Anomalous dynamical scaling in 1D systems with multiparticle collisions

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Introduction

- Dynamical correlations and transport in low-dimensional $d \leq 2$ may be anomalous: spatial constraints alter transport properties
- Universality and dynamical scaling:
  - Connection with Lèvy processes
  - Connection with the Kardar-Parisi-Zhang problem
- Simulation of simple models: deterministic and stochastic

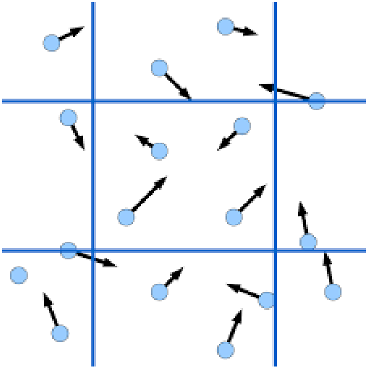
Multi-Particle Collision (MPC)

Malevanets and Kapral (1999) mesoscopic dynamics: stochastic and *local* protocol that redistributes particle velocities, while preserving the global conserved quantities

Three steps:

1. N particles is partitioned in N_c cells.
2. In each simulation cell: the particle velocities are rotated around a random axis passing through the center of mass; the rotation angles are assigned in a way that the invariant quantities are locally preserved.
3. All particles are propagated freely, or under the effect of an external force if present.

Multi-Particle Collision (MPC)



Widely used alternative to MD to simulate complex fluids (e.g. polymers in solution, colloids), flow simulations etc.

MPC for a 1D fluid

1. In each cell i: N_i particles with momentum P_i and kinetic energy K_i;
2. Collision rule: with a given rate r_i, draw a random w_j for each particle from a Maxwellian distribution at the cell temperature $2K_i$,
3. Let $v_{j,\mathrm{old}} \to v_{j,\mathrm{new}} = a_i w_j + b_i$ where a_i and b_i are determined imposing the conservation laws

$$
\begin{aligned}
P_i &= \sum_{j=1}^{N_i} m_j v_{j,\mathrm{old}} = \sum_{j=1}^{N_i} m_j v_{j,\mathrm{new}} = \sum_{j=1}^{N_i} m_j (a_i w_j + b_i); \\
K_i &= \sum_{i=1}^{N_j} m_j \frac{v_{j,\mathrm{old}}^2}{2} = \sum_{j=1}^{N_i} m_j \frac{v_{j,\mathrm{new}}^2}{2} = \sum_{j=1}^{N_i} m_j \frac{(a_i w_j + b_i)^2}{2}
\end{aligned}
$$

4. Propagate ballistically for a given step Δt

MPC for a 1D fluid

- For a closed system: density, energy and momentum are conserved
- The cell size sets the interaction range
- The collision rates r_i sets the interaction time scale and can be chosen to mimic the for example, a Coulomb-like scattering as

$$r_i = \frac{1}{1 + (K_i/\mathcal{E}_{\rm int})^2}, \tag{1}$$

  where $\mathcal{E}_{\rm int}$ is a typical interaction energy
- Initial conditions: initial velocities extracted from a Maxwellian distribution with kinetic energy per unit mass $\mathcal{E}_0$.
- Collisionality parameter: $\eta = \mathcal{E}_0/\mathcal{E}_{\rm int}$ (large η, almost free particles).
- Easily extended to nonequilibrium

Classical nonlinear oscillators on a lattice

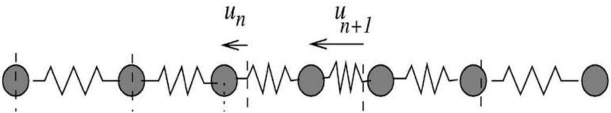
Chain of N coupled oscillators with n.n. coupling: $(p_l = m_l \dot{x}_l)$

$$\mathcal{H} = \sum_{l=1}^{N} \left[\frac{p_l^2}{2m_l} + V(x_{l+1} - x_l) \right] \quad .$$

