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On Stability of Steady States

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Conditions of stability with respect to finite perturbations of a steady transport state are derived on the basis of a statistical theory for a very general type of equations of motion for the state change. Infinitesimal perturbations yield the stability condition of Glansdorff and Prigogine.

1. Introduction

In this paper the question shall be discussed under which conditions a steady state of a physical system is stable with respect to finite perturbations. The steady state shall be a state of transport which can be described by means of thermodynamic variables and includes thermodynamic fluxes such as heat flow and electrical current. The steady state may be far away from thermodynamic equilibrium.

Recently a criterion was given by Glansdorff and Prigogine[1] for the stability of a steady state with respect to small perturbations. These perturbations were considered up to the second order. As is well known from stability problems in other fields, such criteria for small perturbations can totally fail with respect to larger perturbations. It is of great practical importance to know whether a state is stable against a finite perturbation of a certain given extent.

The starting point is a statistical theory, as the microscopic basis of phenomenological macroscopic thermodynamics. The transport states, of which the steady state is a special one, are described by stochastic processes. Stability criteria in this description are criteria for the steady stochastic process. In the following stochastic processes are considered which can be described by differential equations for the probability distribution of first order in time. That means that no memory effects are included.

The stability condition obtained in the following leads to the condition of Glansdorff and Prigogine in the special case that the deviations from the steady state become infinitesimal small. Thus a special result of the following consideration is a statistical foundation of the Glansdorff-Prigogine condition, too.

1 Glansdorff, P., Prigogine, I.: Physica **46**, 344 (1970).

2. Liapunov's Theorem in a Special Case

Let the different transport states of a physical system be uniquely characterized by a set of parameters

$$\xi=(\xi_1, \xi_2, \dots, \xi_f). \tag{2.1}$$

They shall be chosen in such a way that the origin of this parameter space corresponds to the steady state the stability of which is investigated. The change of states with time may be described by a set of differential equations of the type

$$\dot{\xi}_k=f_k(\xi). \tag{2.2}$$

Let be $L(\xi)$ a real function, existing in the whole parameter space ξ and being positive definite

$$L(\xi)\geqq 0 \tag{2.3}$$

such that it vanishes in the origin only. If, moreover, it is concave so that the second variation is positive

$$\delta^{(2)} L=\frac{1}{2}\sum_{kl} \frac{\partial^2 L}{\partial \xi_k \partial \xi_l} \delta \xi_k \delta \xi_l \tag{2.4}$$

in any point ξ, then we can state the following:

If there exists a region in the parameter space which contains the origin in its interior and if

$$\dot{L}(\xi)\leqq 0, \tag{2.5}$$

then the motion is stable whenever it starts in the interior of this region. "Stable" means that the motion does not lead out of a certain limited neighbourhood of the origin. If, moreover, the equality sign in (2.5) is valid in the origin only, then the motion is "asymptotically stable" and leads finally into the origin. If (2.3) and (2.5) are valid in this region, then L is called a Liapunov function.

The proof is nearly obvious. (2.3) and (2.4) grant that $L(\xi)$ is monotonous such that any surface on which L has constant value encloses all surfaces with smaller value of L. (2.5) means that the motion can go only into the interior of the surface on which it starts, or at least remain on it. It never can go out of this region.

The general theorem of Liapunov[2] requires (2.3) only in a certain region round the origin. Then (2.4) is fulfilled at least in the neighbourhood of the origin. In the following we give a function L which has the features (2.3), and (2.4) in the whole parameter space ξ. In this case, we can

2 Lasalle, J., Lefschetz, S.: Stability by Liapunov's direct method. New York: Acad. Press Inc. 1961. German translation: Die Stabilitätstheorie von Ljapunoff. Mannheim: B. I. Hochschultaschenbücher 194.

apply the theorem in a special form and can give the limits of the stability region:

The steady state is stable if there exists a region which includes the origin and in which (2.5) is valid. The steady state is stable with respect to all deviations which lie in this region. The region of stability is limited by the surface with largest possible constant value of L which includes points only where (2.5) is fulfilled.

3. Gain of Information as Liapunov Function

The microstates of the physical system may be characterized by an index i, which can be the symbol of a whole set of numbers. The assumption that the microstates are denumerable is not essential for the following and can be dropped without real difficulty. The assumption, however, which always can be fulfilled in arbitrarily good approximation by dividing the state space in small cells, facilitates the notation.

A macrostate corresponds to a probability distribution

$$p=(p_1, p_2, \ldots)=(p_i). \tag{3.1}$$

A macroscopic change of states with temporal evolution corresponds to a change of the distribution p with time.

