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STABILITY OF A FLOWING SYSTEM USING INFORMATION THEORY

by N. Stankiewicz

Lewis Research Center

Cleveland, Ohio

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16. Abstract

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SUMMARY

The principle of maximum entropy (disorder) is extended to the nonequilibrium situation of viscous flow and a condition for "thermodynamic" stability is found. Violation of this condition coincides with boundary layer separation in a Newtonian fluid.

INTRODUCTION

The concept of maximum entropy is well known in classical thermodynamics, where it is used as the definition of the stable equilibrium condition. However, information theory with its assumption that the disorder of a statistical system is a measure of its entropy can provide a way of extending the maximum entropy (maximum disorder) concept to nonequilibrium situtations.

The application of information theory to a system of particles having only continuous translational degrees of freedom leads to a thermodynamic description of an ideal, classical gas.

For a compound gas including internal degrees of freedom, the method lends itself easily, for example, to the nonequilibrium phenomenon of the two temperature behavior of a plasma (electron heating). In reference 1 this approach is applied to a plasma where the electrons, ions, and neutrals (with internal energy levels) are treated as reacting species. For the case of a quiescent plasma, the Saha equation at the electron temperature holds as expected; however, for the case of a current-carrying plasma, a departure from "Saha equilibrium" occurs. This effect is negligible at ordinary currents but might be important in high-density areas or in some shock phenomena.

The variational method used in information theory directly yields the most probable distribution function consistent with the constraints imposed on the system. In applying the technique to a flowing system, the constraints are the various flow moments of the distribution function. This is in contrast to equilibrium systems where only static constraints are used. The constraints are not numerical constants but may vary from point to point as determined from the hierarchy of flow equations. These flow equations are derived by taking moments of the Boltzmann collision equation. Unfortunately this gives an open set in which each equation involves the next higher flow moment.

In reference 2 the relation between the most probable velocity distribution function and the flow equations is investigated for a specific case in which the system constraints are mass density, momentum density, and stress energy density. Because the form of the distribution function is known from maximizing the entropy, all the required moments can be calculated, thus closing the set of flow equations. For the special case of one-dimensional channel flow, the equations give Newton's law of viscosity and a parabolic flow profile. The distribution function (the ellipsoidal velocity distribution function) is therefore shown to be consistent with a system undergoing viscous flow.

The stability of a system is a natural consideration in equilibrium thermodynamics and also in the study of flowing systems. In equilibrium thermodynamics there is a set of stability conditions (see e.g., Callen, ref. 3) which is derivable from a minimum energy principle. A violation of these conditions indicates that the system is undergoing a phase transition. That is, the system separates into two or more subsystems. Such a breakup is suggestive of the onset of boundary layer separation in a flowing system.

This study was undertaken to find the stability conditions for a flowing system using the variational principle of maximum entropy and to determine whether a violation of these conditions coincides with a physically recognizable event.

The analysis will be limited to the special case of a system whose particles have an ellipsoidal velocity distribution function. This case is consistent with a flowing system undergoing viscous dissipation.

SYMBOLS

d^3v	$dv_1\ dv_2\ dv_3$
F	phase space density
f	distribution function
h	Planck's constant
m	particle mass
n	particle number density
S	entropy density
v_i	i^{th} component of particle velocity
Γ_{ij}	Lagrange multiplier conjugate to $n\langle v_i v_j\rangle$

δ variation of

μ_i Lagrange multiplier conjugate to $n\langle v_i \rangle$

ψ Legendre transformation of entropy

ω degeneracy

Ω Lagrange multiplier conjugate to n

$\langle \rangle$ average value of

ANALYSIS

The variational equation which gives the ellipsoidal distribution function is

$$\delta S = \Omega \delta n + \sum_i \mu_i \delta\left(n\langle v_i \rangle\right) + \sum_{i,j} \Gamma_{ij} \delta\left(n\langle v_i v_j \rangle\right) \tag{1}$$

where Ω, μ_i, and Γ_{ij} are Lagrange multipliers. The entropy is defined as (ref. 1)

$$S = -\omega\left(\frac{m}{h}\right)^3 \int f(\ln f - 1)\, dv^3 \tag{2}$$

and the constraints are

$$n = \omega\left(\frac{m}{h}\right)^3 \int f\, dv^3 \tag{3}$$

$$n\langle v_i \rangle = \omega\left(\frac{m}{h}\right)^3 \int f v_i\, dv^3 \tag{4}$$

$$n\langle v_i v_j \rangle = \omega\left(\frac{m}{h}\right)^3 \int f v_i v_j\, dv^3 \tag{5}$$

The integrals are carried out over all velocities from $-\infty$ to $+\infty$.

The variation δ in equation (1) operates on the distribution function f. With the substitution of equations (2) to (5), this yields the ellipsoidal distribution function

$$f = \exp\left(-\Omega - \sum_{i} \mu_i v_i - \sum_{i,j} \Gamma_{ij} v_i v_j\right) \tag{6}$$

The relation between f and the density F in phase space is

$$F = \omega\left(\frac{m}{h}\right)^3 f \tag{7}$$

The maximum density in phase space is $\omega(m/h)^3$ for the completely degenerate gas, for which case $f = 1$.