Equations of motion :

$$m_n \ddot{x}_n = -F_n + F_{n-1} \quad ; \qquad F_n = -V'(x_{n+1} - x_n)\,,$$

- Boundary conditions e.g. periodic $x_{N+1} = x_0 + L$.
- Displacement from eq. position $x_n = na + u_n$, $L = Na$ chain length
- Symmetry $u_n \to u_n + cst$: momentum conservation, $\sum_l p_l$ const.
- "Acoustic dispersion" in the harmonic limit



Conservation laws

$$L = \sum_{n=1}^{N} (x_{n+1} - x_n) \equiv \sum_{n=1}^{N} r_n$$

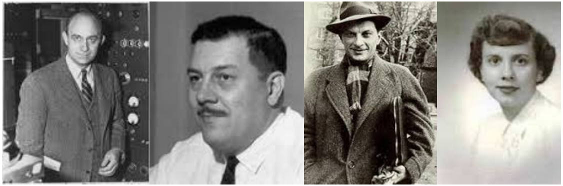
$$P = \sum_{N=1} m\dot{x}_n \equiv \sum_{n=1}^{N} p_n$$

$$E = \sum_{n=1}^{N} \left[\frac{p_n^2}{2m_n} + V(r_n) \right] \equiv \sum_{n=1}^{N} e_n$$

- Microcanonical equilibrium: (L, P, E) (usually $P = 0$)
- Local conservaton laws of densities (r_n, p_n, e_n)
- Local currents

Example: the Fermi-Pasta-Ulam (FPU) model

$$V(z) \;=\; \frac{1}{2}\,(z-a)^2 + \frac{\alpha}{3}\,(z-a)^3 + \frac{\beta}{4}\,(z-a)^4$$



Historically known as "FPU-$\alpha + \beta$ model"

Dynamical correlation functions: structure factors

- For FPU: Fourier transform of displacements

$$u(q,t) = \frac{1}{N}\sum_{l=1}^{N} u_l \exp(-iql). \tag{2}$$

- For MPC: Fourier transform of the particle density

$$\rho(q,t) \;=\; \frac{1}{N}\sum_{n} \exp(-iqx_n) \quad ,$$

Dynamical structure factor

$$S(q,\omega) \;=\; \left\langle \left|\rho(q,\omega)\right|^2 \right\rangle \quad .$$

Information about "collective modes".

Dynamical correlation functions: Green-Kubo integrands

Total energy current $J = \sum_n j_n$, Kubo integrand

$$\langle J(t)J(0)\rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T J(t')J(t'+t)dt'$$

- Response to a weak perturbation
- Onsagers regression hypothesis: spontaneous fluctuations in equilibrium regress back to equilibrium according to the same relaxation equation that describes the macroscopic relaxation (due to external perturbation) -
- By observing equilibrium fluctuations, one can learn about dynamical properties.

Dynamical correlation functions: Green-Kubo integrands

- In practice $\langle ... \rangle$ is an ensemble average over many MD trajectories
- Choice of ensemble: microcanonical with zero momentum
- Current power spectrum

$$C(\omega) = \left| \int J(t) e^{-i\omega t} \right|^2$$

- Wiener-Khintchine theorem

$$C(\omega) = \int \langle J(t) J(0) \rangle e^{-i\omega t} \, dt$$

- Equivalent but more efficient: for n data points $n \ln n$ instead of n^2

Microscopic expression for currents

To compute correlations of energy, momentum and density current $C_{\mathcal{E}}$, C_P and C_ρ an expression in terms of microscopic variables is needed:

- For FPU:

$$J_{\mathcal{E}}(t) = \frac{1}{2} \sum_{i=1}^{N} (\dot{u}_{i+1} + \dot{u}_i)\, F_i. \tag{3}$$

