Relations between various entropy concepts and the quasi-potentials of classical kinetic theories

Subtitle : entropy and path large deviations for classical kinetic theories

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Works about path large deviations for classical kinetic theories:

a) Dilute gases (Boltzmann): F.B.
b) Plasma and systems with long range interactions: O. Feliachi and F.B.
c) Kinetic theory for wave (weak) turbulence: J. Guioth, Y. Onuki, G. Eyink and F.B.

Clay institute, About Entropy in Large Classical Particle Systems, September 2023

Outline

I) Introduction: entropy concepts, from Clausius up to the dynamical meaning of entropy for kinetic theories

II) Path large deviations and macroscopic reversibility: revisiting the irreversibility paradox

III) Path large deviations for kinetic theories: the example of particles with long range interactions

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Entropies

1. Clausius entropy: the thermodynamics entropy for macroscopic systems. Clausius entropy S_C has an operational definition (through thermodynamic processes and the first and second laws of thermodynamics).
2. Boltzmann equilibrium entropy:

$$S_{B,N}(E,V) = k_B \log \Omega_N(E,V),$$

3. Gibbs equilibrium entropies:

$$S_{G,N} = -k_B \int_{\Lambda_N(V)} \mathrm{d}^N \mathrm{q} \mathrm{d}^N \mathrm{p}\, \rho_N \log \rho_N$$

One can prove that

$$S_{B,N}(E_N(\beta)) < S^c_{G,N}(\beta).$$

Which of the equilibrium Boltzmann entropy or the canonical Gibbs entropy $S^c_{G,N}(\beta)$ should be identified with Clausius entropy S_C?

Equilibrium Entropies in The Thermodynamic Limit

- We consider the thermodynamic limit

$$s(e) = \lim_{N\to\infty} \frac{k_B}{N} \log \Omega_N(Ne) = \lim_{N\to\infty} \frac{1}{N} S_N(Ne),$$

  and

$$f(\beta) = \lim_{N\to\infty} -\frac{1}{N} \frac{\log Z_N(\beta)}{\beta}.$$

- Then (using Laplace principle, or large deviation theory), we prove that the free energy is the Legendre–Fenchel transform of the entropy:

$$f(\beta) = \inf_e \{e - Ts(e)\}.$$

- Equilibrium Boltzmann and Gibbs entropies do coincide at the thermodynamic limit.
- Entropies and free energies, are up to constants, large deviation rate functions.

Clausius Entropy is not Equal to Equilibrium Ensemble Entropies

- For the Hamiltonian dynamics, starting from a non-equilibrium state, Gibbs entropy remains constant:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\Lambda_N(V)} \mathrm{d}^N\mathrm{q}\,\mathrm{d}^N\mathrm{p}\,\rho_N \log \rho_N\right) = 0.$$

- This is in contrast with the second law of thermodynamics that states that entropy should increase.
- Clausius entropy, can be identified in the thermodynamic limit, with Boltzmann macrostate entropy.
- One can explain, for instance using large deviation theory, that:

1. Boltzmann macrostate entropy does increase for most initial condition and can be identified with Clausius entropy.
2. It coincides with the equilibrium ensemble entropies at equilibrium and at the thermodynamic limit.

Boltzmann's macrostate entropy

- **Microstates:** $X = \left\{(\mathbf{r}_n, \mathbf{p}_n)_{1 \leq n \leq N}\right\}$

- **Macrostates:** M describes in a coarse-grained way the macroscopic state of a system. As an example, we divide the 6 dimensional $\mu-$space $\left\{\mathbf{r}, \mathbf{p}\right\}$ into K cells, where K is large but still $K \ll N$ and specify the number of particles in each cell.

- **Boltzmann's macrostate entropy:**

$$S_B(X) = S_B\left(M(X)\right) \text{ with}$$

$$S_B(M) = k_B \log |\Gamma_M| .$$

(Time's arrow and Boltzmann's entropy, **Joel L. Lebowitz,** 2008, Scholarpedia)

Boltzmann's macrostate entropy and times arrow

$$S_B(M) = k_B \log |\Gamma_M| .$$

- Boltzmann argued that due to the large differences in the sizes of Γ_M, $S_B(X_t)$ will **typically** increase in a way which explains and describes qualitatively the evolution towards equilibrium of macroscopic systems.

