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Entropy Methods for the Boltzmann Equation

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Foreword

One of the major contributions of Ludwig Boltzmann to science has been the connection between time irreversibility and the increase of entropy as a well-defined quantity associated to the macroscopic state of a system. His ideas are at the basis of most studies in non-equilibrium statistical mechanics, and many non-equilibrium processes are still now physically understood in terms of their *entropy production*.

More recently entropy and entropy production have become mathematical tools used in the context of kinetic and hydrodynamic limits, when deriving the macroscopic behavior of systems from the interaction dynamics of their (many) microscopic elementary constituents at the atomic or molecular level.

In this volume, we have put together two surveys on some recent results in this direction. The first text, by Cedric Villani, illustrates the use of entropy in the analysis of convergence to equilibrium for solutions of the Boltzmann equation. The second text, by Fraydoun Rezakhanlou, discusses the Boltzmann–Grad limit, in which the Boltzmann equation is derived from the dynamics of a large number of hard spheres. Both entropy and entropy production play a major role in these problems.

To illustrate the relevance of entropy in both the kinetic theory of gases and the dynamics of a large number N of hard spheres, we shall recall below two fairly classical, and yet fundamental properties of Boltzmann’s entropy.

The first property, which is a particular case of the Gibbs principle, is a variational characterization of Maxwellian equilibrium distributions in the kinetic theory of gases. Call $f \equiv f(x, v)$ the single-particle phase space density of molecules that are located at the position x with velocity v . (Here, both x and v run through the Euclidian space \mathbf{R}^3 for simplicity.) The following mechanical observables are easily defined in terms of the density f (and the mass m of each molecule):

$$\begin{aligned}
\iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(x, v) dx dv &= \text{number of molecules}, \\
\iint_{\mathbf{R}^3 \times \mathbf{R}^3} mv f(x, v) dx dv &= \text{total momentum}, \\
\iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{1}{2} m |v|^2 f(x, v) dx dv &= \text{total energy}.
\end{aligned}$$

Boltzmann's notion of entropy defined in terms of the density f is $-H(f)$, where the functional $H(f)$ is defined as

$$H(f) = \iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(x, v) \ln f(x, v) dx dv.$$

Consider the following minimization problem:

$$\inf H(f) \text{ with constraints } \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \begin{pmatrix} 1 \\ mv \\ \frac{1}{2} m |v|^2 \end{pmatrix} f(x, v) dx dv = \begin{pmatrix} N \\ P \\ E \end{pmatrix},$$

where $N, E \geq 0$ and $P \in \mathbf{R}^3$ are given.

There are obvious compatibility conditions to be verified by N, P, E for the set of functions f satisfying the constraints to be non-empty: for instance, by the Cauchy-Schwartz inequality, one should have

$$|P|^2 \leq 2mNE.$$

Forgetting momentarily the obvious constraint $f \geq 0$, we write the Euler equation for this minimization problem as

$$\begin{aligned}
DH(f) \cdot \delta f &= \iint_{\mathbf{R}^3 \times \mathbf{R}^3} (\ln f(x, v) + 1) \delta f(x, v) dx dv \\
&= a \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \delta f(x, v) dx dv \\
&\quad + b \iint_{\mathbf{R}^3 \times \mathbf{R}^3} mv \delta f(x, v) dx dv \\
&\quad + c \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \frac{1}{2} m |v|^2 \delta f(x, v) dx dv,
\end{aligned}$$

where $a, c \in \mathbf{R}$ and $b \in \mathbf{R}^3$ are the Lagrange multipliers associated to the constraints of total number of molecules, total energy and total momentum. Since this equality must hold for each smooth, compactly supported δf , it follows that:

$$\ln f(x, v) + 1 = a + b \cdot (mv) + c \frac{1}{2} m |v|^2,$$

or, in other words,

$$f(x, v) = e^{(a-1)+b \cdot (mv)+c \frac{1}{2} m |v|^2}.$$

Notice that the minimizing function f so defined is positive: we therefore verify a posteriori that there was no need for any Lagrange multiplier associated with the constraint $f \geq 0$ a.e..

