Remarks on Entropy and Equilibrium States

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Abstract—We show here that a large class of density functions $0 \leq f_{\infty}(v) = f_{\infty}(|\psi|^2(v)), v \in \Omega \subseteq \mathbb{R}^N$ induces a unique "natural" entropy. As a consequence, given the equilibrium distribution $f_{\infty}$ of a kinetic equation which conserves the mass, one obtains at once the unique entropy functional monotone nonincreasing with time along the solution, independently of the dynamics. Application of this result to classical theory of rarefied gases permits to improve a theorem of McKean in [1].

1. INTRODUCTION

Spatially homogeneous problems of kinetic theory are described in terms of a density $f = f(v, t)$, where $v \in \Omega \subseteq \mathbb{R}^N, N \geq 1, t \in \mathbb{R}_+$. The unknown function $f$ obeys the general partial differential equation (of first order in the time variable)

$$\frac{\partial f}{\partial t} = Q(f),$$

where $Q(f)$ is an operator defining the (collision) dynamics of $f(t)$. The standard physical requirements on the nonnegative initial density $f_0(v) = f(v, t = 0)$ are the boundedness of mass and energy

$$\int_{\Omega} [1 + |\psi|^2(v)] f_0(v) dv < \infty,$$

where $\psi$ is a $C^1$-function of the velocity variable with $|\psi(v)| \to \infty$ as $|v| \to \infty$. Under these constraints, in general, the equation $Q(f) = 0$ is solvable, and defines the (unique) class of equilibrium distribution functions. For many systems, the convergence of the solution to equilibrium is then concluded using the time monotonicity of the physical entropy, which expression is usually derived from the structure of the operator $Q(f)$.

Maybe the most classical example is provided by the spatially homogeneous Boltzmann equation [2,3]

$$\frac{\partial f}{\partial t} = Q_B(f, f).$$

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$Q_B$ is the so-called Boltzmann collision operator,

$$Q_B(f,f) = \int_{\mathbb{R}^N} dv \int_{S^{N-1}} dw B(v-v_\ast,w) (f'f_\ast' - ff_\ast),$$

(1.4)

where $dw$ is the normalized measure on $S^{N-1}$, $f' = f(v')$, and so on, and

$$v' = v - (v - v_\ast)w, \quad v_\ast' = v_\ast - (v - v_\ast)w$$

(1.5)

are the postcollisional velocities of two particles that collide with respective velocities $v$ and $v_\ast$, according to the laws of elastic collision. The functions $f_\infty$ which give a vanishing collision integral, are the Maxwellian equilibrium distributions

$$f_\infty(v) = \exp\left\{-\frac{1}{2}v^2(v)\right\},$$

(1.6)

where $\psi(v)$ is polynomial of degree one in $v$. For initial data satisfying (1.2), the convergence of the solution towards the equilibrium can be shown as a consequence of Boltzmann $H$-theorem [3]. This celebrated theorem says that, under the dynamics induced by $Q_B(f,f)$, the convex functional

$$H(f)(t) = \int_{\Omega} f(v,t) \log f(v,t) dv$$

(1.7)

in nonincreasing in time if $f(t)$ is the solution of equation (1.3). Moreover, given any constant $u \in \mathbb{R}^N$, under the constraints

$$\int_{\Omega} f(v) dv = m, \quad \int_{\Omega} |v-u|^2 f(v) dv \leq E,$$

(1.8)

the $H$-functional reaches the minimum (which by strong convexity is unique), in correspondence to the Maxwellian (1.6) in which $\psi$ is chosen to satisfy (1.8) both with the equality sign. This minimum property is known as the Gibbs Lemma [4]. In the Gibbs Lemma, the energy is included in the constraints.

In the sequel, we will adopt a different point of view, and the energy will be considered part of the entropy. In other words, the “dissipativity” property of the kinetic system in our point of view comes out from the joint action of entropy and energy. Consequently, the “natural” entropy to look for has the form

$$H^*(f) = \int_{\Omega} \{\psi^2(v)f(v) + \Phi[f(v)]\} dv,$$

(1.9)

where $\Phi$ is a (strongly) convex function ($\Phi(r) = r \log r$ for the Boltzmann equation). A remarkable consequence of this choice is that this “natural” entropy is completely independent of the structure of the operator $Q(f)$, being $\Phi$ uniquely determined by the form of the equilibrium distribution. This simply means that Boltzmann’s $H$-functional (1.7) is the unique convex functional naturally coupled to the Maxwellian distribution (1.6). Any other kinetic equation which admits the Maxwellian as equilibrium distribution, has $H^*(f)$ as natural entropy. This is the case of the BGK model [2], of the linear Fokker-Planck equation [2] or of the Landau equation [5], where the collision operators vanish whenever $f_\infty$ is a Maxwellian distribution.