- For MPC: define J_ξ, associated to each conserved quantity ξ, at cell level as

$$J_\xi(t) = \sum_{i=1}^{N_c} \left[\xi_i(t) - \xi_{i-1}(t - \Delta t)\right]. \tag{4}$$

Nonlinear fluctuating hydrodynamics

[Spohn,2014]

- Effective dynamics of the 3 conserved quantities

$$r_n = u_{n+1} - u_n; \qquad \dot{u}_n; \qquad e_n$$

- Fluctuations around the equilibrium values

$$r_n = \ell + U_1; \qquad \dot{u}_n = U_2; \qquad e_n = e + U_3$$

- Write hydrodynamic equations up to second order for $U = (U_1, U_2, U_3)$

$$\dot{U} = -\partial_x \left[AU + UGU + \partial_x CU + B\xi \right]$$

Coupled, noisy Burgers equation (or Kardar-Parisi-Zhang equations)

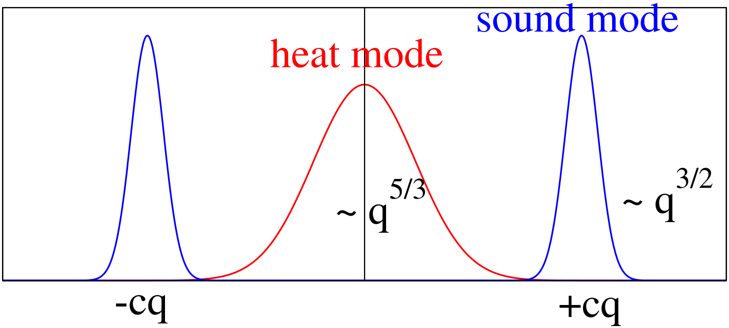
Nonlinear fluctuating hydrodynamics:predictions

- Linear limit: two propagating sound modes and one diffusive heat mode
- 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.
- Universal dynamical exponents (again!)
- Predictions for the scaling functions too e.g. compute the function h such that

$$S(q,\omega) \sim f_{KPZ}((\omega - \omega_{max})/q^{3/2})$$

- Correlation of the heat mode is Lévy-stable distribution function
- Confirmation of two universality classes

Modes correlations

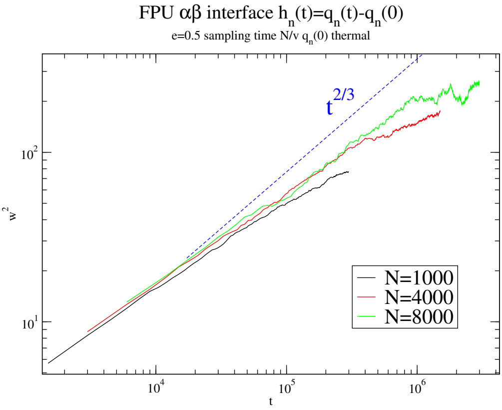


Correlations of observables should be a combination of these.

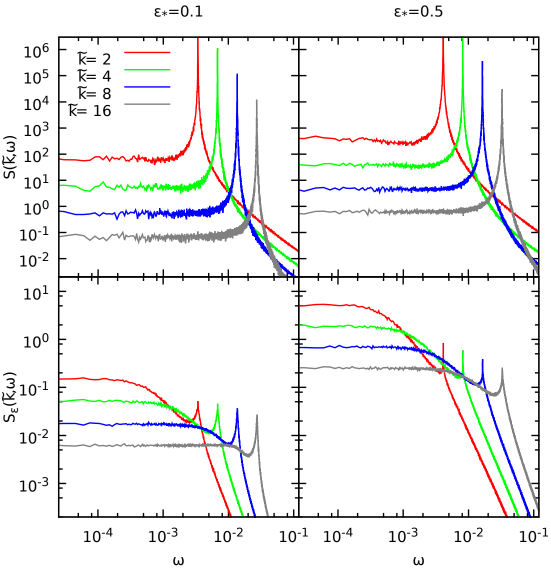
Numerical check: interface roughening

$$h_n(t) \equiv u_n(t) - u_n(0); \qquad w^2 \equiv \frac{1}{N}\langle \sum_n (h_n - \langle h_n \rangle)^2 \rangle$$