This expression can be put in the more familiar form of a Maxwellian density

$$f(x, v) = \frac{N}{(2\pi k\theta)^{3/2}} e^{-m|v-u|^2/2k\theta}$$

by putting

$$a = 1 + \ln N - \frac{3}{2} \ln(2k\theta) - \frac{m|u|^2}{2k\theta}, \quad b = \frac{1}{k\theta} u, \quad c = -\frac{1}{k\theta},$$

where k is the Boltzmann constant. The bulk velocity u and temperature θ are related to the total momentum P and the total energy E by the formulas

$$P = Nmu \quad \text{and} \quad E = N\left(\frac{1}{2}m|u|^2 + \frac{3}{2}k\theta\right).$$

This computation shows that Maxwellian distributions are the critical points of the Boltzmann entropy on the affine manifold of densities f corresponding to a prescribed total number of molecules, total momentum and total energy.

By the strict convexity of the map $f \mapsto f \ln f$, one easily concludes that this critical point is in fact a global minimum of H .

To summarize: Maxwellian distributions maximize the Boltzmann entropy under the constraints of a fixed total number of molecules, total momentum and total energy.

Besides, the strict convexity of H implies that the relative entropy

$$H(f) - \inf H$$

defines some kind of distance from f to the set of Maxwellian distributions.

The second property of the entropy which we want to discuss is a variational characterization of chaotic densities. Let $F \equiv F(z_1, \dots, z_N)$ be the N -body phase space probability density of a system of particles. Here, $z_i = (x_i, v_i)$ consists of the position x_i and velocity v_i of the i th particle; obviously z_i runs through $\mathbf{R}^3 \times \mathbf{R}^3$. We denote $Z_N = (z_1, \dots, z_N)$ and $\hat{Z}_N^i = (z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_N)$. To the density F is associated the family of its marginals

$$F_i(z_i) = \int_{(\mathbf{R}^3 \times \mathbf{R}^3)^{N-1}} F(Z_N) d\hat{Z}_N^i, \quad i = 1, \dots, N.$$

Consider the following minimization problem: to find

$$\inf H(F) \text{ under the constraints } F_i = f$$

where f is a given a.e. non-negative function in $L^1(\mathbf{R}^3 \times \mathbf{R}^3)$. Since

$$F \geq 0 \text{ a.e. and } \int_{(\mathbf{R}^3 \times \mathbf{R}^3)^N} F(Z_N) dZ_N = 1,$$

the function f should satisfy

$$f \geq 0 \text{ a.e. and } \int_{\mathbf{R}^3 \times \mathbf{R}^3} f(z) dz = 1$$

in order for the set of constraints to define a non-empty set of probability densities F .

Neglecting again the obvious constraint $F \geq 0$ a.e., we write the Euler equation for the minimization problem above as

$$\begin{aligned} \text{DH}(F) \cdot \delta F &= \int_{(\mathbf{R}^3 \times \mathbf{R}^3)^N} (\ln F(Z_N) + 1) \delta F(Z_N) dZ_N \\ &= \sum_{1 \leq i \leq N} \int_{(\mathbf{R}^3 \times \mathbf{R}^3)^N} a_i(z_i) \delta F(Z_N) dZ_N. \end{aligned}$$

Since this equality must be satisfied by each smooth, compactly supported δF , one must have

$$\ln F(Z_N) + 1 = \sum_{1 \leq i \leq N} a_i(z_i)$$

i.e.

$$F(z_1, \dots, z_N) = \exp \left(\sum_{i=1}^N a(z_i) - 1 \right).$$

In other words, F is of the form

$$F(z_1, \dots, z_N) = \prod_{i=1}^N \phi_i(z_i), \quad \text{with } \phi_i = \exp(a_i - \frac{1}{N}).$$

Writing

$$F(z_1, \dots, z_N) = \prod_{i=1}^N \int_{\mathbf{R}^3 \times \mathbf{R}^3} \phi_i(z) dz \prod_{i=1}^N \psi_i(z_i)$$

with

$$\psi_i = \frac{\phi_i}{\int_{\mathbf{R}^3 \times \mathbf{R}^3} \phi_i(z) dz},$$

we see that, on account of the normalization condition on F , one has

$$\prod_{i=1}^N \int_{\mathbf{R}^3 \times \mathbf{R}^3} \phi_i(z) dz = 1$$

and

$$\psi_i = f \text{ for each } i = 1, \dots, N.$$

In other words, the only critical point F for this minimization problem is the chaotic density

$$F(z_1, \dots, z_N) = \prod_{i=1}^N f(z_i).$$

Hence, chaotic densities are the only critical points of the Boltzmann entropy on the affine manifold of probability densities with all their marginals equal to a given probability density f .

