Fluctuations in conservative systems and SPDEs

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joint work with Ben Fehrman [arxiv, Invent. Math. 2023+]

and Daniel Heydecker [arxiv]

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Content

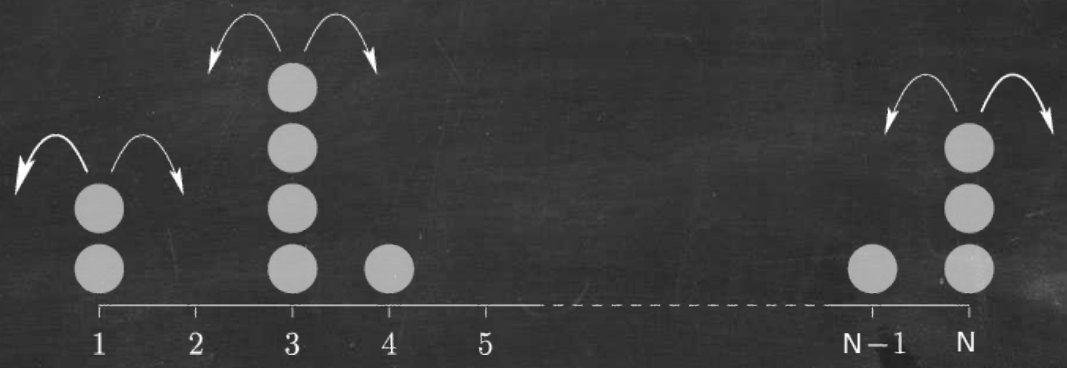
From interacting particle systems to conservative SPDEs

From large deviations to parabolic-hyperbolic PDE with irregular drift

Parabolic-hyperbolic PDE with irregular drift

From interacting particle systems to conservative SPDEs

The zero range process (could also consider simple exclusion, independent particles, ..).



- State space $\mathbb{M}_N := \mathbb{N}_0^{\mathbb{T}_N}$, i.e. configurations $\eta : \mathbb{T}_N \to \mathbb{N}_0$: System in state η if container k contains $\eta(k)$ particles.
- Local jump rate function $g : \mathbb{N}_0 \to \mathbb{R}_0^+$.
- Translation invariant, asymmetric, zero mean transition probability

$$p(k,l) = p(k-l), \quad \sum_k kp(k) = 0.$$

- Markov jump process $\eta(t)$ on $\mathbb{M}_N$.
- $\eta(k,t) =$ number of particles in box k at time t.

- **Hydrodynamic limit?** Multi-scale dynamics

- Empirical density field: $\mu^N(x,t) := \frac{1}{N}\sum_k \delta_{\frac{k}{N}}(x)\eta(k, tN^2)$.
- [Hydrodynamic limit - Ferrari, Presutti, Vares; 1987]

$$\mu^N(t) \rightharpoonup^* \bar{\rho}(t)\, dx$$

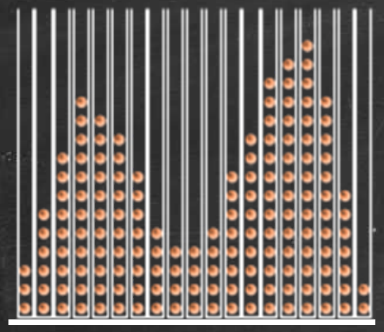
with

$$\partial_t \bar{\rho} = \partial_{xx}\Phi(\bar{\rho})$$

with Φ the mean local jump rate $\Phi(\rho) = \mathbb{E}_{\nu_\rho}[g(\eta(0))]$.
- Loss of information:
  - Fluctuations, rare events / large deviations?
  - Model / Approximation error: $\mu^N = \bar{\rho} + O(N^{-\frac{1}{2}})$.

Fluctuating Hydrodynamics?