The coupling of the equilibrium distribution with its entropy is linked to a minimization problem for (1.9). We will introduce this link in Section 2. In Section 3, we present some consequences of this approach. In particular, we give an improvement of a theorem of McKean [1] concerning uniqueness of Boltzmann’s $H$-functional as nonincreasing entropy for Kac caricature of the Maxwellian gas [6].
2. A MINIMIZATION PROBLEM AND ITS DUAL

In this section, we will derive sufficient conditions for an equilibrium state \( f_\infty(v), v \in \Omega \) to be uniquely coupled with a natural entropy of the form (1.9). This problem is strictly connected to the research of the extremal points of the functional \( H^*(f) \), when \( f \) belongs to the manifold

\[
F_m = \left\{ f \geq 0, \ f \in L^1(\Omega), \ \int_{\Omega} f(v) \, dv = m \right\}.
\]  

(2.1)

Given any monotone nonincreasing (nondecreasing) function \( \rho(r) : \mathbb{R} \rightarrow \mathbb{R}, \rho^{-1} \) will denote its pseudoinverse function.

In the following, we will consider entropies

\[
H^*(f) = \int_{\Omega} \left\{ |\psi|^2(v)f(v) + \Phi[f(v)] \right\} \, dv,
\]

(2.2)

where \( |\psi|^2(v) \) is a \( C^1 \)-function of \( v \), and \( \Phi(r), r > 0 \) is a smooth (strongly) convex function. We have the following.

**Theorem 2.1.** Let \( f \in F_m \). If there exists a constant \( \lambda_m \) such that the function

\[
f_\infty \left( |\psi|^2 \right) = [\Phi']^{-1} (-|\psi|^2 - \lambda_m)
\]

(2.3)

belongs to \( F_m \), then \( f_\infty \) is an extremal of \( H^*(f) \), and, for all \( f \in F_m \),

\[
H^*(f) \geq H^*(f_\infty).
\]

(2.4)

Moreover, if \( \Phi \) is strongly convex, the equality holds if and only if \( f = f_\infty \).

Conversely, let \( f_\infty = f_\infty(|\psi|^2) \in F_m \) be nonincreasing with respect to \( |\psi|^2 \). Then, there exists a constant \( \lambda_m \) such that the (unique) genuinely nonlinear convex function \( \Phi_{\lambda_m} \) belonging to the one-parameter set of convex functions defined by

\[
\Phi_{\lambda}(r) = -\int f_{\infty}^{-1}(r) \, dr + \lambda r
\]

(2.5)

is the natural entropy associated to \( f_\infty \). If \( f_\infty \) is strictly decreasing, \( \Phi_{\lambda} \) is strictly convex.

**Proof.** Let

\[
G(f) = |\psi|^2 f + \Phi[f].
\]

(2.6)

Expanding \( G(f) \) in Taylor's series of \( f \) up to order two in a neighborhood of the equilibrium state \( f_\infty \) given by (2.3), we obtain

\[
G(f) = G(f_\infty) + G'(f_\infty)(f - f_\infty) + \frac{1}{2} G''(\tilde{f})(f - f_\infty)^2.
\]

(2.7)

By (2.3),

\[
G'(f_\infty) = |\psi|^2 + \Phi'(f_\infty) = -\lambda_m \text{ a.e.}
\]

(2.8)

Hence, since both \( f \) and \( f_\infty \) belong to \( F_m \),

\[
\int_{\infty} G'(f_\infty)(f - f_\infty) \, dv = 0.
\]

(2.9)

On the other hand, since \( G(f) \) is convex, (2.7) implies (2.4). Also the statement concerning uniqueness of the minimum is derived from (2.7).
The second half of the theorem follows by remarking that, when $f_\infty$ is nonincreasing in its argument, (2.8) can be written as
\[
\Phi'(r) = -f_\infty^{-1}(r) - \lambda \text{ a.e.} \quad (2.10)
\]
From (2.10), relation (2.5) follows by integration. Since $f_\infty$ is nonincreasing, $\Phi'$ is nondecreasing, which gives convexity.

