

Hamilton's action principle and thermodynamics of irreversible processes — a unifying procedure for reversible and irreversible processes

K.-H. Anthony*

Universität Paderborn, Theoretische Physik, D-33095 Paderborn, Germany

Received 20 September 1999

In memory of my dear teacher and friend, Prof. Dr. Ekkehard Kröner[†] (19 April 2000).

Abstract

Thermodynamics of irreversible processes can be included into the framework of Lagrange formalism. This formalism presents a unified method for reversible and irreversible processes. As a remarkable fact the first and the second law of thermodynamics are *derived in* Lagrange formalism by means of straightforward procedures. The whole information on the dynamics of a system is included in one function only, namely in its Lagrangian.

In this paper the theory is presented in two courses. The first one offers an almost qualitative insight into the structure of the theory; the second one is concerned with the associated mathematics in some detail. The theory is illustrated by three representative examples: the style of the paper is chosen as to stimulate the discussions at a workshop and a school on the state-of-art of non-equilibrium thermodynamics of complex fluids, Oxford, 2000. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Hamilton's action principle; Lagrange formalism; Thermodynamics

1. Lagrange formalism — retrospection and perspectives towards thermodynamics of irreversible processes

Lagrange formalism (LF) in the true meaning of the word is based on Hamilton's action principle. It is well established in a lot of physical disciplines as far as reversible processes is concerned, e.g. in mechanics, quantum mechanics, electrodynamics and nuclear physics. It is a powerful tool for constructing theories as well as for solving approximately particular problems. However, traditionally there is a missing link with regard to thermodynamics of irreversible processes (TIP). One is considerably faced with the opinion, that TIP is principally outside the scope of LF. In the author's opinion this is but an unproved dogma. This paper will show that TIP can be involved into the framework of LF.

* Tel.: +49-5251-602338 (O)/+49-5255-1717 (R); fax: +49-5251-603435 (O)/+49-5255-7945 (R).

E-mail addresses: anthony@phys.uni-paderborn.de, anthony.schwaney@t-online.de (K.-H. Anthony).

1.1. Hamilton's action principle — Lagrange formalism

Lagrange formalism and Hamilton's action principle are commonly known from classical mechanics of conservative, i.e. non-dissipative point systems [1,2]. Referring the system to a finite set $q = \{q_j, j = 1, \dots, f\}$ of generalized coordinates the real physical motion $q(t)$ in the time interval $[t_1, t_2]$ is distinguished as a solution of *Hamilton's action principle*:

$$J = \int_{t_1}^{t_2} L(q, \dot{q}, t) dt = \text{extremum} \quad (1.1)$$

with respect to free variations $\delta q(t)$ of the real motion $q(t)$ keeping fixed its values at the beginning and the end of the motion: $\delta q(t_{1,2}) = 0$.

J is called the *action integral* of the motion. Depending on the special situation of the actual motion it may be a minimum or a maximum. The kernel L of the variational problem is the *Lagrange function* (*Lagrangian*) of the system. In the case of potential forces it is defined by

$$L = T - U, \quad (1.2)$$

where T and U are the kinetic and potential energies of the system. The *Euler–Lagrange equations*,

$$\frac{d}{dt} \frac{dL}{d\dot{q}_k} - \frac{dL}{dq_k} = 0, \quad k = 1, \dots, f \quad (1.3)$$

are the fundamental equations of motion; they are necessary conditions for an extremum of the action J . The Legendre transform of L , called *Hamilton's function*, is another prominent quantity in LF:

$$H(q, \dot{q}, t) = \sum_{j=1}^f \frac{dL}{d\dot{q}_j} \dot{q}_j - L(q, \dot{q}, t). \quad (1.4)$$

It is physically associated with the mechanical energy of the system.

Generalizing this concept in a natural way it may be taken over into field theory [3]. Let a physical system operate in the region V of the three-dimensional space, referred to the coordinates $x = \{x^1, x^2, x^3\}$, and let its processes be defined by the set $\psi = \{\psi_j, j = 1, \dots, f\}$ of fundamental-field variables. For simplicity let us assume the volume V to be constant in time.¹ Then a real physical process $|\psi(t)\rangle = \{\psi(x, t)\} = \{\psi_j(x, t), j = 1, \dots, f\}$ ² running in the time interval $[t_1, t_2]$ is distinguished as a solution of *Hamilton's action principle*:

$$J_{(1)} = \int_{t_1}^{t_2} \int_V \ell(\psi, \partial_t \psi, \nabla \psi, x, t) dV dt = \text{extremum} \quad (1.5)$$

with respect to free variations $\delta \psi(x, t)$ of the real process $\psi(x, t)$ keeping fixed its values at the beginning and the end of the process in the volume V and on its boundary ∂V : $\delta \psi(x, t_{1,2}) = 0$.

¹ A time-dependent volume occurring in the dynamics of a deformable body implies a lot of formal difficulties. $V(t)$ can be taken into account by means of coordinate systems being dragged along either with the deformed body or at least with its outer shape. These details get important, e.g. in plasticity theory which can be involved into LF, too [4].

² The notation $|\psi(t)\rangle$ indicates the system's "state vector" in analogy with the customs in quantum mechanics.

Now, the kernel ℓ of the variational problem is the *Lagrange density function* associated with the system; again it is called the *Lagrangian* of the system. The integral $J_{(1)}$ is called *action integral*; in the subsequent context the index (1) indicates “action integral of the first kind”. In contrast to Eq. (1.2) it cannot be defined from partial energies, in general. The construction of the Lagrangian is now a main task of the theory. In field theory we have to forget about the expression (1.2) which as a sort of mystery is widely spread, even outside mechanics. The *Euler–Lagrange equations* (LEqs),

$$\partial_\alpha \frac{\partial \ell}{\partial (\partial_\alpha \psi_k)} - \frac{\partial \ell}{\partial \psi_k} = 0, \quad k = 1, \dots, f, \quad (1.6)$$

are the *fundamental field equations* of the system. Instead of ordinary differential equation (1.3) we are now dealing with partial differential equations. Formula (1.4) is replaced by the *Hamilton density function*

$$h(\psi, \partial_t \psi, \nabla \psi, x, t) = \sum_{j=1}^f \frac{\partial \ell}{\partial (\partial_t \psi_j)} \partial_t \psi_j - \ell(\psi, \partial_t \psi, \nabla \psi, x, t), \quad (1.7)$$

which within LF is interpreted as the *energy density* of the system.

In Eq. (1.6) and occasionally throughout the paper the following notations are used:

$$\begin{aligned} x &= \{x^\alpha\} = \{x^0 = t, x^1, x^2, x^3\}, \\ \partial_t &= \frac{\partial}{\partial t} = \partial_0 = \frac{\partial}{\partial x^0}, \\ \partial_\alpha &= \frac{\partial}{\partial x^\alpha}, \quad \nabla = \{\partial_1, \partial_2, \partial_3\}. \end{aligned} \quad (1.8)$$

Summation convention is used only for summation over the indices α of space–time coordinates. All other summations are denoted explicitly.

The Lagrangians L and ℓ in Eqs. (1.1) and (1.5) depend on the fundamental variables q and ψ , respectively, and on all its first derivatives, i.e. we are dealing with *first-order Lagrange formalism*. The formalism could be generalized to higher order. However, by appropriately substituting derivatives by auxiliary variables and by taking account of the substitutions in the variational procedure by means of Lagrange multipliers, the formalism indirectly may always be reduced to the first order in taking a detour.

In the action integrals (1.1) and (1.5) the Lagrangians L and ℓ are instantaneous. At time t they depend on the actual state $q(t)$ and $\psi(x, t)$. So, we are dealing with *instantaneous theories*; no after-effects (hysteresis) are contained in the theory. As a consequence and at a first glance this formalism seemingly does not allow of TIP for materials with memory, which of course are a main topic in TIP. However, keeping in mind that phenomenological after effects are due to *hidden variables*, which cannot be immediately manipulated, the task arises to physically identify these variables and to *raise them into the position of phenomenological variables*, i.e. to add them to the set ψ of relevant, fundamental field variables in order to establish an instantaneous theory. So, subsuming TIP in LF includes *the problem of finding the appropriate set of fundamental field variables*. It will be shown, that the answer may be quite unusual from the traditional point of view of TIP.³ In principle one could introduce the Lagrangian as a memory functional. However, such a procedure would destroy the appeal of LF.

³ Along the line of the LF as presented here we have proposed a phenomenological field theory of plastic deformation. Plasticity is microscopically due to dislocation dynamics, which gives rise to deformation hysteresis accompanied by dissipation. So, dislocations are an example for well identified hidden variables, which are enclosed as complex variables into the set ψ of fundamental field variables [4].

Furthermore, on the basis of an action principle of the form Eq. (1.5) we are dealing with a *local theory*. The Lagrangian at site x depends on the states $\psi(x, t)$ at that site.

The Lagrangian as an *individual structure of a system* contains all information on the dynamics of the system. *Once a Lagrangian is given, a system is completely defined* irrespective of its physical existence in real world.⁴ So, we are confronted with the problem of finding the correct Lagrangian for a physically given system.

$$\text{Additive terms} \quad \partial_t g(q, t) \text{ and } \partial_\alpha g^\alpha(\psi, x, t) \quad (1.9)$$

in L and ℓ with arbitrary functions g and g^α are irrelevant for the ELeqs (1.3) and (1.6), respectively. This implies, that the solutions of Hamilton's principle are not affected by the terms (1.9), i.e. these terms are irrelevant for the “*kinematics*” of the system. However, in general they are relevant for the “*dynamics*” of the system. Eq. (1.9)₂ gives rise to additional terms in the energy density (1.9). The concepts “*kinematics*” and “*dynamics*” and its difference will get apparent during the course of this paper.

Looking at the arguments of the Lagrangians in Eqs. (1.1) and (1.5) the variables q and ψ are associated with the *internal eigendynamics* of the system whereas the explicit variables t and (x, t) are due to the *intervention of the outer world into the system*. The dynamics of the outer world does not take part in the variational procedure of Hamilton's principle. Its variables are strictly controlled from outside, giving rise to the explicit dependence of the Lagrangian on the variables t or (x, t) , respectively.⁵ This paper is confined to *TIP of isolated systems* which by no means interact with their outer world. This implies the special structure

$$\ell = \ell(\psi, \partial_t \psi, \nabla \psi) \quad (1.10)$$

of the Lagrangian and

$$\text{vanishing physical fluxes of any kind,} \quad (1.11)$$

where the fluxes already imply a good deal of the theory (see below).

Let us now focus our interest on field theory exclusively. To construct the Lagrangian (1.10) for a given system we may proceed in the following two different ways:

1. Following physical intuition an *ansatz* for the Lagrangian gives rise to a cyclic procedure of try and error. Its consequences obtained from LF have to fit the given system in every respect, i.e. not only with respect to the desired fundamental field equations but also with respect to all relevant balance and constitutive equations.
2. The *inverse problem of variational calculus* aims at the construction of a Lagrangian associated with a given set of field equations [6–9]. Two different problems have to be distinguished as follows:
 - 2.1. The ELeqs as the fundamental field equations have to reproduce the given set of field equations. There is no special care taken to the relevant balance equations of the system. Let us call this procedure the *inverse problem of the first kind* (IP1).

⁴ This statement coincides methodically with the same statement in rational thermodynamics. Once a relevant set of balance equations and the constitutive equations for the associated densities, flux densities and production rate densities are given, a physical system is defined irrespective of its physical existence [5].

⁵ For example, the explicit time dependence of L in Eq. (1.1) is usually due to an explicitly time dependent potential $U(q, t)$ in Eq. (1.2), which is controlled from outside of the system.

- 2.2. The given set of fundamental field equations is supplemented by a set of fundamental balance equations, such as the energy balance, the balance of linear momentum, mass balance, etc. The procedure of item 2.1 is now supplemented by the requirement that LF also reproduces the given set of balance equations. Let us call it the *inverse problem of the second kind* (IP2) [10].

The IP1 can be solved if and only if the given set of field equations (differential equations) is *self-adjoint*. This property implies a set of differential identities which define criteria for the existence of a Lagrangian. In general a given set of differential equations is not self-adjoint. If there is no self-adjointness present one tries to replace the given set of field equations by an equivalent, self-adjoint set. (In this context, it is for instance important to look at the given equations in the right order.) Unfortunately, there is no general procedure which in any case succeeds. However, in any case we formally succeed by properly doubling the set ψ of fundamental field variables accompanied by properly supplementing the fundamental set of field equations. Of course, from the physical point of view we have to interpret the additional field variables and field equations.

It is a remarkable fact that the solution of the IP1 is not unique. One easily can show examples for the fact that a whole sequence of Lagrangians result in the same set of field equations although they are essentially different, i.e. they do not differ by a term (1.9). However, within LF they result in different dynamics, i.e. in different balance equations for energy, linear momentum, etc. [11]. So, there is good reason in LF to distinguish carefully between the kinematics of a system and its dynamics. The solutions $\psi(x, t)$ of the fundamental field equations (1.6) define the kinematics a system, whereas its dynamics takes care of all its relevant balance equations in the sense of LF, too. Different systems may exhibit identical kinematics but completely different dynamics. The dynamics, however, is the essential key for physically characterizing a system. Measuring a system and the coupling of different systems is physically associated with the exchange of balanced quantities like energy, linear momentum, mass, etc. Within LF we call these quantities *observables*.

So, from the physical point of view the procedure of finding a Lagrangian by means of IP1 is too poor. Nevertheless, LF in literature is often confined to this procedure (see e.g. [12]). The result is but a formal variational principle, which may have its merits, e.g. for solving problems approximately by means of direct variational methods. In general, it is no Hamilton's action principle in the true sense. The latter one, however, is necessary for *unifying theories of different systems on the level of LF*, or to *couple different systems on this level*. For example, gauge field theory is running along this line.

As a result of these considerations one obviously is referred to the *IP2 taking account of the complete unifying structure of LF in the sense of the true Hamilton's action principle*. We shall consequently follow this line in the case of TIP.

2. Lagrange formalism

2.1. Why Lagrange formalism, especially in thermodynamics of irreversible processes?

- In theoretical physics a theory for the dynamics of a system is regarded to be *closed* if its Hamilton's action principle is known. In this respect traditional forms of TIP exhibit a missing link.
- LF is the *most concise form of a dynamical theory*. All information on the dynamics of the system is involved in one function only, namely in its Lagrangian. This statement contrasts with traditional TIP which is based on a more or less big set of balance and constitutive equations.

- A *methodical unification* of different systems is a matter of economics in theoretical physics. The structure of LF is universal; it applies methodically in the same way to any system.
- The *coupling of different physical systems* must be done on the same methodical level. Because of its unified structure LF is particularly distinguished in this respect. Gauge field theory is a prominent example for this statement. The coupling of reversible and irreversible (dissipative) processes is a most attractive challenge for LF on the phenomenological level.
- Hamilton's action principle is particularly distinguished for *approximately solving of problems*. Instead of solving a boundary and initial value problem for partial differential equations the problem can be solved approximately by means of direct variational methods on the basis of Hamilton's variational principle (Ritz procedure, finite elements method).

2.2. Methodical unification of reversible and irreversible processes — complex field variables in thermodynamics of irreversible processes

Traditionally TIP is regarded to be outside the scope of LF. A formal reason for this statement is the missing of self-adjointness of the traditionally used set of fundamental field equations. Nevertheless, the statement is but an unproved dogma, which probably results from a lot of failures in the past. For instance one may ask: Which of the given equations have to be regarded as the ELEqs? A priori the answer is quite open! Within LF it is more natural *to look at the traditionally used set of balance equations as the universal Noether-balances of the system*, i.e. to establish LF for TIP along the line of the IP2, keeping the form of the ELEqs initially open.

Because of superior and universal invariance requirements TIP has to be included into LF and it really can be done by using *complex valued, fundamental field variables* instead of the traditional variables like temperature, mass densities and velocities. The traditional variables are derived as secondary quantities from the primary, fundamental variables. As a qualitative rule *complex variables have to be introduced for those phenomena of a thermodynamical system which are involved in irreversibilities*, or — more precisely — which give rise to entropy production.

Complex variables are well established in field theory. The most prominent example is Schrödinger's matter field in quantum mechanics. Another example is the order parameter in the Ginsburg–Landau theory of superconductivity. In both cases we are dealing with classical fields, although the systems are quantum mechanical ones. The quantum mechanical nature of a system is due to the particular form of the Lagrangian and to particular interpretations rather than to the choice of complex variables! In the same way *we are subsequently dealing with classical field theory when using complex field variables*. This unusual approach does not contradict traditional approaches of TIP. On the contrary the latter ones are involved into LF; they are methodically unified within this approach.

Let us regard the basic thermodynamical processes *heat flow, diffusion, and chemical reactions* embedded into a *flowing, material carrier*. In a simplified form these processes will be taken as representative examples throughout this paper. They are associated with the following *complex valued, fundamental field variables*:

1. The *field of thermal excitation or thermion field*⁶ [13–19]

$$\chi(x, t) = \sqrt{T(x, t)} \exp(i\xi(x, t)) \quad (2.1)$$

⁶ The term “thermion field” is due to a canonical quantization of the field χ [19].

is basic for thermal processes. It gives rise to the definition of the positive definite *absolute temperature*

$$T(x, t) = \chi^*(x, t) \cdot \chi(x, t) \geq 0 \quad (2.2)$$

as a secondary quantity. It further contains the *thermal phase* $\xi(x, t)$ which is *associated with the deviation of the process from local equilibrium* (see below). The term “excitation field” is a reminiscence to the microscopic picture of the phenomenological temperature:

$$\begin{aligned} \chi \neq 0 &\Leftrightarrow T \neq 0, \text{ i.e. thermal excitation is present,} \\ \chi = 0 &\Leftrightarrow T = 0, \text{ i.e. no thermal excitation is present.} \end{aligned} \quad (2.3)$$

2. Let $\{S_k, k = 1, \dots, N\}$ be a set of diffusing and chemically reacting constituents according to the chemical reaction equation:

$$\nu_1 S_1 + \nu_2 S_2 + \dots + \nu_m S_m \rightleftharpoons \nu_{m+1} S_{m+1} + \dots + \nu_N S_N + [Q], \quad (2.4)$$

where $[Q]$ denotes the heat production for a gross reaction from left to right; ν_i are the stoichiometric coefficients. Each constituent S_k is associated with a complex valued *matter field* [15],

$$\psi_k(x, t) = \sqrt{n_k(x, t)} \exp(i\varphi_k(x, t)), \quad (2.5)$$

which gives rise to the definition of the positive definite *partial mass density* as a secondary quantity (measured in moles for the sake of TIP):

$$n_k(x, t) = \psi_k^*(x, t) \cdot \psi_k(x, t) \geq 0. \quad (2.6)$$

Again the *matter phase* $\varphi_k(x, t)$ is associated with the deviation of the process from local equilibrium (see below).