Microscopic scale: Particles

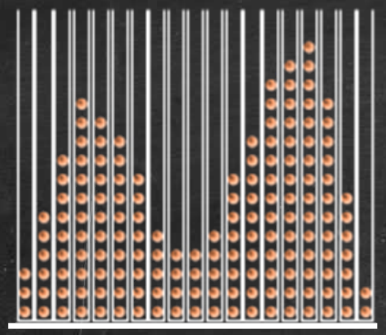


Gridsize = $\frac{1}{N}$

Macroscopic scale: PDEs

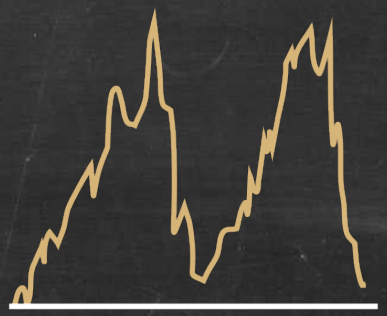
Mean dynamics

Microscopic scale: Particles



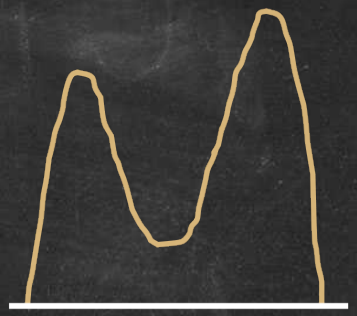
Gridsize = $\frac{1}{N}$

Mesoscopic scale: Conservative SPDEs



Fluctuation correction

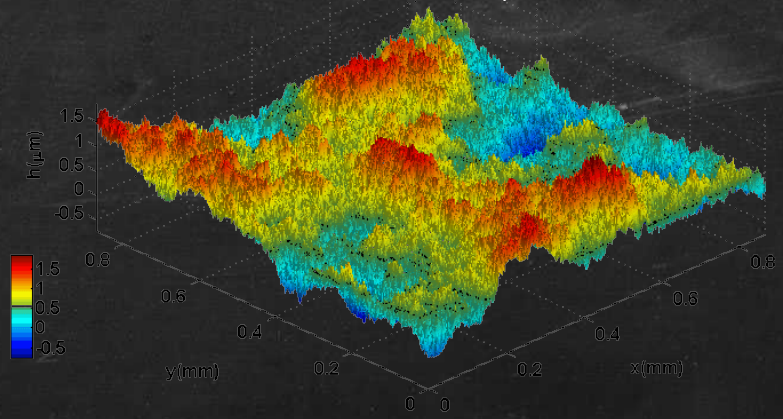
Macroscopic scale: PDEs



Mean dynamics

Ansatz: Conservative SPDEs

$$\partial_t \rho^N = \partial_{xx}\Phi(\rho^N) + N^{-\frac{1}{2}}\partial_x\left(\Phi^{\frac{1}{2}}(\rho^N)\xi^N\right),$$



with ξ^N noise, spatially correlated with decorrelation length $\frac{1}{N}$, and white in time,

Informally, correct large deviations:

- Recall
$$\partial_t \rho^N = \partial_{xx}\left(\Phi(\rho^N)\right) + N^{-\frac{1}{2}}\partial_x\left(\Phi^{\frac{1}{2}}(\rho^N)\xi^N\right).$$

- Rare events: (Im-)probability to observe a fluctuation ρ:
$$\mathbb{P}[\rho^N \approx \rho] = e^{-N\,I(\rho)} \quad N \text{ large}$$

- Informally applying the contraction principle to the solution map
$$F : N^{-\frac{1}{2}}\xi \mapsto \rho$$
yields as a rate function
$$I(\rho) = \inf\{I_\xi(g) : F(g) = \rho\}.$$

- Schilder's theorem for Brownian sheet suggests
$$I_\xi(g) = \int_0^T \int_{\mathbb{T}} |g|^2 \, dxdt.$$

- Get
$$I(\rho) = \inf\left\{\int_0^T \int_{\mathbb{T}} |g|^2 \, dxdt : \partial_t \rho = \partial_{xx}\left(\Phi(\rho)\right) + \partial_x\left(\Phi^{\frac{1}{2}}(\rho)g\right)\right\}.$$

Model / Approximation error:

$$\partial_t \rho^N = \partial_{xx}\Phi(\rho^N) + \partial_x \left(\Phi^{\frac{1}{2}}(\rho^N) N^{-\frac{1}{2}} \xi^N\right).$$

Central limit theorems predict

$$\rho^N = \bar{\rho} + N^{-\frac{1}{2}} Y^1 + O(N^{-1})$$
$$\mu^N = \bar{\rho} + N^{-\frac{1}{2}} Y^1 + O(N^{-1}).$$

Conclude: Higher order of approximation

$$\mu^N = \rho^N + O(N^{-1}).$$

Challenges:

- Well-posedness of conservative SPDEs (2013–): [Lions, Perthame, Souganidis; 2013, 2014], [G., Souganidis; 2015, 2017], [Fehrman, G.; 2021], [Dareiotis, G.; 2020], [Fehrman, G.; 2022].
- Large deviations: [Fehrman, G.; 2022], [Mariani, 2010]
- Expansions / quantified central limit theorems: [Dirr, Fehrman, G.; 2021], Linear case [Cornalba, Fischer, Ingmanns, Raithel]; [Djurdjevac, Kremp, Perkowski].