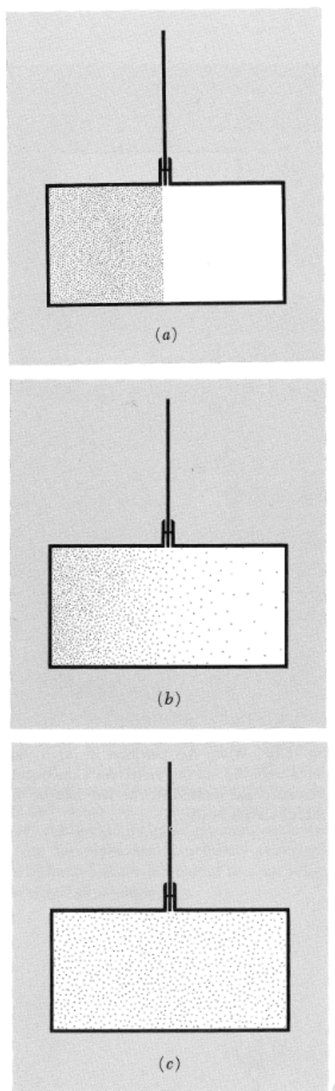
- **Maxwell:** «the second law is drawn from our experience of bodies consisting of an immense number of molecules. ... it is continually being violated, ..., in any sufficiently small group of molecules ... . As the number ... is increased ... the probability of a measurable variation ... may be regarded as practically an impossibility. »

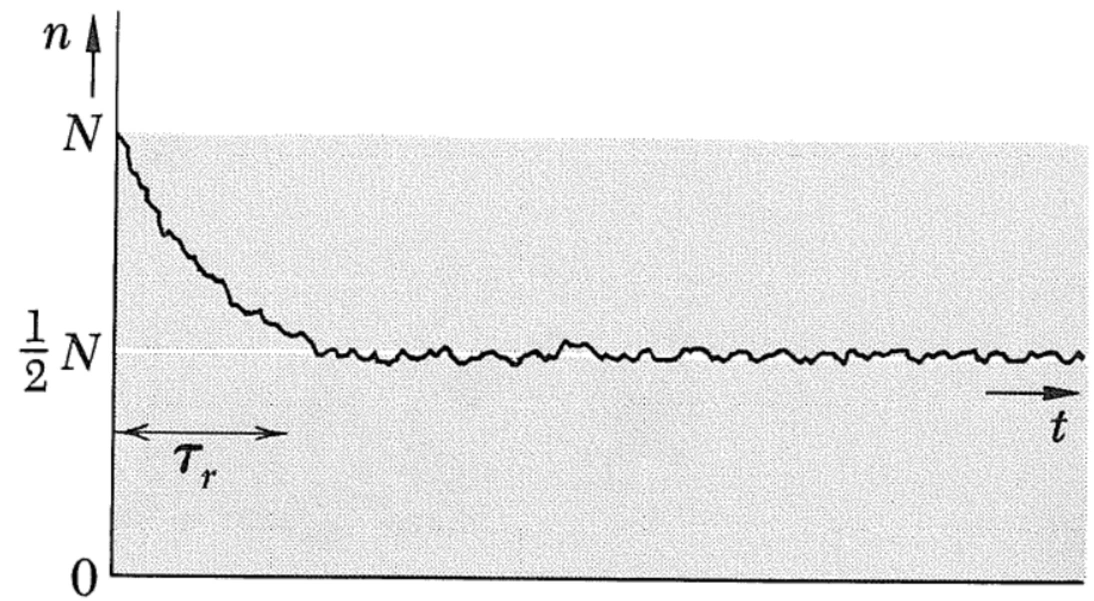
- **Gibbs (quoted by Boltzmann):** « In other words, the impossibility of an uncompensated decrease of entropy seems to be reduced to an improbability. »

- In the limit of a large number of degrees of freedom, Clausius' entropy for a macroscopic description of a physical system can be identified with Boltzmann's macrostate entropy.

(Time's arrow and Boltzmann's entropy, **Joel L. Lebowitz,** 2008, Scholarpedia)

What about entropy and dynamics beyond typical relaxation?





(Figures: Reif)

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

What about entropy and dynamics beyond typical relaxation?

- Boltzmann's macrostate entropy is directly related to the probability in phase space, independently of dynamics.

- **Entropy has also a dynamical meaning.** For instance in stochastic thermodynamics, entropy variation appears as the ratio of the probability of forward paths to the probability of backward paths.

- **For systems in detailed balance, or generalized detailed balance:**

$$\frac{\mathbb{P}\left(\{X(t)\}_{\{t_i \le t \le t_f\}}\right)}{\mathbb{P}\left(\left\{\bar{X}_R(t)\right\}_{\{t_i \le t \le t_f\}}\right)} = \exp\left(\frac{\Delta S}{k_B}\right)$$

- For kinetic theories can we get path probabilities and the dynamical meaning go entropy?