3. The processes 1 and 2 are running within a *material carrier*, e.g. in a deforming solid or in a material flow. The material carrier may be the representative of the sum of all diffusing and chemically reacting substances, e.g. in a mixture of reacting gases, or it may be a different material into which the partial processes heat flow, diffusion and chemical reaction are embedded. In any case it is a *representative of the convective motion of the whole system*. It is associated with a *matter field* [4,10]

$$\Psi(x, t) = \sqrt{\rho(x, t)} \exp(i\Phi(x, t)), \quad (2.7)$$

which gives rise to the definition of the positive definite *carrier's mass density*:

$$\rho(x, t) = \Psi^*(x, t) \cdot \Psi(x, t) \geq 0. \quad (2.8)$$

To get full generality a material flow has to be further associated with a complex *circulation field*

$$Z(x, t) = \sqrt{\Lambda(x, t)} \exp(iM(x, t)). \quad (2.9)$$

The *matter phase* $\Phi(x, t)$ and the circulation field are involved into the definition of the convective *flow velocity*, whereas the circulation field is exclusively responsible for the *vorticity* of the flow (see below). The matter field $\Psi(x, t)$ is basic for thermodynamics in a material system. Thermodynamics can happen only where $\Psi \neq 0$.

The complex field variables define the set ψ of *fundamental field variables* for the respective systems. In TIP these are preferred above each other choice of variables. For example, we may equally well chose

the moduli and the phases of the complex variables as field variables. These, however, are not called “fundamental”; we have to be careful in this respect (see below).

Each of the systems 1–3 is irreversible. Especially material flow is accompanied with friction which gives rise to dissipation of mechanical energy. In any case the irreversible processes are associated with entropy production. How to model this in LF? It is obvious that the quantities (2.2), (2.6) and (2.8) are invariant with respect to *regauging of the complex field variables*:

$$\psi, \psi^* \Rightarrow \tilde{\psi} = \psi \exp(i\varepsilon), \quad \tilde{\psi}^* = \psi^* \exp(-i\varepsilon) \quad (2.10)$$

(ψ represents in turn the variables χ , ψ_k and Ψ). This transformation will be the key for the entropy concept within LF, especially for the entropy production due to the irreversibility of the processes [16]. Here the choice of complex variables for dissipative and — more general — for irreversible processes finds one of its reasonings.

2.3. Lagrange formalism and thermodynamics of irreversible processes — the universal structure of the theory

In Figs. 1 and 2 the flow chart of LF is given [17]. The symbols [(...)] refer to the figures. In this section, I shall comment on the most complex structure rather qualitatively. Furthermore, the diagram may serve as a guide through the formal structure given in Section 3.

The whole theory is based on three fundamentals:

- [(1)] *Hamilton’s action principle* (1.5), which in the total context will be denoted as *action principle of the first kind*. Its integral kernel is given by
- [(2)] the Lagrangian of the system. Being interested in thermodynamics of isolated systems we assume the restricted form (1.10). Making a special ansatz for the Lagrangian the site [(2)] is that one, where an individual structure of the particular system is coming into the play. All other structures are universal. At site [(2)] *the dynamics of the system is implicitly, but finally defined*. Especially irreversibility is taken into account by a *Lagrangian which fails of time reversal invariance*. The action principle of the first kind and the Lagrangian have to be subjected to
- [(3)] a set of *universal invariance requirements*. All of them are methodically founded and obligatory for all physics and there is no exception for thermodynamics. Formally the invariance requirements are represented by a *G-parametric Lie-group*,

$$\begin{aligned} x^\alpha &\Rightarrow \tilde{x}^\alpha = f^\alpha(x, \varepsilon), \quad \alpha = 0, \dots, 3, \\ \psi^k &\Rightarrow \tilde{\psi}^k = F^k(\psi, x, \varepsilon), \quad k = 1, \dots, f, \end{aligned} \quad (2.11)$$

which transforms *real* processes $|\psi(t)\rangle$ into different *real* processes $|\psi(t; \varepsilon)\rangle$. In Eq. (2.11) the abbreviations (1.8) for the time–space variables x and $\varepsilon = \{\varepsilon_K, K = 1, \dots, G\}$ for the set of group parameters are used. The one-element of the group is identified with $\varepsilon = 0$.

The most important universal invariance requirements are associated with the following Lie-groups:⁷

- Time translational invariance:

$$t \Rightarrow \tilde{t} = t + t_0, \quad \forall t_0 \in R. \quad (2.12)$$

⁷ $t_0, \vec{x}_0, \alpha_1, \alpha_2, \alpha_3, \varepsilon$ are the group parameters of the subsequent special groups.

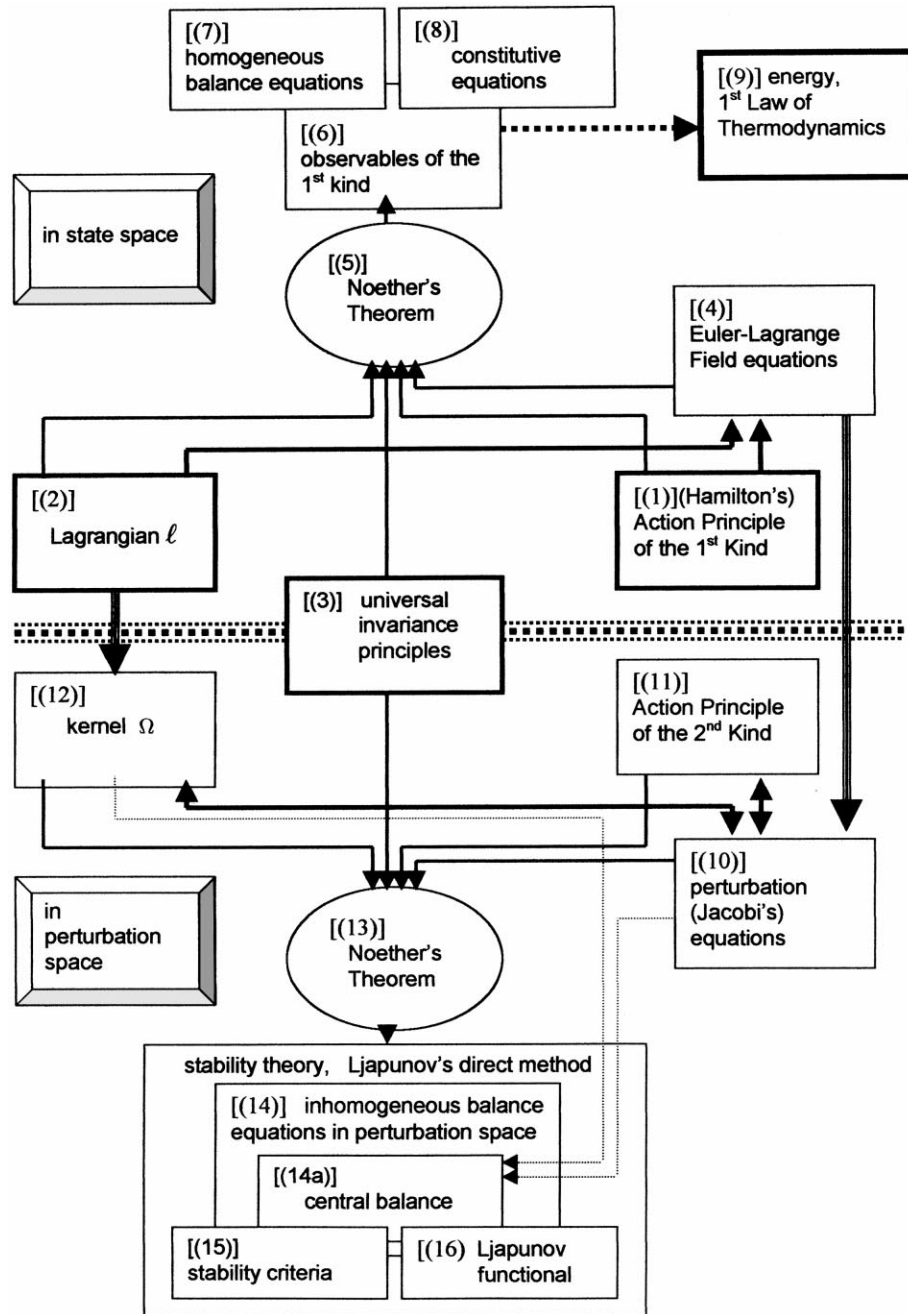


Fig. 1. Structure of Lagrange formalism and stability theory as an implication, especially for thermodynamics of irreversible processes.

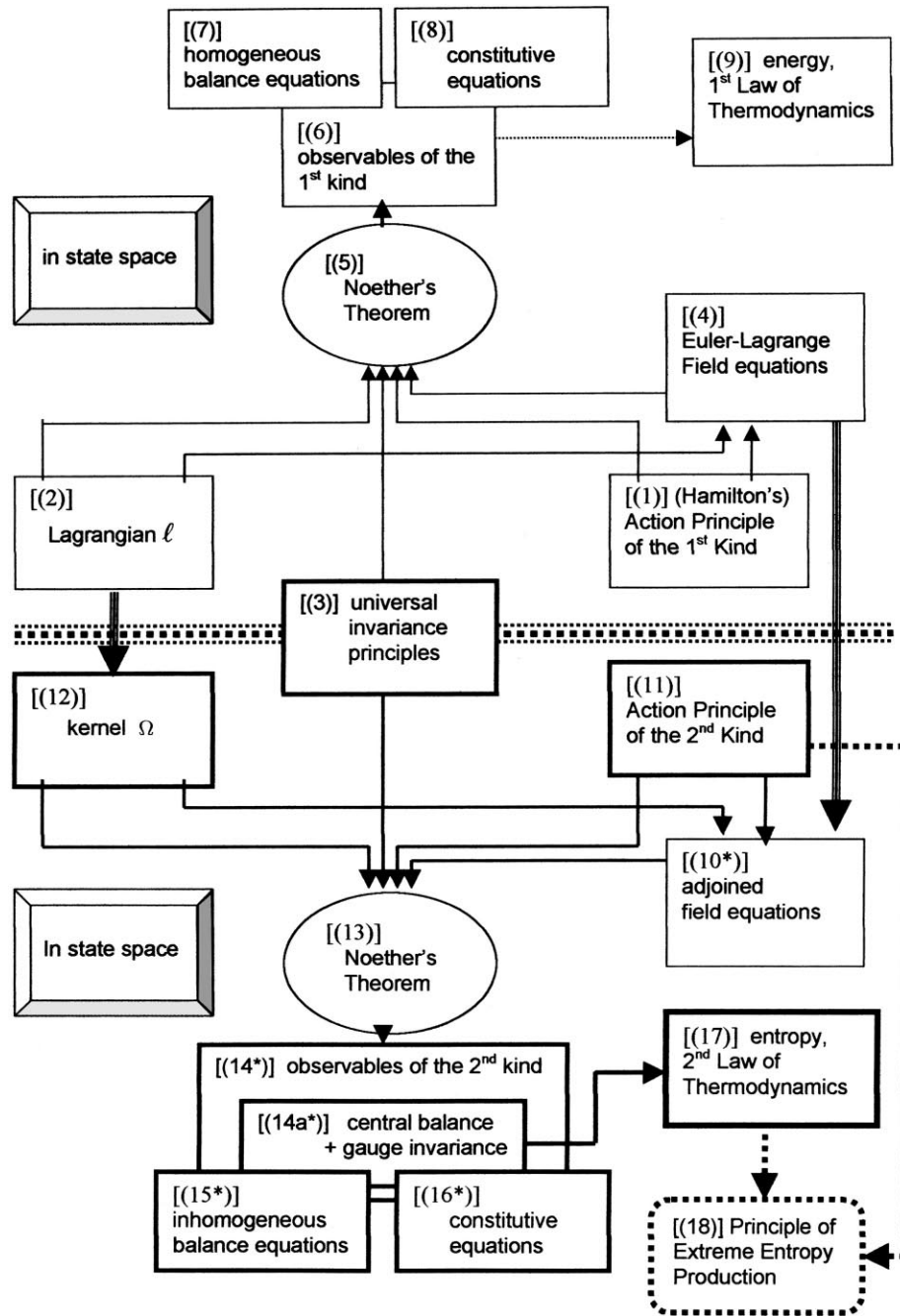


Fig. 2. Extended Lagrange formalism, especially for thermodynamics of irreversible processes.

Each real process being arbitrarily shifted in time by t_0 results in a real process again. In other words, each process can be reproduced at any instant, or, the time continuum is homogeneous with respect to any physics, or, no instant is physically preferred from any other instant. Obviously time translational invariance is the mathematical correlate of the most fundamental principle of physics: ‘physical processes have to be reproducible’. It is a *methodical principle*!

- Space translational invariance:

$$\vec{x} \Rightarrow \vec{\tilde{x}} = \vec{x} + \vec{x}_0, \forall \vec{x}_0 \in R^3. \quad (2.13)$$

Repeat the sermon for Eq. (2.12) analogously in the spatial sense. It is again a methodical principle!⁸

- Rotational invariance:

$$\vec{x} \Rightarrow \vec{\tilde{x}} = \underline{R}(\alpha_1, \alpha_2, \alpha_3) \cdot \vec{x}. \quad (2.14)$$

Each real process being subjected to a rigid rotation \underline{R} in space results in a real process again. The α_i may, for example, be the three Euler’s angles. There is no direction in space physically distinguished from any other direction.

Obviously these invariance requirements apply to isolated systems, only. However, the isolation of a system may cause problems. If necessary the isolation can be realized either by joining the system with its relevant physical environment in order to create a bigger, isolated system, or by enlarging the system internally by means of supplementary variables in the set ψ of fundamental field variables. An example for the first procedure is a gravitating environment which by no means can be screened from a system and which, as a consequence, has to be joined with the system. Of course, this procedure is also accompanied with enlarging the set ψ , here by the gravitation field as an additional variable. The second procedure is realized, for example, when mechanics is generalized towards thermo-mechanics. A mechanical system with friction (dissipation) cannot be isolated within pure mechanics; for such a system there exists no explicitly time-independent Lagrangian depending on mechanical variables, only. The mechanical energy is leaving the system to an undefined nowhere. However, the isolation is possible by adding thermal variables. Then dissipation is an irreversible energy transfer from mechanical to thermal degrees of freedom.

So far invariance transformations have been applied to the space and time variables, only. The processes are rigidly transposed in space and time. However, the behavior of the field variables ψ_k under universal invariance transformations is no trivial problem. Of course, in general they will be affected depending on their special nature (e.g. scalar, vector, tensor, spinor, real or complex field, etc.).⁹

The next example for an invariance requirement applies to the field variables exclusively. The use of complex field variables suggests *gauge invariance*:¹⁰

$$\psi \Rightarrow \tilde{\psi} = \psi \exp(i\varepsilon), \quad \psi^* \Rightarrow \tilde{\psi}^* = \psi^* \exp(-i\varepsilon), \quad \varepsilon \in R, \forall \text{ complex variables}. \quad (2.15)$$

As a *common gauge transformation* it applies to all complex fields simultaneously. Each real process results after regauging in a new real process. The reasoning for gauge invariance in the case of TIP is

⁸ Both, the time and the space translational invariance imply theoretically and experimentally the procedure of “parallel transport” of physical information. Here we are dealing with the flat (Euclidean) space–time of non-relativistic physics.

⁹ For details I refer to the chapter “Duality of Representation” in [10].

¹⁰ See the comments for Eq. (2.10).

rather involved. After a long way through LF it finally results in the entropy concept. In the context of TIP gauge invariance is regarded as a *universal requirement*.

Having established the fundamentals [(1)], [(2)], [(3)], LF as a straightforward procedure can be started. Performing the variation in the action principle [(1)] of the first kind we get for a given Lagrangian [(2)] the

[(4)] *Euler–Lagrange equations* (1.6) as the *fundamental field equations* of the system in the volume V .

Depending on the particular situation at the boundary they are supplemented by particular boundary conditions due to free or bounded variation of the fields at the boundary.

On the basis of the three fundamentals [(1)]–[(3)] and using the fundamental field equations [(4)], [(5)] *Noether’s theorem* can be established for the processes of the system [3,20]. Each group parameter ε_K of the Lie-group (2.11) of invariance transformations is associated with an

[(6)] *observable*¹¹ of the first kind $A_{(\varepsilon_K)}$, which is implicitly defined by means of a respective

[(7)] *homogeneous Noether’s balance equation*:

$$\varepsilon_K \Rightarrow A_{(\varepsilon_K)}^I : \quad \partial_t a_{(\varepsilon_K)}^I + \operatorname{div} \vec{J}_{(\varepsilon_K)}^I = 0. \quad (2.16)$$

By Noether’s theorem the density $a_{(\varepsilon_K)}^I$ and the associated flux density $\vec{J}_{(\varepsilon_K)}^I$ are uniquely defined from the Lagrangian ℓ giving rise to the

[(8)] *constitutive equations* of the respective observable of the first kind:

$$\ell \Rightarrow \begin{cases} a_{(\varepsilon_K)}^I = a_{(\varepsilon_K)}^I(\psi, \partial_t \psi, \nabla \psi), \\ \vec{J}_{(\varepsilon_K)}^I = \vec{J}_{(\varepsilon_K)}^I(\psi, \partial_t \psi, \nabla \psi). \end{cases} \quad (2.17)$$

Due to the first-order Lagrangian ℓ they depend on the field variables ψ and on their first-order derivatives.