Nonequilibrium statistical mechanics - fluctuating gradient flows

- Many physical systems can be described by a competition between the relaxation of an energy E and friction in terms of a mobility M
- Gradient flow on an (infinite dimensional) "Riemannian manifold" [Jordan, Kinderlehrer, Otto, 1998]

$$\partial_t \rho = -M(\rho)\frac{\partial E}{\partial \rho}(\rho).$$

- For example

$$\partial_t \rho = \Delta\Phi(\rho) = \nabla \cdot (\Phi(\rho)\nabla \log(\Phi(\rho))) = -M(\rho)\frac{\partial E}{\partial \rho}(\rho)$$

with $-M(\rho)(\cdot) = \mathrm{div}(\Phi(\rho)\nabla\cdot)$, $\frac{\partial E}{\partial \rho} = \log(\Phi(\rho))$ generalized Boltzmann entropy.
- Formal non-equilibrium stationary Gibbs state $\mu = \frac{1}{Z}e^{-\varepsilon E(\rho)}$.
- Detailed-balance: Fluctuating gradient flow ([Öttinger 2005], fluctuating hydrodynamics [Spohn 1991])

$$\partial_t \rho = -M(\rho)\frac{\partial E}{\partial \rho}(\rho) + \sqrt{\varepsilon}M^{\frac{1}{2}}(\rho)\xi.$$

- Decorrelation length $\approx$ typical particle distance / grid-size: $\xi \to \xi^\delta$
- For example

$$\partial_t \rho = \Delta\Phi(\rho) + \nabla \cdot (\Phi^{\frac{1}{2}}(\rho)\,\xi^\delta)$$

Examples

- E.g. symmetric simple exclusion process:
  [Giacomin, Lebowitz, Presutti, 1999]

$$\partial_t \rho = \Delta \rho + \sqrt{\varepsilon} \nabla \cdot (\sqrt{\rho(1-\rho)}\, \xi^\delta).$$

- More generally:

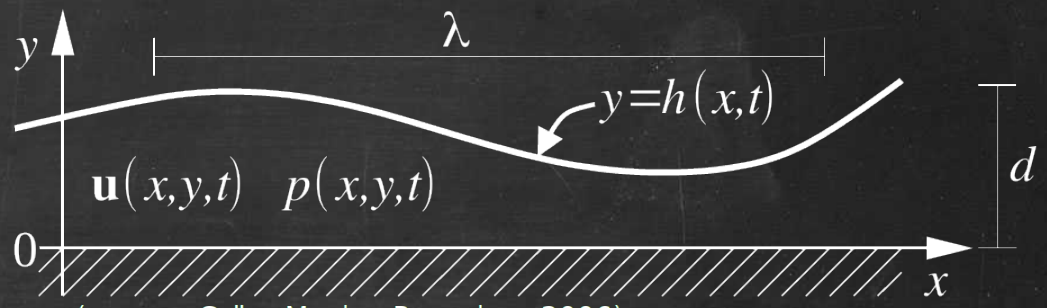
$$\partial_t \rho = \Delta \Phi(\rho) + \nabla \cdot \nu(\rho) + \sqrt{\varepsilon} \nabla \cdot (\sigma(\rho)\, \xi^\delta).$$

- Fluctuating incompressible Navier-Stokes-Fourier

$$\begin{aligned} \partial_t v =& \Delta v + v \cdot \nabla v + \nabla \cdot (\sqrt{T} \xi_1) \\ \partial_t T =& \Delta T + \nabla \cdot (vT) + |\nabla_{sym} v|^2 + \nabla \cdot (T\, \xi_1) + \nabla \cdot (\sqrt{T} \nabla v\, \xi_2). \end{aligned}$$

Stochastic thin films

$$\partial_t h = -\mathrm{div}(h^m \nabla \Delta h) + \mathrm{div}(h^{m/2}\xi)$$



(source: Grün, Mecke, Rauscher, 2006)