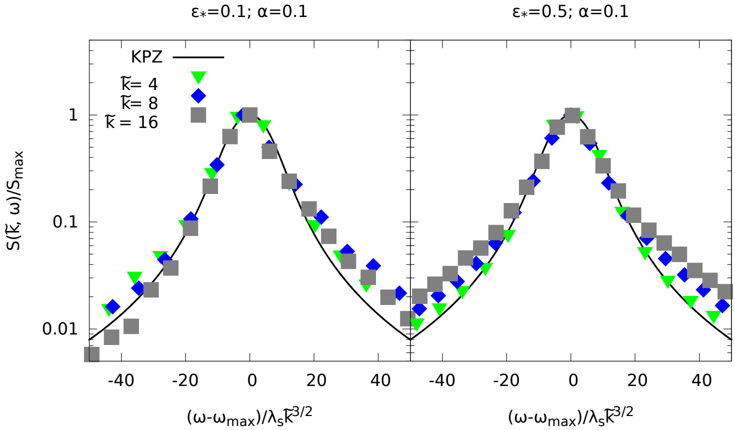
Stroboscopic observation: $t_n = nN/v$



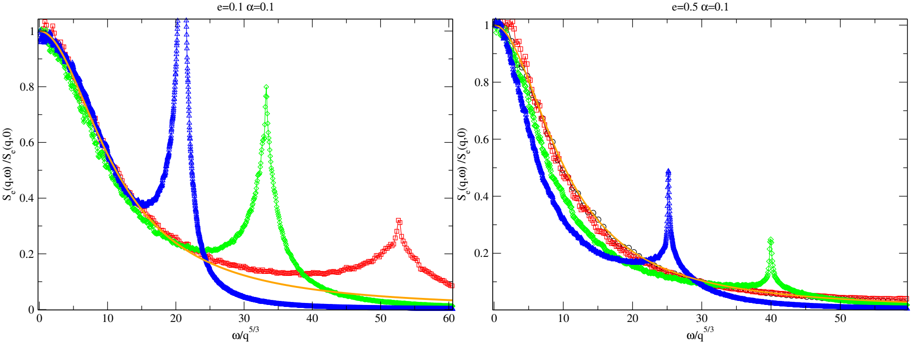
Numerics: structure factors, FPU



FPU Sound peaks: KPZ scaling

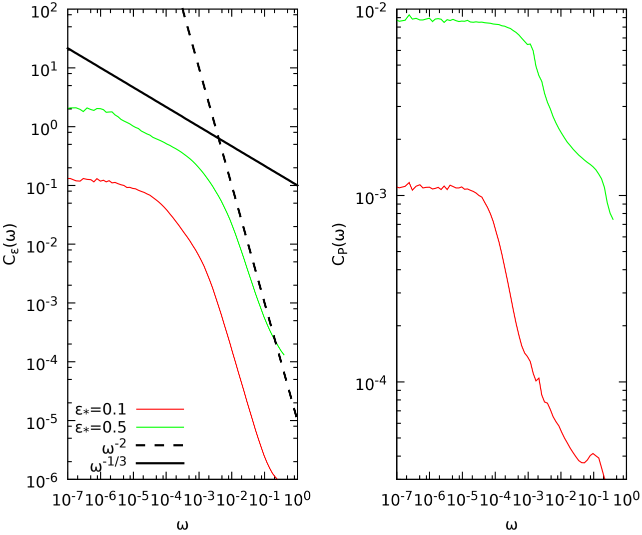


FPU Heat peaks: Lévy scaling



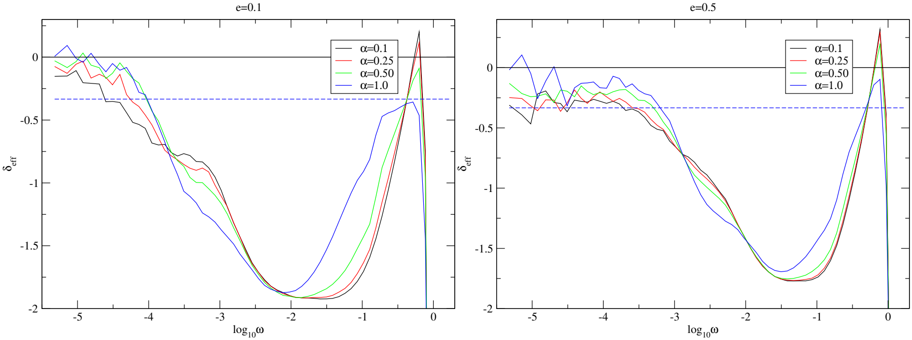
Lévy peak: Lorenzian with width $q^{5/3}$