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:

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

- What is ε? Can we compute H?
- 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.

Example: macroscopic fluctuation theory, sometimes derived from microscopic Markov dynamics.

Can we derive path large deviations for classical kinetic theories ?

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

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

- 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

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

- C. Leonard, 1995. F. Rezakhanlou, 1998: stochastic model 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 $\mathscr{O}\left(e^{-N}\right)$.

Path large deviations for kinetic theories

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

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

- What is ε? Can we compute H?
- 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, Annales Henry Poincaré.

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III) Path large deviations for kinetic theories: the example of particles with long range interactions

2. Macroscopic reversibility for the empirical measure through path large deviations: Revisiting the irreversibility paradox
   - Properties and symmetries for path large deviations
   - Time reversal symmetry of path large deviations
   - The irreversibility paradox
3. Path large deviations for particles with long-range interactions (Landau and Balescu–Lenard–Guernsey equation)
   - Particles with long range interactions, the Vlasov, the Landau and the Balescu–Lenard–Guernsey equations
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   - Hamiltonian for the Balescu–Lenard–Guernsey equation

Which Properties Must we Expect for Large Deviations for Kinetic Theories?

- We expect a large deviation principle for the empirical distribution dynamics

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

- What are the expected properties of H? From thermodynamics and statistical physics?
- First the kinetic equation has to be the most probable evolution. This is a law of large numbers.

$$\frac{\partial f}{\partial t}=\frac{\delta H}{\delta p}[f,p=0]=\mathrm{Kinetic}[f]$$

Conserved Quantities

- If C is equal to either the mass

$$M = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, f,$$

or the momentum

$$\mathbf{P} = \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \mathbf{v} f,$$

or the kinetic energy

$$E = \frac{1}{2}\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \mathbf{v}^2 f,$$

H should have the symmetries related to the conservation law:

$$\text{for any } f \text{ and } p,\ \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{v}\, \frac{\delta H}{\delta p(\mathbf{v})}[f,p]\frac{\delta C}{\delta f(\mathbf{v})} = 0.$$

The Quasipotential has to be the Entropy Constrained by the Conserved Quantities

- Quasipotential definition:

$$P_{s,\varepsilon}[f] \equiv \mathbb{E}[\delta(f_\varepsilon - f)] \underset{\varepsilon \downarrow 0}{\asymp} \exp\left(-\frac{U[f]}{\varepsilon}\right),$$

- We expect from equilibrium statistical that

$$U[f] = \begin{cases} -S[f] \text{ if } M[f] = 1, \ \mathbf{P}[f] = 0, \text{ and } E[f] = E_0 \\ -\infty \text{ otherwise.} \end{cases}$$

- This is true up to additive and/or multiplicative constants.

Large Deviation Structure, Lyapunov Functionals and Entropy

As a consequence of the large deviation structure, we can immediately conclude that

1. the entropy increases along the relaxation paths (solution of the kinetic equation),
2. the entropy decreases along the fluctuation paths.

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Definition of Detailed Balance for Stochastic Processes

- We consider a time homogeneous stationary stochastic process $\{X(t)\}_{0\leq t<\infty}$ (for instance a continuous time Markov process).
- P_S is the stationary probability distribution function, and P is the two point transition probability distribution function

$$P_S(x) = \mathbb{E}\left[\delta\left(x - X(t)\right)\right] \text{ and } P\left(y,T;x,0\right) = \mathbb{E}_x\left[\delta\left(y - X(T)\right)\right].$$

- The definition of time reversibility for this process is

$$\text{for any } (x,y,T),\; P\left(y,T;x,0\right)P_S(x) = P\left(x,T;y,0\right)P_S(y).$$

  This is called the detailed balance condition.
- If the N-particle dynamics is time-reversible (for instance Hamiltonian), we expect the stochastic process of the empirical distribution to be time reversible. How does this translate at the level of the path large deviations?

