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Positivity of Entropy Production and Phase Density in the Chapman–Enskog Expansion

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Nomenclature

C_k = peculiar velocity, $c_k - v_k$, m/s
$C_{\max}$ = upper bound for peculiar velocity, m/s
c_k = microscopic velocity, m/s
f = phase density, s^3/m^6
f_M = Maxwell distribution, s^3/m^6
Kn = Knudsen number, $\eta / Lp\sqrt{(k/m)T}$
k = Boltzmann's constant, 1.3804×10^{-23} J/K
L = typical length scale, m
m = particle mass, kg
p = pressure, N/m^2
$\mathcal{S}$ = collision term, s^2/m^6
T = temperature, K
t = time, s
v_i = center of mass velocity, m/s
x_k = space variable, m
$\partial v_{\langle i}/\partial x_{j\rangle}$ = symmetric and trace free part of the velocity gradient, 1/s
η = viscosity, kg/ms
ξ = dimensionless velocity
ρ = mass density, kg/m^3
σ = entropy production, J/K
Φ = nonequilibrium part of phase density
$\phi^{(n)}$ = expansion coefficients of Φ

Introduction

IN a recent paper Comeaux et al.[1] showed that the entropy production according to the Burnett equations may become negative. This result stands in contradiction to Boltzmann's H-theorem, which states that the entropy production is positive for any distribution function f. In this Note we show that the negative production of entropy results from the use of approximative solutions of the Boltzmann equation outside their proper range and improper mathematics, that is, a series expansion that does not converge outside that range.

The behavior of rarefied gases is well described by the Boltzmann equation[2,3]

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \mathcal{S} \tag{1}$$

where f is defined such that $f\,\mathrm{d}\boldsymbol{c}\,\mathrm{d}\boldsymbol{x}$ gives the number of particles with velocities in $(c_i, c_i + \mathrm{d}c_i)$ in the space element $(x_i, x_i + \mathrm{d}x_i)$ at time t. The collision term $\mathcal{S}(f, f)$ describes the change of f as a result of collisions among the particles; the particular form of $\mathcal{S}$ can be found in the literature.[2,3]

Being a nonlinear integro-differential equation, the Boltzmann equation cannot be solved analytically and must either be treated numerically or with approximations. The latter is usually done by the Chapman–Enskog method[3] or by Grad's moment method.[4,5]

The Chapman–Enskog method uses a series expansion into powers of the Knudsen number Kn, with the Euler equations as solution of order zero, the Navier–Stokes equation as first-order correction, and the so-called Burnett equations for the second-order approximation. Thus, from the derivation it is clear that the equations—Euler, Navier–Stokes, or Burnett—have only a finite range of applicability (defined by the Knudsen number) and cannot serve for the description of any processes in a gas. Besides, the Burnett equations become unstable for steep gradients.[6]

Boltzmann's celebrated H-theorem[2,3] states that the entropy production

$$\sigma = -k \int \mathcal{S} \ln f \,\mathrm{d}\boldsymbol{c} \tag{2}$$

is positive for all phase densities f. The proof relies on the particular form of the collision term $\mathcal{S}$ and can be found in the cited literature.

Thus, the findings in Ref. 1, a negative entropy production, are in contradiction to the H-theorem. This discrepancy will be discussed in the following.

Positivity of Phase Density and Entropy Production

The Chapman–Enskog method is an expansion in terms of the Knudsen number Kn, which gives the ratio between the mean free path of a gas particle and a typical macroscopic length scale. The method yields the phase density[2,3]

$$f = f_M(1 + \Phi) \qquad \text{where} \qquad \Phi = Kn\phi^{(1)} + Kn^2\phi^{(2)} + \cdots \tag{3}$$

$$f_M = (\rho/m)\sqrt{m/2\pi kT}^{\,3} \exp[-(m/2kT)C^2] \tag{4}$$

The $\phi^{(n)}$ are products between polynomials in the peculiar velocity and derivatives in space and time of temperature and velocity.[3] The simplest example is given by the first Chapman–Enskog expansion for Maxwell molecules where[3,1]

$$\Phi = -\frac{\eta}{p(k/m)T} C_i C_j \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \frac{15}{4}\frac{\eta}{pT}\left(1 - \frac{1}{5}\frac{m}{kT}C^2\right) C_k \frac{\partial T}{\partial x_k} \tag{5}$$

The phase densities for higher-order expansions (Burnett, Super-Burnett) can be found in the literature.

Because of its definition as a number density in phase space, the phase density ought to be positive, and, moreover, the definition in Eq. (2) only makes sense for positive f. The Chapman–Enskog expression, Eq. (3), however, will become negative because Φ will fall below (-1) for large C.

In the proper range of applicability, the gradients of temperature and velocity are rather small, and Φ falls below (-1) only for very large C. However, Φ is always multiplied by the Maxwellian (4).

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which suppresses the negative contributions for the large velocities in question.

