s_\ell^2)^{1/2}(1-s_{\ell+1}^2)^{1/2}\sin r_\ell\ . \end{aligned}$$

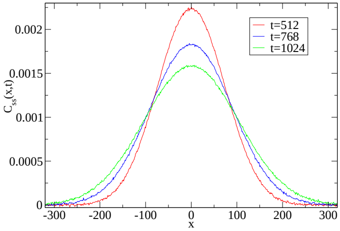
$r_\ell = \theta_{\ell+1} - \theta_\ell$.

Equilibrium distribution $->$ $e^{-\beta(H-\mu\sum_\ell s_\ell)}$.
Equilibrium currents IDENTICALLY zero:$\langle j^s\rangle = \langle j^\epsilon\rangle = 0$.

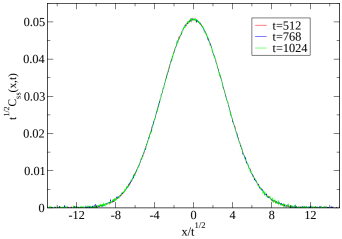
Hence we expect diffusive hydrodynamic equations.

Numerical tests: $\beta = 1.0,\ \mu = 0.3\ ,\quad C_{ss}(x,t) = \langle s_x(t) s_0(0) \rangle_{eq}$.

$s - s$ correlations



Diffusive scaling



Low temperature: effective symmetry breaking

At low temperatures, one expects the *xy*-plane symmetry to be broken.
Small fluctuations around a chosen θ^* and $r_\ell = \theta_{\ell+1} - \theta_\ell = \nabla\theta$ is a new "conserved" variable.

Clearly $\dot{r}_\ell = -\nabla j^r$ with $j^r = \dot{\theta} = \partial H/\partial s$.

Equilibrium measure is now $-> \sim \; e^{-\beta(H - \mu \sum_\ell s_\ell - \nu \sum_\ell r_\ell)}$.

Equilibrium currents are now NON-ZERO. Magic Identity (Mendl,Spohn, 2016) gives

$$\langle j^r \rangle_{eq} = \langle -\partial H/\partial s \rangle_{eq} = -\mu, \qquad \langle j^s \rangle_{eq} = \langle -\partial H/\partial r \rangle_{eq} = -\nu \;, \qquad \langle j^\epsilon \rangle_{eq} = \mu\nu \;.$$

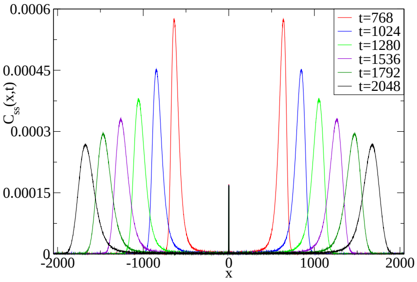
— This is useful for computing linear and nonlinear coefficients in FHT equations.

Fluctuating hydrodynamics then predicts two KPZ sound modes and one Levy heat mode. [SPECIAL CASE: $\mu = 0$, two diffusive sound modes, one Levy heat mode]

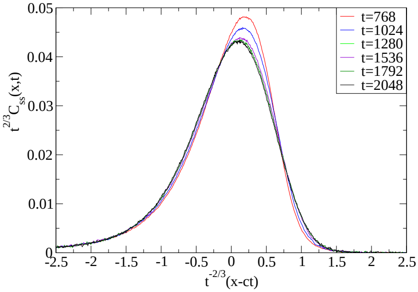
Low temperature correlations

Numerical tests: $\beta = 8.0,\ \mu = 0.3,\ N = 4096$

$s - s$ correlations

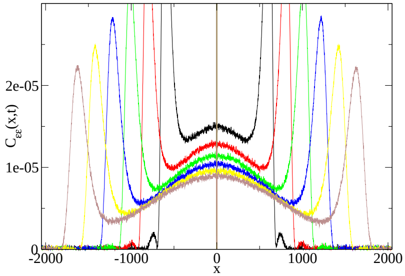


KPZ-scaling

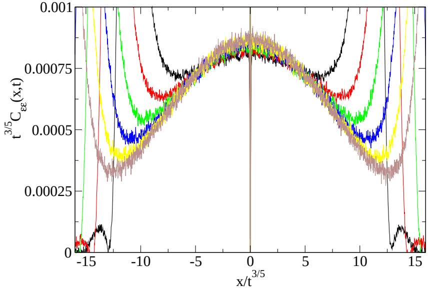


Speed of sound: $c = 0.819....$

$\epsilon - \epsilon$ correlations



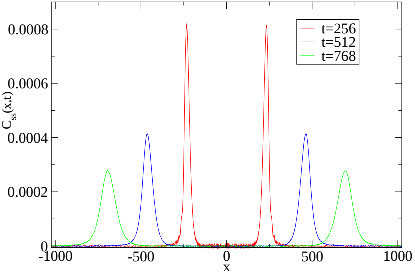
Levy-5/3 scaling



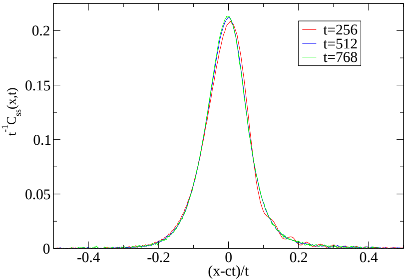
Still need to go to normal modes to see scaling clearly — *i.e* look at linear combinations of the basic fields.

Very low-temperature: integrable dynamics

s − *s* correlations



Ballistic scaling



Ballistic scaling implies integrability at low temperatures — but probably not harmonic ?

Numerical methods

- We implemented an effective finite-time version of the dynamics, which preserves the conservation laws exactly [Damle (unpublished notes)]. Possible to study large system sizes and large times.
- Dynamics is a variant of symplectic algorithms, normally written for (X, P) systems, implemented here for spin dynamics.
- Similar to odd-even dynamics which conserves ONLY energy exactly — alternately odd and even sites updated in parallel.
- Can check that in the limit of small update times, dynamics is equivalent to the exact Poisson-bracket dynamics.

Conclusions

- Equilibrium space-time correlations of conserved variables in one-dimensional interacting systems.
  Very detailed theoretical predictions [Spohn, JSP (2014)] allow direct comparision with microscopic simulations.

- Fermi-Pasta-Ulam chains, Rotor chain and integrable models.

  A new class is investigated here — classical spin chains.

- Simulations for *XXZ* chain verify the scaling predictions quite well. [Preliminary results- work in progress]
  High temperatures - Diffusive scaling
  Low temperatures - Anomalous scaling

  — Levy scaling for heat mode

  — KPZ scaling for sound-mode

  Very low temperatures - Ballistic scaling

  Open questions:

- Derivation of hydrodynamic equations (Diffusion matrix ?).
- Understanding strong finite size effects seen in simulations.