Detailed Balance Condition for Large Deviations

- **Detailed balance condition** for path large deviations:

$$\text{for any x and } \dot{x},\; L(x,\dot{x}) - L(x,-\dot{x}) = \dot{x}.\nabla U,$$

  or equivalently

$$\text{for any x and p, } H(x,-p) = H(x,p+\nabla U).$$

- I is the time-reversal symmetry involution. We assume that I is self adjoint for the scalar product $I(x).p = I(p).x$. ***Generalized detailed balance*** condition: if $U(x) = U(I[x])$ and

$$L(x,\dot{x}) - L(x,-I[\dot{x}]) = I[\dot{x}].\nabla U$$

  or equivalently

$$H(I[x],-I[p]) = H(x,p+\nabla U).$$

- All the large deviation Hamiltonians for kinetic theories verify this large deviation detailed balance condition.

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Dynamical Large Deviations and the Irreversibility Paradox of Kinetic Theories

- We expect a large deviation action which is time-reversal symmetric with respect to the entropy.
- The time reversal symmetry is not broken neither by the mesoscopic description nor by the Stosszahlansatz!
- However the most-probable evolution (or the average, due to the law of large number) is irreversible. It increase entropy.
- Fluctuation paths are time reversed relaxation paths **(non-linear Onsager relations)**.
- The picture is clear and simple. There is no more any paradox. Any path is possible. The probability of any path is quantified.

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Particles with Mean–Field Interactions

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

- 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 $g_N\left(\mathbf{r},\mathbf{v},t\right) = \frac{1}{N}\sum_{n=1}^{N} \delta\left(\mathbf{r}-\mathbf{r}_n(t);\mathbf{v}-\mathbf{v}_n(t)\right)$ formally solves the Klimontovich equation

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

- 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.

The Vlasov Equation

- We suppose an ensemble of initial conditions $\{g_N\}$ where each g_N is close to g_0.
- Law of large numbers: "for almost all initial conditions" $\lim_{N\to\infty} g_N = g$ where g solves the Vlasov equation

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

- This is actually a stability result for the Vlasov (Klimontovich) equation (Braun and Hepp, 1977 for smooth interactions).
- This equation is Hamiltonian, conserves the energy and an infinite number of Casimir conserved quantities.
- It could still converge to the Boltzmann distribution in a weak sense, but it does not.

Stationary Solutions of the Vlasov Equation

- The Vlasov equation has an infinite number of stable stationary solutions, for instance homogenous solutions $g(\mathbf{r},\mathbf{v}) = f_0(\mathbf{v})$ such that for any $\mathbf{k}$ and $\omega \in \mathbf{R}$, $\varepsilon(\mathbf{k},\omega) > 0$ with

$$\varepsilon[f_0](\mathbf{k},\omega) = 1 - \hat{W}(k)\int \mathrm{d}\mathbf{v}\,\frac{\mathbf{k}.\frac{\partial f_0}{\partial \mathbf{v}}(\mathbf{v})}{\mathbf{k}.\mathbf{v} - \omega - \mathbf{i}0^{+}}$$

- ε is called the dielectric susceptibility and plays the role of a dispersion relation for the linearized dynamics.
- $\hat{W}$ is the Fourier transform of W.
- Those stable homogeneous distributions $f_0(\mathbf{v})$ play the role of attractors for the Vlasov equation.

Stationary Solutions of the Vlasov Equation

- The Vlasov equation has an infinite number of stable stationary solutions: homogeneous distributions $f_0(\mathbf{v})$.
- Those stable homogeneous distributions $f_0(\mathbf{v})$ play the role of attractors for the Vlasov equation.
- What will happen for the N particle dynamics if we start from an ensemble of initial conditions $\{f_N\}$ which is close to a homogeneous stable $f_0(\mathbf{v})$?
- The distribution are stable on the Vlasov time scale (of order 1), however an evolution will occur on a time scale of order $\tau = N$. This evolution is governed by the Balescu–Guernsey–Lenard equation.

The Balescu–Guernsey–Lenard Equation

- We suppose an ensemble of initial conditions $\{g_N\}$ where each g_N is close to a stable homogeneous $f_0(\mathbf{v})$.
- Law of large numbers: after time rescaling $t = N\tau$, "for almost all initial conditions", $\lim_{N\to\infty} g_N = f$, where f solves the Balescu–Lenard–Guernsey equation

$$\frac{\partial f}{\partial \tau} = LB[f] \text{ with } LB[f] = \frac{\partial}{\partial \mathbf{v}}.\int d\mathbf{v}_2 \overleftrightarrow{B}[f](\mathbf{v},\mathbf{v}_2)\left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}}\right)$$

with

$$\overleftrightarrow{B}[f](\mathbf{v}_1,\mathbf{v}_2) = \frac{\pi}{L^3}\int_{-\infty}^{+\infty} d\omega \sum_{\mathbf{k}} \delta(\omega - \mathbf{k}.\mathbf{v}_1)\,\delta(\omega - \mathbf{k}.\mathbf{v}_2)\,\frac{\mathbf{k}\mathbf{k}\hat{W}(\mathbf{k})^2}{|\varepsilon[f](\omega,\mathbf{k})|}.$$

- First derived by R.L. Guernsey (1960). (or Bogolyubov?)
- For smooth enough W, there is an exact derivation of the Balescu-Guernsey-Lenard equation in the sense of theoretical physicists (see Lifshitz–Pitaevskii's book on kinetic theory, or Nicholson's book on plasma).

