Path large deviations for kinetic theories: beyond the Boltzmann, the Landau, the Balescu–Guernsey–Lenard, and the weak turbulence kinetic equations

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With O. Feliachi (Boltzmann eq. and plasma).
With J. Guioth, Y. Onuki and G. Eyink (wave turbulence).

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Outline

1. Introduction
   - Path large deviations theory
   - Motivations for path large deviations for kinetic theories
2. Path large deviations for particles with long-range interactions (Landau and Balescu–Lenard–Guernsey equation)
   - Particles with long range interactions, the Landau and the Balescu–Lenard–Guernsey equations
   - Path large deviations for quadratic forms of Gaussian processes using the Szegö–Widom theorem
   - Hamiltonian for the Balescu–Lenard–Guernsey equation

Outline

Large Deviation Theory

- Large deviation theory is a general framework to describe probability distributions in asymptotic limits

$$P(x,\varepsilon) = \mathbb{P}\left[X_\varepsilon = x\right] \underset{\varepsilon \ll 1}{\asymp} \mathrm{e}^{-\frac{\mathscr{F}[x]}{\varepsilon}}.$$

For equilibrium statistical mechanics, $\mathscr{F}$ is the free energy, and $\varepsilon = k_B T/N$.

Maths: Cramer 30', Sanov 50', Lanford 70', Freidlin–Wentzell 70' and 80', Varadhan, ... In parallel with theoretical physicists.

Feng and Kurtz book for stochastic processes.

Path Large Deviation Theory

$$f_N(\mathbf{r},\mathbf{v},t) \equiv \frac{1}{N}\sum_{n=1}^{N}\delta\left(\mathbf{v}-\mathbf{v}_n(t)\right)\delta\left(\mathbf{r}-\mathbf{r}_n(t)\right).$$

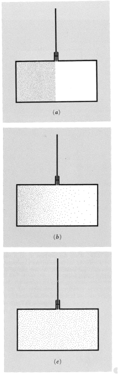
- For many kinetic theories one expects:

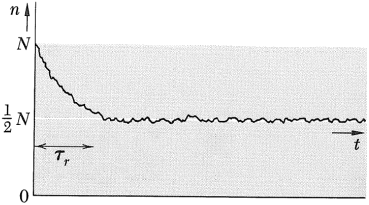
$$\mathbb{P}\left[\{f_N(t)\}_{0\leq t<T} = \{f(t)\}_{0\leq t<T}\right] \underset{\varepsilon\downarrow 0}{\asymp} \exp\left(-\frac{\sup_p \int_0^T \mathrm{d}t \left\{\int \dot{f}\, p\, \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v} - H[f,p]\right\}}{\varepsilon}\right).$$

- What is ε? Can we compute H?
- This is a statistical field theory for the effective large scale dynamics.
- H summarizes all the relevant statistical information. This is the Holy Grail of any modern statistical mechanician.
- This gives the most probable evolution, the Gaussian fluctuations (stochastic differential or partial differential equations) and the rare events beyond Gaussian fluctuations.

Outline

Motivation 1: Joule Expansion and Large Deviations



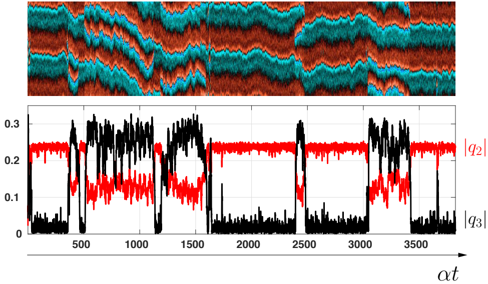


(Figures: Reif)

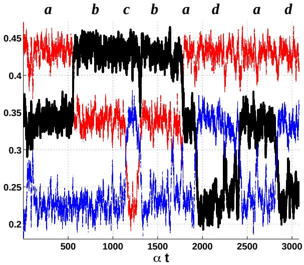
- What is the probability of a dynamical rare fluctuation? The answer is not known within the classical statistical equilibrium framework.

