The Discrete Boltzmann Equation : The Regular Plane Model with Four Velocities

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Abstract. For a simple discrete model of Boltzmann equation, we study the derivatives of *H*-Boltzmann function, and prove that all derivatives of odd order are negative, instead all derivatives of even order are postive. These result is a first and small generalisation of the classical *H*-Boltzmann theorem.

We consider a discrete model of the Boltzmann equation with the the four following velocities : $\boldsymbol{\xi}_1 = \boldsymbol{c}(1,0)$, $\boldsymbol{\xi}_2 = \boldsymbol{c}(0,1)$, $\boldsymbol{\xi}_3 = \boldsymbol{c}(-1,0)$, $\boldsymbol{\xi}_4 = \boldsymbol{c}(0,-1)$. The only binary collisions are $(\boldsymbol{\xi}_1, \boldsymbol{\xi}_3) \leftrightarrow (\boldsymbol{\xi}_2, \boldsymbol{\xi}_4)$. Denoting by $\boldsymbol{N_i(t)}$ the density of molecules with velocity ξ_i , and by $\boldsymbol{H(t)} = \sum_{\boldsymbol{i}=1}^{4} \boldsymbol{N_i(t)} \boldsymbol{Log} \left| \boldsymbol{N_i(t)} \right|$, the *H*-Boltzmann functional, we prove the following result :

$$(-1)^{\boldsymbol{k}} \frac{\boldsymbol{d^k H(t)}}{\boldsymbol{dt^k}} \geq 0$$

This result was published by Harris in 1967, [1], but unfortunately the proof of Harris was erroneous, as he has recognized in two e-mails. In the first e-mail, sent to Li-Shi Luo (on October 13, 2003) he writes : " I am impressed how elegant your proof is, ... It is a truly wonderful piece of work and I am glad to see the matter resolved after so many years of thinking about it ". In the second e-mail, sent to Henri Cabannes (on October 20, 2003) he writes : " Congratulations on your proof which I am in great admiration of ..... . I would be interested to see for which, if any, other models a proof can be found ". Harris passed away last May 2004, at the age of 67 ! We have given an exact proof, last novembre, in reference [2], which is the section 3.1.3 of Lecture Notes on The Discrete Boltzmann Equation.

3.1.3 The *H*-Boltzmann Function

The first derivative of the H-Boltzmann function is negative. It is interesting to note that for the regular plane four velocities model, it is true that the successive derivatives of the H-Boltzmann function alternate in sign [45]:

$$(-1)^k \frac{d^k H}{dt^k} \geq 0, \qquad k = 1,\, 2,\, \ldots . \tag{3.1.3-1}$$

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As a consequence of the first Euler equation, when the densities are independent of the space variables, the total density n is a constant. Letting $n_i = N_i/n$ and $\tau = cSnt$, we can write the kinetic equations (3.1.1-1) as:

$$\frac{dn_i}{d\tau} = n_{i+1}n_{i+3} - n_i n_{i+2}, \qquad i = 1, 2, 3, 4, \quad \text{with } (n_1 + n_2 + n_3 + n_4) = 1. \tag{3.1.3-2}$$

In the above equation we are considering $n_k = n_l$ when $k \equiv l \pmod 4$. From equations (3.1.3-2) we deduce:

$$\frac{d^k n_i}{d\tau^k} = (-1)^{k+1}\frac{dn_i}{d\tau}, \qquad i = 1, 2, 3, 4. \tag{3.1.3-3}$$

The H-Boltzmann function is:

$$H = \sum_{i=1}^{4} N_i \ln(N_i) = n\ln(n) + n\sum_{i=1}^{4} n_i \ln(n_i),$$

and because n is a positive constant, the derivatives with respect to t of H have the same sign as the derivatives with respect to τ of:

$$h(\tau) = \sum_{i=1}^{4} n_i(\tau)\ln(n_i(\tau)). \tag{3.1.3-4}$$

By taking successive derivatives we obtain:

$$\begin{aligned}
\frac{dh}{d\tau} &= \sum_{i=1}^{4} \ln(n_i)\frac{dn_i}{d\tau} = (n_1 n_3 - n_2 n_4)\ln\left(\frac{n_2 n_4}{n_1 n_3}\right) \le 0, \\
\frac{d^2 h}{d\tau^2} &= \sum_{i=1}^{4}\left\{\ln(n_i)\frac{d^2 n_i}{d\tau^2} + \frac{1}{n_i}\left(\frac{dn_i}{d\tau}\right)^2\right\} \\
&= -\frac{dh}{d\tau} + \sum_{i=1}^{4} A_i, \qquad A_i := \frac{1}{n_i}\left(\frac{dn_i}{d\tau}\right)^2 \\
\frac{d^{k+2}h}{d\tau^{k+2}} &= -\frac{d^{k+1}h}{d\tau^{k+1}} + \frac{d^k A}{d\tau^k}, \qquad \text{with } A := \sum_{i=1}^{4} A_i.
\end{aligned}$$

The initial values of the densities $\{N_i\}$ are positive, and so is the initial value of A and the derivative $\frac{d^2h}{d\tau^2}$.

