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Concavity of thermostatic entropy and convexity of Lax's mathematical entropy

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Abstract

It is shown that for any real gas in chemical equilibrium, the convexity proposed by Lax is equivalent to the concavity of the entropy considered as thermodynamic potential and the positivity of temperature.

Résumé

Nous montrons que pour tout gaz réel à l'équilibre chimique, la convexité introduite par Lax est équivalente à la concavité de l'entropie considérée comme potentiel thermodynamique et à la positivité de la température.

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1) Introduction

Gas dynamics is based on conservation laws of physics and an assumption of local thermostatic equilibrium (for instance, see Germain [5]) leading to the Euler equations in the case where viscosity and heat conduction are neglected. These equations are included in the general category of nonlinear hyperbolic systems for which Lax suggested a general concept of mathematical entropy in [4, 10]. In the case of a polytropic ideal gas, it is well known [7, 8, 11] that this concept can be interpreted by the usual thermostatic concept of entropy. In this note, we show that for any real gas in chemical equilibrium, the convexity proposed by Lax is equivalent to the concavity of the entropy considered as a thermodynamic potential. Below, we recall the bases of thermostatics and gas dynamics in the next two sections (in order to define the mathematical framework of our analysis), then, in the last section, we analyse the relations between thermostatic entropy and Lax's entropy.

2) Thermostatic equilibrium

In this section, we recall a few essential properties of real gases in thermochemical equilibrium. These properties are established in the classical works of Landau-Lifchitz [9], Callen [1] and Germain [5], for instance.

The thermodynamic properties of a gas with mass M , internal energy E enclosed in volume V are completely determined by these three parameters (M, V, E) . In effect, the thermostatic entropy S is a function of the triplet (M, V, E) :

$$(1) \quad S = \Sigma(M, V, E).$$

We assume that Σ can be differentiated; its first derivatives (and second derivatives when defined) are used to compute all the thermodynamic properties of the gas.

We recall the two fundamental properties of entropy Σ .

Hypothesis 1. Function Σ is first-order homogeneous (entropy is an extensive variable):

$$(2) \quad \Sigma(\lambda M, \lambda V, \lambda E) = \lambda \Sigma(M, V, E), \quad \forall \lambda > 0.$$

Hypothesis 2. Function Σ is superadditive:

$$(3) \quad \Sigma(M + M', V + V', E + E') \geq \Sigma(M, V, E) + \Sigma(M', V', E').$$

This last property expresses the second principle of thermodynamics: when two masses of gas are mixed, the entropy of the resulting system is always higher than or equal to the sum of the entropies of the constituents. From this, we easily infer the following result.

Proposition 1. Function $]0, +\infty[^3 \ni (M, V, E) \mapsto \Sigma(M, V, E)$ is concave.

We remark that temperature T is the inverse of the derivative of the entropy with respect to the internal energy:

$$(4) \quad \frac{1}{T} = \frac{\partial \Sigma}{\partial E}(M, V, E).$$

3) Gas dynamics

The Euler gas dynamics equations express conservation of mass, momentum and energy. They take the form of a nonlinear hyperbolic system of conservation laws:

$$(5) \quad \frac{\partial U}{\partial t} + \operatorname{div} f(U) = 0.$$

Below, in order to simplify the notations, we will restrict ourselves to the case of a single space variable x , but the extension to more than one dimension is straightforward. The conserved variables U and the flux $f(U)$ are expressed as follows (see for instance Germain [5]):

$$(6) \quad U = \left(\rho, q \equiv \rho u, \varepsilon \equiv \rho e + \frac{1}{2} \rho u^2 \right)^t,$$

$$(7) \quad f(U) = \left(\rho u, \rho u^2 + p, \varepsilon u + p u \right)^t.$$

The pressure p introduced in the expression of the flux (7) is defined by the relation $p = (\gamma - 1) \rho e$ in the case of an ideal gas with constant specific heats in a ratio γ (polytropic gas). For a real gas, we have the following general result.

Proposition 2. The pressure p and the specific entropy $s \equiv \frac{\Sigma}{M}$ are defined as functions of the conservative variables U alone.

