The Boltzmann equation and corresponding extremal problems

Lev Sakhnovich

99 Cove ave., Milford, CT, 06461, USA
E-mail: lsakhnovich@gmail.com

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Abstract

We start with some global Maxwellian function $M$, which is a stationary solution (with the constant total density $\rho$) of the Boltzmann equation, and we denote the number of the corresponding space variables by $n$. The notion of distance between the global Maxwellian function and an arbitrary solution $f$ (with the same total density $\rho$ at the fixed moment $t$) of the Boltzmann equation is introduced. In this way we essentially generalize the important Kullback-Leibler distance, which was used before. An extremal problem to find a solution of the Boltzmann equation, such that $\text{dist}\{M, f\}$ is minimal in the class of solutions with the fixed values of energy and of $n$ moments, is solved.

1 Introduction.

The well-known Boltzmann equation for the monoatomic gas has the form

$$\frac{\partial f}{\partial t} = -\zeta \cdot \nabla_x f + Q(f, f),$$

(1.1)
where \( t \in \mathbb{R} \) stands for time, \( x = (x_1, ..., x_n) \in \Omega \) stands for space coordinates, \( \zeta = (\zeta_1, ..., \zeta_n) \in \mathbb{R}^n \) is velocity, and \( \mathbb{R} \) denotes the real axis. The collision operator \( Q \) is defined by the relation
\[
Q(f, f) = \int_{\mathbb{R}^n} \int_{S^{n-1}} [f(\zeta')f(\zeta') - f(\zeta)f(\zeta') \cdot B(\zeta - \zeta', \sigma)] d\sigma d\zeta,
\]
where \( B(\zeta - \zeta', \sigma) \geq 0 \) is the collision kernel. Here we used the notation
\[
\zeta' = (\zeta_\star + \zeta)/2 + \sigma|\zeta - \zeta'|/2, \quad \zeta'\star = (\zeta_\star + \zeta)/2 - \sigma|\zeta - \zeta'|/2,
\]
where \( \sigma \in S^{n-1} \), that is, \( \sigma \in \mathbb{R}^n \) and \( |\sigma| = 1 \). The solution \( f(t, x, \zeta) \) of Boltzmann equation (1.1) is the distribution function of gas. We start with some global Maxwellian function \( M \), which is the stationary solution (with the total density \( \rho \)) of the Boltzmann equation. The notion of distance between the global Maxwellian function and an arbitrary solution \( f \) (with the same value \( \rho \) of the total density at the fixed moment \( t \)) of the Boltzmann equation is introduced. In this way we essentially generalize the Kullback-Leibler distance \[4\], which was fruitfully used before (see further references in the recent papers \[2, 9, 12\]). Our approach enables us to treat also the non-homogeneous case. An extremal problem to find a solution of the Boltzmann equation, such that \( \text{dist}\{M, f\} \) is minimal in the class of solutions with the fixed values of energy and of \( n \) moments, is solved.

Some necessary preliminary definitions and results are given in Section 2. An important functional, which attains maximum at the global Maxwellian function is introduced in Section 3. The distance between solutions and the corresponding extremal problem are studied in Section 4.

We use the notation \( C^1_0 \) to denote the class of differentiable functions \( f(\zeta) \), which tend to zero sufficiently rapidly when \( \zeta \) tends to infinity.

## 2 Preliminaries: main definitions and results

In this section we present some well-known notions and results connected with the Boltzmann equation. The distribution function \( f(t, x, \zeta) \) is non-negative:
\[
f(t, x, \zeta) \geq 0,
\]
and so the entropy
\[
S(t, f) = -\int_{\Omega} \int_{\mathbb{R}^n} f(t, x, \zeta) \log f(t, x, \zeta) d\zeta dx
\]

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is well-defined.

**Definition 2.1** A function $\phi(\zeta)$ is called a collision invariant if it satisfies the relation

$$
\int_{\mathbb{R}^n} \phi(\zeta) Q(f, f)(\zeta) d\zeta = 0 \quad \text{for all } f \in C^1_0.
$$

(2.3)

It is well-known (see [11]) that there are the following collision invariants:

$$
\phi_0(\zeta) = 1, \quad \phi_i(\zeta) = \zeta_i \quad (i = 1, 2, \ldots, n), \quad \phi_{n+1}(\zeta) = |\zeta|^2.
$$

(2.4)

