Convexity of gas-dynamic entropy

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This note shows (A) that gas-dynamic entropy of a single species of a gas is a strictly convex function of the state variables of the gas (1) for the Boltzmann model and (2) for moment closures that minimize mathematical entropy and (B) that the entropy of a plasma can be defined to be a convex function of its state variables.

1 Definitions

Discrete variables.
s := generic species index
i := ion species index
e := electron species index
D := number of dimensions of space (3)

Parameters.
ϵ_0 := permittivity of free space
μ_0 := permeability of free space

Independent variables.
t := position in space
$\mathbf{x}$:= position in space
$\mathbf{v}$:= particle velocity

State variables.
$\mathbf{E}(t,\mathbf{x})$:= electric field
$\mathbf{B}(t,\mathbf{x})$:= magnetic field
$f_\mathrm{s}(t,\mathbf{x},\mathbf{v})$:= particle number density of species s

Derived variables.
S := generic entropy
S^gas := gas-dynamic entropy
S^tot := total entropy
$\mathcal{E}$:= generic energy
$\mathcal{E}^\mathrm{tot}$:= total energy
$\mathcal{E}^\mathrm{gas}$:= gas-dynamic energy
$\mathcal{E}^\mathrm{em}$:= electromagnetic energy

2 Boltzmann model

The Boltzmann equation asserts conservation (or balance) of particles in phase space,

$$\partial_t f_\mathrm{s} + \nabla_\mathbf{x}\cdot(\mathbf{v} f_\mathrm{s}) + \nabla_\mathbf{v}\cdot(\mathbf{a} f_\mathrm{s}) = \mathcal{C}_\mathrm{s},$$

where $q_\mathrm{s} = \pm e$ is particle charge, m_s is particle mass, $\mathbf{a} = \frac{q_\mathrm{s}}{m_\mathrm{s}}(\mathbf{E}+\mathbf{v}\times\mathbf{B})$ is the (Lorentz law) acceleration, and $\mathcal{C}_\mathrm{s}$ is the collision operator.

For simplicity, we consider the case of two species. Then the state variables for the Boltzmann model are f_i, f_e, $\mathbf{E}$, and $\mathbf{B}$.

I claim that a strictly convex entropy for the Boltzmann system is

$$S^\mathrm{tot} := S^\mathrm{gas} + \kappa\mathcal{E}^\mathrm{tot},$$

where

$$\mathcal{E}^\mathrm{tot} = \mathcal{E}^\mathrm{gas} + \mathcal{E}^\mathrm{em}$$

and κ is an arbitrary positive (for mathematical entropy) constant.

To verify this claim it is enough to show that

1. electromagnetic energy is strictly convex in $\mathbf{E}$ and $\mathbf{B}$,
2. gas-dynamic energy is flat (linear) in f_i and f_e, and
3. the gas-dynamic entropy is strictly convex in f_i and f_e.

To demonstrate convexity (for a continuous or Lebesgue-measurable function) it is sufficient to prove midpoint convexity. That is, to show that the entropy is a convex function of the conserved state variables we need that the entropy of the average of two states is less than the average of their entropies.

Firstly, the electromagnetic energy is

$$\epsilon_0 E^2/2 + B^2/(2\mu_0);$$

thus, the electromagnetic energy is a norm, so it is convex in its variables.

Secondly, the gas-dynamic energy is

$$\mathcal{E}_i + \mathcal{E}_e,$$

where the gas-dynamic energies of each species are defined to be

$$\mathcal{E}_i = (m_i/2)\int_v v^2 f_i \quad \text{and}$$
$$\mathcal{E}_e = (m_e/2)\int_v v^2 f_e.$$

The thermal gas-dynamic energy is flat, since

$$\int_v v^2(f_1+f_2) = \int_v v^2(f_1) + \int_v v^2(f_2) \quad (\forall f_1, f_2).$$

Thirdly, the gas-dynamic entropy is defined by the relations

$$\begin{aligned}
&\eta(f) := f \ln f + \alpha f, \\
&S(f) := \int_v \eta(f), \\
&S_i := S(f_i), \\
&S_e := S(f_e), \\
&S^{\text{gas}} = S_i + S_e,
\end{aligned}$$

where α is an arbitrary universal constant. (We will see that choosing $\alpha := (\ln(2\pi) - 1)D/2$, where D is the number of spatial dimensions, yields an entropy consistent with the common gas-dynamic formulas.) Since η is convex ($\eta''(f) = 1/f > 0$), so is S and so is the gas-dynamic entropy.

To confirm that S^{tot} is actually an entropy, one needs to confirm that (1) in the absence of collisions entropy remains constant and (2) in the presence of collisions entropy does not increase. Since flow in phase space is incompressible, we can rewrite the Boltzmann equation as

$$\partial_t f_{\text{s}} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_{\text{s}} + \mathbf{a} \cdot \nabla_{\mathbf{v}} f_{\text{s}} = \mathcal{C}_{\text{s}}.$$

Multiplying by $\eta'(f)$,

$$\begin{aligned}
&\partial_t \eta_{\text{s}} + \mathbf{v} \cdot \nabla_{\mathbf{x}} \eta_{\text{s}} + \mathbf{a} \cdot \nabla_{\mathbf{v}} \eta_{\text{s}} = \eta' \mathcal{C}_{\text{s}}, \quad \text{i.e,} \\
&\partial_t \eta_{\text{s}} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} \eta_{\text{s}}) + \nabla_{\mathbf{v}} \cdot (\mathbf{a} \eta_{\text{s}}) = \eta' \mathcal{C}_{\text{s}}.
\end{aligned}$$

Integrating over velocity space,

$$\partial_t S_{\text{s}}^{\text{gas}} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} S_{\text{s}}^{\text{gas}}) = \int_{\mathbf{v}} \eta' \mathcal{C}_{\text{s}},$$

that is,

$$\partial_t S_{\text{s}}^{\text{gas}} + \nabla \cdot (\mathbf{u}_{\text{s}} S_{\text{s}}^{\text{gas}}) + \nabla \cdot (\mathbf{c}_{\text{s}} S_{\text{s}}^{\text{gas}}) = \int_{\mathbf{c}} \eta' \mathcal{C}_{\text{s}},$$

where $\mathbf{u}$ denotes bulk fluid velocity and $\mathbf{c} : \mathbf{v} - \mathbf{u}$ denotes thermal particle velocity.