Proof of Proposition 2. The second identity of (6) allows the internal specific energy e to be defined as a function of U :

$$(8) \quad e = \frac{\varepsilon}{\rho} - \frac{q^2}{2\rho}.$$

In addition, considering the homogeneity of Σ , the specific entropy s depends only on the density and the specific internal energy:

$$(9) \quad s = \sigma(\rho, e) \equiv \Sigma\left(1, \frac{1}{\rho}, e\right) = \frac{1}{M} \Sigma\left(M, \frac{M}{\rho}, M e\right).$$

We then define the pressure by the usual thermostatic properties:

$$(10) \quad p = T \frac{\partial \Sigma}{\partial V}\left(1, \frac{1}{\rho}, e\right).$$

This last expression can be evaluated by function σ alone and the conservative variables by the following relation:

$$(11) \quad p = -\rho^2 \frac{\frac{\partial \sigma}{\partial \rho}(\rho, e)}{\frac{\partial \sigma}{\partial e}(\rho, e)}.$$

□

4) Mathematical entropy

In [4, 10], P. Lax proposes a concept of mathematical entropy for any hyperbolic system of conservation laws (5). It is a function $\eta(U)$ which has the following properties: there exists an entropy flux $\xi(U)$ such that

$$(12) \quad d\xi(U) = d\eta(U) \cdot df(U) \quad \text{for any } U$$

$$(13) \quad U \longmapsto \eta(U) \quad \text{is convex.}$$

For any hyperbolic system of conservation laws (1), nothing *a priori* ensures the existence or uniqueness of a mathematical entropy η satisfying relations (12) and (13).

In the case of gas dynamics, a function $\eta(U)$ satisfying equations (12), (13) and which is nonaffine has the form

$$(14) \quad \eta(U) = -\rho s(U)$$

as is suggested by Friedrichs and Lax in [4], where $s(U)$ was defined in (8) and (9). Below, we shall call this ‘‘Lax’s entropy’’.

Property (12) results from the additional conservation law

$$(15) \quad \frac{\partial}{\partial t}(\rho s(U)) + \frac{\partial}{\partial x}(\rho u s(U)) = 0$$

satisfied for regular solutions of (5), as remarked by Godunov in [6].

The convexity of Lax’s entropy (14) has been thoroughly studied (for instance Harten [7], Hughes, Franca and Mallet [8] and Tadmor [11]) in the case of a polytropic ideal gas for which function Σ has the following particular form

$$(16) \quad \Sigma(M, V, E) = M C_v \left(\log \frac{E M_0}{E_0 M} + (\gamma - 1) \log \frac{V M_0}{V_0 M} \right).$$

In the case of any real gas, Wagner demonstrated [12] that this property was equivalent to the property of convexity of the opposite of the specific entropy ($-s$) with respect to the variables $(\frac{1}{\rho}, u, e + \frac{u^2}{2})$ of the Lagrangian gas dynamics. But, at our knowledge, the convexity of Lax’s entropy does not seem to have been established generally for suitable physical hypotheses. When thermochemical equilibrium is assumed reached, we have the following property.

Proposition 3. The convexity of function $\eta(U)$ defined in (14) is equivalent to the concavity of function $\Sigma(M, V, E)$ and the positivity of the temperature.

Proof of Proposition 3. We first assume Σ to be concave and T to be positive, *i.e.* $\Sigma(M, V, \cdot)$ to be nondecreasing. We compute Lax’s entropy (14) taking (9) then (2) into account. This yields:

$$\eta(U) = -\rho s(U) = -\rho \Sigma \left(1, \frac{1}{\rho}, e \right)$$

$$(17) \quad \eta(U) = -\Sigma(\rho, 1, \rho e).$$

We define two states U_1, U_2 , and we study $\eta((1-t)U_1 + tU_2)$, $0 \leq t \leq 1$. With the notations introduced in (6), the internal energy $\rho e(t)$ associated with state $(1-t)U_1 + tU_2$ equals, considering (8):

$$(18) \quad \rho e(t) = (1-t)\varepsilon_1 + t\varepsilon_2 - \frac{1}{2} \frac{((1-t)q_1 + tq_2)^2}{(1-t)\rho_1 + t\rho_2}$$

and, remarking that mapping $]0, +\infty[\times \mathbb{R} \ni (\rho, q) \mapsto \frac{q^2}{\rho}$ is convex, we deduce

$$(19) \quad \rho e(t) \geq (1-t)\varepsilon_1 + t\varepsilon_2 - \frac{1}{2} \left((1-t) \frac{q_1^2}{\rho_1} + t \frac{q_2^2}{\rho_2} \right).$$

As function Σ is non decreasing with respect to the third argument, we deduce the following inequality from (19)

$$(20) \quad \eta((1-t)U_1 + tU_2) \leq -\Sigma \left((1-t)\rho_1 + t\rho_2, 1, (1-t) \left(\varepsilon_1 - \frac{q_1^2}{2\rho_1} \right) + t \left(\varepsilon_2 - \frac{q_2^2}{2\rho_2} \right) \right)$$

which, considering the concavity of Σ and relation (17), establishes the concavity of Lax's entropy.