Due to the universal invariance requirements (2.12)–(2.14) we get along this procedure universal definitions for the usual *observables energy, linear and angular momentum*. Once and for all and for each physical system the following relations between universal invariance requirements and observables of the first kind are stated in LF:

time translational invariance \Rightarrow energy,
space translational invariance \Rightarrow linear momentum,
rotational invariance \Rightarrow angular momentum.

According to the homogeneous Noether-balance equations (2.16) the total amounts A of these observables are conserved as it has to be for an isolated system:

$$\frac{dA}{dt} = \frac{d}{dt} \int_V a(\cdots) dV = - \int_{\partial V} \vec{J}_{(a)}(\cdots) dF = 0. \quad (2.18)$$

See Eq. (1.11). Especially in the case of TIP the Noether’s energy balance is the

¹¹ “Observables” are commonly known from quantum mechanics. They are defined by Hermitian operators, the real eigenvalues of which are identified with the possible outcome of measurements. In the context of LF and TIP the term “observable” is chosen with regard to the fact that measurement is finally associated with the exchange of conserved quantities like energy, linear and angular momentum between the system and the measuring apparatus (norm-system). At this point we meet again the universality of these quantities for each system.

[(9)] first law of thermodynamics. At this point Noether's procedure meets the Hamiltonian (1.7). Within LF the first law is no a priori law of nature but a straightforwardly deduced result. As compared with the traditional view the axiomatic basis of thermodynamics concerning the first law is shifted to the existence of Hamilton's action principle and to the methodically justified time translational invariance. From the point of view of LF the universality of Noether's energy is the deeper reason for the fact that "energies" in different systems, e.g. in mechanics, electrodynamics, thermodynamics, are one and the same entity, which may be exchanged between different systems. At this point the existence of the universal mechanical heat equivalent (427 mkp/kcal) finds its reasoning.

So far we have been concerned with the traditional part of LF, only. As a new feature it applies to TIP. This traditional part completely works within state space, i.e. in the function space spread by the set of ψ fundamental field variables. We now proceed to a less known part of LF which, however, is quite generally useful in field theory and which is particularly significant for TIP. The lower half of the flow chart is covered twice. In Fig. 1 it is concerned with stability theory which operates in perturbation space. In Fig. 2 this part is applied to special classes of "perturbations" which are associated with the invariance group and which give rise to further structures of LF in *state space*! This extended LF results in a natural way in the *entropy concept of TIP*.

Let us look at a one-parameter class of real processes $|\psi(t; \pi)\rangle = \{\psi_k(x, t; \pi), k = 1, \dots, f\}$ in the range $-\pi_0 < \pi < +\pi_0$ of the real *perturbation parameter* π . $\psi_k(x, t; \pi)$ is assumed to be continuously differentiable with respect to π . Referred to the *reference process* $|\psi(t)\rangle = |\psi(t; \pi = 0)\rangle$ the processes $|\psi(t; \pi)\rangle$ are regarded as perturbed processes. The exact perturbation is approximated by its main linear part,

$$\Delta|\psi(t; \pi)\rangle = |\psi(t; \pi)\rangle - |\psi(t)\rangle \underset{\text{linear}}{\approx} \left. \frac{\partial|\psi(t; \pi)\rangle}{\partial\pi} \right|_{\pi=0} \cdot \pi, \quad (2.19)$$

giving rise to the definition of the set of functions

$$|\eta(t)\rangle = \left. \frac{\partial|\psi(t; \pi)\rangle}{\partial\pi} \right|_{\pi=0} = \left\{ \eta_k(x, t) = \left. \frac{\partial\psi_k(x, t; \pi)}{\partial\pi} \right|_{\pi=0}, \quad k = 1, \dots, f \right\}, \quad (2.20)$$

which is an element of the accompanying tangent space associated with the state space, or — in physical terms — which is an element of the accompanying *perturbation space* associated with the reference process at time t (see Fig. 3). Let us call $|\eta(t)\rangle$ the *generator of the class* $|\psi(t; \pi)\rangle$. It is a representative of the real perturbation (2.19) of the reference process $|\psi(t)\rangle$.

It should be noticed that we are not dealing with perturbations of the system but of the processes! The Lagrangian is kept fixed! The perturbation parameter π is, for example, associated with a perturbation of the initial values.

For each parameter π the processes $|\psi(t; \pi)\rangle$ are solutions of the ELeqs. Thus, using the definition (2.20) we obtain from [(4)] the

[(10)] *perturbation or Jacobi's equations*¹² associated with the reference process $|\psi(t)\rangle$ of the system. These equations are linear, partial differential equations for the generators $|\eta(t)\rangle$. Having the form of ELeqs they can be associated with a variational principle which is called the

¹² These equations are often called "variational equations". However, one should carefully distinguish between (virtual) variations, applied to a variational problem, and (real) perturbations within a class of real processes. So, the term "perturbation equations" is preferred.

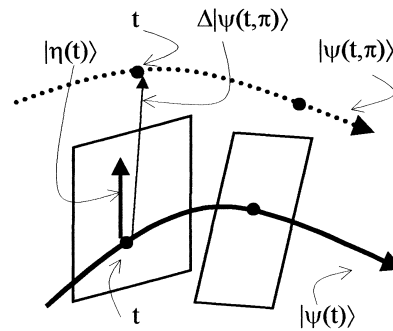


Fig. 3. Accompanying tangent- or perturbation-space at the trajectory $|\psi(t)\rangle$ of the process. Perturbation: $\Delta|\psi(t; \pi)\rangle$; generator: $|\eta(t)\rangle$.

[(11)] *action principle of the second kind*:

$$J_{(2)} = \int_{t_1}^{t_2} \int_V 2\Omega(\psi, \partial_t \psi, \nabla \psi; \eta, \partial_t \eta, \nabla \eta) dV dt = \text{extremum} \quad (2.21)$$

with respect to free variations $\delta\eta(x, t)$ of the generator $\eta(x, t)$, keeping fixed its values at the beginning and the end of the process in the volume V and on its boundary ∂V : $\delta\eta(x, t_{1,2}) = 0$.

For a given reference process $|\psi(t)\rangle$ Eq. (2.21) defines in the perturbation space an action principle for the admissible generators $|\eta(t)\rangle$. In Eqs. (2.20) and (2.21) the reference process $|\psi(t)\rangle$ plays the role of control variables. It does not take part in the variational procedure (2.21). The

[(12)] *integral kernel* Ω is uniquely defined from the Lagrangian ℓ of the system. It contains the complete information on the admissible generators, i.e. on all possible perturbations of a given reference process. The perturbation equations [(10)] are the “Euler–Lagrange equations” in perturbation space associated with the variational principle (2.21), [(11)].

As an obvious consequence of these considerations the structures [(10)]–[(12)] contain all information on the *stability* or *instability* of the real processes $|\psi(t)\rangle$ of a system, too. Thus, it should be possible to establish *Ljapunov’s direct method of stability theory* [16,21] within LF.

Stability theory is interested in the behavior of the perturbations $|\Delta\psi(t; \pi)\rangle$ for $t \rightarrow \infty$.¹³ A (reference) process $|\psi(t)\rangle$ is called *asymptotically stable*, if each perturbation tends to zero. If there exists at least one perturbation which is leaving the reference process the latter one is called unstable. The situation is qualitatively demonstrated by means of Fig. 4. Being representatives of perturbation classes $|\Delta\psi(t; \pi)\rangle$ the generators $|\eta(t)\rangle$ have to be submitted to the same criteria, i.e. we have to ask for the asymptotic behavior of the solutions $|\eta(t)\rangle$ of the perturbation equations [(10)]. Ljapunov’s direct method is a most powerful tool to *decide between stable and unstable processes without solving the perturbation equations explicitly*. It can be based on LF! That’s the topic of the remaining structures in Fig. 1.

[(3)] Of course, the *universal invariance principles* have to be applied to the perturbations $|\Delta\psi(t; \pi)\rangle$, too, i.e. to its associated generators $|\eta(t)\rangle$ as well as formerly to the reference processes $|\psi(t)\rangle$.

Thus, we may establish a formalism in perturbation space (lower half in Fig. 1) which as a mirror

¹³ For simplicity only the “asymptotic stability” will be discussed here.

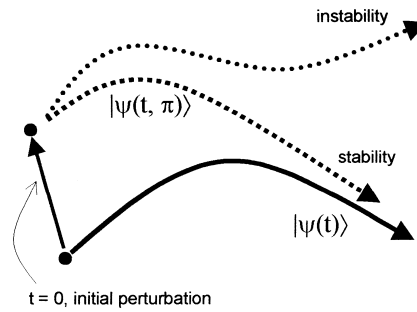
Fig. 4. Stability and instability of a process $|\psi(t)\rangle$.

image works in the same way as the formalism in the upper half of Fig. 1. The invariance principles [(3)] apply to the total dynamics of a system and thus especially to action principle of the second kind and its kernel Ω .

On the basis of the structures [(10)]–[(12)]

[(13)] *Noether's theorem can be applied in perturbation space*, too. It offers a variety of options to establish a

[(14)] *stability theory in the sense of Ljapunov's direct method*. Each group parameter of the invariance group of Ω is associated with an inhomogeneous balance equation for the generators $|\eta(t)\rangle$ of perturbations of the reference process $|\psi(t)\rangle$. These balance equations offer

[(15)] *stability criteria* to be used in Ljapunov's method. Especially the density functions involved in the balance equations offer various options for the definition of

[(16)] *Ljapunov-functionals*.

An interesting side branch is associated with the *algebraic structure of the kernel Ω* . It is homogenous of the second degree with respect to its arguments $\eta, \partial_t \eta, \nabla \eta$ giving immediately rise to a prominent inhomogeneous balance equation in perturbation space without using Noether's theorem [(10)] + [(12)] \Rightarrow [(14a)]:

$$\partial_t \omega(\psi, \partial \psi; \eta, \partial \eta) + \text{div } \vec{J}_{(\omega)}(\cdots) = \sigma_{(\omega)}(\cdots). \quad (2.22)$$

This balance is called

[(14a)] *central balance* in perturbation space. It takes especially part in Ljapunov's theory and will be basic for the entropy concept.

The lower half of the flow chart in Fig. 1 will now be covered with a *second layer of structures which refer to the state space again*. The result is given in the lower part of Fig. 2. One should keep in mind that the chart in Fig. 2 is completely referred to the state space.

Applying the invariance transformations (2.11) to a real process $|\psi(t)\rangle$ we obtain in quite a natural way as many process classes $|\psi(t; \pi)\rangle$ as there are group parameters available in the full Lie-group of invariance transformations. In turn the group parameters have to be interpreted as perturbation parameter, $\varepsilon_K \Rightarrow \pi, K = 1, \dots, G$, keeping fixed the $(G - 1)$ residual group parameters. In this context the generators $|\eta(t)\rangle$ of the classes $|\psi(t; \pi)\rangle$ of perturbations coincide with the *generators of the invariance transformations* (2.11) in the group theoretical sense. The perturbation equations [(10)] applied to these generators are transposed into state space, again [(10*)]. We call them *adjoint* to the fundamental field equations [(4)]. On the other hand, each group parameter gives rise to a Noether procedure [(13)]. Thus,

there is a G^2 -fold covering of the structures [(13)]–[(16)] in Fig. 1. Taking further account of the central balance (2.22), [(14a)], and applying it to each of the before mentioned G process classes we get another G -fold covering of the structures [(13)]–[(16)]. Summing up we get for each real process $|\psi(t)\rangle$ a set of [(14*)] $(G^2 + G)$ observables of the second kind, which are implicitly defined by [(15*)] inhomogeneous balance equations,

$$\partial_t a'' + \text{div } \vec{J}_{(a)}'' = \sigma_{(a)}'', \quad (2.23)$$

and by

[(16*)] *constitutive equations*

$$a'' = a''(\psi, \partial\psi, \partial\partial\psi), \quad \vec{J}_{(a)}'' = \vec{J}_{(a)}''(\psi, \partial\psi, \partial\partial\psi), \quad \sigma_{(a)}'' = \sigma_{(a)}''(\psi, \partial\psi, \partial\partial\psi) \quad (2.24)$$

for the densities, flux densities, and production rate densities. These are uniquely defined by the Noether procedure [(13)] or by the central balance (2.22), [(14a)]. In general, they depend on the field variables ψ , and its first and second derivatives. However, the arguments $\partial\partial\psi$ may disappear in several distinguished cases.

Among the observables of the second kind there is the

[(17)] *entropy*. It is due to the central balance (2.22), [(14a)], and to the common gauge transformation (2.15) applied to the set of all complex field variables. We get the *first part of the second law of thermodynamics*,

$$\partial_t s + \text{div } \vec{J}_{(s)} = \sigma_{(s)} \quad (2.25)$$

which is fulfilled by each real process $|\psi(t)\rangle$. The density s , flux density $J_{(s)}$ and production rate density $\sigma_{(s)}$ of the entropy depend on the same variables ψ and $\partial\psi$ as the Lagrangian does. Concerning the *second part of the second law*,

$$\text{entropy production rate density } \sigma_{(s)} \geq 0, \quad (2.26)$$

it is *most probable, that this relation is correlated with Ljapunov's stability of the processes*. For this purpose Ljapunov's stability theory [(14)], [(14a)], [(15)] and [(16)] of Fig. 1 has to be combined with the theory of the observables of the second kind [(14*)], [(14a*)], [(15*)] and [(16*)] in Fig. 2.

The second law of thermodynamics is a straightforward outcome of LF similar to the first law. As compared with traditional axiomatics the axiomatic basis of the second law is shifted in LF to the existence of Hamilton's action principle, to the gauge invariance of the theory and (probably) to confining the system to Ljapunov's stability.

In traditional TIP a 'principle of least entropy production' is frequently discussed [12,22]. It asserts that the *instantaneous total* entropy production is a minimum for stationary non-equilibrium processes as compared with virtually varied stationary processes. This principle is not proved generally. The prove is confined to a few particular processes with linear constitutive equations for the fluxes. In contrast with the traditional situation there exists a

[(18)] *principle of extreme entropy production* in LF which holds for TIP quite generally. It applies to any irreversible process. However, instead of the instantaneous total entropy production the '*total entropy production during the course $[t_1, t_2]$ of the process*' has to be considered. Formally the variational principle is degenerated to some extent as compared with usual variational principles.

It is closely connected with the action principle of the second kind (2.21), [(11)].¹⁴ The traditional principle of least entropy production is involved as a special case.

3. Lagrange formalism and thermodynamics of irreversible processes — the mathematics (examples: material flow, heat conduction, diffusion and chemical reactions)

The general formulae and structures will now be realized by three examples:

Example I. Isothermal flow of a hydroelastic, ideal fluid (IF).

Example II. Heat conduction (HC).

Example III. Heat conduction + diffusion + chemical reactions (HC–D–CR).

By these examples the theory is evaluated for a reversible process I and for irreversible processes II and III. It will be demonstrated that LF works in the same, unified manner for TIP as well as for reversible physics [13–18].¹⁵

The symbols [(n)] refer the reader to Figs. 1 and 2 and its interpretations in Section 2.3.

The traditional approach of TIP for the Examples II and III is incorporated into LF by taking into account the traditional *principle of local equilibrium* (PLE) [22]. The processes are assumed to run locally through equilibrium states. Formally the PLE is firstly based on the ad hoc generalization of Gibbs' fundamental form of thermostatics,

$$dU = T dS - p dV + \sum_{j=1}^N \mu_j dN_j \Rightarrow d_t U = T d_t S - p d_t V + \sum_{j=1}^N \mu_j d_t N_j, \quad (3.1)$$

and secondly on the use of the state functions from thermostatics which are related by

$$U = TS - pV + \sum_{j=1}^N \mu_j N_j. \quad (3.2)$$

Switching over to local densities these equations have to be substituted by

$$du = T ds + \sum_{j=1}^N \mu_j dn_j \Rightarrow \partial_t u = T \partial_t s + \sum_{j=1}^N \mu_j \partial_t n_j, \quad (3.3)$$

and

$$u = Ts - p + \sum_{j=1}^N \mu_j n_j. \quad (3.4)$$

¹⁴ A detailed presentation would go beyond the frame of this paper. The reader is referred to [15] and to forthcoming publications.

¹⁵ The coupling of these processes, e.g. in order to describe realistic fluid dynamics would break the frame and the intention of this paper. See [10] and forthcoming papers.

U, S, V, N_j are the total energy, entropy, volume and partial masses of chemical constituents S_j (given in moles) of a homogeneous system, u, s, n_j the respective densities ($u = U/V$, etc.), and p and μ_j the hydroelastic pressure and the chemical potentials of the constituents S_j .

3.1. The action principle of the first kind [(1)] and the Lagrangian [(2)]

The system of f degrees of freedom is described by the set

$$\psi = \{\psi_k, k = 1, \dots, f\} \quad (3.5)$$

of fundamental field variables. In the case of complex variables both the variable and its complex conjugate are numbered as two separate degrees of freedom among the set ψ . They can equally well be substituted by its moduli and phases giving rise to the set ψ' of field variables. The phases have to be dimensionless.

Example I. Complex matter and circulation fields (2.7)–(2.9):

$$\psi = \{\Psi, \Psi^*, Z, Z^*\} \quad \text{or equivalently} \quad \psi' = \{\rho, \Phi, \Lambda, M\}. \quad (3.6)$$

Example II. Complex thermion fields (2.1) and (2.2):

$$\psi = \{\chi, \chi^*\} \quad \text{or equivalently} \quad \psi' = \{T, \xi\}. \quad (3.7)$$

Example III. Complex thermion and matter fields (2.1), (2.2), (2.5) and (2.6):

$$\psi = \{\chi, \chi^*, \psi_k, \psi_k^*, k = 1, \dots, N\} \quad \text{or equivalently} \quad \psi' = \{T, \xi, n_k, \varphi_k, k = 1, \dots, N\}. \quad (3.8)$$

The action principle of the first kind (1.5), [(1)], is based on a *local, instantaneous* Lagrangian [(2)],

$$\ell = \ell(\psi, \partial_t \psi, \nabla \psi) = \ell(\psi_k, \partial_t \psi_k, \nabla \psi_k, k = 1, \dots, f). \quad (3.9)$$

Being associated with the physical action it has to be real valued, even in the case of complex valued field variables!

