On the sign of successive time derivatives of Boltzmann's H function

1970 J. Phys. A: Gen. Phys. 3 331

(http://iopscience.iop.org/0022-3689/3/4/002)

J. Phys. A: Gen. Phys., 1970, Vol. 3. Printed in Great Britain

On the sign of successive time derivatives of Boltzmann's *H* function

W. MAASS

Institut für Theoretische Physik I, Universität Marburg/L., Renthof 7, Germany

MS. received 4*th February* 1970

Abstract. It has been conjectured in the literature that for the Boltzmann equation: (i) Boltzmann's H has the property of possessing successive (semi-) definite time derivatives with alternating sign, (ii) this property is suitable for selecting H from further possibly existing (Lyapunov) functions with (semi-) definite first time derivative. For simple models of the Boltzmann equation the conjecture (i) has been confirmed.

We show at first that, in contradiction to (ii), for Maxwell's model of a discrete velocity gas the corresponding variant of H is not the unique Lyapunov function having the above property (i) and suitable to define a 'non-equilibrium entropy' with respect to the (spatially homogeneous) Boltzmann equation of this model. Secondly, in the case of the complete spatially inhomogeneous Boltzmann equation, $\ddot{H}$ is generally not (semi-)definite in contradiction to the above-mentioned conjecture (i).

1. Introduction

In the framework of macroscopic–kinetic theories of matter the possibility of introducing a 'non-equilibrium entropy' is based on the existence of an 'H theorem'. The mathematical importance of H with regard to the basic kinetic equation consists of the fact that a Lyapunov functional, constructed eventually from H, has a (semi-) definite time derivative. Such a functional yields stability statements (in the sense of Lyapunov) for the equation of motion (Zubov 1964). With this viewpoint equations in statistical physics have been investigated, e.g. by Maass (1969), Hofelich (1969), Maass (to be published).

It should be emphasized that we start here from the existence of a basic kinetic equation and define the corresponding 'entropy' by a Lyapunov functional of this equation. This procedure is different from the information theoretical approach to statistical mechanics where the entropy is defined as 'missing information' with reference to a given probability distribution in Γ space (Landsberg 1961, Jaynes 1963, Katz 1967).

The question arises as to the uniqueness of an 'entropy' defined in this way. For the kinetic model of Boltzmann's equation McKean (1966) has proposed the reduction of the set of competing functionals by requiring that the successive time derivatives of the functional in question should alternate in sign. Boltzmann's H has been conjectured to satisfy this requirement. This conjecture has been verified by Harris (1967) for Maxwell's model of a discrete velocity gas, and by Simons (1969) for the spatially homogeneous linearized Boltzmann equation.

In § 2 we consider the Maxwell model and construct the Lyapunov functional $\tilde{L}$ which differs essentially from Boltzmann's H_{model} Harris (1967) and has successive time derivatives alternating in sign, just as H_{model}.

In § 3 we show for the complete spatially inhomogeneous Boltzmann equation that the second time derivative of Boltzmann's H is generally not (semi-)definite. We conclude that McKean's rule is then not satisfied.

2. Maxwell's model of a discrete velocity gas

The truncated Boltzmann equation considered by Harris (1967) has the form

$$\begin{aligned} \dot{n}_1 &= n_2 n_4 - n_1 n_3 \\ \dot{n}_2 &= -\dot{n}_1 \\ \dot{n}_3 &= \dot{n}_1 \\ \dot{n}_4 &= -\dot{n}_1 \end{aligned} \tag{1}$$

with

$$0 < n_i(t) < 1 \qquad (i = 1, \ldots, 4)$$

$$\sum_{i=1}^{4} n_i = 1, \qquad n_0 \equiv (n_{0i}) = (\tfrac{1}{4}) \ \text{(equilibrium)}$$

and corresponds to the motion of the particles along two orthogonal axes. We notice that because $\ddot{n}_i = -\dot{n}_i$ the general solution of (1) is

$$n_i(t) = n_i(0) + \dot{n}_i(0)\{1 - \exp(-t)\}.$$

The system of equations (1) written in the form

$$\dot{n}_i = f_i(n_1, \ldots, n_4) \qquad (i = 1, \ldots, 4) \tag{2}$$

is asymptotically stable in the large relative to n_0.

Corresponding to the method of Zubov (1964), Lyapunov functionals $L\{n\}$ can be constructed by solving the following equation for L:

$$\sum_{i=1}^{4} \frac{\partial L}{\partial n_i} \dot{n}_i = \varphi(n)\,(1+L)\left(1 + \sum_{i=1}^{4} f_i^2\right)^{1/2} \tag{3}$$

having regard to the conditions

(i) the functions $L(n)$ and $\varphi(n)$ are continuous (in E_4)

(ii) $-1 < L(n) < 0, \qquad \varphi(n) > 0 \qquad \text{for } n \neq n_0$

(iii) $\lim\limits_{n \to n_0} \begin{pmatrix} L(n) \\ \varphi(n) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

(iv) $L = -1$ on the boundary of the region of asymptotic stability.