Fluctuating gradient flow structure

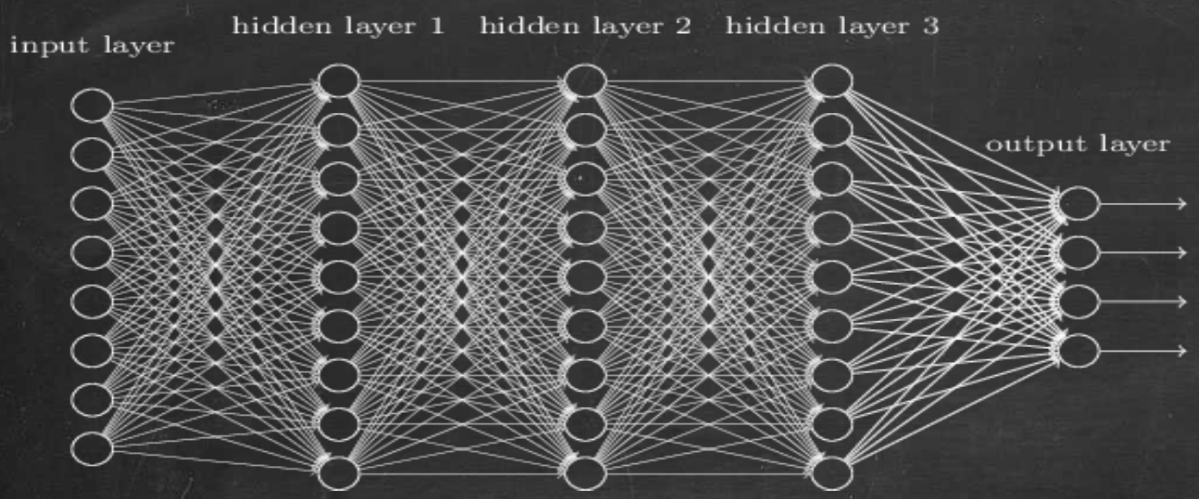
$$\partial_t h = -M(\rho)\frac{\partial E}{\partial h}(h) + M^{\frac{1}{2}}(h)\xi,$$

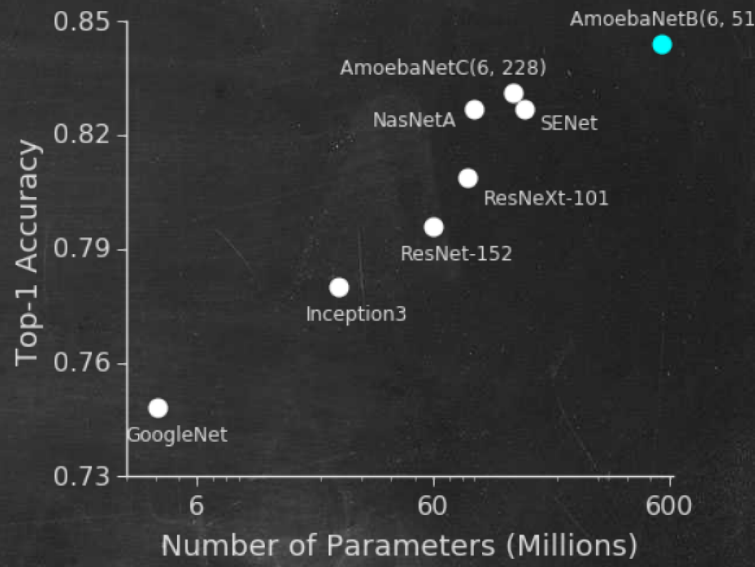
with $E(h) = \frac{1}{2}\int |\nabla h|^2 dx$ and $M(h) = \mathrm{div}(h^m \nabla \cdot)$,
Relevance to include thermal fluctuations:

- Improved prediction of empirical film rupture time scales
  [Grün, Mecke, Rauscher 2006]
- Corrected spreading rate of droplets
  [Davidovitch, Moro, Stone 2005]

Machine learning

Feed-forward neural network





Collecting all parameters $\theta = (\theta_1, \ldots, \theta_M) \in \mathbb{R}^M$
Stochastic gradient descent / empirical risk minimization

$$\theta_{n+1} = \theta_n - \eta \nabla_\theta l(\theta_n, \omega_n),$$

Scaling limits: Small learning rate η, overparametrization $M \to \infty$.
Empirical distribution $\mu_t^M := \frac{1}{M} \sum_i \delta_{\theta_t^i} \to \mu_t$ solution to

$$\partial_t \mu_t = \mathrm{div}(\nabla V(\mu_t, \cdot)\mu_t) + D^2 : (A(\mu_t, \cdot)\mu_t) + \sqrt{\sigma}\mathrm{div}(T(\mu_t, \cdot)\mu\,\xi),$$

where ξ is space-time white noise and V, A, T_μ are non-local operators, see [Chen, Rotskoff, Bruna, Vanden-Eijnden, 2020].