Example I. The pure mechanics of the ideal fluid is described by the Lagrangian [4,10]

$$\begin{aligned} \ell_{\text{IF}} &= \ell(\Psi, \Psi^*, Z, Z^*, \partial \Psi, \partial \Psi^*, \partial Z, \partial Z^*) \\ &= - \left\{ \left[\frac{1}{2i} (\Psi^* \partial_t \Psi - \Psi \partial_t \Psi^*) + \frac{1}{2i} \Psi \Psi^* (Z^* \partial_t Z - Z \partial_t Z^*) \right] \right. \\ &\quad \left. + \frac{1}{2} \Psi \Psi^* \left[\frac{1}{2i} \frac{1}{\Psi \Psi^*} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) + \frac{1}{2i} (Z^* \nabla Z - Z \nabla Z^*) \right]^2 + \Psi \Psi^* W(\Psi \Psi^*) \right\}, \end{aligned} \quad (3.10)$$

or equivalently, using the variables (3.6)₂, by the Lagrangian [23]

$$\ell_{\text{IF}} = \ell'(\rho, \Lambda, \partial\rho, \partial\Phi, \partial\Lambda, \partial M) = -\rho \left[(\partial_t \Phi + \Lambda \partial_t M) + \frac{1}{2}(\nabla \Phi + \Lambda \nabla M)^2 + W(\rho) \right]. \quad (3.11)$$

$W(\rho)$ is the specific hydroelastic energy. This Lagrangian is closely related with Hamilton–Jacobi theory of point-mechanics. (Compare Eq. (3.11) with the Hamilton–Jacobi equation of point-mechanics [1].) The phase functions Φ and M have to be dimensionless. This implies a dimension factor in Eqs. (3.10) and (3.11), which for simplicity is substituted by 1. The Lagrangian being gauge invariant (see Eq. (2.10)) does not depend on the phase variables, but on its derivatives only.

Example II. For simplicity the specific heat c and the tensor $\underline{\lambda}$ of heat conductivity are assumed to be independent of temperature. We are dealing here with the linear theory of heat conduction. The process is embedded in a rigid material [13–15]

$$\begin{aligned} \ell_{\text{HC}} &= \ell(\chi, \chi^*, \partial\chi, \partial\chi^*) \\ &= -c\chi\chi^* - \frac{c}{\omega} \left[\frac{1}{2i}(\chi^* \partial_t \chi - \chi \partial_t \chi^*) + \partial_t g(\chi\chi^*) \right] \\ &\quad + \frac{\underline{\lambda}}{\omega} \cdot \left[\frac{1}{2i} \{ (\chi^* \nabla \chi) \otimes (\chi^* \nabla \chi) - (\chi \nabla \chi^*) \otimes (\chi \nabla \chi^*) \} + \frac{T_0}{2(\chi\chi^*)^2} \nabla(\chi\chi^*) \otimes \nabla(\chi\chi^*) \right], \end{aligned} \quad (3.12)$$

or equivalently,

$$\ell_{\text{HC}} = \ell'(T, \xi, \partial T, \partial \xi) = -\frac{1}{\omega} \{ cT \partial_t [\xi - \xi^0(t, T)] + (-\underline{\lambda} \cdot \nabla T) \cdot \nabla [\xi - \xi^0(\dots)] + \partial_t g(T) \}. \quad (3.13)$$

The abbreviations

$$\xi^0(t, T) = -\omega t + \frac{T_0}{2T}, \quad (3.14)$$

and

$$g(T) = \frac{T_0}{2T} \int_{T_0/T}^1 \frac{p(\vartheta T)}{\vartheta^2} d\vartheta, \quad (3.15)$$

are used. Because of gauge invariance the phase variable ξ again does not appear in the argument. Here $p(T)$ will turn out to be the hydroelastic pressure (see below), which in the present context must be regarded as a rigid body reaction of the material background. Of course, the term $\partial_t g(t)$ as a total time derivative in Eqs. (3.12) and (3.13) is irrelevant for the ELeqs. However, it will be *relevant for the entropy concept!* The yet unspecified function $p(T)$ will finally be fitted to the PLE (3.3) and (3.4) (see Section 3.11), which in the present context of pure heat conduction reduces to

$$\partial_t u = T \partial_t s, \quad p = Ts - u. \quad (3.16)$$

ω is a yet unspecified dimensional factor which drops out of the relevant equations.

The second bracket $[\dots]$ in Eq. (3.12) is a symmetric tensor of rank 2. This implies that the heat conductivity tensor $\underline{\lambda}$ in front of the bracket is symmetric. Physically this correlates with *Onsager's reciprocity relation* as applied to heat flow [22].

Example III. This example is based on general constitutive relations. It demonstrates that the method is not restricted to linear TIP. In order to avoid an overloaded presentation only the simpler form of the Lagrangian is given using the moduli and the phases as basic variables. We look at the chemical reaction (2.4) between diffusing constituents S_j . The reaction gives rise to heat supply and thus to heat flow. The whole process is embedded into a rigid material background. The Lagrangian reads [15]

$$\begin{aligned} \ell_{\text{HC-D-CR}} = \ell'(T, \xi, n_k, \varphi_k, k = 1, \dots, N) \\ = -\frac{1}{\omega} \left\{ u(T, n_k, k = 1, \dots, N) \partial_t (\xi - \xi^0(t, T)) \right. \\ + \sum_{j=1}^N n_j \partial_t [\mu_j(T, n_k, k = 1, \dots, N) \alpha_j] \\ + \vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) \cdot \nabla [\xi - \xi^0(\dots)] \\ + \sum_{j=1}^N \vec{J}_j(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) \cdot \nabla [\mu_j(\dots) \alpha_j] \\ \left. + R(T, n_k, \alpha_k, k = 1, \dots, N) + \partial_t g(T, n_k, k = 1, \dots, N) \right\}, \end{aligned} \quad (3.17)$$

with the following abbreviations:

$$\xi^0(t, T) = -\omega t + \frac{T_0}{2T}, \quad (3.18)$$

$$\varphi_j^0(t, T, n_j) = -\omega t + \gamma \frac{n_j}{2T}, \quad \gamma \text{ is a dimensional constant}, \quad (3.19)$$

$$\alpha_j = [\varphi_j - \varphi_j^0(t, T, n^j)] - [\xi - \xi^0(t, T)] = [(\varphi_j - \xi)] - [\varphi_j^0(t, T, n^j) - \xi^0(t, T)], \quad (3.20)$$

$$g(T, n_k, k = 1, \dots, N) = \frac{T_0}{2T} \int_{T_0/T}^1 \frac{p(\vartheta T, \vartheta n_k, k = 1, \dots, N)}{\vartheta^2} d\vartheta. \quad (3.21)$$

Again ω is a dimensional factor which does not enter into the relevant equations. Later on the yet unspecified functions entering into Eq. (3.17) will find the following interpretations:

$u(T, n_k, k = 1, \dots, N)$: density of internal energy,

$\mu_j(T, n_k, k = 1, \dots, N)$: chemical potential of constituent S_j ,

$\vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N)$: flux density of internal energy,

$\vec{J}_j(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N)$: diffusion flux density of constituent S_j ,

$R(T, n_k, \alpha_k, k = 1, \dots, N)$: reaction potential, which takes into account the chemical reaction (2.4).

It is endowed with the property

$$R(T, n_k, \alpha_k = 0, k = 1, \dots, N) = 0 \text{ for each choice of } T \text{ and } n_k. \quad (3.22)$$

It especially gives rise to heat supply and to mass creation and annihilation during a chemical reaction.

Comparing Eqs. (3.15)¹⁶ and (3.21) the form of the term $\partial_t g(\dots)$ in Eq. (3.17) is still preserved. The yet unspecified pressure $p(T, n_k, k = 1, \dots, N)$ again has to be interpreted as a rigid body reaction. According to the extended dynamics of the present system the set of its arguments is now enhanced. In Section 3.11 the function $p(\dots)$ will again be fitted to the PLE (3.3) and (3.4) which now appears in its full extension:

$$\partial_t u = T \partial_t s + \sum_{j=1}^N \mu_j \partial_t n_j, \quad p = Ts - u + \sum_{j=1}^N \mu_j n_j. \quad (3.23)$$

Proceeding from Eqs. (3.13)–(3.17), $(\xi - \xi^0)$ is further preserved; it is supplemented by analogous terms $(\varphi_j - \varphi_j^0)$ (see Eq. (3.20)). The phase functions ξ and φ_i are referred to the reference functions $\xi^0(t, T)$ and $\varphi_j^0(t, T, n_j)$, (see Eqs. (3.14), (3.18) and (3.19)), which later on will be associated with the PLE (see Section 3.10). Taking account of the PLE the LF for TIP is furthermore fitted to the well established thermostatics, i.e. to the equilibrium states as a special class of processes within LF.

As a remarkable feature the reference functions $\xi^0(t, T)$ and $\varphi_j^0(t, T, n_j)$ get singular at $T = 0$. In physical terms this is interpreted as the *third law of thermodynamics*: There is no physical way to get at the absolute zero point.

In LF this law is coming into the play by fitting the Lagrangians to the PLE and not by inherent structures of LF as in the case of the first and second laws.

The Lagrangians of the three examples are all real valued. Furthermore, they are invariant with respect to a common re-gauging (2.10) of the complex field variables. In the formulae (3.11) and (3.13) this feature corresponds with the fact, that the Lagrangians do not depend on the phase functions $\{\Phi, M\}$ and ξ , respectively, but on its derivatives, only.¹⁷ In Eq. (3.17) the phase functions ξ and φ_j , occur explicitly. However, the combinations $(\xi - \varphi_j)$ ensure gauge invariance (see Eq. (3.20)).

The Lagrangians $\{(3.10), (3.11)\}$ and $\{(3.12), (3.13)\}$, and Eq. (3.17) define reversible and irreversible dynamics, respectively. The dynamics of a system is called reversible, if time reversal transforms each real process into another real process. The “movie” is running the other way round, so to speak. This implies time reversal invariance of the Lagrangian. We come back to this topic in Section 3.5.

3.2. The Euler–Lagrange equations [(4)]

The Euler–Lagrange equations

$$\partial_\alpha \frac{\partial \ell}{\partial (\partial_\alpha \psi^k)} - \frac{\partial \ell}{\partial \psi^k} = 0, \quad k = 1, \dots, f, \quad (3.24)$$

are due to free variation of the fields $\psi_k(x, t)$ within the volume V of the system. They must be supplemented by *boundary conditions*, which fit with the special situation of the system. In the case of a *totally closed system* they can be obtained from the variational principle, too. They are due to free variations of the fields $\psi_k(x, t)$ at the boundary ∂V the system:¹⁸

¹⁶ The strange form of this function is chosen in order to coincide with Eq. (3.21) in Example III. Of course, Eq. (3.15) can be simplified.

¹⁷ Gauge transformation (2.10) in an alternative form: phase variable \Rightarrow phase variable $+$ ε .

¹⁸ Performing the variation in Eq. (1.5) implies a partial integration which via Gauss’ theorem leads to a surface integral containing the term (3.25).

$$\vec{n} \cdot \frac{\partial \ell}{\partial (\nabla \psi_k)} = 0, \quad k = 1, \dots, f. \quad (3.25)$$

\vec{n} is the outer unit normal vector of the boundary. Closing a system is physically characterized by vanishing fluxes $\vec{J}_{(a)}$ of the relevant observables A across the boundary (see Eqs. (2.16)–(2.18)):

$$\vec{n} \cdot \vec{J}_{(a)} = 0. \quad (3.26)$$

From Noether's theorem (Section 3.3) it gets apparent that Eq. (3.25) results in Eq. (3.26) with one exception, only.¹⁹ Thus, *closing a system from its surrounding is associated with free variation of field variables at the boundary* of the system.

Example I. The ELEqs due to the variations $\delta\psi$, $\delta\psi^*$, δZ and δZ^* and in Eq. (3.10) are rather complicated and hard to be estimated. There is a part which looks like Schrödinger's equation. The remaining terms, however, are terribly non-linear and coupled. Turning over to Eq. (3.11) the situation gets much simpler. *Euler–Lagrange equations* associated with the variations $\delta \dots$:

$$\delta p : \quad (\partial_t \Phi + \Lambda \partial_t M) + \frac{1}{2}(\nabla \Phi + \Lambda \nabla M)^2 + \left(W(\rho) + \rho \frac{\partial W(\rho)}{\partial \rho} \right) = 0, \quad (3.27)$$

$$\delta \Phi : \quad \partial_t \rho + \text{div}(\rho(\nabla \Phi + \Lambda \nabla M)) = 0, \quad (3.28)$$

$$\delta \Lambda : \quad \rho(\partial_t M + (\nabla \Phi + \Lambda \nabla M) \cdot \nabla M) = 0, \quad (3.29)$$

$$\delta M : \quad \partial_t(\rho \Lambda) + \text{div}((\nabla \Phi + \Lambda \nabla M) \Lambda) = 0, \quad (3.30)$$

Defining the *flow velocity* by

$$\vec{v} = \nabla \Phi + \Lambda \nabla M, \quad (3.31)$$

Eq. (3.27) is recognized as *Bernoulli's law* generalized for the ideal, hydroelastic fluid and Eq. (3.28) as the *mass balance equation*. Using the substantial derivative

$$D_t = \partial_t + \vec{v} \cdot \nabla, \quad (3.32)$$

the Eqs. (3.29) and (3.30) together with Eq. (3.28) result in

$$D_t M = 0 \quad \text{and} \quad D_t \Lambda = 0, \quad (3.33)$$

which are equivalent with *Helmholtz law* of vortex dynamics:

$$\vec{\omega} = \frac{1}{2} \text{curl} \vec{v} = \frac{1}{2} \nabla \Lambda \times \nabla M = \frac{1}{2} \nabla Z^* \times \nabla Z \Rightarrow \partial_t \vec{\omega} + \text{curl}[\vec{\omega} \times \vec{v}] = 0. \quad (3.34)$$

The (non-trivial) *boundary conditions* (3.25) for the isolated flow are

$$\delta \Phi : \quad \vec{n} \cdot [\rho(\nabla \Phi + \Lambda \nabla M)] = 0, \quad (3.35)$$

$$\delta M : \quad \vec{n} \cdot [\Lambda \rho(\nabla \Phi + \Lambda \nabla M)] = 0. \quad (3.36)$$

¹⁹ The exception concerns linear momentum. It will not be reported in this paper.

Together with Eq. (3.31) both imply *material closure* of the flow:

$$\vec{n} \cdot (\rho \vec{v}) = 0. \quad (3.37)$$

In the present context the interpretation of expression (3.31) as the flow velocity is due to the mass balance (3.28):²⁰ (mass flux density)/(mass density). On the other hand, in three dimensions each vector field \vec{v} can locally be represented by the ansatz (3.31) [27]. The quantities Φ , Λ , and M are called *Clebsch- or Monge-potentials*.

Example II. Again the ELEqs associated with the variation of the complex thermion fields χ and χ^* are terribly complicated. So, we turn over to the form (3.13) of the Lagrangian.

Euler–Lagrange equations:

$$\delta \xi : \quad c \partial_t T - \underline{\lambda} \cdots \nabla \otimes \nabla T = 0, \quad (3.38)$$

$$\delta T : \quad \frac{\partial \xi^0(t, T)}{\partial T} [c \partial_t T - \underline{\lambda} \cdots \nabla \otimes \nabla T] + [c \partial_t (\xi - \xi^0(\cdots)) + \underline{\lambda} \cdots \nabla \otimes \nabla (\xi - \xi^0(\cdots))] = 0. \quad (3.39)$$

Taking account of Eq. (3.38), Eq. (3.39) results in

$$c \partial_t (\xi - \xi^0(t, T)) + \underline{\lambda} \cdots \nabla \otimes \nabla (\xi - \xi^0(\cdots)) = 0. \quad (3.40)$$

One should keep in mind that the couple of Eqs. (3.38) and (3.39) is self-adjoint; the equivalent couple (3.38) and (3.40), however, is not self-adjoint!

Obviously Eq. (3.38) is *Fourier's law of heat conduction*. Within LF it is supplemented by Eq. (3.40) which is solved by

$$\xi = \xi^0(t, T) = -\omega t + \frac{T_0}{2T}. \quad (3.41)$$

In Section 3.11 it will get apparent that this particular solution is associated with the PLE.

The *boundary conditions* for the isolated system are

$$\delta \varphi : \quad \vec{n} \cdot (-\underline{\lambda} \nabla T) = 0, \quad (3.42)$$

$$\delta T : \quad \vec{n} \cdot \left[-\underline{\lambda} \nabla (\xi - \xi^0(\cdots)) + (-\underline{\lambda} \nabla T) \frac{T_0}{2T^2} \right] = 0. \quad (3.43)$$

Eq. (3.42) ensures *thermal closure* of the system; there is no heat flux across the boundary (see Section 3.3). Eq. (3.43) is fulfilled on the base of Eqs. (3.42) and (3.41).

Due to Eqs. (2.1) and (3.41) a heat conduction process following the local equilibrium is associated with the *thermion wave*:

$$\chi(x, t) = \sqrt{T(x, t)} \exp \left[i \left(-\omega t + \frac{T_0}{2T(x, t)} \right) \right], \quad (3.44)$$

where $T(x, t)$ is a solution of Eqs. (3.38) and (3.42). It is the physical carrier of heat transport.

²⁰ See also Eqs. (3.102)–(3.105) and the related text.

Example III. Half of the ELeqs are too voluminous to be written down here in detail. Their essential structure will be reported only.