The notions of density $\rho(t, x)$, total density $\rho(t)$, mean velocity $u(t, x)$, energy $E(t, x)$, and total energy $E(t)$ are introduced via formulas:

$$
\rho(t, x) = \int f(t, x, \zeta) d\zeta, \quad \rho(t) = \int_{\Omega} \rho(t, x) dx,
$$

(2.5)

$$
u(t, x) = (1/\rho(x, t)) \int \zeta f(t, x, \zeta) d\zeta,
$$

(2.6)

$$
E(t, x) = \int \frac{|\zeta|^2}{2} f(t, x, \zeta) d\zeta, \quad E(t) = \int_{\Omega} \int_{\mathbb{R}^n} \frac{|\zeta|^2}{2} f(t, x, \zeta) d\zeta dx.
$$

(2.7)

The function

$$
f = \left( \rho/(2\pi T)^{n/2} \right) \exp \left( -|\zeta - u|^2/(2T) \right).
$$

(2.8)

is called the global Maxwellian and is a function of the mass density $\rho > 0$, bulk velocity $u = (u_1, \ldots, u_n)$ and temperature $T$. We assume that the domain $\Omega$ is bounded and so its volume is bounded too:

$$
\text{Vol}(\Omega) = V_\Omega < \infty.
$$

(2.9)

Therefore, the function

$$
M(\zeta) = \left( \rho/(V_\Omega(2\pi T)^{n/2}) \right) \exp \left( -|\zeta - u|^2/(2T) \right)
$$

(2.10)

is a global Maxwellian with the constant total density $\rho$.

**Proposition 2.2** [11] The global Maxwellian function $M(\zeta)$ is the stationary solution of the Boltzmann equation (1.1).

Boltzmann proved in [1] the fundamental result below:

**Theorem 2.3** Let $f \in C^1_0$ be a non-negative solution of equation (1.1). Then the following inequality holds:

$$
\frac{dS}{dt} \geq 0.
$$

(2.11)
3 Extremal problem

Similar to the cases considered in [7,8], an important role is played by the functional

\[ F(f) = \lambda E + S, \quad \lambda = -1/T, \]  

where \( S \) and \( E \), respectively, are defined by formulas (2.2) and (2.7). The parameters \( \lambda = -1/T \) and \( \rho \) are fixed. Now, we use the calculus of variations (see [3]) and find the function \( f_{\text{max}} \) which maximizes the functional (3.1) on the class of functions with the same \( \rho(t) = \rho \) at the fixed moment \( t \). The corresponding Euler's equation takes the form

\[ \frac{\delta}{\delta f} \left[ \frac{\lambda |\zeta|^2}{2} f - f \log f + \mu f \right] = 0. \]  

(3.2)

Here \( \frac{\delta}{\delta f} \) stands for the functional derivative. Our extremal problem is conditional and \( \mu \) is the Lagrange multiplier. Hence, we have

\[ \lambda \frac{|\zeta|^2}{2} - 1 - \log f + \mu = 0. \]  

(3.3)

From the last relation we obtain

\[ f = C e^{-|\zeta|^2/(2T)}. \]  

(3.4)

Formulas (2.10) and (3.4) imply that

\[ f = M(\zeta) = \frac{\rho}{V_\Omega (2\pi T)^{n/2}} e^{-|\zeta|^2/2T}. \]  

(3.5)

We have the inequality

\[ \frac{\delta^2}{\delta f^2} F = -1/f < 0. \]  

(3.6)

**Corollary 3.1** The global Maxwellian function \( M(\zeta) \), which is defined by formula (3.4), gives the maximum of the functional \( F \) on the class of functions with the same value \( \rho \) of the total density \( \rho(t) \) at the fixed moment \( t \).
In view of (2.2), (2.7), and (3.1) we see that

$$\left(F(f)\right)(t) = -\int_{\Omega} \int_{\mathbb{R}^n} \left(\frac{|\zeta|^2}{2T} + \log f(t, x, \zeta)\right) f(t, x, \zeta) d\zeta dx.$$  \hspace{1cm} (3.7)

It follows from (2.5), (3.5), and (3.7) that

$$F(M) = -\rho \log \left(\frac{\rho}{V_{\Omega}(2\pi T)^{n/2}}\right).$$  \hspace{1cm} (3.8)

Therefore, Corollary 3.1 can also be proved without using the calculus of variation (see [10]). Indeed, taking into account relations (3.5), (3.7), and (3.8) and the fact that the total densities of $M$ and $f$ are equal, we have

$$F(M) - F(f) = \int_{\Omega} \int_{\mathbb{R}^n} M \left(1 - \frac{f}{M} + \frac{f}{M} \log \frac{f}{M}\right) d\zeta dx.$$  \hspace{1cm} (3.9)

Using inequality $1 - x + x \log x > 0$ for $x > 0, x \neq 1$, we derive from (3.9) that

$$F(M) - F(f) > 0 \quad (f \neq M).$$  \hspace{1cm} (3.10)

**Remark 3.2** Since the extremal problem is conditional, the connection between the energy and entropy can be interpreted in terms of game theory. The functional (3.1) defines this game. The global Maxwellian function $M(\zeta)$ is the solution of it. A game interpretation of quantum and classical mechanics problems is given in the papers [7, 8].