By using again the strict convexity of the functional H , we see that this critical point is in fact the minimum point.

Therefore, chaotic densities maximize the Boltzmann entropy among all probability densities with all their marginals equal to a given probability density f .

Again, the strict convexity of H implies that the relative entropy

$$H(F) - \inf H$$

measures the distance from F to the set of chaotic distributions.

The two properties of the entropy described above pertain to the two topics addressed in this volume.

Indeed, the first text, by Cédric Villani, concerns the use of the entropy and entropy production as a tool in order to estimate the speed of convergence to a (uniform) Maxwellian equilibrium density. As was explained above, the relative entropy measures the *distance* of a non-equilibrium state to equilibrium; entropy production is another way to measure that distance. Finding how these two measures of the distance to equilibrium are related is one of the major arguments in estimating the speed of approach to equilibrium in the kinetic theory of gases.

In spatially inhomogeneous non-equilibrium states it is then useful to work with *local entropy* and *local entropy production*. Cédric Villani carefully explains the mathematical difficulties arising in this problem: the system can be locally close to equilibrium, and have small total entropy production, while still being far from the set of *global* equilibria.

In Villani's own words, "local equilibrium states are your worst enemies" if you want to prove (and estimate) convergence to global equilibrium. In order to obtain this global convergence, the system should locally move out of the "local equilibrium" and Cédric Villani discusses various tools and conjectures on this mostly open problem.

This convergence problem is another aspect that shows the inadequacy of the notion of local equilibrium in order to understand non-equilibrium phenomena. Also transport in stationary non-equilibrium states (like the heat conductivity when the system is under a gradient of temperature imposed by external thermostats) cannot be explained in terms of local equilibrium states. Such local equilibrium states can only be a zeroth-order approximation of the real non-equilibrium state, and only further order approximations can explain transport and convergence to equilibrium.

The Boltzmann–Grad limit is the process by which the Boltzmann equation, which governs the evolution of the single-particle phase space density of the molecules of a monatomic gas, is derived from the N -body molecular dynamics. Hence, this limit necessarily involves the approximation of the N -body phase space density by chaotic densities whose single-body marginal is a solution of the Boltzmann equation. Therefore, the second property of entropy recalled above obviously plays a role in this limit.

The text by Fraydoun Rezakhanlou discusses various aspects of the Boltzmann–Grad limit. This is a classical open problem in mathematical physics, where little progress has been made since the seminal work of Lanford in 1975 (extended by Illner and Pulvirenti in 1986).

Rezakhanlou recalls the main conjecture, that can be formulated as a law of large numbers in a non-equilibrium situation, and also formulates the corresponding conjectures about small and large fluctuations about this limit. Then he propose a stochastic version of the hard sphere dynamics. Stochasticity helps in proving molecular chaos (the *Stosszahlansatz*) which is the key argument in all derivations of this type of limits.

We hope that these surveys, addressing two very different issues in the statistical mechanics of non-equilibrium processes with similar methods based on the concept of entropy as defined by Boltzmann, will convince the reader of the versatility of that notion.

We conclude this brief overview with a few words about the origin of these texts. In the fall term of 2001, we organized a four-month session supported by the Centre Émile Borel on “Hydrodynamic Limits” at the Institut Henri Poincaré in Paris. Various events were proposed in this period, including an international congress focussed on the state of the art as well as open problems and perspectives in the subject of hydrodynamic limits. This congress was dedicated to Claude Bardos in recognition of his fundamental contributions to this subject. In addition, several research courses were given during that period, among these the courses by Cedric Villani and Fraydoun Rezakhanlou whose notes are gathered together in this volume.

We express our deepest gratitude to both directors of Institut Henri Poincaré, Profs. Michel Broué and Alain Comtet, for the warm hospitality so generously offered to all participants in this session.

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Finally, the tragic events of September 11 2001 regreably struck the family of one of our guests; we are especially grateful to Mrs Annie Touchant and Mrs. Sylvie Lhermitte of the Centre Emile Borel for their kind assistance and support in these sad circumstances.

Paris, December 2006

François Golse
Stefano Olla

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