Two examples will clarify how Theorem 2.1 works. First, let the equilibrium state be given by the Maxwellian (1.6). In this context, "Maxwellian" simply means that $f_\infty$ is exponentially decaying as $|\psi(v)|^2$, where $\psi(\psi)$ is a function of $v |\psi(v)| \to \infty$ as $|v| \to \infty$. Then, (2.5) takes the form
\[
\Phi_\lambda(r) = + \int \log r \, dr + \lambda r = r \log r + (\lambda - 1)r. \quad (2.11)
\]
Choosing $\lambda = 1$, we obtain $\Phi(r) = r \log r$, namely Boltzmann's $H$-functional. In this case,
\[
H^*(f) = \int_{\Omega} \left\{ |\psi|^2 f(v) + f(v) \log f(v) \right\} dv
= \int_{\Omega} \left\{ -\log e^{-|\psi|^2} f(v) + f(v) \log f(v) \right\} dv = \int_{\Omega} f(v) \log \frac{f(v)}{f_\infty(v)} dv,
\]
and $H^*(f)$ coincides with the classical relative entropy considered in information theory [7,8]. This equality holds only for Maxwellians.

The second example refers to the equilibrium distribution
\[
\text{foo} \left( |v|^2 \right) = \frac{1}{\Gamma(p-1)} \frac{C - \frac{p-1}{2p} |v|^2}{|v|^{p-1}}, \quad v \in \mathbb{R}^N \quad (2.12)
\]
for a constant $C$ such that $f_\infty$ has mass equal to $m$. As usual, $g_+$ indicates the positive part of $g$.

Equation (2.12) is the Barenblatt-Pattle profile, namely the self-similar solution of the porous medium equation [9]
\[
\frac{\partial u}{\partial t} = \Delta u^p, \quad p > 1, \quad (2.13)
\]
at a fixed time $t = 1$. If we apply Theorem 2.1 with $\Omega$ equal to the support of (2.12), $f_\infty(|v|^2)$ can be inverted, and from (2.5) we obtain
\[
\Phi_\lambda(r) = \frac{2}{p-1} r^p + \left( \frac{2pC}{p-1} \right) r. \quad (2.14)
\]
Choosing $\lambda = -\left( \frac{2pC}{p-1} \right)$ we conclude that the associated entropy is
\[
H^*(f) = \int_{\Omega} \left\{ |v|^2 f(v) + \frac{2}{p-1} f^p(v) \right\} dv. \quad (2.15)
\]
The entropy functional (2.15) has been introduced by Newman in [10], and subsequently used by Carrillo and Toscani [11] to study the asymptotic behaviour of the solution of equation (2.13). We remark that to obtain $H^*(f)$ in the previous situation, we need to restrict the support in order that the equilibrium distribution be invertible. On the other hand, one time we have the associated entropy, since $H^*(f_\infty)$ is bounded whenever $\Omega = \text{Supp}\{f_\infty\}$, the minimization problem is meaningful for any $\Omega \subseteq \mathbb{R}^N$. In fact, it can be easily verified that Theorem 2.1 applied to
\[
H^*(f) = \int_{\mathbb{R}^N} \left\{ |v|^2 f(v) + \frac{2}{p-1} f^p(v) \right\} dv, \quad (2.16)
\]
gives $H^*(f) \geq H^*(f_\infty)$, where $f_\infty$ is given by (2.12).
3. CONSEQUENCES

Theorem 2.1 has some immediate consequences. Let us consider equation (1.1), with $Q(f)$ given by the linear expression

$$Q(f) = \sigma (f_\infty - f),$$

where $\sigma$ is a positive constant. Let $f_\infty \in F_m$ satisfy the hypotheses of Theorem 2.1. If the initial value $f_0(v) \in F_m$, given the natural entropy associated to $f_\infty$, and supposing that on $\Omega$,

$$H^*(f) = \int_\Omega \{ |\psi|^2(v)f(v) + \Phi[f(v)] \} \, dv = c < \infty,$$

one obtains

$$\frac{d}{dt} H^*(f) = \sigma \int_\Omega \{ |\psi|^2 + \Phi'(f) \} (f_\infty - f) \, dv = \sigma \int_\Omega \{ |\psi|^2 + \Phi'(f_\infty) \} (f_\infty - f) \, dv$$

$$+ \sigma \int_\Omega \{ \Phi'(f) - \Phi'(f_\infty) \} (f_\infty - f) \, dv = -\sigma \int_\Omega \{ \Phi'(f) - \Phi'(f_\infty) \} (f - f_\infty) \, dv,$$

since, by (2.8) the first integral vanishes. It follows that, provided $H^*(f_0)$ is finite, the natural entropy associated to $f_\infty$ is monotone nonincreasing with time along the solution to our linear kinetic equation. By theorem 2.1 follows also that this entropy is unique in the class of entropies of type (1.9) such that $H^*(f_\infty)$ is finite. Suppose in fact that there exists another convex function $\Phi_1$ such that