Thus, entropy is conserved in the absence of collisions; we will require the net production of mathematical entropy by the collision operators to be negative:

$$\int_{\mathbf{v}} \eta' \mathcal{C}_{\text{i}} + \int_{\mathbf{v}} \eta' \mathcal{C}_{\text{e}} \leq 0.$$

In particular, interspecies collisions must satisfy this inequality and intraspecies collisions must satisfy $\int_{\mathbf{v}} \eta' \mathcal{C}_{\text{s}} \leq 0$.

The 5-moment and 10-moment closures minimize mathematical entropy over all distributions with a given set of moments. To see that the entropy of an entropy-minimizing closure is convex, consider two states q_1 and q_2 and let $f_1 \neq f_2$ be the corresponding entropy-minimizing distributions. The moments of the averaged distribution $(f_1 + f_2)/2$ are the moments of the averaged state $(q_1 + q_2)/2$, so taking $S(\cdot)$ as "the entropy of",

$$\begin{aligned}
&(S(q_1) + S(q_2))/2 \\
&= (S(f_1) + S(f_2))/2 \\
&> S((f_1 + f_2)/2) \\
&\geq S((q_1 + q_2)/2),
\end{aligned}$$

as needed.

3 Verification of convexity for 5-moment gas

Of course one may also directly verify the convexity of the entropy for the 5- and 10-moment closures.

Here is a physical experiment that argues that entropy is a a convex function of density and thermal energy in the 5-moment case. Put equal amounts of gas in containers of equal volume and allow them to exchange all conserved variables freely. Symmetry dictates that in equilibrium the gas in both containers will be in the same state, and since the state variables are conserved their final values will be the average of their initial values. The total entropy must decrease, so the final entropies must be less than the average of the initial entropies.

To show more generally that entropy is a convex function of density, momentum, and total energy contemplate a completely inelastic collision between two equal volumes followed by the experiment above. The collision adds heat, decreasing the total mathematical entropy. (And then the subsequent equilibration of the two volumes further decreases the mathematical entropy.)

Mathematically, making the definitions

$A :=$ average of two values,
$n :=$ density,
$\mathbf{M} :=$ momentum,
$E :=$ total energy,
$U :=$ thermal energy,
$K :=$ kinetic energy,
$S :=$ entropy,

and noting

Property	Name
$AS(n, U) < S(An, AU)$	(strict convexity of entropy in n and U),
$U = E - K$	(linearity of thermal energy in E and K),
$AK(n, \mathbf{M}) >= K(An, A\mathbf{M})$	(convexity of kinetic energy in n and $\mathbf{M}$),
$AK(n_0, M) > K(n_0, A\mathbf{M})$	(strict convexity of kinetic energy in $\mathbf{M}$),
$S_U < 0$	(monotonicity of entropy in thermal energy),
$U_K > 0$	(monotonicity of thermal energy in kinetic energy),

we verify convexity by

Statement/Expression	Reason
$AS(n, U)$	
$\geq S(An, AU)$	(convexity of S in n and U)
$= S(An, U(AE, AK))$	(linearity of U in E and K)
$\geq S(An, U(AE, K(An, AM)))$	(convexity of K and monotonicity of U and S)
$= S(An, AE, AM)$	

as needed for convexity. For strict convexity, the first inequality is strict if $n_1 \neq n_2$ or $U_1 \neq U_2$ (e.g. $E_1 \neq E_2$ and $\mathbf{M}_1 \neq \mathbf{M}_2$) and the second inequality is strict if $\mathbf{M}_1 \neq \mathbf{M}_2$ but $n_1 = n_2$.

To see that kinetic energy is semidefinite, taking
$K = M^2/(2n)$,
$\mathbb{I} := D\text{x}D$ identity matrix, and
$'$:= transpose,

the Hessian of $K(n, \mathbf{M})$ is

$$\text{Hessian}(K) = \begin{bmatrix} \mathbb{I}/n & -\mathbf{M}/n^2 \\ -\mathbf{M}'/n^2 & M^2/n^3 \end{bmatrix};$$

a block determinant computation gives $\det(\text{Hessian}(K)) = \det((M^2\mathbb{I} - \mathbf{MM})/n^4) = 0$, since $(M^2 I - \mathbf{MM}) \cdot \mathbf{M} = 0$ shows that 0 is an eigenvalue. Since $\mathbb{I}$ is positive definite, we may conclude that Hessian(K) is semidefinite.

For the strict convexity of an ideal gas,

$$\begin{aligned}(\gamma - 1)S &= -n \ln((\gamma - 1)U/n^\gamma) \\ &= -n \ln(\gamma - 1)) - n \ln U + \gamma n \ln n\end{aligned}$$

has Hessian

$$\begin{bmatrix} \gamma/n & -1/U \\ -1/U & n/U^2 \end{bmatrix}$$

with determinant $(\gamma - 1)/U^2$, which is positive as long as $\gamma > 1$.