We now assume η to be convex. We first demonstrate the concavity of Σ . We choose two states U_1 and U_2 , with zero momentum:

$$(21) \quad q_1 = q_2 = 0.$$

Inequalities (19) and (20) are then equalities and we deduce the following estimate from the convexity of η :

$$(22) \quad \Sigma((1-t)\rho_1 + t\rho_2, 1, (1-t)\varepsilon_1 + t\varepsilon_2) \geq (1-t)\Sigma(\rho_1, 1, \varepsilon_1) + t\Sigma(\rho_2, 1, \varepsilon_2)$$

which, considering the homogeneity of Σ , establishes the required inequality through an elementary calculation detailed below:

$$\begin{aligned} & \Sigma((1-t)M_1 + tM_2, (1-t)V_1 + tV_2, (1-t)E_1 + tE_2) \\ &= ((1-t)V_1 + tV_2) \Sigma \left(\frac{(1-t)V_1}{(1-t)V_1 + tV_2} \frac{M_1}{V_1} + \frac{tV_2}{(1-t)V_1 + tV_2} \frac{M_2}{V_2}, 1, \frac{(1-t)V_1}{(1-t)V_1 + tV_2} \frac{E_1}{V_1} + \frac{tV_2}{(1-t)V_1 + tV_2} \frac{E_2}{V_2} \right) \\ &\geq ((1-t)V_1 + tV_2) \left[\frac{(1-t)V_1}{(1-t)V_1 + tV_2} \Sigma \left(\frac{M_1}{V_1}, 1, \frac{E_1}{V_1} \right) + \frac{tV_2}{(1-t)V_1 + tV_2} \Sigma \left(\frac{M_2}{V_2}, 1, \frac{E_2}{V_2} \right) \right] \\ &= (1-t)\Sigma(M_1, V_1, E_1) + t\Sigma(M_2, V_2, E_2). \end{aligned}$$

We now show that the temperature is positive, *i.e.* that $\Sigma(M, V, \cdot)$ is a nondecreasing function. For this, we introduce $\Delta E > 0$ and we define two states, U_1 and U_2 , as follows:

$$(23) \quad \begin{cases} \rho_1 = \rho, q_1 = \sqrt{8\rho\Delta E}, \varepsilon_1 = E + 4\Delta E \\ \rho_2 = \rho, q_2 = 0, \varepsilon_2 = E. \end{cases}$$

State $(1-t)U_1 + tU_2$ has an internal energy per unit volume computed according to relation (18), *i.e.*

$$(24) \quad \rho e(t) = E + 4t(1-t)\Delta E.$$

Futhermore, considering (17) and (23), we have

$$(25) \quad (1-t)\eta(U_1) + t\eta(U_2) = -\Sigma(\rho, 1, E), \quad \forall t \in [0, 1].$$

The convexity of η expressed by taking $t = \frac{1}{2}$ therefore results in the inequality

$$(26) \quad \Sigma(\rho, 1, E + \Delta E) \geq \Sigma(\rho, 1, E)$$

which, considering the homogeneity (2), establishes the required property. \square

Remark. In [2], we demonstrated the following less general result: if the temperature is positive and the specific internal energy e is a regular function (of class \mathcal{C}^2 , excluding any phase transition) of the (specific entropy s , specific volume $\tau \equiv \frac{1}{\rho}$) pair, the convexity

of function $(s, \tau) \mapsto e(s, \tau)$ is equivalent to that of Lax's entropy. The property of positivity of the temperature for gases in chemical equilibrium is a classical result. For the establishment of this property based on purely physical arguments, the reader is referred, for instance, to Landau and Lifchitz [9]. This last property was also used by Friedrichs and Lax in [4]. The convexity of Lax's entropy was probably already known by Godunov, who introduced in [6] the entropy variables φ , *i.e.* the gradient of (14) with respect to the conservative variables (the bijectivity of the mapping $U \mapsto \varphi$ results immediately from the strict convexity of η). For an extension of the analysis concerning mixing of two gases without mutual interaction, we refer the reader to [3].

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