Numerics for SPDEs? [1] Consider

$$\partial_t \rho = \Delta \Phi(\rho) + \nabla \cdot (\Phi^{\frac{1}{2}}(\rho)\, \xi^{\delta})$$

with ξ space time white noise.

Difficulty:

- Irregularity of space-time white noise: Solution is not known to take values in a function space.
- L^p-based estimates fail.
- L^2-based finite elements not a good choice

Idea: H^{-1}-based finite elements.

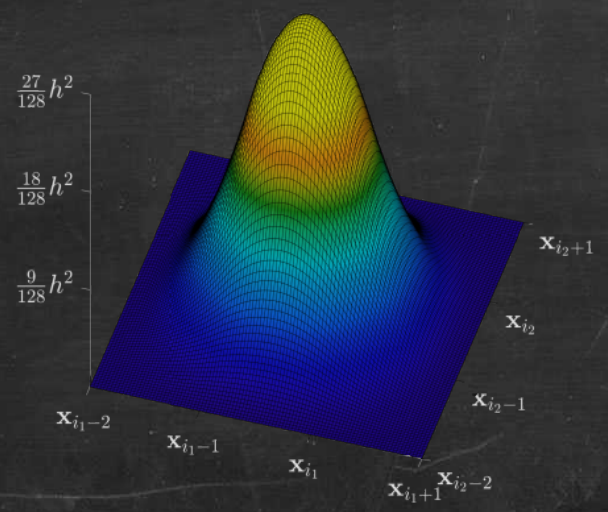
But, standard basis (e.g. piecewise constant) have non-sparse mass matrix

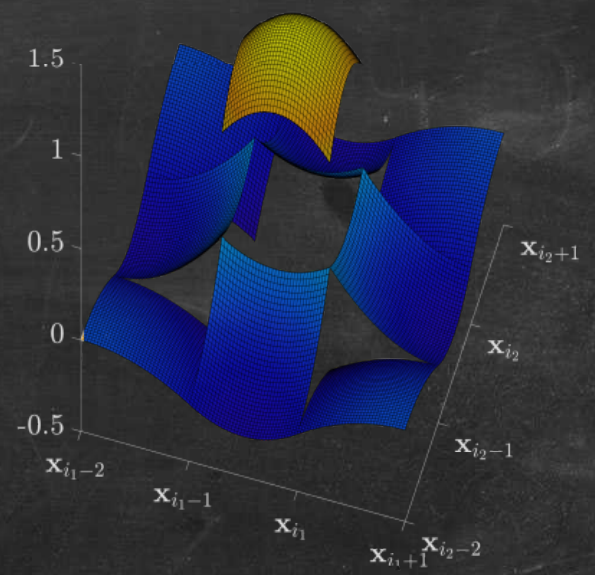
$$(M_h)_{i,j} = (\varphi_i, \varphi_j)_{H^{-1}} = (\varphi_i, (-\Delta)^{-1} \varphi_j)_{L^2}.$$

[1] [Banas, G., Vieth, 2020]

Solution:

1. 1d [Emmrich, Siska, CMS, 2012]
2. all dimensions d [Banas, G., Vieth, 2020]: Construction of H^1 basis functions $\psi_i(x)$, $i \in \{1, \ldots, J\}^d$ with $\phi_i = -\Delta\psi_i$ both with small support.





From large deviations to parabolic-hyperbolic PDE with irregular drift

Rare events: (Im-)probability to observe a fluctuation ρ:

$$\mathbb{P}[\mu^N \approx \rho] = e^{-N\, I(\rho)} \quad N \text{ large}$$

A bit more precisely, for every open set O,

$$\mathbb{P}[\mu^N \in \bar{O}] \lesssim e^{-N \inf_{\rho \in \bar{O}} I(\rho)}$$

$$e^{-N \inf_{\rho \in O} I(\rho)} \lesssim \mathbb{P}[\mu^N \in O]$$

Zero range process

$$I(\rho) = \inf\{\int_0^T \int_{\mathbb{T}} |g|^2 \, dxdt \; : \underbrace{\partial_t \rho = \partial_{xx}\Phi(\rho) + \partial_x(\Phi^{\frac{1}{2}}(\rho) g)}_{\text{"skeleton equation"}}\}.$$