$$H^*(f) = \int_\Omega \{ |\psi|^2(v)f(v) + \Phi_1[f(v)] \} \, dv$$

is monotone nonincreasing along the solution $f(t)$. Then, given any initial datum $f \in F_m$, or $H^*(f)$ is unbounded, which implies $H^*(f) > H^*(f_\infty)$, or $H^*(f) = c$. In this case, since the solution is given by

$$f(v, t) = \exp\{-\sigma t\}f(v) + [1 - \exp\{-\sigma t\}]f_\infty(v), \quad (3.2)$$

given any convex function $\Psi(r)$

$$\Psi(f(t)) \leq \exp\{-\sigma t\}\Psi(f) + [1 - \exp\{-\sigma t\}]\Psi(f_\infty). \quad (3.3)$$

Hence, coupling (3.3) with Fatou’s Lemma, when both $H^*(f)$ and $H^*(f_\infty)$ are bounded,

$$\lim_{t \to \infty} H^*(f(t)) = H^*(f_\infty). \quad (3.4)$$

Finally, for all $f \in F_m$

$$\int_\Omega \{ |\psi|^2(v)f(v) + \Phi_1[f(v)] \} \, dv \geq \int_\Omega \{ |\psi|^2(v)f_\infty(v) + \Phi_1[f_\infty(v)] \} \, dv, \quad (3.5)$$

with $\Phi_1$ different from the natural entropy. This is in contradiction with Theorem 2.1. If $f_\infty$ is a Maxwellian equilibrium distribution (1.6), the linear operator (3.1) is nothing but the BGK collision operator of the kinetic theory of rarefied gases [3]. So we proved that the relative entropy given by Boltzmann’s $H$-functional is the unique entropy nonincreasing along the solution to this model.

In [1], McKean proved that Boltzmann’s $H$-functional is the only decreasing functional of Kac’s caricature of the Maxwellian gas. His proof makes use of the form of the collision operator, and of a certain dual of Gibbs Lemma. In addition, the initial datum is required to be bounded from below and above in terms of two Maxwellians. By means of Theorem 2.1, the uniqueness of Boltzmann’s $H$-functional (in the class of all entropies of type (1.9)) follows simply assuming that the initial distribution possesses moments of order $2+\delta$, $\delta > 0$, and $H^*(\cdot)$ is lower semicontinuous.
In fact, under the hypothesis of existence of $2 + \delta$ moments, the solution to Kac equation converges exponentially to equilibrium in a metric equivalent to weak*-convergence of measures [12]. Hence, repeating step by step the arguments we used for BGK linear models, (3.5) follows by convexity and lower semicontinuity. On the other hand, since the energy is conserved, 

$$E = \int_{\Omega} v^2 f(v, t),$$

is the unique convex functional which reaches the minimum in correspondence to the Maxwellian distribution.

In view of some recent results on entropy dissipation for the spatially homogeneous Boltzmann equation (1.3) [13], one can conclude that, under the hypotheses that guarantee the convergence to zero of the relative entropy

$$H^*(f) = \int_{\Omega} f(v) \log \frac{f(v)}{f_{\infty}(v)} dv,$$

Boltzmann's $H$-functional is the only decreasing functional (in the class $H^*$) along the solution to Boltzmann equation.

A last consequence of the result of Section 2 is concerned with the use of (1.9) in the study of $L^1$-convergence of kinetic equations towards equilibrium. By Theorem 2.1, given any (strongly) convex function $\Phi$ in $H^*(f)$, there exists a (unique) function $f_{\infty}$ such that, for all densities $f$ with the same mass of $f_{\infty}$, $H^*(f) \geq H^*(f_{\infty})$. Thus, one can define the relative entropy as the difference

$$H^*(f) - H^*(f_{\infty}).$$

In many cases, this relative entropy (3.8) bounds from above the square of $L^1$-distance between $f$ and $f_{\infty}$. The case $\Phi(r) = r \log r$, in which $H^*(f)$ coincides with the classical relative entropy, falls into the classical Csiszar-Kullback inequalities [7,8,10]. The same bound holds for $\Phi(r) = [2/(m - 1)] r^m$, studied in [11]. A general result of the type

$$\|f - f_{\infty}\|_{L^1}^2 \leq c_\Phi [H^*(f) - H^*(f_{\infty})]$$

is at the moment not available.

REFERENCES