The Landau Equation

- The Landau equation is an approximation the Balescu–Guernsey–Lenard equation neglecting collective effects, or equivalently assuming $\varepsilon(\mathbf{k},\omega) = 1$.
- Landau equation:

$$\frac{\partial f}{\partial \tau} = \frac{\partial}{\partial \mathbf{v}} \cdot \int d\mathbf{v}_2 \overleftrightarrow{B}(\mathbf{v},\mathbf{v}_2)\left(-\frac{\partial f}{\partial \mathbf{v}_2} f(\mathbf{v}) + f(\mathbf{v}_2)\frac{\partial f}{\partial \mathbf{v}}\right),$$

where $\overleftrightarrow{B}$ does not depend on f:

$$\overleftrightarrow{B}(\mathbf{v}_1,\mathbf{v}_2) = \frac{\pi}{L^3}\int_{-\infty}^{+\infty} d\omega \sum_{\mathbf{k}} \delta(\omega - \mathbf{k}.\mathbf{v}_1)\,\delta(\omega - \mathbf{k}.\mathbf{v}_2)\,\frac{\mathbf{k}\mathbf{k}\hat{W}(\mathbf{k})^2}{|\varepsilon[f](\omega,\mathbf{k})|} = \frac{1}{2}\int d\mathbf{q}\, w(\mathbf{v}_1,\mathbf{v}_2;\mathbf{q})\mathbf{q}\otimes\mathbf{q},$$

see Lifshitz–Pitaevskii's book on kinetic theory, or Nicholson's book on plasma.

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

- We decompose

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

with the projection over homogeneous distributions:

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

- The dynamics (Klimontovich equation) then reads

$$\frac{\partial f_N}{\partial t} = \frac{1}{NL^3}\int \mathrm{d}\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right) \text{ and}$$

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

Derivation of the BGL eq. 2: Quasilinear approximation

$$\frac{\partial f_N}{\partial t} = \frac{1}{NL^3}\int d\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right) \text{ and}$$

$$\frac{\partial \delta g_N}{\partial t} = -\mathbf{v}.\frac{\partial \delta g_N}{\partial \mathbf{r}} + \frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial f_N}{\partial \mathbf{v}} + \frac{1}{\sqrt{N}}\left[\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}} - \frac{1}{L^3}\int d\mathbf{r}\left(\frac{\partial V[\delta g_N]}{\partial \mathbf{r}}.\frac{\partial \delta g_N}{\partial \mathbf{v}}\right)\right].$$

- Neglecting the non-linear terms in the second equation and rescaling time $\tau = t/N$, gives the quasilinear approximation

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

- Solving this set of equations with the Bogoliubov hypothesis (averaging a slow/fast set of equation) gives the Balescu–Guernsey–Lenard equation.

Beyond the Law of Large Numbers: The Large Deviation Action.

- We expect a large deviation principle for the empirical distribution dynamics

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

- Why is N the large deviation parameter?
- Expected properties of H? First the Lenard–Balescu equation should be the most probable evolution

$$\frac{\partial f}{\partial \tau} = LB[f] = \frac{\delta H}{\delta p}\left[f, p = 0\right].$$

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).

3. Path large deviations for particles with long-range interactions (Landau and Balescu–Lenard–Guernsey equation)
   - Particles with long range interactions, the Vlasov, 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

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.

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

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

(see F. Bouchet, R. Tribe, and **O. Zaboronski** - Physical Review E, 2023)

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

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

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

(see F. Bouchet, R. Tribe, and **O. Zaboronski** - Physical Review E, 2023)

3. Path large deviations for particles with long-range interactions (Landau and Balescu–Lenard–Guernsey equation)
   - Particles with long range interactions, the Vlasov, the Landau and the Balescu–Lenard–Guernsey equations
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   - Hamiltonian for the Balescu–Lenard–Guernsey equation

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

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

with

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

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.

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

- 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, Annales Henry Poincaré.