Theorem ([Large deviation principle, Kipnis, Olla, Varadhan; 1989 & Benois, Kipnis, Landim; 1995])

For every open set $O \subseteq D([0,T], \mathcal{M}_+)$ we have

$$\mathbb{P}[\mu^N \in \bar{O}] \lesssim e^{-N \inf_{\rho \in \bar{O}} I(\rho)}$$

$$\mathbb{P}[\mu^N \in \bar{O}] \lesssim e^{-N \inf_{\rho \in \bar{O}} I(\rho)}$$

$$e^{-N \inf_{\rho \in O} J(\rho)} \lesssim \mathbb{P}[\mu^N \in O]$$

where $J = \overline{I_{|A}}$ and A is the set of nice fluctuations $\mu = \rho\, dx$ with ρ a solution to

$$\partial_t \rho = \partial_{xx} \Phi(\rho) + \partial_x (\Phi^{\frac{1}{2}}(\rho) g)$$

for some $\underline{g \in C^{1,3}_{t,x}}$.

This is a frequently observed problem: E.g. Fluctuations around Boltzmann equation [Rezakhanlou 1998], [Bodineau, Gallagher, Saint-Raymond, Simonella 2020].
Counter-examples for Boltzmann [Heydecker; 2021].

Difficult: Open problem for the zero range process since [Benois, Kipnis, Landim; 1995]

Parabolic-hyperbolic PDE with irregular drift

Skeleton equation

$$\partial_t \rho = \partial_{xx}\Phi(\rho) + \partial_x(\Phi^{\frac{1}{2}}(\rho)\underbrace{g}_{\in L^2_{t,x}}).$$

How difficult is the well-posedness?

- Difficulty: Stable a-priori bound? L^p framework does not work.
- Do we expect non-concentration of mass / well-posedness?

Scaling and criticality of the skeleton equation

- We consider, $\Phi(\rho) = \rho^m$,

$$\partial_t \rho = \partial_{xx}\rho^m + \partial_x(\rho^{\frac{m}{2}} g)$$

  with $g \in L^q_t L^p_x$ and $\rho_0 \in L^r_x$.
- Via rescaling ("zooming in"):
  - $p = q = 2$ is critical.
  - $r = 1$ is critical, $r > 1$ is supercritical.

Recall: [Le Bris, Lions; CPDE 2008], [Karlssen, Risebro, Ohlberger, Chen, ...]

$$\partial_t \rho = \frac{1}{2}\partial_{xx}(\sigma\sigma^* \rho) + \partial_x(\rho\, g)$$

needs $g \in W^{1,1}_{loc,x}$, $\operatorname{div} g \in L^\infty$.

Overview of ingredients of the proof:

- **Part 1:** Apriori-bounds; entropy-entropy dissipation estimates
- **Part 2:** Extending the concepts of DiPerna-Lions, Ambrosio, Le Bris-Lions to nonlinear PDE (but going beyond).
- **Part 3:** Uniqueness for renormalized entropy solutions (variable doubling): New treatment of kinetic dissipation measure. Exploit finite *singular* moments.

Theorem (The skeleton equation, Fehrman, G. 2022)

Let $g \in L^2_{t,x}$, ρ_0 non-negative and $\int \rho_0 \log(\rho_0) dx < \infty$. There is a unique weak solution to

$$\partial_t \rho = \Delta \Phi(\rho) + \nabla \cdot (\Phi^{\frac{1}{2}}(\rho) g).$$

The map $g \mapsto \rho$, $L^2_{t,x} \to L^1_{t,x}$, is weak-strong continuous. E.g. including all $\Phi(\rho) = \rho^m$, $m \in [1, \infty)$.

Theorem (LDP for zero range process, G., Heydecker, 2023)

The rescaled zero range process satisfies the <u>full</u> large deviations principle with rate function

$$I(\rho) = \|\partial_t \rho - \partial_{xx} \Phi(\rho)\|_{H^{-1}_{\Phi(\rho)}}.$$

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Advertisement: Two open PostDoc positions at Bielefeld University (CRC 1283, and ERC CoG "FluCo") in stochastic analysis, in particular,

- stochastic PDEs
- non-equilibrium statistical mechanics
- mathematics of machine learning
- stochastic dynamics.