Euler–Lagrange equations:

$$\delta\xi : \quad \partial_t u_{(Q)} + \nabla \cdot \vec{J}_{(Q)} = \zeta_{(Q)}, \quad (3.45)$$

$$\delta\varphi_k : \quad \partial_t u_{(\text{Ch})_k} + \nabla \cdot \vec{J}_{(\text{Ch})_k} = \zeta_{(\text{Ch})_k}, \quad k = 1, \dots, N, \quad (3.46)$$

$$\delta T : \quad \text{partial differential equation, homogeneous with respect to } (\xi - \xi^0) \text{ and } (\varphi_k - \varphi_k^0) \text{ and its first and second derivatives.} \quad (3.47)$$

$$\delta n_k, k = 1, \dots, N : \quad \text{partial differential equation, homogeneous with respect to } (\xi - \xi^0) \text{ and } (\varphi_k - \varphi_k^0) \text{ and its first and second derivatives.} \quad (3.48)$$

The abbreviations used in Eqs. (3.45) and (3.46) and its physical interpretations, which are due to Noether's theorem (see Sections 3.3 and 3.4), can be taken from the following list.

$$\text{Internal energy density : } u(T, n_k, k = 1, \dots, N), \quad (3.49)$$

$$\text{chemical potential of the constituent } S_i : \quad \mu_i(T, n_k, k = 1, \dots, N), \quad (3.50)$$

thermal part of the internal energy density :

$$u_{(Q)}(T, n_k, k = 1, \dots, N) = u(T, n_k, k = 1, \dots, N) - \sum_{j=1}^N n_j \mu_j(T, n_k, k = 1, \dots, N), \quad (3.51)$$

chemical part of the internal energy density associated with constituent S_i :

$$u_{(\text{Ch})_i}(T, n_k, k = 1, \dots, N) = n_i \mu_i(T, n_k, k = 1, \dots, N), \quad (3.52)$$

$$\text{total flux density of the internal energy : } \vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N), \quad (3.53)$$

$$\text{diffusion flux density of the constituent } S_i : \quad \vec{J}_i(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N), \quad (3.54)$$

$$\text{heat flux density : } \vec{J}_{(Q)}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) = \vec{J}(\dots) - \sum_{j=1}^N \mu_j \vec{J}_j(\dots), \quad (3.55)$$

flux density of the chemical part of the internal energy associated with constituent S_j :

$$\vec{J}_{(\text{Ch})_j}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) = \mu_j \vec{J}_j(\dots), \quad (3.56)$$

energy production rate density associated with constituent S_j due to the chemical reaction :

$$\zeta_{(\text{Ch})_j}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) = \frac{\partial R(T, n_k, \alpha_k, k = 1, \dots, N)}{\partial \alpha_j} + n_j \partial_t \mu_j(\dots) + \vec{J}_j \nabla \mu_j(\dots), \quad (3.57)$$

density of heat supply due to chemical reaction :

$$\zeta_{(Q)}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) = - \sum_{j=1}^N \zeta_{(\text{Ch})_j}(\dots). \quad (3.58)$$

It should be noticed that in the energy production rates (3.57) and (3.58) the reaction potential plays an essential part!

Eqs. (3.47) and (3.48) are fulfilled by the particular solution

$$\xi = \xi^0(t, T) = -\omega t + \frac{T_0}{2T}, \quad (3.59)$$

$$\varphi_j = \varphi_j^0(t, T, n_j) = -\omega t + \gamma \frac{n_j}{2T}, \quad j = 1, \dots, N, \quad (3.60)$$

which on the base of solutions $T(x, t)$ and $n_k(x, t)$ of Eqs. (3.45) and (3.46) is again associated with the PLE, as in Example II.

The *boundary conditions* (3.25) for the isolated system are given by

$$\delta\xi : \quad \vec{n} \cdot \vec{J} - \sum_{j=1}^N \vec{n} \cdot \vec{J}_j \mu_j = 0, \quad (3.61)$$

$$\delta\varphi_k : \quad \vec{n} \cdot \vec{J}_j \mu_j = 0, \quad j = 1, \dots, N. \quad (3.62)$$

Similar to Example II those conditions associated with δT and δn_i , are fulfilled on the base of Eqs. (3.61) and (3.62) for processes running through local equilibrium states. Eqs. (3.61) and (3.62) really define an isolated system. Using Eq. (3.55) the heat and mass fluxes vanish across the boundary:

$$\vec{n} \cdot \vec{J}_{(Q)} = 0, \quad \vec{n} \cdot \vec{J}_j = 0, \quad j = 1, \dots, N. \quad (3.63)$$

Obviously Eq. (3.45) is a generalization of Fourier's law of heat conduction including chemical heat production ($\zeta_{(Q)} >, =, < 0$). The total rate of heat production is defined from the heat production rate density $\zeta_{(Q)}$:

$$[\dot{Q}(t)] = \int_V \zeta_{(Q)}(\dots) dV. \quad (3.64)$$

For a cross reaction running in the time interval $[t_1, t_2]$ the term

$$[Q] = \int_{t_1}^{t_2} [\dot{Q}(t)] dt = \int_{t_1}^{t_2} \int_V \zeta_{(Q)}(\dots) dV dt \quad (3.65)$$

finally is the gross heat production of the chemical reaction (2.4).

According to Eq. (3.58) the energy production rates balance mutually,

$$\zeta_{(Q)} + \sum_{j=1}^N \zeta_{(\text{Ch})_j} = 0, \quad (3.66)$$

which together with Eqs. (3.45), (3.46), (3.51) and (3.55) results in the *balance equation of the internal energy*

$$\partial_t u(\dots) + \nabla \cdot \vec{J}(\dots) = 0, \quad (3.67)$$

and thus on the level of the ELeqs in the *first law of thermodynamics*.

Performing the differentiations involved in Eq. (3.46) via the terms (3.52) and (3.56) we get an equivalent form of the field equations (3.46):

$$\partial_t n_j(x, t) + \nabla \cdot \vec{J}_j(\dots) = \sigma_j(\dots), \quad j = 1, \dots, N. \quad (3.68)$$

These are the *diffusion-reaction-equations* associated with the constituents S_j in the chemical reaction (2.4). The *partial mass production rate densities* due the reaction are given by

$$\sigma_j(T, n_k, \alpha_k, k = 1, \dots, N) = \frac{1}{\mu_j(T, n_k, k = 1, \dots, N)} \frac{\partial R(T, n_k, \alpha_k, k = 1, \dots, N)}{\partial \alpha_j}, \quad j = 1, \dots, N. \quad (3.69)$$

The form of the reaction potential is still open within LF; it has to be fitted to further physical structures. The phenomenological *principle of multiple proportions*

$$\sigma_1 : \sigma_2 : \dots : \sigma_N = \nu_1 : \nu_2 : \dots : \nu_N \quad (3.70)$$

is solved by

$$\sigma_j = \nu_j r(T, n_k, \alpha_k, k = 1, \dots, N), \quad j = 1, \dots, N, \quad (3.71)$$

where the function

$$r = r(T, n_k, \alpha_k, k = 1, \dots, N) \quad (3.72)$$

defines a *constitutive equation for the reaction velocity* r of the chemical reaction. The stoichiometric coefficients ν_i have to be taken with plus or minus signs according to their position on the right- or left-hand side of Eq. (2.4), respectively.

Let M_j be the molar mass of constituent S_j . Then the gross mass balance

$$\sum_{j=1}^N M_j \nu_j = 0 \quad (3.73)$$

of the chemical reaction leads via Eq. (3.71) to the condition

$$\sum_{i=1}^N M_i \sigma_i = 0, \quad (3.74)$$

and thus together with Eq. (3.69) to a constraint for the reaction potential,

$$\sum_{j=1}^N \frac{M_j}{\mu_j} \frac{\partial R(T, n_k, \alpha_k, k = 1, \dots, N)}{\partial \alpha_j} = 0, \quad (3.75)$$

and via Eqs. (3.69) and (3.71) for a given constitutive equation (3.72) to a set of differential equation for the reaction potential:

$$\frac{\partial R(T, n_k, \alpha_k, k = 1, \dots, N)}{\partial \alpha_j} = v_j \mu_j(T, n_k, k = 1, \dots, N) r(T, n_k, \alpha_k, k = 1, \dots, N),$$

$$j = 1, \dots, N. \quad (3.76)$$

Formally the reaction velocity $r(\dots)$ is an integrating factor for the “vector field” $\{v_j \mu_j(\dots), j = 1, \dots, N\}$. A solution of Eq. (3.76) for the case of a linear relation between the reaction velocity (3.72) and the affinity of the chemical reaction can be found in [15].

With regard to the complex field variables (2.1) and (2.5) the diffusion-reaction-process is associated with a *thermion wave* and *N matter waves*

$$\chi(x, t) = \sqrt{T(x, t)} \exp \left[i \left(-\omega t + \frac{T_0}{2T(x, t)} \right) \right],$$

$$\psi_k(x, t) = \sqrt{n_k(x, t)} \exp \left[i \left(-\omega t + \frac{n_k(x, t)}{2T(x, t)} \right) \right], \quad k = 1, \dots, N. \quad (3.77)$$

Again they are the physical carriers of thermodynamical energy transport. (For simplicity we choose $\gamma = 1$).

3.3. Invariance transformations and Noether's theorem for the action principle of the first kind [(3, 5)]

Given a Lagrangian (3.9) and a G -parameter Lie-group (2.11) of combined transformations in time and space (represented by $x = \{x^0 = t, x^1, x^2, x^3\}$) and in the state space (represented by the set $\psi = \{\psi_k, k = 1, \dots, f\}$):

$$x^\alpha \Rightarrow \tilde{x}^\alpha = f^\alpha(x^\beta, \varepsilon_K), \quad \alpha = 0, \dots, 3,$$

$$\psi_k \Rightarrow \tilde{\psi}_k = F_k(\psi_l, x^\beta, \varepsilon_K), \quad k = 1, \dots, f. \quad (3.78)$$

$\varepsilon = \{\varepsilon_K, K = 1, \dots, G\}$ is the set of group parameters with $\varepsilon = 0$ representing the one-element of the group. Here and in the following equations the range of the indices l, β, K at the arguments is evident from the respective sets ψ, x, ε . This group is called *invariance group of the Lagrangian* (or of the system) if the *invariance criterion*

$$\ell(\psi_k, \partial_\alpha \psi_k) \equiv \text{Det}_{x, \psi, \partial \psi, \varepsilon} |\partial_\alpha f^\beta(x, \varepsilon)| \ell(F_k(\psi, x, \varepsilon), F_{\alpha k}(\psi, \partial \psi, x, \varepsilon)) + \partial_\alpha \tilde{\mathcal{E}}^{(I)\alpha}(\psi, x, \varepsilon) \quad (3.79)$$

is fulfilled with a particular four-vector $\tilde{\mathcal{E}} = \tilde{\mathcal{E}}^{(I)\alpha}(\psi, x, \varepsilon)$. The term $F_{\alpha k}$ is defined by the following equation:²¹

$$F_{\alpha k}(\psi, \partial \psi, x, \varepsilon) = \left. \frac{\partial f_\beta^{-1}(\tilde{x}, \varepsilon)}{\partial \tilde{x}^\alpha} \right|_{\tilde{x} \Rightarrow x} (I) \partial_\beta F_k(\psi, x, \varepsilon). \quad (3.80)$$

²¹ This expression results from Eq. (3.78)₂ by evaluating the term $\partial_\alpha \tilde{\psi}_k(\tilde{x})$.

The criterion ensures, that a real process $|\psi\rangle$ is transformed into another real process $|\tilde{\psi}\rangle$ again:²²

$$|\psi\rangle = \{\psi_k(x^\alpha)\} \Rightarrow |\tilde{\psi}\rangle = \left\{ \tilde{\psi}_k(x^\alpha, \varepsilon_k) = F_k(\psi_l(x^\beta), x^\beta, \varepsilon_K) \Big|_{x^\beta = f_\beta^{-1}(\tilde{x}^\alpha, \varepsilon_K)} \Big|_{\tilde{x} \Rightarrow x}, k=1, \dots, f \right\}. \quad (3.81)$$

From Eq. (3.79) follows *Noether's theorem in state space* [20]:

Each group parameter of the invariance group of a system is associated with a homogeneous balance equation, the density and flux density of which are defined from the Lagrangian:

$$\varepsilon_K \Rightarrow \partial_\alpha \Lambda_{(K)}^{(I)} = 0 \Leftrightarrow \begin{cases} \partial_t a_{(K)}^{(I)} + \nabla \cdot \vec{J}_{(K)}^{(I)} = 0, \\ a_{(K)}^{(I)} = \Lambda_{(K)}^{(I)}, \vec{J}_{(K)}^{(I)} = \left\{ \Lambda_{(K)}^{(I)1}, \Lambda_{(K)}^{(I)2}, \Lambda_{(K)}^{(I)3} \right\}, \end{cases} \quad (3.82)$$

$$\Lambda_{(K)}^{(I)} = \left(\Theta_\beta^{(I)} \frac{\partial f^\beta(x, \varepsilon)}{\partial \varepsilon_K} - \sum_{i=1}^f \frac{\partial \ell(\psi, \partial \psi)}{\partial (\partial_\alpha \psi_i)} \frac{\partial F_i(\psi, x, \varepsilon)}{\partial \varepsilon_K} - \frac{\partial \Xi^\alpha(\psi, x, \varepsilon)}{\partial \varepsilon_K} \right) \Big|_{\varepsilon=0}. \quad (3.83)$$

In the first term the canonical energy-momentum-tensor in state space is involved:

$$\Theta_\beta^{(I)} = \sum_{i=1}^f \frac{\partial \ell(\psi, \partial \psi)}{\partial (\partial_\alpha \psi_i)} \partial_\beta \psi_i - \delta_\beta^\alpha \ell(\psi, \partial \psi). \quad (3.84)$$

The balance equation is fulfilled by each real process.

3.4. Observables of the first kind [(6)]–[(8)] — the first law of thermodynamics [(9)]

Let us apply Noether's theorem to the most simple but nevertheless to the most important, universal time translational invariance (2.12). The one-parameter Lie-group is given by

$$\begin{aligned} \tilde{t} = t + t_0 &\Rightarrow \tilde{x}^0 = x^0 + \varepsilon =: f^0(x, \varepsilon), \\ \tilde{x}^\alpha &= x^\alpha =: f^\alpha(x, \varepsilon), \quad \alpha = 1, 2, 3, \\ \tilde{\psi}_k &= \psi_k =: F_k(\psi, x, \varepsilon), \quad k = 1, \dots, f. \end{aligned} \quad (3.85)$$

Only the independent time variable is affected. The invariance criterion (3.79) evaluated for the group (3.85) results in the statement that the Lagrangian may not depend explicitly on time,

$$\frac{\partial \ell}{\partial t_{\text{ex}}} = 0 \Rightarrow \ell = \ell(\psi, \partial \psi), \quad (3.86)$$

as we have already assumed in Eq. (1.10). Thus, Noether's theorem (3.82)–(3.84) evaluated for Eq. (3.85) gives rise to the definition of the observable of the first kind, called *energy*:

$$\varepsilon = t_0 \Rightarrow \partial_t u + \nabla \cdot \vec{J}_{(u)} = 0, \quad (3.87)$$

²² Both processes are solutions of Hamilton's principle simultaneously. Comparing the variational principles for both processes and taking account of the ambiguity (1.9) the criterion can be established. One should further keep in mind, that we are concerned with transformations in space and time and not with coordinate transformations. In a fixed reference frame the process is "deformed". That is also the reason for the final substitution ($\tilde{x} \Rightarrow x$) at the end of formula (3.81).

$$\Lambda_{(\varepsilon)}^0 = \Theta_0^0 = u \Rightarrow \text{energy density : } u = u(\psi, \partial\psi) = \sum_{j=1}^f \frac{\partial \ell(\psi, \partial\psi)}{\partial (\partial_t \psi_j)} \partial_t \psi_j - \ell(\psi, \partial\psi), \quad (3.88)$$

$$\{\Lambda_{(\varepsilon)}^1, \Lambda_{(\varepsilon)}^2, \Lambda_{(\varepsilon)}^3\} = \{\Theta_0^1, \Theta_0^2, \Theta_0^3\} = \vec{J}_{(u)}$$

$$\Rightarrow \text{energy flux density : } \vec{J}_{(u)} = \vec{J}_{(u)}(\psi, \partial\psi) = \sum_{j=1}^f \frac{\partial \ell(\psi, \partial\psi)}{\partial (\nabla \psi_j)} \partial_t \psi_j. \quad (3.89)$$

In the case of thermodynamics *Noether's energy balance* is interpreted as the *first law of thermodynamics*. Eqs. (3.88) and (3.89) are the associated *constitutive equations*.

Example I. The Lagrangian will be taken in the form (3.11).

$$\text{Energy density : } u = \frac{1}{2} \rho (\nabla \Phi + \Lambda \nabla M)^2 + \rho W(\rho) = \frac{1}{2} \rho \vec{v}^2 + \rho W(\rho), \quad (3.90)$$

$$\text{energy flux density : } \vec{J}_{(u)} = -\rho (\nabla \Phi + \Lambda \nabla M) (\partial_t \Phi + \Lambda \partial_t M) = \vec{v} \left(\frac{1}{2} \rho \vec{v}^2 + \rho W(\rho) \right) + \vec{v} p(\rho), \quad (3.91)$$

where

$$p(\rho) = \rho^2 \frac{\partial W(\rho)}{\partial \rho} \quad (3.92)$$

is the hydroelastic pressure.²³ The ELeq (3.27) and the definition (3.31) has been used. The four terms in Eqs. (3.90) and (3.91) are in turn the well-known densities of the kinetic and elastic energies, the convective part of the energy flux density and the power $\vec{v} p(\rho)$ of the elastic forces.

Example II. The Lagrangian is taken in the form (3.13). To begin with Noether's expressions (3.88) and (3.89) for the present case,²⁴

$$u = cT - \frac{1}{\omega} \underline{\lambda} \cdot \nabla T \otimes \nabla [\xi - \xi^0(\dots)], \quad (3.93)$$

$$\vec{J}_{(u)} = \frac{1}{\omega} \underline{\lambda} \cdot \nabla T \partial_t \xi + \frac{1}{\omega} \underline{\lambda} \cdot \left(\nabla [\xi - \xi^0(\dots)] + \frac{T_0}{2T^2} \nabla T \right) \partial_t T, \quad (3.94)$$

we get the well-known formulae for heat transport, if the particular solution (3.41) is taken into account:

$$\text{internal energy density : } u = cT, \quad (3.95)$$

flux density of the internal energy = heat flux density (in the present context):

$$\vec{J}_{(u)} = -\underline{\lambda} \cdot \nabla T. \quad (3.96)$$

²³ This expression results from Noether's momentum balance, which is due to the spatial translation group (2.13). The pressure is 1/3 of the trace of the momentum flux tensor (stress tensor).