Motivation 2: Effective Description of Turbulent Flows

Rare transitions for quasigeostrophic jets



Bistability between 2 and 3 jets



Between 3 jet states

F. Bouchet, J. Rolland and E. Simonnet, Phys. Rev. Lett. 2018 and JAS 2021

Motivation 3: Large Deviations and the Geometric Structure of Kinetic Equations

- In many cases (diffusion, Vlasov–Mac-Kean, and so on), kinetic equations can be seen as Gradient dynamics

$$\frac{\partial f}{\partial t} = -\mathrm{Grad}_f \mathscr{F},$$

where the gradient is with respect to the Wasserstein distance (Otto-Villani).

- Where does this structure come from?
- From large deviation theory. The metric is given by the dynamical large deviation Hamiltonian, $\mathscr{F}$ is the quasipotential. There is then a natural generalization

$$\frac{\partial f}{\partial t} = -\mathrm{Grad}_f \mathscr{F} + \mathscr{G} \text{ with } \left(\mathrm{Grad}_f \mathscr{F}, \mathscr{G}\right) = 0.$$

Boltzmann Equation for dilute gases

$$\frac{\partial f}{\partial t}+\mathbf{v}.\frac{\partial f}{\partial \mathbf{r}}=\int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{v}_1'\mathrm{d}\mathbf{v}_2'\, w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v},\mathbf{v}_2)\left[f\left(\mathbf{v}'_1,\mathbf{r}\right)f\left(\mathbf{v}_2',\mathbf{r}\right)-f\left(\mathbf{v},\mathbf{r}\right)f\left(\mathbf{v}_2,\mathbf{r}\right)\right].$$

- A cornerstone of physics.
- The irreversibility paradox and the 19^{th} century controversy (Loschmidt, Zermelo, Poincaré).
- Classical explanation of the paradox by Boltzmann, theoretical physicists of the 20th century, Lanford work (1973).
- It is a very active contemporary subject both in physics and mathematics.

The Boltzmann Equation is a Law of Large Numbers

- We consider the empirical distribution

$$f_N(\mathbf{r},\mathbf{v},t) = \frac{1}{N}\sum_{n=1}^{N} \delta\left(\mathbf{r}-\mathbf{r}_n(t),\mathbf{v}-\mathbf{v}_n(t)\right)$$

- We consider an ensemble of initial conditions $\{\mathbf{r}_n,\mathbf{v}_n\}_{1\leq n\leq N}$ where each $f_N(t=0)$ is close to f_0.
- The Boltzmann equation is a law of large numbers:

$$\lim_{N\to\infty} f_N(t) = f(t),$$

where f solves the Boltzmann equation with $f(t=0)=f_0$.
- For large enough N, "for almost all initial conditions" and for a finite time, $f_N(t)$ remains close to $f(t)$ where f solves the Boltzmann equation with $f(t=0)=f_0$.
- We should study the probabilities of f_N, beyond the law of large numbers. May be Gaussian fluctuations, but even more interesting large deviations.

Path Large Deviations for the Boltzmann Equation

- Dynamical large deviations for the empirical distribution:

$$P\left[\{f_N(t)\}_{0\leq t<T}=\{f(t)\}_{0\leq t<T}\right]\underset{\varepsilon\downarrow 0}{\asymp}\exp\left(-\frac{\sup_p\int_0^T\mathrm{d}t\left\{\int\dot{f}p\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}-H_B[f,p]\right\}}{\varepsilon}\right).$$

  ε is the inverse of the number of particles in a volume of size the mean free path.