To fix our arguments, we introduce a velocity bound $C_{\max}$ defined such that $f \simeq 0$ for $C > C_{\max}$ and demand that

$$\Phi > -1 \qquad \text{for} \qquad C < C_{\max} \tag{6}$$

Because of the polynomial structure of Φ, this requirement is tantamount to

$$|\Phi| < 1 \qquad \text{for} \qquad C < C_{\max} \tag{7}$$

With this in mind, we turn the attention to the entropy production Eq. (2). Because of conservation of mass, momentum, and energy, $\int \mathcal{S} \ln f_M \, \mathrm{d}\boldsymbol{c} = 0$ (Ref. 7), and we find the entropy production as

$$\sigma = -k \int \mathcal{S} \ln(1 + \Phi) \, \mathrm{d}\boldsymbol{c} \tag{8}$$

This equation makes sense under the assumption that $C_{\max}$ is a suitable bound for the collision term $\mathcal{S}$ as well so that $\mathcal{S}$ is negligible above $C_{\max}$, where the argument of the logarithm becomes negative.

The condition of Eq. (7) is the prerequisite for expanding the logarithm into a Taylor series, namely,

$$\begin{aligned}\sigma &= -k \int \mathcal{S}\left(\Phi - \frac{\Phi^2}{2} + \cdots\right) \mathrm{d}\boldsymbol{c}\\ &= -k \int \mathcal{S}\left\{Kn\phi^{(1)} + Kn^2\left[-\frac{1}{2}\left(\phi^{(1)}\right)^2 + \phi^{(2)}\right] + \cdots\right\} \mathrm{d}\boldsymbol{c}\end{aligned} \tag{9}$$

We emphasize that the series does not converge if $|\Phi| \geq 1$. In other words, the series expansion is wrong if the requirement of Eq. (7) is violated.

Thus, if Eq. (7) holds, everything turns out well. In particular, we are allowed to compute the entropy production by means of the expansion in Eq. (9). On the other hand, if Eq. (7) is not fulfilled, the expansion is not allowed and will, if used, give incorrect results, for example, a negative value for the entropy production. This, indeed, is the explanation for the results of Ref. 1, where the preceding expansion is used, but the finite radius of convergence is left out of consideration.

Clearly, the condition of Eq. (7) is not easy to evaluate, in particular because one has to provide the bound $C_{\max}$ first. As an example, we consider the first Chapman–Enskog expansion for Maxwell molecules of Eq. (5). In this case the condition of Eq. (7) can be written as

$$\frac{\eta}{p}\left|\xi_i \xi_j \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right| \leq 1, \qquad \frac{15}{4}\frac{\eta}{p\sqrt{(m/k)T}}\left|\xi_k\left(1 - \frac{\xi^2}{5}\right)\frac{\partial T}{\partial x_k}\right| \leq 1 \tag{10}$$

where ξ_i is a suitable dimensionless velocity with absolute value of the order of $C_{\max}/\sqrt{[(k/m)T]}$. The first of these conditions resembles the conditions of Ref. 1 for positive entropy production in the Burnett case, and we can consider our preceding arguments as the explanation of these conditions.

For the first-order expansion, however, only the first term in the series (9) is required for the entropy production

$$\sigma = -k \int \mathcal{S}\Phi \, \mathrm{d}\boldsymbol{c} \tag{11}$$

which turns out to be positive for all gradients of temperature and velocity.[3] Because the expansion is not allowed if the conditions of Eqs. (7) or (10) are violated, this result must be seen as a mere coincidence. See also Ref. 8, where the authors show that the realizability of some moments of the first-order Chapman–Enskog phase density is not ensured if the gradients become to steep.

Finally, we would like to point out that the computation of the entropy production from Grad's moment method faces similar problems.

Conclusions

We summarize our results as follows:

1) The Chapman–Enskog method does not ensure the positivity of the phase density in general. This poses no problem if the method is applied in the permitted range of processes.

2) A negative entropy production may occur as a result of a negative phase density and improper mathematics (nonconverging series).

3) Therefore, a negative entropy production shows that the approximation is overstressed and as such serves as an indicator for the applicability of the model.[1]

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Resolution of Magnetogasdynamic Phenomena Using a Flux-Vector Splitting Method

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Nomenclature

A_p = Powell's flux-vector Jacobian
$\hat{a}$ = homogeneity variable
$\boldsymbol{B}$ = magnetic field vector
$\boldsymbol{b}$ = unsplit flux
C = left eigenvector matrix
C^{-1} = right eigenvector matrix
c_v = constant-volume specific heat
$\boldsymbol{F}$ = x-direction flux vector
p = pressure
R = gas constant
R_n = nose radius
S = transformation Jacobian from conservative to primitive variables
$\boldsymbol{S}$ = cell-face surface area
S^{-1} = transformation Jacobian from primitive to conservative variables
T = temperature
$\boldsymbol{U}$ = conservative variables vector

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