²⁴ One should keep in mind the term $(-\omega t)$ in the function ξ^0 (Eq. (3.18)).

These expressions, however, are associated in traditional linear TIP with the PLE. This fact justifies the already mentioned statement, that the particular solution (3.41) is associated with those processes which locally run through equilibrium states. The system is regarded to be out of equilibrium only globally. These considerations give rise to the statement, that the *phase function ξ in the thermion field χ is associated with the deviation of the process from local equilibrium*. However, asking for a theory of processes running outside of local equilibrium touches a difficult question, which cannot be answered on the base of the Lagrangian (3.12) and (3.13) (see Section 4).

Inserting the constitutive relations (3.95) and (3.96) into the Noether-balance (3.87) we find Fourier's law of heat conduction (3.38) again, but on the different methodical level of Noether's energy.

Example III. Noether's expressions (3.88) and (3.89) applied to Eq. (3.17) become

$$u = u(T, n_k, k = 1, \dots, N) + \frac{1}{\omega} \left\{ \vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) \cdot \nabla[\xi - \xi^0(\dots)] \right. \\ \left. + \sum_{j=1}^N \vec{J}_j(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) \cdot \nabla[\mu_j(\dots)\alpha_j] + R(T, n_k, \alpha_k, k = 1, \dots, N) \right\}, \quad (3.97)$$

$$\vec{J}_{(u)} = \vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N) - \frac{1}{\omega} \left\{ \vec{J}(\dots) \cdot \partial_t[\xi - \xi^0(\dots)] \right. \\ \left. + \sum_{j=1}^N \vec{J}_j(\dots) \partial_t[\mu_j(\dots)\alpha_j] + (\vec{D} \otimes \vec{J}(\dots, \nabla T, \nabla n_k, \dots)) \cdot \nabla[\xi - \xi^0(\dots)] \right. \\ \left. + \sum_{i=1}^N (\vec{D} \otimes \vec{J}_j(\dots, \nabla T, \nabla n_k, \dots)) \nabla(\mu_j, \alpha_j) \right\}. \quad (3.98)$$

Taking account of the particular solutions (3.59) and (3.60) we arrive again at the formulae from traditional TIP:

$$\text{internal energy density : } u = u(T, n_k, k = 1, \dots, N), \quad (3.99)$$

$$\text{flux density of the internal energy : } \vec{J}_{(u)} = \vec{J}(T, n_k, \nabla T, \nabla n_k, k = 1, \dots, N). \quad (3.100)$$

Following the same arguments as in Example II the phase functions ξ and φ_k in the thermion and matter fields ξ and ψ_k are again associated with the *deviations of the processes from local equilibrium*.

The operator \vec{D} used in Eq. (3.98) is defined by

$$\vec{D} = \partial_t T \frac{\partial}{\partial(\nabla T)} + \sum_{j=1}^N \partial_t n_j \frac{\partial}{\partial(\nabla n_j)}. \quad (3.101)$$

Let us next apply Noether's theorem to gauge invariance. The field variables are all assumed to be complex. In the set $\psi = \{\psi_1, \dots, \psi_{f/2}, \psi_{(f/2)+1}, \dots, \psi_f\}$ the first half denotes the complex variables,

the second half the associated complex conjugates. Then the group (3.78) reads

$$\begin{aligned}\tilde{x}^\alpha &= x^\alpha =: f^\alpha(x, \varepsilon), \quad \alpha = 0, 1, 2, 3, \\ \tilde{\psi}_k &= \psi_k \exp(i\varepsilon) =: F_k(\psi, x, \varepsilon), \quad k = 1, \dots, \frac{1}{2}f, \\ \tilde{\psi}_k &= \psi_k \exp(-i\varepsilon) =: F_k(\psi, x, \varepsilon), \quad k = \left(\frac{1}{2}f + 1\right), \dots, f.\end{aligned}\tag{3.102}$$

Let us assume that this group fulfills the invariance criterion (3.79) with $\mathcal{E} = 0$, which is the case for the Examples I–III. Then Noether's theorem results in the balance

$$\varepsilon \Rightarrow \partial_t \mu + \nabla \cdot \vec{J}_{(\mu)} = 0,\tag{3.103}$$

with the density

$$\mu = \mu(\psi, \partial\psi) = - \left\{ \sum_{j=1}^{f/2} \frac{\partial \ell(\psi, \partial\psi)}{\partial (\partial_t \psi_j)} i \psi_j + \text{c.c.} \right\}\tag{3.104}$$

and the flux density

$$\vec{J}_{(\mu)} = \vec{J}_{(\mu)}(\psi, \partial\psi) = - \left\{ \sum_{j=1}^{f/2} \frac{\partial \ell(\psi, \partial\psi)}{\partial (\nabla \psi_j)} i \psi_j + \text{c.c.} \right\}.\tag{3.105}$$

Applying these formulae to the Examples I–III we find the mass balance in the case I (ideal fluid) and the energy balance again in the cases II and III (thermodynamics). The interpretation of the Noether balance associated with gauge invariance is no unified one. This is no bad luck because, on the one hand, the gauge invariance is no universal, methodically justified requirement. Strictly speaking it is an individual invariance of the particular system. Only within thermodynamics we look at the gauge invariance as a universal requirement because of its relevance for the entropy. On the other hand, the “mass balance” in Example I strictly speaking is an “energy balance” because of the dimensional prefactor in Eqs. (3.10) and (3.11) which has been neglected²⁵ for simplicity. However, this prefactor already contains rudimentally a mass–energy–frequency equivalence known from relativity and quantum mechanics: $mc^2 = E = \hbar\omega$. These items will get essential for coupling the Lagrangian of Example I with those of Examples II and III, i.e. if thermodynamical processes are embedded into a deformable material body.

3.5. Reversibility and irreversibility

The invariance criterion (3.79) holds as well for discrete invariance groups. Then the continuously varying group parameters ε have to be replaced by one discretely varying index which numbers the group elements. The main point of the criterion is the same. A real process is transformed into another real process (of course, there is no more a Noether's theorem). Let us look at the time reversal transformation for Example 1:²⁶

$$t \Rightarrow -t, \quad \{\Psi, \Psi^*, Z, Z^*\} \Rightarrow \{\Psi^*, \Psi, Z^*, Z\}.\tag{3.106}$$

²⁵ This procedure is quite usual in literature, too.

²⁶ This transformation is well known in quantum mechanics.

Obviously the Lagrangian (3.10) and (3.11) is invariant with respect to this transformation, i.e. a real process $\{\Psi(x, t), Z(x, t)\}$ is transformed into another real process $\{\tilde{\Psi}(x, t), \tilde{Z}(x, t)\} = \{\Psi^*(x, -t), Z^*(x, -t)\}$. The truth of this statement can also be seen by inserting Eq. (3.106) into the ELEqs (3.27)–(3.30). It implies *reversibility* of the system.

Obviously an analogous procedure does not work for the Examples II and III (Lagrangians (3.12), (3.13) and (3.17)). These are *irreversible systems*.

3.6. Perturbation equations and the action principle of the second kind [(10, 11, 12)]

Given a one-parameter class of real processes $|\psi(t; \pi)\rangle = \{\psi_k(x, t; \pi), k = 1, \dots, f\}$ which are based on the reference process $|\psi(t)\rangle = |\psi(t; \pi = 0)\rangle$. Let us ask for the fundamental equations for the associated generator (2.20):

$$|\eta(t)\rangle = \left. \frac{\partial |\psi(t; \pi)\rangle}{\partial \pi} \right|_{\pi=0}. \quad (3.107)$$

Inserting $|\psi(t; \pi)\rangle$ into the ELEq (3.24) and applying the operation $(\partial/\partial \pi \dots)|_{\pi=0}$ we find a set of f linear, second-order partial differential equations for the generator $|\eta(t)\rangle$. These take the remarkable form

$$\partial_\alpha \frac{\partial \Omega(\dots)}{\partial (\partial_\alpha \eta_k)} - \frac{\partial \Omega(\dots)}{\partial \eta_k} = 0, \quad k = 1, \dots, f, \quad (3.108)$$

with a *kernel* Ω defined from the Lagrangian:

$$2\Omega(\psi, \partial\psi|\eta, \partial\eta) = \sum_{i,j=1}^f \left[\frac{\partial^2 \ell(\psi, \partial\psi)}{\partial \psi_i \partial \psi_j} \eta_i \eta_j + 2 \frac{\partial^2 \ell(\psi, \partial\psi)}{\partial \psi_i \partial (\partial_\alpha \psi_j)} \eta_i \partial_\alpha \eta_j + \frac{\partial^2 \ell(\psi, \partial\psi)}{\partial (\partial_\alpha \psi_i) \partial (\partial_\beta \psi_j)} \partial_\alpha \eta_i \partial_\beta \eta_j \right]. \quad (3.109)$$

The same procedure applied to the boundary conditions (3.25) results in the *boundary conditions for the generator* on ∂V :

$$\vec{n} \cdot \frac{\partial \Omega}{\partial (\nabla \eta_k)} = 0, \quad k = 1, \dots, f. \quad (3.110)$$

They belong to the isolated system.

Two kinds of field variables are involved; the arguments in Ω are accordingly separated by a vertical bar in Eq. (3.109): ψ denotes the given reference process and η the associated generator which has to be determined by Eqs. (3.108) and (3.110).

In literature the Eq. (3.108) are called *Jacobi's equations*. With regard to our present context the notation *perturbation equations* is preferred. They involve all information on all possible perturbations of a given reference process and thus on its stability or instability.

Obviously the perturbation equations (3.108) and the boundary conditions (3.110) have the form of ELEqs for an isolated system. Thus, we introduce the associated *action principle of the second kind*:

$$J_{(2)} = \int_{t_1}^{t_2} \int_V 2\Omega(\psi, \partial_t \psi, \nabla \psi) |\eta, \partial_t \eta, \nabla \eta| dV dt = \text{extremum} \quad (3.111)$$

by free variation $|\delta\eta(t)\rangle$ of the generator $|\eta(t)\rangle$ within the volume V and on its boundary ∂V , keeping fixed its values at the beginning and the end of the process: $|\delta\eta(t_{1,2})\rangle = 0$.

The variational procedure does not affect the given reference process $|\psi(t)\rangle$ which formally plays the role of control variables.

A four-divergence $(1.9)_2$ in the Lagrangian enters into the kernel Ω , too. This holds especially for the terms in $\partial_t g(\dots)$ in Eqs. (3.12), (3.13) and (3.17). As a consequence these terms enter into the entropy concept (see Sections 3.10 and 3.11).

As a very important fact the kernel Ω in the form (3.109) is not form invariant with respect to a transformation $\psi \Rightarrow \psi'$ of the field variables. Let the kernel Ω' be defined in the same way (Eq. (3.109)) with respect to the variables ψ' and the associated generators η' . Then

$$\Omega(\psi, \partial\psi|\eta, \partial\eta) \neq \Omega'(\psi', \partial\psi'|\eta', \partial\eta'), \quad (3.112)$$

i.e. the kernel Ω of the action principle of the second kind is ambiguous! This fact is due to the second partial derivatives of the Lagrangian in Eq. (3.109). The situation in state space is analogous to that one of differential geometry in ordinary Euclidean space:

Starting from a scalar (invariant) function $f(x, y, z)$ the set of partial derivatives $\{\partial_x f, \partial_y f, \partial_z f\}$ is an invariant object, namely a vector, called the gradient of f : ∇f . However, the $(3, 3)$ -matrix $(\partial_\alpha \partial_\beta f)$ of second order, partial derivatives is no more an invariant object. In order to obtain a second rank tensor as an invariant object the partial derivatives have to be substituted by covariant derivatives, i.e. instead of ordinary differential calculus, one has to deal with Ricci or covariant differential calculus. However, these things get essential only if curvilinear coordinates are taken into account. If differential geometry is exclusively referred to Cartesian coordinates we may forget about all these complications.

Coming back to Eq. (3.112), in order to define an invariant object Ω based on second derivatives of the Lagrangian one should introduce in state space a “covariant Ricci-calculus”, which of course causes a lot of mathematical trouble. However, preferring once and for all one particular set ψ of field variables above all other sets ψ' we arrive at the same goal. In LF for TIP these things get essential. Looking at Eqs. (3.12), (3.13) and (3.17) there are given two forms ℓ and ℓ' of the Lagrangian: ℓ being based on the set of complex field variables is more complicated than ℓ' , which is based on the set of moduli and phases. Both forms of the Lagrangian are equivalent, although ℓ' is preferred for doing calculations. However, which form has to be taken from the principle point of view to define the kernel Ω ? For the sake of stability theory both forms can be taken. On Ω as well as on Ω' a stability theory may be established (see Section 3.9), each choice leading to a particular stability analysis. However, the concept of entropy has to be invariant with respect to the choice of the set of field variables. The following statement turned out to be successful: ‘the concept of entropy has to be based on the set of complex field variables’!

Referring to the analogy mentioned above the complex field variables define so to speak the “Cartesian frame” in state space. This set is called the set of fundamental field variables.

The transformation of Ω associated with a transformation of the field variables is particular important for practical use. In detail, let $\psi = \{\psi_k, k = 1, \dots, f\}$ and $\psi' = \{\psi_{k'}, k' = 1, \dots, f\}$ be different sets of field variables in state space and $\eta = \{\eta_k, k = 1, \dots, f\}$ and $\eta' = \{\eta_{k'}, k' = 1, \dots, f\}$ the associated generators in perturbation space. Then the following formalism holds:

$$\psi \Leftrightarrow \psi': \quad \psi_{j'} = \psi_{j'}(\psi_j, j = 1, \dots, f), j' = 1, \dots, f \Rightarrow \eta_{j'} = \sum_{j=1}^f \frac{\partial \psi_{j'}(\psi)}{\partial \psi_j} \eta_j, \quad (3.113)$$

referred to ψ : $\ell(\psi, \partial\psi) \Rightarrow \Omega(\psi, \partial\psi|\eta, \partial\eta)$,

referred to ψ' : $\ell'(\psi', \partial\psi') \Rightarrow \Omega'(\psi', \partial\psi'|\eta', \partial\eta')$,

$$2\Omega(\psi, \partial\psi|\eta, \partial\eta) = \left[2\Omega'(\psi', \partial\psi'|\eta', \partial\eta') + \partial_\alpha \left(\sum_{i', i, j=1}^f \frac{\partial \ell'(\psi', \partial\psi')}{\partial (\partial_\alpha \psi_{i'})} \frac{\partial^2 \psi_{i'}(\psi)}{\partial \psi_i \partial \psi_j} \eta_i \eta_j \right) \right] \Big|_{\psi' \Rightarrow \psi}. \quad (3.114)$$

Eq. (3.114) is due to a rather lengthy calculation. As a remarkable fact the second term on the right is a complete four-divergence, which on the one hand will be quite convenient for calculating entropy quantities. On the other hand, because of this term the ambiguity of Ω in the action principle of the second kind (3.111) does not affect the Jacobi equations (3.108) (see Eq. (1.9) and the related statements)!

Example II. Starting from the identifications²⁷

$$\psi = \{\psi_1, \psi_2\} = \{\chi, \chi^*\} \quad \text{and} \quad \psi' = \{\psi_{1'}, \psi_{2'}\} = \{T, \xi\}$$

$$\eta = \{\eta_1, \eta_2\} = \{\eta_\chi, \eta_{\chi^*}\} \quad \text{and} \quad \eta' = \{\eta_{1'}, \eta_{2'}\} = \{\eta_T, \eta_\xi\}$$

and applying Eq. (3.109) to Eq. (3.13) we get the kernel Ω' which is based on the set ψ' of field variables:

$$2\Omega'(T, \partial T, \partial \xi|\eta_T, \partial \eta_\xi) = -\frac{1}{\omega} \left\{ \left[\left(\frac{cT_0}{T^3} + \frac{d^3 g(T)}{dT^3} \right) \partial_t T - 3 \frac{T_0}{T^4} \underline{\lambda} \cdot \nabla T \otimes \nabla T \right] \eta_T \eta_T \right. \\ \left. - \frac{T_0}{T^2} \underline{\lambda} \cdot \nabla \eta_T \otimes \nabla \eta_T - 2 \underline{\lambda} \cdot \nabla \eta_T \otimes \nabla \eta_\xi \right\}. \quad (3.115)$$

With Eq. (3.114) we finally arrive at $\Omega(\psi, \partial\psi|\eta, \partial\eta)$ which, however, looks rather lengthy.