- The large deviation Hamiltonian is $H_B=H_C+H_T$, with H_T the free transport part, and with the collision part H_c given by

$$H_C[f,p]=\frac{1}{2}\int\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}_{1,2,1',2'}\,w(\mathbf{v}_1',\mathbf{v}_2';\mathbf{v}_1,\mathbf{v}_2)f(\mathbf{r},\mathbf{v}_1)f(\mathbf{r},\mathbf{v}_2)\left\{\mathrm{e}^{\left[p(\mathbf{r},\mathbf{v}_1)+p(\mathbf{r},\mathbf{v}_2)-p\left(\mathbf{r},\mathbf{v}_1'\right)-p\left(\mathbf{r},\mathbf{v}_2'\right)\right]}-1\right\}.$$

- C. Leonard, 1995. F. Rezakhanlou, 1998: stochastic models with Boltzmann like behavior.
- F. Bouchet, 2020, for dilute gases.
- T. Bodineau, I. Gallagher, L. Saint-Raymond and S. Simonella, 2020, for a mathematical proof for short times.
- D. Heydecker, 2022, and G. Basile, D. Benedetto, L. Bertini and E. Caglioti, 2022: energy non-conserving solutions with probability $\mathcal{O}\left(e^{-N}\right)$.

Outline

Particles with Mean–Field Interactions

$$\frac{\mathrm{d}\mathbf{r}_n}{\mathrm{d}t} = \mathbf{v}_n \text{ and } \frac{\mathrm{d}\mathbf{v}_n}{\mathrm{d}t} = -\frac{1}{N}\sum_{m=1}^{N}\frac{\mathrm{d}W}{\mathrm{d}\mathbf{x}}\left(\mathbf{r}_n - \mathbf{r}_m\right). \left(\mathbf{r}_n \in \mathbb{R}^d \textit{ or } \mathbf{r}_n \in \mathbb{T}^d\right).$$

- Energy
$$H_N = \frac{1}{2}\sum_{n=1}^{N}\frac{\mathbf{v}_n^2}{2} + \frac{1}{2N}\sum_{n,m=1}^{N} W\left(\mathbf{r}_n - \mathbf{r}_m\right).$$
- The empirical distribution $g_N(\mathbf{r},\mathbf{v},t) = \frac{1}{N}\sum_{n=1}^{N}\delta\left(\mathbf{r}-\mathbf{r}_n(t);\mathbf{v}-\mathbf{v}_n(t)\right)$ formally solves the Klimontovich equation

$$\frac{\partial g_N}{\partial t} + \mathbf{v}.\frac{\partial g_N}{\partial \mathbf{r}} - \frac{\mathrm{d}V[g_N]}{\mathrm{d}\mathbf{r}}.\frac{\partial g_N}{\partial \mathbf{v}} = 0 \text{ with } V[g_N](\mathbf{r}) = \int \mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{v}\, W\left(\mathbf{r}-\mathbf{r}'\right) g_N(\mathbf{r},\mathbf{v}).$$

- Coulomb interaction: $W(\mathbf{r}) = -1/\mathbf{r}^2$ and N is the number of particles in a volume of the size of the Debye length. N is related to the plasma parameter Γ.

Derivation of the Balescu–Lenard–Guernsey eq. 1: Projection on homogeneous distributions

- We decompose

$$g_N(\mathbf{r},\mathbf{v},t) \equiv \frac{1}{N}\sum_{n=1}^{N}\delta\left(\mathbf{r}-\mathbf{r}_n(t);\mathbf{v}-\mathbf{v}_n(t)\right) = f_N(\mathbf{v},t) + \frac{1}{\sqrt{N}}\delta g_N(\mathbf{r},\mathbf{v},t),$$

with the projection over homogeneous distributions:

$$f_N(\mathbf{v},t) = \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\, g_N(\mathbf{r},\mathbf{v},t) = \frac{1}{NL^3}\sum_{n=1}^{N}\delta(\mathbf{v}-\mathbf{v}_n(t)).$$

- After rescaling time $\tau = t/N$, at leading order in N we obtain

$$\begin{aligned}\frac{\partial f_N}{\partial \tau} &= \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right),\\ \frac{\partial \delta g_N}{\partial \tau} &= N\left(-\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f_N}{\partial \mathbf{v}}\right).\end{aligned}$$

Our plan to compute explicitly H

1. Justify a slow fast dynamics and describe path large deviations for slow/fast dynamics.
2. Compute path large deviations for quadratic observables of Gaussian processes using Szegö–Widom theorems.
3. Compute explicitly functional determinants and determinants over infinite dimensional space.
4. Write the formula for H and verify all its symmetry properties (time reversal symmetries, conservation laws, entropy and quasipotential).
5. Justify the quasi-linear approximation (or check the self-consistency of this hypothesis).