Because S is a maximum consistent with the constraints of the system, its second order variation must be negative, that is,

$$\delta^2 S < 0 \tag{8}$$

This condition must be satisfied for stability. However, it is convenient mathematically to work out the stability conditions using a Legendre transformation of the entropy, namely,

$$\psi = S - \Omega n - \sum_{i} \mu_i n \langle v_i \rangle - \sum_{i,j} \Gamma_{ij} n \langle v_i v_j \rangle \tag{9}$$

Then

$$\delta\psi = -n\delta\Omega - \sum_{i} n\langle v_i \rangle \delta\mu_i - \sum_{i,j} n\langle v_i v_j \rangle \delta\Gamma_{ij} \tag{10}$$

It is a property of Legendre transformations (see ref. 4) to preserve the variational principle. Thus the function ψ is also an extremal but minimized, that is,

$$\delta^2\psi = 0 \tag{11}$$

It can be shown, using equations (2) to (6) and the transformation of equation (9) that

$$\psi \equiv n \tag{12}$$

Therefore, from equation (10)

$$\left(\frac{\partial n}{\partial \Omega}\right)_{\mu, \Gamma} = -n; \quad \left(\frac{\partial n}{\partial \mu_i}\right)_{\Omega, \Gamma} = -n\langle v_i\rangle; \quad \left(\frac{\partial n}{\partial \Gamma_{ij}}\right)_{\Omega, \mu} = -n\langle v_i v_j\rangle \tag{13}$$

These relations can be verified by carrying out the partial derivatives on equation (3) and using the distribution function in equation (6).

The second order variation of $n(\equiv\psi)$ is then (ref. 3)

$$\delta^2 n = \frac{1}{2}\Bigg[\left(\frac{\partial^2 n}{\partial \Omega^2}\right)(\delta\Omega)^2 + 2\sum_{i}\left(\frac{\partial^2 n}{\partial \mu_i \partial \Omega}\right)\delta\Omega\delta\mu_i$$

$$+ 2\sum_{i,j}\left(\frac{\partial^2 n}{\partial \Gamma_{ij}\partial \Omega}\right)\delta\Gamma_{ij}\delta\Omega + \sum_{i,j,k}\left(\frac{\partial^2 n}{\partial \mu_i^2}\right)(\delta\mu_i)^2$$

$$+ \sum_{i,j\neq i}\left(\frac{\partial^2 n}{\partial \mu_i \partial \mu_j}\right)\delta\mu_i\delta\mu_j + 2\sum_{i,j,k,}\left(\frac{\partial^2 n}{\partial \mu_i \partial \Gamma_{jk}}\right)\delta\mu_i\delta\Gamma_{jk}$$

$$+ \sum_{i,j}\left(\frac{\partial^2 n}{\partial \Gamma_{ij}^2}\right)(\delta\Gamma_{ij})^2 + \sum_{\substack{i,j,k,l \\ (i,j)\neq(k,l)}}\left(\frac{\partial^2 n}{\partial \Gamma_{ij}\partial \Gamma_{kl}}\right)\delta\Gamma_{ij}\delta\Gamma_{kl}\Bigg] \tag{14}$$

The coefficients of the variations in equation (14) form a 10 by 10 matrix. (There are 10 independent Lagrange multipliers: Ω, three components of the vector μ, and six elements of the symmetric tensor Γ.) The quadratic form of equation (14) is greater than zero (see eq. (11)), if the determinant of the matrix is positive definite. A necessary and sufficient condition for positive definiteness requires that the leading principal minors are positive (see e.g., ref. 5).

Because the matrix is of order 10, there will be 10 independent conditions for stability that can be found. However, the rows and columns of the matrix can be arranged in many ways without disturbing the value of its determinant. As a consequence, only the principal minors of order one and two need be considered; all other minors will give redundant conditions.

The 10 basic stability conditions are then found to be

$$\frac{\partial^2 n}{\partial \Omega^2} > 0 \tag{15}$$

$$\frac{\partial^2 n}{\partial \mu_i^2} > 0; \; i = 1, 2, 3 \tag{16}$$

$$\left(\frac{\partial^2 n}{\partial \Omega^2}\right)\left(\frac{\partial^2 n}{\partial \mu_i^2}\right) - \left(\frac{\partial^2 n}{\partial \Omega \, \partial \mu_i}\right)^2 > 0; \; i = 1, 2, 3 \tag{17}$$

$$\left(\frac{\partial^2 n}{\partial \Omega^2}\right)\left(\frac{\partial^2 n}{\partial \mu_i \partial \mu_j}\right) - \left(\frac{\partial^2 n}{\partial \Omega \, \partial \mu_i}\right)\left(\frac{\partial^2 n}{\partial \Omega \, \partial \mu_j}\right) > 0; \; i \neq j = 1, 2, 3 \tag{18}$$

Using the definition of n in equation (3) and the distribution function from equation (6) and carrying out the partial derivatives, the stability conditions then are

$$n > 0 \tag{15a}$$

$$n \langle v_i^2 \rangle > 0 \tag{16a}$$

$$n^2 \left(\langle v_i^2 \rangle - \langle v_i \rangle^2 \right) > 0 \tag{17a}$$

$$n^2 \left(\langle v_i v_j \rangle - \langle v_i \rangle \langle v_j \rangle \right) > 0 \tag{18a}$$

Equations (15a) and (16a) are trivial and are always satisfied. Equation (17a) is a condition that the mean random energy for each direction be positive. This is equivalent to the condition that the temperature be positive and is consistent with the ideal gas assumption. For real gases the analogous condition should be that the temperature be greater than a temperature at which a change of phase occurs.

The shear stress is defined in kinetic theory as $mn \left(\langle v_i v_j \rangle - \langle v_i \rangle \langle v_j \rangle \right)$ and must be positive according to equation (18a) if the flow is to remain stable. For Newtonian fluids the shear stress at the wall is proportional to the velocity gradient and a violation of equation (18a) will occur whenever the gradient vanishes or changes sign. The vanishing of the velocity gradient at the wall is recognized in fluid dynamics as the onset of boundary layer separation.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, January 8, 1970,
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