FPU currents



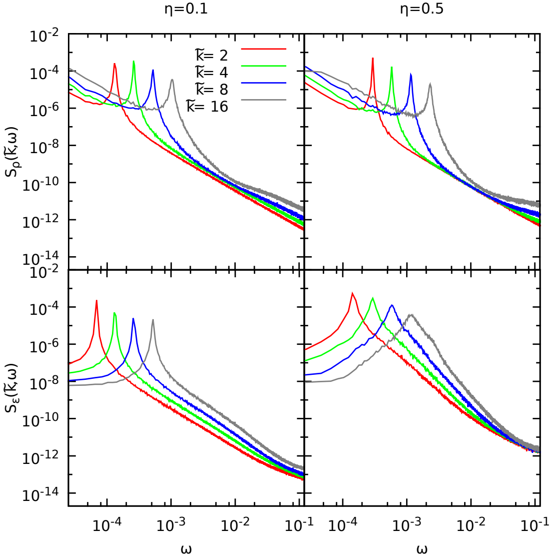
FPU energy flux correlator, log derivatives

$$\delta_{\text{eff}}(\omega) \; = \; \frac{d \ln S}{d \ln \omega} \quad .$$

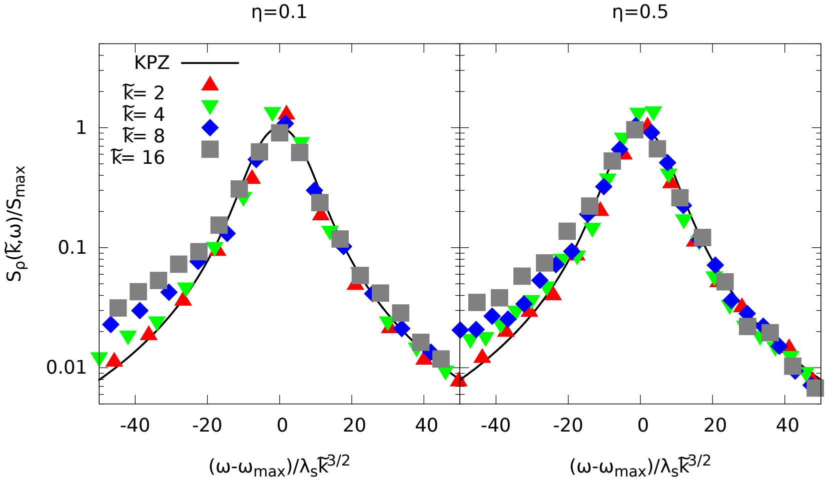


Why this difference despite the convincing KPZ scaling in the other observables? Yet an open issue ....