Outline

Quasilinear Dynamics and Large Deviation Principle

- With time rescaling $\tau = t/N$, we have the slow/fast dynamics

$$\frac{\partial f_N}{\partial \tau} = \frac{1}{L^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right),$$

$$\frac{\partial \delta g_N}{\partial \tau} = N\left\{-\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f_N}{\partial \mathbf{v}}\right\}.$$

- Then we have the large deviation principle

$$\mathbf{P}(f_N = f) \underset{N\to\infty}{\asymp} \exp\left[-NL^3 \mathrm{Sup}_p \int_0^T \left(\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p]\right)\right], \text{ with}$$

$$H[f,p] = \lim_{T\to\infty}\frac{1}{T}\log \mathbb{E}_f\left[\exp\left(\frac{1}{L^3}\int_0^T \mathrm{d}\tau \int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}\, p(\mathbf{v}) \int \mathrm{d}\mathbf{r}' \frac{\partial V[\delta g_N]}{\partial \mathbf{r}'}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right].$$

- This is the large deviation for time averages of quadratic functionals of a Gaussian process.

Large deviations for quadratic functionals of stationary Gaussian processes

- Let Y_t be a stationary Gaussian process with values on $\mathbb{C}^n$. We denote $C(t) = \mathbb{E}(Y_t^* \otimes Y_0)$ and assume $\mathbb{E}(Y_t \otimes Y_0) = 0$.
- Let M is an Hermitian matrix of size $n \times n$.
- Then

$$\log \mathbb{E} \exp\left(\int_0^T \mathrm{d}t\, Y_t^{*\mathsf{T}} M Y_t\right) \underset{T\to\infty}{\sim} -\frac{T}{2\pi}\int \mathrm{d}\omega \log \det_{\mathscr{M}_{n,n}}\left(I_n - M\tilde{C}(\omega)\right), \quad (1)$$

where $\tilde{C}(\omega) = \int_{\mathbb{R}} \mathrm{e}^{i\omega t} C(t)\,\mathrm{d}t$ is the Fourier transform of C.

Gaussian integration of quadratic functionals

- Let Y_t be a stationary Gaussian process with values on $\mathbb{C}^n$. We denote $C(t) = \mathbb{E}(Y_t^* \otimes Y_0)$ and assume $\mathbb{E}(Y_t \otimes Y_0) = 0$.
- Then

$$\log \mathbb{E} \exp\left(\int_0^T \mathrm{d}t\, Y_t^{*\mathsf{T}} M Y_t\right) = -\log \det_{\mathscr{F}([0,T],\mathbb{C}^n)} \left(\mathrm{Id} - \overline{MC}_T\right),$$

where $\overline{MC}_T$ is the integral operator over $\mathscr{F}([0,T],\mathbb{C}^n)$ defined by

$$\text{If } X \in \mathscr{F}([0,T],\mathbb{C}^n) \text{ then } \overline{MC}_T(t)[X] = \int_0^T MC(t-s)X(s)\mathrm{d}s.$$

The Szegö–Widom theorem

- Let $\bar{K}_T$ be an integral operator on $\mathscr{F}([0,T],\mathbb{C}^n)$ defined by

$$\bar{K}_T X(t) = \int_0^T K(t-s)X(s)\,\mathrm{d}s,$$

where $K \in \mathscr{F}([0,T],\mathbb{C}^n)$ is called the kernel of the operator $\bar{K}_T$.