3.7. Invariance transformations and Noether's theorem for the action principle of the second kind [(3, 13, 14)]

In the context of the action principle of the second kind the invariance group (3.78) has to be supplemented by transformations for the generator $\eta = \{\eta_k, k = 1, \dots, f\}$ of a perturbation. These a fortiori result from Eq. (3.78) when applying Eq. (2.20):

$$\begin{aligned} x^\alpha &\Rightarrow \tilde{x}^\alpha = f^\alpha(x^\beta, \varepsilon_K), \quad \alpha = 0, \dots, 3, \\ \psi_k &\Rightarrow \tilde{\psi}_k = F_k(\psi_l, x^\beta, \varepsilon_k), \quad k = 1, \dots, f, \\ \eta_k &\Rightarrow \tilde{\eta}_k = G_k(\psi_l, \eta_l, x^\beta, \varepsilon_K) = \sum_{j=1}^f \frac{\partial F_k(\dots)}{\partial \psi_j} \eta_j, \quad k = 1, \dots, f, \end{aligned} \quad (3.116)$$

($\varepsilon = 0$ is the one-element of the group). Being based on the preceding structures of LF this group is automatically an invariance group of the kernel Ω of the action principle of the second kind, i.e. the *invariance criterion*

²⁷ Examples I and III are too lengthy for the sake of this paper. They are left to the reader's exercise.

$$\begin{aligned} \Omega(\psi_k, \partial_\alpha \psi_k | \eta_k, \partial_\alpha \eta_k) &\equiv_{x, \psi, \partial \psi, \eta, \partial \eta, \varepsilon} \\ \text{Det}[\partial_\alpha f^\beta(x, \varepsilon)] \Omega(F_k(\psi, x, \varepsilon), F_{\alpha k}(\psi, \partial \psi, x, \varepsilon) | G_k(\psi, \eta, x, \varepsilon), G_{\alpha k}(\psi, \partial \psi, \eta, \partial \eta, x, \varepsilon)) \\ &+ \partial_\alpha \Xi^{(II)}(\psi, \eta, x, \varepsilon) \end{aligned} \quad (3.117)$$

is automatically fulfilled with a particular four-vector $\Xi^{(II)} = \{\Xi^{\alpha(II)}(\psi, \eta, x, \varepsilon)\}$. The terms $F_{\alpha k}$ and $G_{\alpha k}$ are defined by

$$\begin{aligned} F_{\alpha k}(\psi, \partial \psi, x, \varepsilon) &= \frac{\partial f_\beta^{-1}(\tilde{x}, \varepsilon)}{\partial \tilde{x}^\alpha} \Big|_{\tilde{x} \Rightarrow x} \partial_\beta F_k(\psi, x, \varepsilon), \\ G_{\alpha k}(\psi, \partial \psi, \eta, \partial \eta, x, \varepsilon) &= \frac{\partial f_\beta^{-1}(\tilde{x}, \varepsilon)}{\partial \tilde{x}^\alpha} \Big|_{\tilde{x} \Rightarrow x} \partial_\beta G_k(\psi, \eta, x, \varepsilon). \end{aligned} \quad (3.118)$$

The criterion (3.117) gives rise to *Noether's theorem in perturbation space*:

Each group parameter of the invariance group of a system is associated with an inhomogeneous balance equation, the density, flux density and production rate density of which are defined from the kernel Ω and thus from the Lagrangian:²⁸

$$\varepsilon_K \Rightarrow \partial_\alpha \Lambda_{(K)}^{(II)} = \sigma_{(K)}^{(II)} \Leftrightarrow \partial_t a_{(K)}^{(II)} + \nabla \cdot \vec{J}_{(K)}^{(II)} = \sigma_{(K)}^{(II)} \quad (3.119)$$

$$\begin{aligned} a_{(K)}^{(II)} &= a_{(K)}^{(II)}(\psi, \partial \psi | \eta, \partial \eta) = \Lambda_{(K)}^0, \quad \vec{J}_{(K)}^{(II)} = \vec{J}_{(K)}^{(II)}(\psi, \partial \psi | \eta, \partial \eta) = \left\{ \Lambda_{(K)}^1, \Lambda_{(K)}^2, \Lambda_{(K)}^3 \right\}, \\ \sigma_{(K)}^{(II)} &= \sigma_{(K)}^{(II)}(\psi, \partial \psi | \eta, \partial \eta). \end{aligned} \quad (3.120)$$

$$\Lambda_{(K)}^{(II)} = \left(\Theta_\beta^{(II)} \frac{\partial f^\beta(x, \varepsilon)}{\partial \varepsilon_K} - \sum_{i=1}^f \frac{\partial \Omega(\psi, \partial \psi | \eta, \partial \eta)}{\partial (\partial_\alpha \eta_i)} \frac{\partial G_i(\psi, \eta, x, \varepsilon)}{\partial \varepsilon_K} - \frac{\partial \Xi^\alpha(\psi, \eta, x, \varepsilon)}{\partial \varepsilon_K} \right) \Big|_{\varepsilon=0}, \quad (3.121)$$

$$\begin{aligned} \sigma_{(K)}^{(II)} &= - \sum_{j=1}^f \left\{ \left[\frac{\partial \Omega}{\partial \psi_j} - \partial_\alpha \frac{\partial \Omega}{\partial (\partial_\alpha \psi_j)} \right] \left[\partial_\beta \psi_j \frac{\partial f^\beta}{\partial \varepsilon_K} - \frac{\partial F_j}{\partial \varepsilon_K} \right] \right. \\ &\quad \left. + \partial_\alpha \left[\frac{\partial \Omega}{\partial (\partial_\alpha \psi_j)} \left(\partial_\beta \psi_j \frac{\partial f^\beta}{\partial \varepsilon_K} - \frac{\partial F_j}{\partial \varepsilon_K} \right) \right] \right\} \Big|_{\varepsilon=0}. \end{aligned} \quad (3.122)$$

In the first term of Eq. (3.121) the *canonical energy-momentum-tensor of perturbation space* is involved:

$$\Theta_\beta^{(II)} = \sum_{j=1}^f \frac{\partial \Omega(\psi, \partial \psi | \eta, \partial \eta)}{\partial (\partial_\alpha \eta_j)} \partial_\beta \eta_j - \delta_\beta^\alpha \Omega(\dots). \quad (3.123)$$

²⁸ Apply the operator $(\partial, \partial \varepsilon_K \dots)|_{\varepsilon=0}$ to Eq. (3.117) and use the Jacobi equations (3.108) and Eleqs (3.24).

The balance equations (3.120) are fulfilled by the generator $|\eta(t)\rangle$ of any perturbation of a given reference process $|\psi(t)\rangle$.

Example 1 (Time translational invariance (Eq. (3.85) supplemented)). The four-vector $\Xi^{(II)}$ in the criterion (3.117) is assumed to vanish, which is the case for our Examples I–III. The group (3.116) is specified to

$$\begin{aligned}\tilde{t} &\Rightarrow t + t_0 \Rightarrow \tilde{x}^0 = x^0 + \varepsilon =: f^0(x, \varepsilon), \\ \tilde{x}^\alpha &= x^\alpha =: f^\alpha(x, \varepsilon), \quad \alpha = 1, 2, 3, \\ \tilde{\psi}_k &= \psi_k =: F_k(\psi, x, \varepsilon), \quad k = 1, \dots, f, \\ \tilde{\eta}_k &= \eta_k =: G_k(\psi, x, \varepsilon), \quad k = 1, \dots, f.\end{aligned}\quad (3.124)$$

Applying Eqs. (3.120)–(3.123) to Eq. (3.124) we get the balance

$$\partial \mathcal{G} + \nabla \cdot \vec{J}_{(\mathcal{G})} = \sigma_{(\mathcal{G})} \quad (3.125)$$

with the density, flux density, and production rate density

$$\mathcal{G} = \mathcal{G}(\psi, \partial \psi | \eta, \partial \eta) = \overset{(II)}{\Theta}_0^0 = \sum_{i=1}^f \frac{\partial \Omega(\psi, \partial \psi | \eta, \partial \eta)}{\partial (\partial_t \eta_i)} \partial_t \eta_i - \Omega(\dots), \quad (3.126)$$

$$\vec{J}_{(\mathcal{G})} = \vec{J}_{(\mathcal{G})}(\psi, \partial \psi | \eta, \partial \eta) = \left\{ \overset{(II)}{\Theta}_0^1, \overset{(II)}{\Theta}_0^2, \overset{(II)}{\Theta}_0^3 \right\} = \sum_{i=1}^f \frac{\partial \Omega(\psi, \partial \psi | \eta, \partial \eta)}{\partial (\nabla \eta_i)} \partial_t \eta_i, \quad (3.127)$$

$$\sigma_{(\mathcal{G})} = \sigma_{(\mathcal{G})}(\psi, \partial \psi | \eta, \partial \eta) = - \sum_{i=1}^f \left\{ \frac{\partial \Omega}{\partial \psi_i} \partial_t \psi_i + \frac{\partial \Omega}{\partial (\partial_\alpha \psi_i)} \partial_t \partial_\alpha \psi_i \right\}. \quad (3.128)$$

Example 2 (Gauge invariance (Eq. (3.102) supplemented)). The four-vector $\Xi^{(II)}$ in the criterion (3.117) is assumed to vanish, which holds for our Examples I–III. The group (3.116) is specified to

$$\begin{aligned}\tilde{x}^\alpha &= x^\alpha =: f^\alpha(x, \varepsilon), \quad \alpha = 0, 1, 2, 3, \\ \tilde{\psi}_k &= \psi_k \exp(i\varepsilon) =: F_k(\psi, x, \varepsilon), \quad k = 1, \dots, \tfrac{1}{2}f, \\ \tilde{\psi}_k &= \psi_k \exp(-i\varepsilon) =: F_k(\psi, x, \varepsilon), \quad k = ((\tfrac{1}{2}f) + 1), \dots, f, \\ \tilde{\eta}_k &= \eta_k \exp(i\varepsilon) =: G_k(\psi, \eta, x, \varepsilon), \quad k = 1, \dots, \tfrac{1}{2}f, \\ \tilde{\eta}_k &= \psi_k \exp(-i\varepsilon) =: G_k(\psi, \eta, x, \varepsilon), \quad k = ((\tfrac{1}{2}f) + 1), \dots, f.\end{aligned}\quad (3.129)$$

Eqs. (3.120)–(3.123) applied to Eq. (3.129) now result in the balance

$$\partial \mathcal{H} + \nabla \cdot \vec{J}_{(\mathcal{H})} = \sigma_{(\mathcal{H})} \quad (3.130)$$

with the density, flux density, and production rate density defined by

$$\mathcal{H} = \mathcal{H}(\psi, \partial \psi | \eta, \partial \eta) = \overset{(II)}{\Lambda}^0 = - \left(\sum_{j=1}^{f/2} \frac{\partial \Omega(\psi, \partial \psi | \eta, \partial \eta)}{\partial (\partial_t \eta_j)} i \eta_j + \text{c.c.} \right), \quad (3.131)$$

$$\vec{J}_{(\mathcal{H})} = \vec{J}_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta) = \left\{ \overset{(I)}{\Lambda^1}, \overset{(II)}{\Lambda^2}, \overset{(III)}{\Lambda^3} \right\} = - \left(\sum_{j=1}^{f/2} \frac{\partial\Omega(\psi, \partial\psi|\eta, \partial\eta)}{\partial(\nabla\eta_j)} i\eta_j + \text{c.c.} \right), \quad (3.132)$$

$$\sigma_{(\mathcal{H})} = \sigma_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta) = \sum_{j=1}^{f/2} \left\{ \frac{\partial\Omega}{\partial\psi_j} i\psi_j + \frac{\partial\Omega}{\partial(\partial_\alpha\psi_j)} i\partial_\alpha\psi_j \right\} + \text{c.c.} \quad (3.133)$$

One should keep in mind that all densities, flux densities and production rate densities mentioned in this chapter are *homogeneous of second degree with respect to the variables η and $\partial\eta$* . The balance equations (3.119), (3.125) and (3.130) are fulfilled by the generator $|\eta(t)\rangle$ of any perturbation of each real process $|\psi(t)\rangle$.

3.8. The central balance in perturbation space [(14a)]

Due to his homogeneity of second degree with respect to the variables η and $\partial\eta$ the kernel Ω (3.109) may be subjected to Euler's formula:

$$2\Omega(\psi_k, \partial_\alpha\psi_k|\eta_k, \partial_\alpha\eta_k) = \sum_{j=1}^f \left(\frac{\partial\Omega(\dots)}{\partial\eta_j} \partial\eta_j + \frac{\partial\Omega(\dots)}{\partial(\partial_\alpha\eta_j)} \partial_\alpha\eta_j \right). \quad (3.134)$$

Substituting the first term by means of the perturbation equations (3.108) and condensing the whole expression into a four-divergence we get the *central balance in perturbation space*,

$$\partial\varpi + \nabla \cdot \vec{J}_{(\varpi)} = \sigma_{(\varpi)}, \quad (3.135)$$

with the density, flux density, and production rate density defined by

$$\varpi = \varpi(\psi, \partial\psi|\eta, \partial\eta) = \sum_{j=1}^f \frac{\partial\Omega(\dots)}{\partial(\partial_t\eta_j)} \eta_j, \quad (3.136)$$

$$\vec{J}_{(\varpi)} = \vec{J}_{(\varpi)}(\psi, \partial\psi|\eta, \partial\eta) = \sum_{j=1}^f \frac{\partial\Omega(\dots)}{\partial(\nabla\eta_j)} \eta_j, \quad (3.137)$$

$$\sigma_{(\varpi)} = \sigma_{(\varpi)}(\psi, \partial\psi|\eta, \partial\eta) = 2\Omega(\psi, \partial\psi|\eta, \partial\eta). \quad (3.138)$$

This balance (3.135) is *universal*; it holds within LF for each system! It is due to the algebraic structure of the kernel Ω and is not related with the universal invariance groups of the system. It is fulfilled by the generator $|\eta(t)\rangle$ of any perturbation of each real process $|\psi(t)\rangle$.

One should keep in mind, that the formulae (3.135)–(3.138) hold for any choice of the fundamental field variables ψ . However, they are not form invariant! Turning over to a different set ψ' of field variables the formula (3.114) has to be taken into account; all the quantities (3.136)–(3.138) will be affected.

3.9. Stability theory — Ljapunov's direct method within Lagrange formalism [(14, 14a, 15, 16)]

In Section 2.3 the generator $|\eta(t)\rangle$ (Eq. (2.20)) has been introduced as a representative for the perturbation $\Delta|\Psi(t; \pi)\rangle$ of a reference process $|\Psi(t)\rangle = |\Psi(t; \pi = 0)\rangle$ (π is a perturbation parameter). Dynamical stability or instability of the reference process are associated with the behavior of the perturbations $\Delta|\Psi(t; \pi)\rangle$ for increasing time. In linear approximation the decision on stability or instability will be done by means of the generator. For the sake of TIP the following considerations will be confined to asymptotic stability.

Let us introduce in perturbation space $\eta = \{\eta_k, k = 1, \dots, f\}$ a norm $\|\eta\|$. Then, with respect to this norm asymptotic stability or instability of a reference process $|\Psi(t)\rangle$ is defined by

$$\begin{aligned} \text{asymptotic stability :} & \quad \text{for, each generator} \quad \|\eta(\cdot, t)\| \rightarrow 0 \quad \text{for} \quad t \rightarrow \infty, \\ \text{asymptotic instability :} & \quad \text{at least for one generator} \quad \|\eta(\cdot, t)\| \rightarrow \infty \quad \text{for} \quad t \rightarrow \infty. \end{aligned} \quad (3.139)$$

In principle we are free to choose a particular norm. For the sake of TIP two simple “Euclidean” norms are useful:

$$\|\eta(\cdot, t)\|_{(1)} = \sqrt{\int_V \sum_{j=1}^f \eta_j^*(x, t) \eta_j(x, t) dx^3}, \quad (3.140)$$

$$\|\eta(\cdot, t)\|_{(2)} = \sqrt{\int_V \sum_{j=1}^f [\eta_j^*(x, t) \eta_j(x, t) + \partial_t \eta_j^*(x, t) \partial_t \eta_j + \nabla \eta_j^*(x, t) \cdot \nabla \eta_j(x, t)] dx^3}. \quad (3.141)$$

Eq. (3.141) is much stronger than Eq. (3.140); via the derivatives it includes spatial and temporal fluctuations of the perturbation. Both are instantaneous functionals of the generator. They are written in a form which immediately applies to the case of complex field variables; we are dealing with a “Euclidean” norm, so to speak.

By means of Ljapunov's direct method [21] the decision (3.139) can be done *without solving the perturbation equations* (3.108)!²⁹ In addition to the given norm $\|\eta\|$ one looks for another functional $\mathcal{L}[\eta]$ which fulfills the following properties:

$$1. \quad \mathcal{L}[\eta] \text{ positive definite, i.e. } \mathcal{L}[\eta] \geq 0 \text{ for } \|\eta\| \geq 0, \quad (3.142)$$

$$2. \quad \mathcal{L}[\eta] \geq m(\|\eta\|), \quad (3.143)$$

where $m(\dots)$ is a monotonically increasing function,

$$3. \quad \frac{d\mathcal{L}[\eta(\cdot, t)]}{dt} < 0, \quad (3.144)$$

along each trajectory $|\eta(t)\rangle$ in perturbation space.

These properties taken together define a *stability criterion*.

If such a functional can be found the reference process $|\Psi(t)\rangle$ is asymptotically stable with respect to the norm $\|\eta\|$. $\mathcal{L}[\eta]$ is called a *Ljapunov functional*.

$\mathcal{L}[\eta]$ is understood to depend on the variables η or on $\{\eta, \partial\eta\}$ if the norm (3.140) or (3.141) is taken, respectively. As an essential point of the method the relation (3.144) has to be verified by means of the perturbation equations (3.108) and its dynamical contents without solving them explicitly.

²⁹ That is the most charming feature of Ljapunov's ingenious idea.

In general the Ljapunov functional is introduced into the theory by assumption, i.e. by a procedure of try and error. However, stability and instability are inherent properties of the system. Thus, *there should exist a procedure within LF, which allows of constructing Ljapunov functionals completely from the dynamical structure of the system*. In doing so it may happen that the functional depends also on the reference process $|\Psi(t)\rangle$:

$$\mathcal{L}[\eta] \Rightarrow \mathcal{L}[\psi|\eta]. \quad (3.145)$$

Then it may further happen, that the Ljapunov-indicatrix

$$\mathcal{L}[\psi(\cdot, t)|\eta] = 1 \quad (3.146)$$

is blowing up with increasing time as compared with the Euclidean indicatrix $||\eta|| = 1$. To avoid this situation the constraint (3.143) has been introduced. Of course, this constraint is obsolete if \mathcal{L} does not depend on ψ .