### 4 Distance

Let $f(t, x, \zeta)$ be a nonnegative solution of the Boltzmann equation (1.1). We assume that $T$ and the value $\rho = \rho(t)$ at some moment $t$ are fixed. According to (3.10) we have

$$F(M) - F(f) \geq 0,$$  \hspace{1cm} (4.1)

where the global Maxwellian function $M(\zeta)$ is defined in (3.5). The equality in (4.1) holds if and only if $f(t, x, \zeta) = M(\zeta)$. Hence, we can introduce the following definition of distance between the solution $f(t, x, \zeta)$ and the global Maxwellian function $M(\zeta)$:

$$\text{dist}\{M, f\} = F(M) - F(f).$$  \hspace{1cm} (4.2)
Remark 4.1 In the spatially homogeneous case, if not only the total densities $\rho_M$ and $\rho_f$ of $M$ and $f$ are equal, but the energies $E_M$ and $E_f$ are equal too, then our definition (4.2) of distance coincides with the Kullback-Leibler distance (see [12]). However, our approach enables us to treat also the non-homogeneous case.

Next, we study the case $E_M \neq E_f$ and start with an example.

Example 4.2 Let $T_1 \neq T$ and consider the global Maxwellian function

$$M_1(\zeta) = \frac{\rho}{V\Omega(2\pi T_1)^{n/2}} \exp \left( -\frac{|\zeta|^2}{2T_1}\right).$$

(4.3)

Direct calculation shows that

$$E_1 = E_{M_1} = \rho n T_1/2 \neq E, \quad (4.4)$$

$$F(M_1) = -\rho \left( \log \left( \frac{\rho}{V\Omega(2\pi T_1)^{n/2}} \right) - n(1 - T_1/T)/2 \right). \quad (4.5)$$

It follows from (3.8) and (4.5) that

$$\text{dist}\{M, M_1\} = -\rho n \left( \log(T_1/T) - T_1/T + 1 \right)/2. \quad (4.6)$$

We introduce the class $C(\rho, E_1, U)$ of non-negative functions $f(t, x, \zeta)$ with the given total density $\rho$ (see (2.8)), total energy

$$\int_{\Omega} \int_{\mathbb{R}^n} \frac{|\zeta|^2}{2} f(t, x, \zeta) d\zeta dx = E_1, \quad (4.7)$$

and total moments $U = (U_1, U_2, ..., U_n)$, where

$$U_k = \int_{\Omega} \int_{\mathbb{R}^n} \zeta_k f(t, x, \zeta) d\zeta dx. \quad (4.8)$$

Recall that the global Maxwellian function $M$ is defined by (3.3).

**Extremal problem.** Find a function $f$, which minimizes the functional $\text{dist}\{M, f\}$ on the class $C(\rho, E_1, U)$.

The corresponding Euler’s equation takes the form

$$\frac{\delta}{\delta f} \left[ (\lambda + \nu) \frac{|\zeta|^2}{2} f - f \log f + \mu f + f \sum_k \gamma_k \zeta_k \right] = 0. \quad (4.9)$$
Recall that our extremal problem is conditional, and \( \mu, \nu, \gamma_k \) are the Lagrange multipliers. Hence, we have

\[
(\lambda + \nu)\frac{|\zeta|^2}{2} - \log f - 1 + \mu + \sum_k \gamma_k \zeta_k = 0. \tag{4.10}
\]

From the last relation we obtain

\[
f = C \exp \left( (\lambda + \nu)\frac{|\zeta|^2}{2} + \sum_k \gamma_k \zeta_k \right). \tag{4.11}
\]