- Then

$$\log \det_{\mathscr{F}([0,T],\mathbb{C}^n)} \left(\mathrm{Id} + \bar{K}_T\right) \underset{T\to\infty}{\sim} \frac{T}{2\pi}\int \mathrm{d}\omega \log \det_{\mathscr{M}_{n,n}} \left(I_n + \int_{\mathbb{R}} \mathrm{e}^{i\omega t} K(t)\,\mathrm{d}t\right).$$

Large deviations for quadratic functionals of stationary Gaussian processes

- Let Y_t be a stationary Gaussian process with values on $\mathbb{C}^n$. We denote $C(t) = \mathbb{E}(Y_t^* \otimes Y_0)$ and assume $\mathbb{E}(Y_t \otimes Y_0) = 0$.
- Let M is an Hermitian matrix of size $n \times n$.
- Then

$$\log \mathbb{E} \exp\left(\int_0^T \mathrm{d}t\, Y_t^{*\mathsf{T}} M Y_t\right) \underset{T\to\infty}{\sim} -\frac{T}{2\pi}\int \mathrm{d}\omega \log \underset{\mathscr{M}_{n,n}}{\det}\left(I_n - M\tilde{C}(\omega)\right), \quad (2)$$

where $\tilde{C}(\omega) = \int_{\mathbb{R}} \mathrm{e}^{i\omega t} C(t)\,\mathrm{d}t$ is the Fourier transform of C.

Outline

Large Deviation Principle

- We have the large deviation principle

$$\mathbf{P}(f_N = f) \underset{N\to\infty}{\asymp} \mathrm{e}^{-NL^3 \mathrm{Sup}_p \int_0^T \left\{\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \dot{f} p - H[f,p]\right\}}, \text{ with}$$

$$H[f,p] = \lim_{T\to\infty} \frac{1}{T} \log \mathbb{E}_f \left[\exp\left(\frac{1}{L^3}\int_0^T \mathrm{d}\tau \int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{v}\, p(\mathbf{v})\, \frac{\partial V[\delta g_N]}{\partial \mathbf{r}} . \frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right].$$

- This is the large deviation for time averages of quadratic functionals of a Gaussian process.

$$H[f,p] = -\frac{T}{2\pi}\int \mathrm{d}\omega \log \det_{\mathscr{L}_\mathbf{v}} \left(I_n - M\tilde{C}(\omega)\right).$$

Computing determinants on the space of complex functions of the velocity space

- We need to compute the determinant of an operators U that acts on complex-function φ over the velocity space:

$$U[\varphi](\mathbf{v}_1) = \varphi(\mathbf{v}_1) + i\hat{W}(\mathbf{k})\mathbf{k}\cdot\int \mathrm{d}\mathbf{v}_2\mathrm{d}\mathbf{v}_3\,\tilde{C}_{GG}(\mathbf{k},\omega,\mathbf{v}_2,\mathbf{v}_3)\left\{\frac{\partial p}{\partial \mathbf{v}}(\mathbf{v}_2) - \frac{\partial p}{\partial \mathbf{v}}(\mathbf{v}_1)\right\}\varphi(\mathbf{v}_3).$$

- A critical remark: U is the identity plus a rank two linear operator

$$U : \varphi \longmapsto \varphi + (w, Q\varphi)\,v + (v, Q\varphi)\,w,$$

then

$$\det U = 1 + 2\Re\left[(v, Qw)\right] + (v, Qw)(v, Qw)^* - (w, Qw)(v, Qv).$$

- The determinant of U only depends on the two-point correlation function of the quasi-linear problem.

