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A Definition of the H-Functional for Heat Conduction

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Abstract: In this Note a mathematical formulation of a monotonically decreasing functional with respect to time (the H-functional) is derived for physical systems described by the diffusion equation. This returns a condition which is equivalent to the second law of thermodynamics.

The H-theorem is certainly the most debated (and probably the most important) part of Boltzmann's scientific heritage [1,2]. As it is well known, this theorem states that, given a function $f(t,x,v)$ which is a solution of Boltzmann's equation, one can define a functional which is monotonically decreasing in time (the H-functional):

$$H(f) = \int_{\Re_x^n \times \Re_v^n} f \log f \tag{1}$$

with

$$\frac{dH}{dt} \leq 0 \tag{2}$$

The importance of this theorem consists in the fact that it was the first attempt to give an analytical proof of the second law of thermodynamics for some specific model of statistical mechanics. In fact, if one reads the term on the left hand side of Eq. (2) as a negative entropy, the theorem is equivalent to the statement that the physical entropy of an isolated system should not decrease in time.

Since its first formulation, the H-theorem raised some negative criticism, most of which addressed the inconsistency of the irreversibility with respect to time implied by the theorem, because the assumptions appear to be intrinsically time-reversible. This point is the essence, for instance, of Loschmidt's paradox [1], and the debate is still going on, even with attacks to the foundations of Boltzmann's kinetic theory itself [3].

Recently, an active trend of research is represented by the attempt to extend the H-theorem to physical systems other than the ideal gas, for which it was originally derived. These include, for instance, systems described by Fokker-Planck type equations [4-6], or simple models for granular media [7,8]. Roughly speaking, from the physicist's point of view the problem reduces to giving a formulation of Boltzmann's H-functional, and of its rate of decrease, in terms of the relevant physical quantities.

As a matter of fact, a feature of many collisional kinetic systems is their tendency to converge to an equilibrium distribution as time becomes large, and very often convergence is driven by a thermodynamic principle: there is a distinguished Lyapunov functional, called entropy, which attains a stationary point as the system goes towards the equilibrium distribution, under constraints imposed by physical laws.

Here, a formulation of the H-theorem for the conduction of heat is proposed. Starting from the Cauchy problem for the heat equation, and assuming that the initial value $T_0(x) = T(x,0)$ is a probability density in $\Re^n$, one can write:

$$\frac{\partial T}{\partial t} = \alpha \Delta_x T \qquad x \in \Re^n \quad t \geq 0 \tag{3}$$

where the initial value $T_0(x)$ satisfies the following conditions:

$$\int_{\Re^n} T_0(x) d^n x = 1 \tag{4}$$

$$\int_{\Re^n} x T_0(x) d^n x = 0 \tag{5}$$

$$\int_{\Re^n} |x|^2 T_0(x) d^n x = nE < \infty \tag{6}$$

$$\int_{\Re^n} T_0(x) \log(T_0(x)) d^n x = H_0 < \infty \tag{7}$$

Given any smooth convex function $\varphi = \varphi(r)$, with $r \geq 0$, one can multiply both sides of the heat equation by $\varphi' = \varphi'(T_t)$, where T_t is the solution of Eq. (3) at any instant t, and integrate over $\Re^n$:

$$\int_{\Re^n} \frac{\partial \varphi(T_t)}{\partial t} d^n x = \alpha \int_{\Re^n} \varphi'(T_t) \Delta T_t d^n x \tag{8}$$

Finally, one can introduce the vanishing condition at infinity as follows:

$$\lim_{x_j \to \infty} \varphi'(T_t) \frac{\partial T_t}{\partial x_j} = 0 \qquad j \geq 1 \quad t > 0 \tag{9}$$

and a bounding integral condition:

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$$\int_{\Re^n} \varphi''(T_t)\left(\frac{\partial T_t}{\partial x_j}\right)^2 d^n x \le C \tag{10}$$

where C is a suitably large constant.

Now, integration by parts of the right hand side of Eq. (8) is possible, which allows the exchange of integral and derivative on the left hand side of the same equation:

$$\frac{\partial}{\partial t}\int_{\Re^n} \varphi(T_t) d^n x = -\alpha \int_{\Re^n} \varphi''(T_t)(\nabla T_t)^2 d^n x \tag{11}$$

Eq. (11) is the analogous of Boltzmann's H-theorem for the heat equation. This can be shown in few steps by taking:

$$\varphi(T_t) = T_t(x)\log(T_t(x)) d^n x \tag{12}$$

so that Eq. (11) becomes:

$$\frac{\partial}{\partial t}\int_{\Re^n} T_t(x)\log(T_t(x)) d^n x = -\alpha \int_{\Re^n} \frac{|\nabla T_t|^2}{T_t} d^n x \tag{13}$$

Introducing Fisher's functional $\Im(r) = \int_{\Re^n} \frac{|\nabla r|^2}{r} d^n x$ [9], Eq. (13) can be re-written in the following compact form:

$$\frac{\partial H(T_t)}{\partial t} + \alpha \Im(T_t) = 0 \tag{14}$$

The Fisher functional $\Im$ plays the role of entropy production rate during heat conduction. Thus, Eq. (14) represents Boltzmann's H-theorem for systems described by the heat equation.

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