To complete the proof of inequalities (3.1.3-1) it suffices to show that:

$$(-1)^k \frac{d^k A_i}{d\tau^k} \ge 0. \tag{3.1.3-5}$$

This will certainly be true if we can show:

$$(-1)^k \frac{d^k A_i}{d\tau^k} \ge A_i \quad \forall k, \tag{3.1.3-6}$$

because $A_i \ge 0$. The above inequality can be proved by induction.

For $k=1$ we have:

$$-\frac{dA_i}{d\tau} = \frac{1}{n_i}\left\{2\left(\frac{dn_i}{d\tau}\right)^2 + A_i\frac{dn_i}{d\tau}\right\} = A_i\left\{2 + \frac{1}{n_i}\frac{dn_i}{d\tau}\right\}.$$

Equation (3.1.3-2) can be written as:

$$n_i + \frac{dn_i}{d\tau} = n_{i+1}n_{i+3} + n_i(n_{i-1} + n_i + n_{i+1}) \geq 0, \tag{3.1.3-7}$$

which proves inequality (3.1.3-6) for $k=1$. To compute $\frac{d^kA_i}{d\tau^k}$, we differentiate the product n_iA_i in two different ways. First we use formula (3.1.3-3) and then we use Leibniz rule:

$$\begin{aligned}
\frac{d^k(n_iA_i)}{d\tau^k} &= \frac{d^k}{d\tau^k}\left(\frac{dn_i}{d\tau}\right)^2 = (-2)^k\left(\frac{dn_i}{d\tau}\right)^2 \\
\frac{d^k(n_iA_i)}{d\tau^k} &= \sum_{j=0}^{k-1} C_k^j \frac{d^{k-j}n_i}{d\tau^{k-j}}\frac{d^jA_i}{d\tau^j} + n_i\frac{d^kA_i}{d\tau^k},
\end{aligned}$$

where $C_k^j := k!/j!(k-j)!$ is the binomial coefficient. Comparing the last two equations yields:

$$(-1)^k\frac{d^kA_i}{d\tau^k} = \frac{1}{n_i}\left\{2^k\left(\frac{dn_i}{d\tau}\right)^2 + \sum_{j=0}^{k-1}(-1)^jC_k^j\frac{d^jA_i}{d\tau^j}\frac{dn_i}{d\tau}\right\}. \tag{3.1.3-8}$$

We have shown inequality (3.1.3-6) holds for $k=1$, assume that it holds for $(k-1)$, then the above equality leads to:

$$\begin{aligned}
(-1)^k\frac{d^kA_i}{d\tau^k} &\geq A_i\left\{2^k + \frac{1}{n_i}\frac{dn_i}{d\tau}\sum_{j=0}^{k-1}C_k^j\right\} \\
&= A_i\left\{2^k + (2^k-1)\frac{1}{n_i}\frac{dn_i}{d\tau}\right\} \\
&= A_i\left\{1 + (2^k-1)\frac{1}{n_i}\left(n_i + \frac{dn_i}{d\tau}\right)\right\} \\
&\geq A_i.
\end{aligned} \tag{3.1.3-9}$$

This completes the proof of inequality (3.1.3-6), and hence forth inequality (3.1.3-1).

The densities $\{N_i(t)\}$ are monotonic functions of time, and if the initial state is Maxwellian so that $(\bar{n}_1\bar{n}_3 - \bar{n}_2\bar{n}_4) = 0$, then the $\{N_i(t)\}$ are constants.

Conclusion.

To conclude our work and to answer the second Harris's e-mail, we can suggest different possible extensions. First : one can try to extend our results to the three dimensional Broadwell model, with six velocities, or more generally models with 2p velocities ; one can try to prove that the second derivative of ***H*** Boltzmann functional is, at least for those models, always positive. The second suggestion is to study the same problem for the two-dimensional semi-continuous model of Boltzmann equation

$$\frac{\partial N(t;\theta)}{\partial t}=\frac{1}{2\pi}\int_0^{2\pi}\left\{N(t;\phi)N(t;\phi+\pi)-N(t;\theta)N(t;\theta+\pi)\right\}d\phi$$

All the velocities have the same modulus, and arbitrary directions. The unknown function $N(t;\theta)$, a density, depends upon time t and and angle θ, direction of velocity. $N(t;\theta)$ is a periodic function in θ, with period 2π ; when the period is equal to π, the general solution was obtained in parametric form [3], [4], [5]. An interesting problem seems to be the determination of all initial densities $N(0;\theta)$, for which the second derivative of H Boltzmann functional is positive. Our conjecture is that positivity is valid for all solutions.

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