The name "microstate" is used in a very general way. The physical system can be defined e.g. by all particles in a fixed volume. Such a system does not have a fixed phase space but a multiplicity of phase spaces with different particle numbers as it is used e.g. by defining a grand canonical distribution. The generalisation can go even into another direction. The so called microstates need not be given by all dynamical variables of the particles. They can be given by variables the number of which is smaller than that of all dynamical variables, however large compared to the number of macroscopic variables which are used to describe the transport states in view. An example are the particle velocities in the velocity distribution of the Boltzmann equation. Another example would be variables to describe detailed thermal fluctuations in small parts of a system.

We can assume that the "microstates" in this sense are chosen such that the probability distribution p' which corresponds to the steady state is time independent.

In the following we restrict the considerations to stochastic laws of the form

$$\dot{p}_i=\varphi_i(p). \tag{3.2}$$

This restriction excludes memory effects, for which the function φ_i of the distribution p had to be replaced by a functional of the time function $p(t)$. In the special case of a Marcovian process φ_i becomes linear in p.

We shall consider non Marcovian processes, as well, for which φ_i is non linear in p.

The probabilities p_i fulfil the relation

$$\sum_i p_i = 1 \tag{3.3}$$

and therefore are not independent one from another. We can, however, always find independent parameters ξ_k which are linearly connected with the probabilities p_i and characterize, uniquely, the distribution p. We can moreover choose the ξ_k in such a manner that the steady state p' corresponds to the origin of the ξ-space. (3.2) leads to differential equations of the form (2.2).

The quantity

$$K(p, p') = \sum_i p_i \ln \frac{p_i}{p'_i} \tag{3.4}$$

is positive definite and vanishes only if the distributions p and p' are identical.

Moreover, in an expansion of K in powers of a small change δp of p

$$\begin{aligned} \delta K &= K(p+\delta p, p') - K(p, p') \\ &= \sum_i \delta p_i \ln \frac{p_i}{p'_i} + \frac{1}{2} \sum_i \frac{(\delta p_i)^2}{p_i} + \cdots \end{aligned} \tag{3.5}$$

the second order variation is positive,

$$\delta^{(2)} K = \frac{1}{2} \sum_i \frac{(\delta p_i)^2}{p_i} > 0 . \tag{3.6}$$

If we express K as function of the parameters ξ_k

$$K(p, p') = L(\xi), \tag{3.7}$$

it has the features (2.3) and (2.4). Therefore stability condition (2.5) is

$$-\dot{K}(p, p') = -\dot{L}(\xi) \geqq 0 . \tag{3.8}$$

4. Stability Condition Expressed by Thermodynamic Quantities

The entropy of the state p is

$$S(p) = -\sum_i p_i \ln p_i . \tag{4.1}$$

Boltzmann's constant k is made equal to unity by adequate choice of units.

In the following we shall denote the deviation from the steady state by

$$\delta p_i = p_i - p_i' . \tag{4.2}$$

Then

$$K(p' + \delta p, p') = -\delta S - \sum_i \delta p_i \ln p_i' \tag{4.3}$$

and

$$\begin{aligned} -\dot{K}(p' + \delta p, p') &= \delta \dot{S} + \sum_i \delta \dot{p}_i \ln p_i' \\ &= -\sum_i \delta \dot{p}_i \ln \left(1 + \frac{\delta p_i}{p_i'}\right) \\ &= -\sum_i \frac{\delta \dot{p}_i \delta p_i}{p_i'} + \cdots . \end{aligned} \tag{4.4}$$

If δS and $\delta \dot{S}$ are expanded in powers of δp, $\delta \dot{p}$, then it is to be seen that the left side of (4.3) is equal to the non linear part $-\delta_{NL} S$ of $-\delta S$ and that the left side of (4.4) is equal to the non linear part of $\delta \dot{S}$:

$$K(p' + \delta p, p') = -\delta_{NL} S \tag{4.5}$$

$$-\dot{K}(p' + \delta p, p') = \delta_{NL} \dot{S} . \tag{4.6}$$

We state, moreover, that the linear part of $\delta \dot{S}$ contains $\delta \dot{p}$ only and not δp.

Let be M a macroscopic variable which is the mean value of a variable M_i in the microstates i:

$$M = \sum_i p_i M_i . \tag{4.7}$$

Then its derivative with respect to time is

$$\dot{M} = \sum_i \dot{p}_i M_i . \tag{4.8}$$

Macroscopic variables of this kind are called extensive variables in contrast to intensive variables. The latter are parameters of a canonical distribution. If p' is canonical and the M are thermostatic quantities, then $\ln p_i'$ is linear in M_i.