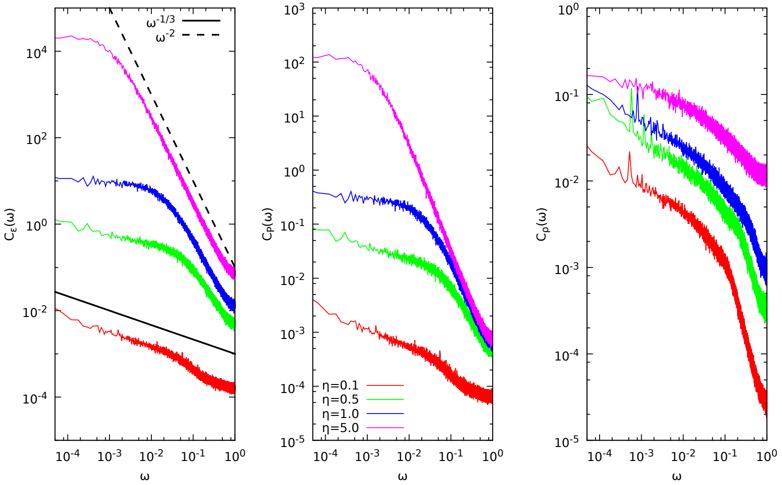
Numerics: structure factors, MPC



MPC Sound peaks: KPZ scaling

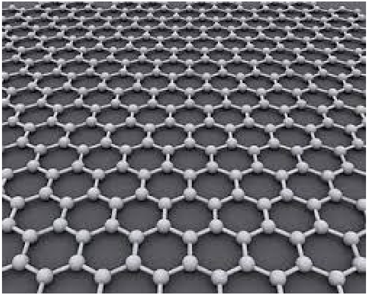


Currents correlator, MPC



$\eta = 0.1$, 0.5, 1 and 5 (bottom to top)

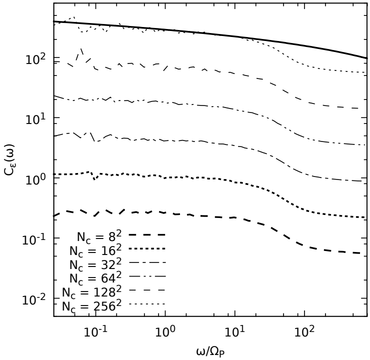
Two-dimensional systems



Less developed theory! one may expect

- Long tail in energy current correlators t^{-1} (with log corrections?)
- $\kappa \sim \log L$

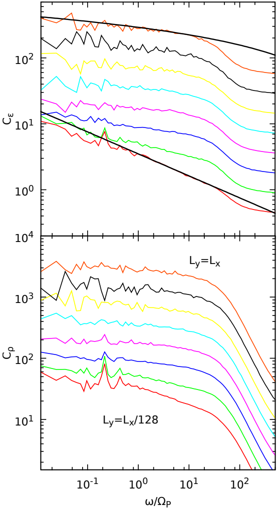
Remark: 2D MPC conserves also angular momentum



Solid: $f(\omega) = \alpha - \beta \log(\omega)$

Remark: Results insensitive to angular momentum conservation

2D $\rightarrow$ 1D dimensional cross-over



Different aspect ratios L_x/L_y: $\omega^{-1/3} \rightarrow -\log(\omega)$ in energy current

Outlook

- MPC dynamics
- Comparison between oscillators chain and 1D-MPC
- Dynamical scaling:
  1. good agreement with KPZ for the structure factors
  2. exponential decay of energy flux correlation instead of power: closeness to some integrable limit?
- Extension to 2D - MPC
  1. dimensional crossover
  2. marginal role of angular momentum conservation

Bibliography

1. P Di Cintio, R Livi, S Lepri, G Ciraolo Physical Review E 95 (4), 043203 (2017)
2. P Di Cintio, R Livi, H Bufferand, G Ciraolo, S Lepri, MJ Straka Physical Review E 92 (6), 062108 (2015)