Choosing

$$\varphi = (n_2 n_4 - n_1 n_3)^2 \{1 + 4(n_2 n_4 - n_1 n_3)^2\}^{-1/2}$$

we get from (3), for example, the functional

$$L = \exp\{-\tfrac{1}{2}(n_2 n_4 - n_1 n_3)^2\} - 1. \tag{4}$$

Because $\ddot{n} = -\dot{n}$, it is easy to see that

$$\dot{L} \geqslant 0, \qquad \ddot{L} \leqslant 0$$

where the equality is valid only for $\dot{n} = 0$. Forming

$$\tilde{L} \equiv \ln(L+1) = -\tfrac{1}{2}(n_2 n_4 - n_1 n_3)^2 \tag{5}$$

we have

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} \tilde{L} = (-2)^n \tilde{L} \qquad (n \text{ integral} \geqslant 1).$$

Comparing (5) with the Lyapunov functional

$$\hat{L} \equiv -c \sum_{i=1}^{4} n_i \ln n_i \qquad (0 < c \leqslant \tfrac{1}{4})$$

which is obtained by choice of

$$\varphi = c(n_2n_4 - n_1n_3) \ln\left(\frac{n_2n_4}{n_1n_3}\right)\left\{1 - c \sum_i n_i \ln\left(\frac{n_i}{n_{0i}}\right)\right\}^{-1} \{1 + 4(n_2n_4 - n_1n_3)^2\}^{-1/2}$$

we see that $\tilde{L}$ has successive time derivatives alternating in sign, just as $\hat{L}.\tilde{L}$ is usable as well as $\hat{L}$ to define a non-equilibrium entropy. We notice that $\hat{L}$ corresponds to Boltzmann's $H_{\text{model}} \equiv \Sigma_i n_i \ln n_i$ (Harris 1967) with respect to the model Boltzmann equation (1).

3. The spatially inhomogeneous Boltzmann equation

Let the particle distribution function $f(\boldsymbol{r}, \boldsymbol{v}; t)$ of an isolated gas system satisfy Boltzmann's equation. For simplicity we assume 'specular reflection' as the boundary condition. On assumption of some physically motivated existence properties of solutions of Boltzmann's equation, the Lyapunov functional

$$H \equiv \int \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{v}\, f \ln\left(\frac{f}{f_0}\right) \tag{6}$$

can be applied to prove uniformly asymptotic stability in the large of the total Maxwell distribution $f_0(v)$ (Maass—to be published).

In the literature the term 'Boltzmann's H function' usually denotes the functional $\int \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{v}\, f \ln f$ which corresponds to H_{model} of § 2. We prefer here the dimensionally correct form (6) which has the same time derivative as $\int \mathrm{d}^3\boldsymbol{r}\, \mathrm{d}^3\boldsymbol{v}\, f \ln f$.

$\dot{H}\{f\} \leqslant 0$ vanishes only if f has the form of a local Maxwell distribution

$$f^{(0)} = \alpha_1 \exp\{-\alpha_2(\boldsymbol{v} - \boldsymbol{\alpha}_3)^2\} \qquad (\alpha_i = \alpha_i(\boldsymbol{r})). \tag{7}$$

$f = f^{(0)} \neq f_0$ is possible, at most, in discrete points of time (Uhlenbeck and Ford 1963). We notice that in the case of spatial homogeneity the set of local Maxwell distributions contracts to the total Maxwell distribution f_0. Let a 'trajectory' of the Boltzmann equation pass through a distribution $f^{(0)} \neq f_0$ at time $t^{(0)} \epsilon [0, \infty)$; for instance, the initial distribution may be prepared to have the form (7).

Because of

$$-\tfrac{1}{2}\dot{H}^2(t) = \int_t^\infty \mathrm{d}\tau\, \dot{H}(\tau)\, \ddot{H}(\tau)$$

we get

$$0 = \int_{t^{(0)}}^\infty \mathrm{d}\tau\, \dot{H}(\tau)\, \ddot{H}(\tau).$$

Taking into account the strict monotony of $H(t)$ ($\dot{H}(t) \leqslant 0$), we see that $\ddot{H}(t)$ has to change the sign in $[t^{(0)}, \infty)$ and cannot be (semi-)definite. Continuity of $\dot{H}(t)$ and $\ddot{H}(t)$ is presumed.

We remark that for the spatially homogeneous Boltzmann equation, in particular for the linearized form considered by Simons (1969), the distributions (7) reduce to f_0 such that the arguments of this section are irrelevant in that case.

Acknowledgments

I wish to thank Professor G. Ludwig for his interest and advice.

References

HARRIS, S., 1967, *J. math. Phys.*, **8**, 2407–10.
HOFELICH, F., 1969, *Z. Phys.*, **226**, 395–408.
JAYNES, E. T., 1963, *Brandeis Summer Lectures on Statistical Physics*, 1962 (New York: Benjamin).
KATZ, A., 1967, *Principles of Statistical Mechanics* (San Francisco: Freeman).
LANDSBERG, P. T., 1961, *Thermodynamics with Quantum Statistical Applications* (New York: Interscience).
MAASS, W., 1969, *Z. Naturf.*, **24a**, 1575–80.
—— *Ann. Phys.*, in the press.
MCKEAN, H. P., 1966, *Archs Ration. Mech. Analysis*, **21**, 343–67.
SIMONS, S., 1969, *J. Phys.* A: *Gen. Phys.*, **2**, 12–3.
UHLENBECK, G. E., and FORD, G. W., 1963, *Lectures in Statistical Mechanics* (Providence: American Mathematical Society).
ZUBOV, V. I., 1964, *Methods of A. M. Lyapunov and their Application* (Groningen: Noordhoff).