We always can characterize macroscopic transport states by an appropriate set of extensive variables including nonstatic quantities like flows. In the following we assume that also for a steady state $\ln p_i'$ is linear in M_i. If we expand δS, $\delta \dot{S}$ in powers of δM, $\delta \dot{M}$, then the non linear part of these expansions is identical with the non linear part of the expansion in powers of δp, $\delta \dot{p}$, as K, $\dot{K}$ have no linear parts. Moreover, the linear part of $\delta \dot{S}$ contains $\delta \dot{M}$ only, and not δM.

In that way we get the result that the non linear parts with respect to the extensive variables are connected with $L(\xi)$:

$$L(\xi) = -\delta_{NL} S \tag{4.9}$$

$$-\dot{L}(\xi) = \delta_{NL} \dot{S}. \tag{4.10}$$

Finally we can state the following:

For all deviations from the steady state there is valid

$$-\delta_{NL} S \geqq 0. \tag{4.11}$$

The equality sign is fulfilled for vanishing deviation only.

A stability region, if it exists, is the largest region round the steady state in the space of the extensive parameters which is limited by a surface with constant value of $\delta_{NL} S$ and in which everywhere is fulfilled:

$$\delta_{NL} \dot{S} \geqq 0. \tag{4.12}$$

5. Relation to Stability Theory of Glansdorff and Prigogine

Glansdorff and Prigogine[1] derived a stability criterion for small deviations from the steady state by thermodynamic arguments. This criterion states that the steady is stable with respect to small deviations if the second order variation of $\dot{S}$ is positive:

$$\delta^{(2)} \dot{S} \geqq 0. \tag{5.1}$$

This criterion is a special result of the more general one given above because it is concerned with infinitesimal small perturbations only.

If, in special cases, the stability region is very small, the practical value of stability with respect to infinitesimal perturbations can be relatively small. The general criterion, however, gives the answer to the question relevant for practice, how large perturbations may be without leading to instability.

Some relations should be given to the well known Glansdorff-Prigogine variation of entropy production, which was introduced 1964 in the theory of stationary states[3].

In an earlier paper[4] it was pointed out that

$$-K(p, p^0) = -\sum_i p_i \ln \frac{p_i}{p_i^0} \tag{5.2}$$

3 Glansdorff, P., Prigogine, I.: Physica **30**, 351 (1964). — Prigogine, I., Glansdorff, P.: Physica **31**, 1242 (1965).

4 Schlögl, F.: Z. Physik **198**, 559 (1967).

is the entropy produced in the interior of a system by a process in which the state p changes spontaneously into the equilibrium state p^0. That suggests to define

$$P = -\dot{K}(p, p^0) \tag{5.3}$$

as entropy production in the interior of the system. For the deviation of P from the state p' to p we get

$$\begin{aligned} \delta P &= -\sum_i \delta \dot{p}_i \ln \frac{p_i' + \delta p_i}{p_i^0} \\ &= \delta_{NL} \dot{S} - \sum_i \delta \dot{p}_i \ln \frac{p_i}{p_i^0} \end{aligned} \tag{5.4}$$

$$\delta_{NL} P = \delta_{NL} \dot{S}. \tag{5.5}$$

Moreover the linear part of δP contains $\delta \dot{p}$ only, but not δp. It, therefore, does not contain δM.

Entropy production is most generally a bilinear form

$$P = X_\nu I^\nu \tag{5.6}$$

of "fluxes" I^ν and "forces" X_ν. The forces X_ν are dependent on static thermodynamic quantities M only, but not on the $\dot{M}$. Therefore the linear part of δP does not contain δX_ν and we get

$$\delta_{NL} P = I^\nu \delta X_\nu. \tag{5.7}$$

This is the well known Glansdorff-Prigogine variation[3].

6. Interpretation of the Result

The quantity K in (3.4) was defined by Rényi[5] as "gain of information" which is necessary to come from p' to p. In earlier papers it was shown[6] that this quantity has an important meaning in thermodynamic statistics, especially in non equilibrium theory, in different respects.

The meaning of K gives an interpretation of the stability conditions which were derived above. This interpretation is not necessary for the derivation. It, however, gives a better insight.

A steady state is a state of the system in which the knowledge of the observer about the system does not change with time. This is true because the probability distribution p' describing this state does not change

5 Rényi, A.: Wahrscheinlichkeitsrechnung. Berlin: VEB Deutscher Verlag der Wissenschaften 1966.

6 Schlögl, F.: Z. Physik **191**, 81 (1966). — Schlögl, F.: Ann. Physics **45**, 155 (1967).

with time. If p' is a stable steady state, and the observer does not know more than that the system initially once was in some unknown state of the stability region, then an unbiased estimate for the momentary state would lead to p'. If the observer, however, knows e.g. by observation the momentary state p, then his excess knowledge is measured by K of (3.4). The spontaneous development of the states after the last observation can only go such that this knowledge does not increase.

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