According to (2.5) we have \( \lambda + \nu < 0 \). Now, we rewrite (4.11) as

\[
f = C_1 \left( -\frac{2\pi}{\lambda + \nu} \right)^{-n/2} \exp \left( \frac{\lambda + \nu}{2} \sum_k \left( \zeta_k + \frac{\gamma_k}{\lambda + \nu} \right)^2 \right), \tag{4.12}
\]

where

\[
C_1 = C \frac{\pi^{n/2}}{\left( -\frac{\lambda + \nu}{2} \right)^{n/2}} \exp \left( -\frac{\sum_k \gamma_k^2}{2(\lambda + \nu)} \right). \tag{4.13}
\]

To calculate the parameters \( \mu, \nu, \gamma_k \) we use again the well-known formulas

\[
\int_{-\infty}^{\infty} e^{-a\xi^2} d\xi = \sqrt{\pi/a}, \quad \int_{-\infty}^{\infty} \xi^2 e^{-a\xi^2} d\xi = \frac{1}{2a} \sqrt{\pi/a}, \quad a > 0. \tag{4.14}
\]

Formulas (2.5), (4.7), (4.8), (4.12), and (4.14) imply that

\[
C_1 = \rho/V_\Omega, \quad \gamma_k/(\lambda + \nu) = -U_k/\rho, \quad -(\lambda + \nu) = T_1^{-1}, \tag{4.15}
\]

where

\[
T_1 = \frac{2}{n\rho} E_1 - \frac{1}{n\rho^2} \sum_k U_k^2. \tag{4.16}
\]

Because of (4.12) and (4.15) we see that \( f \) is just another global Maxwellian function

\[
f = M_1(\zeta) = \frac{\rho}{V_\Omega(2\pi T_1)^{n/2}} \exp \left( -\frac{|\zeta - U/\rho|^2}{2T_1} \right). \tag{4.17}
\]

Moreover, the inequality

\[
\frac{\delta^2}{\delta f^2} \left[ \text{dist}\{M, f\} \right] = 1/f \tag{4.18}
\]

holds, that is, the functional dist\{M, f\} attains its minimum on the function \( f = M_1 \), which satisfies conditions \( \rho(t) = \rho \), (4.7), and (4.8). The following assertion is true.
Proposition 4.3  Let $M$ and $M_1$, respectively, be defined by (3.5) and (4.17). If the function $f$ satisfies conditions $\rho(t) = \rho$, (4.7), (4.8), and $f \neq M_1$, then

$$\text{dist}\{M, f\} > -\frac{n\rho}{2} (\log(T_1/T) - T_1/T + 1) + \frac{|U|^2}{2\rho T_1}.$$ 

References

[1] Boltzmann L., *Lectures on Gas Theory*, Courier Dover Publications, 1995.

[2] Haba Z., *Non-linear relativistic diffusions* Physica A: Statistical Mechanics and its Applications, doi:10.1016/j.physa.2011.03.025

[3] Hahn W., *Theory and Application of Liapunov’s Direct Method*, Englewood Cliffs, NJ: Prentice-Hall, 1963.

[4] Kullback S., Leibler R.A., *On information and sufficiency*, Ann. Math. Stat. 22, 79-86, 1951.

[5] Sakhnovich L.A., *Comparing Quantum and Classical Approaches in Statistical Physics*, Theor. Math. Phys. 123:3, 846-850, 2000.

[6] Sakhnovich L.A., *Comparison of Thermodynamic Characteristics of a Potential Well under Quantum and Classical Approaches*, Funct. Anal. Appl. 36:3, 205-211, 2002.

[7] Sakhnovich L.A., *Comparison of Thermodynamics Characteristics in Quantum and Classical Approaches and Game Theory*, arXiv:10104717, v.2, Physica A to appear.

[8] Sakhnovich L.A., *Laws of thermodynamics and game theory*, arXiv:1105.4633.

[9] Sobczyk K., Holobut P., *Information-theoretic approach to dynamics of stochastic systems*, Probabilistic Engineering Mechanics, doi:10.1016/j.probengmech.2011.05.007

[10] Toscani G., Villani C., *Sharp entropy dissipation bounds and explicit rate of trend to equilibrium for the spatially homogeneous Boltzmann equation*, Comm. Math. Phys. 203:3, 667706, 1999.
[11] Villani C., *A review of mathematical topics in collisional kinetic theory*, in: Handbook of mathematical fluid dynamics, Vol. I, 71305, Amsterdam: North-Holland, 2002.

[12] Villani C., *Entropy production and convergence to equilibrium for the Boltzmann equation*, in: Zambrini J.-C. (ed.), XIVth international congress on mathematical physics. Selected papers, 130-144, Hackensack, NJ: World Scientific, 2005.