The Large Deviation Hamiltonian for the Lenard–Balescu equation

- The large deviation Hamiltonian reads

$$H[f,p]=-\frac{1}{4\pi}\sum_{\mathbf{k}}\int \mathrm{d}\omega\,\log\left\{1-\mathscr{J}[f,p](\mathbf{k},\omega)\right\},$$

with

$$\mathscr{J}[f,p](\mathbf{k},\omega)=4\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\,\frac{\partial p}{\partial \mathbf{v}_1}.\overleftrightarrow{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2).\left\{\frac{\partial f}{\partial \mathbf{v}_2}f(\mathbf{v}_1)-f(\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}_1}\right\}$$
$$+4\pi\int \mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2\left\{\frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_1}-\frac{\partial p}{\partial \mathbf{v}_1}\frac{\partial p}{\partial \mathbf{v}_2}\right\}:\overleftrightarrow{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2)f(\mathbf{v}_1)f(\mathbf{v}_2), \quad (3)$$

where

$$\overleftrightarrow{A}(\mathbf{k},\omega,\mathbf{v}_1,\mathbf{v}_2)=\pi\frac{\mathbf{k}\mathbf{k}\hat{W}(\mathbf{k})^2}{|\varepsilon(\omega,\mathbf{k})|^2}\delta(\omega-\mathbf{k}.\mathbf{v}_1)\,\delta(\omega-\mathbf{k}.\mathbf{v}_2).$$

Conclusion: The Landau and Balescu–Lenard–Guernsey Large Deviation Hamiltonians

- With O. Feliachi, we have derived the Hamiltonian for the path large deviations for the empirical density of systems with long range interactions (related to the BLG equation).
- We have justified the Hamiltonian for the path large deviations for the Landau equation, both from the Boltzmann and from the BLG Hamiltonians.

$$H_{LB}[f,p]=\underbrace{\int \mathbf{dv_1}\, f\left\{\mathbf{b}[f].\frac{\partial p}{\partial \mathbf{v_1}}+\frac{\partial}{\partial \mathbf{v_1}}\left(\overleftrightarrow{D}[\mathbf{f}]\frac{\partial p}{\partial \mathbf{v_1}}\right)+\overleftrightarrow{D}[f]:\frac{\partial p}{\partial \mathbf{v_1}}\frac{\partial p}{\partial \mathbf{v_1}}\right\}}_{H_{MF}[f,p]}-\underbrace{\int \mathbf{dv_1 dv_2}\, f(\mathbf{v_1})f(\mathbf{v_2})\overleftrightarrow{B}[f](\mathbf{v_1},\mathbf{v_2})\frac{\partial p}{\partial \mathbf{v_1}}\frac{\partial p}{\partial \mathbf{v_2}}}_{H_I[f,p]}.$$

- The large deviations are non-Gaussian for BLG and Gaussian for Landau. We can identify a gradient structure for both.
- The Hamiltonians are time reversal symmetric, conserve mass, momentum and energy. Entropy is the quasipotential.

Path large deviations for kinetic theories

$$f_N(\mathbf{r},\mathbf{v},t) \equiv \frac{1}{N}\sum_{n=1}^{N} \delta\left(\mathbf{v}-\mathbf{v}_n(t)\right)\delta\left(\mathbf{r}-\mathbf{r}_n(t)\right).$$

$$\mathbb{P}\left[\{f_N(t)\}_{0\le t<T} = \{f(t)\}_{0\le t<T}\right] \underset{\varepsilon\downarrow 0}{\asymp} \exp\left(-\frac{\sup_p \int_0^T \mathrm{d}t \left\{\int \dot{f}\, p\, \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v} - H[f,p]\right\}}{\varepsilon}\right).$$

- What is ε? Can we compute H?
- Dilute gases (Boltzmann equation): F. Bouchet, JSP, 2020.
- Plasma beyond debye length: O. Feliachi and F. B., JSP, 2021.
- Systems with long range interactions: O. Feliachi and F. Bouchet, JSP, 2022.
- Weak turbulence theory (wave turbulence), homgeneous case: J. Guioth, G. Eyink, and F. Bouchet, 2022, JSP. Inhomogeneous case with random potential: Y. Onuki, J. Guioth, and F. Bouchet, 2023, arXiv:2301.03257.