The *formalism to construct a Ljapunov functional* is based on the balances in perturbation space established in Sections 3.7 and 3.8. Let

$$\partial_t \mathfrak{a}(\psi, \partial\psi|\eta, \partial\eta) + \nabla \cdot \vec{J}_{(\mathfrak{a})}(\psi, \partial\psi|\eta, \partial\eta) = \sigma_{(\mathfrak{a})}(\psi, \partial\psi|\eta, \partial\eta) \quad (3.147)$$

represent either any inhomogeneous balance equation out of the set (3.119) associated with the group parameters ϵ of the invariance group or let it represent the central balance (3.135). In any case the density, the flux density and the production rate density are *homogeneous functions of second degree in η and $\partial\eta$* . From the local balance (3.147) we turn over to the global balance of the system

$$\frac{d}{dt} \mathfrak{A}[\psi(\cdot, t)|\eta(\cdot, t)] = \mathfrak{B}[\psi(\cdot, t)|\eta(\cdot, t)] - \mathfrak{F}[\psi(\cdot, t)|\eta(\cdot, t)], \quad (3.148)$$

where

$$\mathfrak{A}[\psi(\cdot, t)|\eta(\cdot, t)] = \int_V \mathfrak{a}(\psi(x, t), \partial\psi(x, t)|\eta(x, t), \partial\eta(x, t)) dx^3, \quad (3.149)$$

$$\mathfrak{B}[\psi(\cdot, t)|\eta(\cdot, t)] = \int_V \sigma_{(\mathfrak{a})}(\psi(x, t), \partial\psi(x, t)|\eta(x, t), \partial\eta(x, t)) dx^3, \quad (3.150)$$

$$\mathfrak{F}[\psi(\cdot, t)|\eta(\cdot, t)] = - \int_{\partial V} \vec{n} \cdot \vec{J}_{(\mathfrak{a})}(\psi, (x, t), \partial\psi(x, t)|\eta(x, t), \partial\eta(x, t)) dx^2, \quad (3.151)$$

are in turn the total amount of the quantity \mathfrak{a} in the volume V , its total production rate in the volume V , and its total flux across the boundary ∂V . All of them are *quadratic functionals* of the fields $\eta(x, t)$ and $\partial\eta(x, t)$. In general they depend on the fields $\psi(x, t)$ and $\partial\psi(x, t)$ associated with the reference process, too. By definition the global balances (3.148) are fulfilled by the generator $|\eta(t)\rangle$ of any perturbation of a given reference process $|\Psi(t)\rangle$!

If among the functionals $\mathfrak{A}[\psi(\cdot, t)|\eta(\cdot, t)]$ there is at least one which fulfills the stability criterion (3.142)–(3.144) *a Ljapunov functional has been constructed within LF exclusively by means of internal, dynamical structures*:

$$\mathcal{L}[\psi(\cdot, t)|\eta(\cdot, t)] = \mathfrak{A}[\psi(\cdot, t)|\eta(\cdot, t)]. \quad (3.152)$$

The stability criterion has to be tested by means of the global balance (3.148) without solving the perturbation equations:

$$\begin{aligned} \mathfrak{A}[\psi(\cdot, t)|\eta] &\geq 0 \text{ for } \|\eta\| \geq 0, \quad \mathfrak{A}[\psi(\cdot, t)|\eta] \geq m(\|\eta\|), \\ \frac{d\mathfrak{A}[\psi(\cdot, t)|\eta(\cdot, t)]}{dt} &= \mathfrak{B}[\psi(\cdot, t)|\eta(\cdot, t)] - \mathfrak{F}[\psi(\cdot, t)|\eta(\cdot, t)] < 0. \end{aligned} \quad (3.153)$$

Obviously the definiteness properties of the functionals \mathfrak{A} , \mathfrak{B} , \mathfrak{F} are decisive for Eq. (3.153). How to investigate these properties?

- As a remarkable fact a *stability analysis for open systems is involved* into the theory, too, due to the total flux \mathfrak{F} . (The reader is reminded of the fact, that in non-linear open systems there are most important instabilities involved (synergetics, self-organization).) This functional is primarily defined by the surface integral (3.151). By means of the integral theorem of Gauss it may be transformed back into a volume integral which can be joined with the functional \mathfrak{B} . In the case of an isolated system, however, the situation simplifies due to the boundary conditions (3.110):

$$\mathfrak{F}[\psi(\cdot, t)|\eta(\cdot, t)] = 0. \quad (3.154)$$

(Compare the boundary conditions (3.110) with the general expressions (3.120) and (3.121) for Noether's fluxes, or with the flux (3.137) of the central balance, or with the special fluxes (3.127) and (3.132). There is again one exception involved associated with translation group in space.)

- We are left with the problem of deciding on the definiteness of a big variety of functionals \mathfrak{A} and \mathfrak{B} . Let

$$\mathfrak{B}[\psi(\cdot, t)|\eta(\cdot, t)] = \int_V \mathfrak{b}(\psi(x, t), \partial\psi(x, t)|\eta(x, t), \partial\eta(x, t)) dx^3 \quad (3.155)$$

represent these functionals, all of which are homogeneous of degree 2 with respect to the variables $\eta(x, t)$ and $\partial\eta(x, t)$.

Lemma for the definiteness of the functional \mathfrak{B} . Two different cases have to be considered:

1. $b(\psi, \partial\psi|\eta, \partial\eta)$ does not depend on time derivatives $\partial_t\eta$:

$$\mathfrak{B}[\psi|\eta] \geq 0 \quad \text{for } \|\eta\| \geq 0 \Leftrightarrow \sum_{\alpha, \beta=1}^3 \sum_{i, j=1}^f \frac{\partial^2 b(\psi, \partial\psi|\eta, \partial\eta)}{\partial(\partial_\alpha \eta_i) \partial(\partial_\beta \eta_j)} u^\alpha u^\beta v_i v_j > 0 \quad (3.156)$$

for arbitrary “vectors” $u = (u^1, u^2, u^3) \neq 0$ and $v = (v_1, \dots, v_f) \neq 0$.

2. $b(\psi, \partial\psi|\eta, \partial\eta)$ depends on time derivatives $\partial_t\eta$:³⁰

$$\mathfrak{B}[\psi|\eta] \geq 0 \quad \text{for } \|\eta\| \geq 0 \Leftrightarrow \sum_{\alpha, \beta=0}^3 \sum_{i, j=1}^f \frac{\partial^2 b(\psi, \partial\psi|\eta, \partial\eta)}{\partial(\partial_\alpha \eta_i) \partial(\partial_\beta \eta_j)} u^\alpha u^\beta v_i v_j > 0 \quad (3.157)$$

for arbitrary “vectors” $u = (u^0, u^1, u^2, u^3) \neq 0$ and $v = (v_1, \dots, v_f) \neq 0$.

The coefficients in these bi-quadratic forms are independent of η and $\partial\eta$. However, in general they depend on the reference process ψ . The proof of the lemma can be found in [16,24].

³⁰ Remember $\partial_0 = \partial/\partial t$.

Example II. Only a few remarks concerning heat conduction.³¹ Within the class of those processes, which are constraint by the PLE, i.e. which are constraint by the particular solution (3.41)

$$\xi - \xi_0(t, T(x, t)) = 0, \quad (3.158)$$

stability can be shown. It is related with the well-known condition:

$$\text{tensor of heat conductivity coefficients : } \underline{\lambda} \text{ positive definite.} \quad (3.159)$$

However, leaving this class of processes, i.e. going beyond local equilibrium,

$$\xi - \xi_0(t, T(x, t)) \neq 0, \quad (3.160)$$

the processes get unstable. This has been already expected because of Eq. (3.40) which formally is a time reversed heat conduction equation with exploding solutions.³² The deeper physical reason for this unsatisfactory situation can immediately be found. The Lagrangian (3.12) and (3.13) is still a *truncated* one. Thermal inertia is still missing (see Section 4).

3.10. Observables of the second kind [(14*–16*)]

The inhomogeneous balance equations (3.119) — including the special cases (3.125) and (3.130) — and the central balance (3.135) hold for the generator $|\eta(t)\rangle$ of any perturbation $\Delta|\psi(t)\rangle$ of a reference process $|\psi(t)\rangle$. We now turn over to “special perturbations” which are defined by the symmetry group (3.78) of the system. Starting from the real process $|\psi(t)\rangle = \{\psi_k(x, t), k = 1, \dots, f\}$ we get by Eq. (3.81) again a real process $|\psi(t; \varepsilon)\rangle = \{\psi_k(x, t; \varepsilon), k = 1, \dots, f\}$ for each choice of the group parameters ε .³³ Interpreting one special group parameter ε_P as perturbation parameter π and putting all other parameters zero we obtain by means of Eq. (3.81) a one parameter class of *symmetry-induced perturbations* $\Delta|\psi(t; \pi)\rangle_{(\varepsilon_P)}$ of the reference process $|\psi(t)\rangle = \{\psi_i(x, t), i = 1, \dots, f\}$:

$$\begin{aligned} \Delta|\psi(t; \pi)\rangle_{(\varepsilon_P)} &= |\psi(t; \pi)\rangle_{(\varepsilon_P)} - |\psi(t)\rangle, \\ |\psi(t; \pi)\rangle_{(\varepsilon_P)} &= \{\psi_k(x^\alpha; \varepsilon_P = \pi, \varepsilon_K = 0 \text{ for } K \neq P), k = 1, \dots, f\}, \\ \psi_k(x^\alpha; \pi) &= F_k(\psi_l(x^\beta), x^\beta, \varepsilon) \Big|_{x^\beta = f^\beta(\tilde{x}^\alpha; \varepsilon)} \Big|_{\tilde{x} \Rightarrow x} \Big|_{\varepsilon = \{0, \dots, \varepsilon_P = \pi, 0, \dots, 0\}}. \end{aligned} \quad (3.161)$$

By means of Eq. (3.107) this class is associated with the *symmetry-induced generator*

$$|\eta(t)\rangle_{(\varepsilon_P)} = \frac{\partial |\psi(t; \pi)\rangle_{(\varepsilon_P)}}{\partial \pi} \Big|_{\pi=0} = \underline{\eta_{(\varepsilon_P)}} |\psi(t)\rangle = \{\eta_k(x, t)_{(\varepsilon_P)} = \underline{\eta_{(\varepsilon_P)}} \psi_k(x, t), k = 1, \dots, f\}. \quad (3.162)$$

³¹ Exemplifying these methods for the Examples I–III in some detail would go beyond the scope of this paper. The reader is referred to [16] and to forthcoming papers. In [16] the method is demonstrated for Schrödinger’s matter wave (one-particle quantum mechanics) as a reversible system. For heat conduction as an irreversible process first investigations are given for processes running through local equilibrium.

³² Compare with Eq. (3.38).

³³ The sign “~” on ψ is suppressed in the present context.

However, the generator $|\eta(t)\rangle_{(\varepsilon_P)}$ is now related with a linear operator $\eta_{(\varepsilon_P)}$, namely with the generator³⁴ of the invariance group belonging to the group parameter ε_P . $\eta_{(\varepsilon_P)}$ applies to the reference process $|\psi(t)\rangle$. Thus, with $|\eta(t)\rangle_{(\varepsilon_P)}$ we are pulled back into the state space again.

The index (ε_P) in Eqs. (3.161) and (3.162) indicates the special group which underlies the procedure. According to the whole set ε of group parameters there are G possibilities to define a symmetry-induced generator (3.162). Each of them fulfills by definition the perturbation equations (3.108), which, however, in this context are pulled back to the state space, i.e. each of the symmetry induced generators gives rise to a set of f differential equations for the reference process $|\psi(t)\rangle$ (which is primarily a solution of the f ELEqs (3.24)). Thus, in addition to the basic set of ELEqs we have G sets of symmetry-induced equations for the real processes $|\psi(t)\rangle$, i.e. $f \cdot G$ additional equations totally. We call them *adjoint equations* [(10*)]. These may be helpful for solving the ELEqs.

Furthermore, each symmetry-induced generator $|\eta(t)\rangle_{(\varepsilon_P)}$ fulfills by definition the G inhomogeneous Noether balances (3.119). Thus, we obtain G^2 inhomogeneous balance equations which completely operate in state space, i.e. which are fulfilled by each real process $|\psi(t)\rangle$. Taking further into account the central balance (3.135), which by definition is again fulfilled by each symmetry-induced generator, we get another set of G inhomogeneous balance equations for each real process. Thus, in a natural way there are $G(G + 1)$ inhomogeneous balance equations available in LF, each of which defines for the real processes a — traditionally nameless — *observable of the second kind*. These are implicitly defined

- by the balance equations (3.119) or (3.135) and their respective constitutive equations (3.120)–(3.122) or (3.136)–(3.138) for the respective densities, flux densities, and production rate densities, and
- by the symmetry-induced generators (3.162) which have to be inserted into these constitutive equations.

Example 1 (Time translational group (3.124)). Starting from the real process $|\psi(t)\rangle$ we get by means of Eq. (3.161) the symmetry-induced class of perturbations³⁵

$$\Delta|\psi(t; \pi)\rangle_{(\text{time transl})} = |\psi(t - \pi)\rangle - |\psi(t)\rangle, \quad (3.163)$$

which results by means of Eq. (3.162) in the generator

$$|\eta(t)\rangle_{(\text{time transl})} = \left. \frac{\partial|\psi(t - \pi)\rangle}{\partial\pi} \right|_{\pi=0} = -\frac{\partial}{\partial t}|\psi(t)\rangle. \quad (3.164)$$

The associated operator $\eta_{(\text{time transl})} = -\partial/\partial t$ is the well-known generator of time translations.

Example 2 (Gauge group (3.129)). The complex field variables are ordered as in Eq. (3.129). Starting from the real process $|\psi(t)\rangle = \{\psi_1(x, t), \dots, \psi_{f/2}(x, t), \psi_{(f/2)+1}(x, t), \dots, \psi_f(x, t)\}$ the gauge group (3.129) results via Eq. (3.161) in the regauged process

$$|\psi(t, \pi)\rangle_{(\text{gauge})} = \{\psi_1(x, t) \exp(i\pi), \dots, \psi_{f/2}(x, t) \exp(i\pi), \psi_{(f/2)+1}(x, t) \exp(-i\pi), \dots, \psi_f \exp(-i\pi)\} \quad (3.165)$$

and thus via Eq. (3.162) in the induced generator

³⁴ In the usual group theoretical sense.

³⁵ In Eq. (3.124) replace t_0 by π .

$$\begin{aligned}
|\eta(t)\rangle_{(\text{gauge})} &= \{i\psi_1(x, t), \dots, i\psi_{f/2}(x, t), -i\psi_{(f/2)+1}(x, t), \dots, -i\psi_f(x, t)\} \\
&= \begin{pmatrix} i & 0 & \cdot & 0 & 0 & 0 & \cdot & 0 \\ 0 & i & \cdot & 0 & 0 & 0 & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & i & 0 & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 & -i & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 & 0 & -i & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & 0 & 0 & 0 & \cdot & -i \end{pmatrix} \cdot \begin{pmatrix} \psi_1(x, t) \\ \psi_2(x, t) \\ \cdot \\ \psi_{f/2}(x, t) \\ \psi_{(f/2)+1}(x, t) \\ \psi_{(f/2)+2}(x, t) \\ \cdot \\ \psi_f(x, t) \end{pmatrix}. \quad (3.166)
\end{aligned}$$

The quadratic (f, f) -matrix is the associated operator $\underline{\eta}_{(\text{gauge})}$.

Inserting, e.g. Eq. (3.164) into Eq. (3.130)–(3.133) we get a *balance of the second kind*

$$\partial \widetilde{\mathcal{H}} + \nabla \cdot \widetilde{\vec{J}}_{(\mathcal{H})} = \widetilde{\sigma}_{(\mathcal{H})}, \quad (3.167)$$

with the density, flux density, and production rate density *completely defined in state space*:

$$\text{from Eq. (3.131): } \widetilde{\mathcal{H}} = \mathcal{H}(\psi, \partial\psi|\eta, \partial\eta)|_{\eta \Rightarrow -\partial_t \psi, \partial\eta \Rightarrow -\partial \partial_t \psi}, \quad (3.168)$$

$$\text{from Eq. (3.132): } \widetilde{\vec{J}}_{(\mathcal{H})} = \vec{J}_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta)|_{\eta \Rightarrow -\partial_t \psi, \partial\eta \Rightarrow -\partial \partial_t \psi}, \quad (3.169)$$

$$\text{from Eq. (3.133): } \widetilde{\sigma}_{(\mathcal{H})} = \sigma_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta)|_{\eta \Rightarrow -\partial_t \psi, \partial\eta \Rightarrow -\partial \partial_t \psi}. \quad (3.170)$$

The same procedure performed with the same balance (3.130) but with the generator (3.166) results in a *different balance of the second kind*:

$$\partial \widehat{\mathcal{H}} + \nabla \cdot \widehat{\vec{J}}_{(\mathcal{H})} = \widehat{\sigma}_{(\mathcal{H})} \quad (3.171)$$

with the density, flux density, and production rate:

$$\text{from Eq. (3.131): } \widehat{\mathcal{H}} = \mathcal{H}(\psi, \partial\psi|\eta, \partial\eta)|_{\substack{\eta \Rightarrow i\psi, \partial\eta \Rightarrow i\partial\psi \\ \eta^* \Rightarrow -i\psi^*, \partial\eta^* \Rightarrow -i\partial\psi^*}}, \quad (3.172)$$

$$\text{from Eq. (3.132): } \widehat{\vec{J}}_{(\mathcal{H})} = \vec{J}_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta)|_{\substack{\eta \Rightarrow i\psi, \partial\eta \Rightarrow i\partial\psi \\ \eta^* \Rightarrow -i\psi^*, \partial\eta^* \Rightarrow -i\partial\psi^*}}, \quad (3.173)$$

$$\text{from Eq. (3.133): } \widehat{\sigma}_{(\mathcal{H})} = \sigma_{(\mathcal{H})}(\psi, \partial\psi|\eta, \partial\eta)|_{\substack{\eta \Rightarrow i\psi, \partial\eta \Rightarrow i\partial\psi \\ \eta^* \Rightarrow -i\psi^*, \partial\eta^* \Rightarrow -i\partial\psi^*}}. \quad (3.174)$$

The balance (3.171) involves the field variables Ψ and their derivatives up to the second-order whereas Eq. (3.167) involves the derivatives up to the third-order. Both balances are different although they are based on the same original balance (3.130)!

3.11. The second law of thermodynamics [(14a*, 17)]

Among the observables of the second kind we consider that one which is based on the central balance equation (3.135) and on the gauge-symmetry-induced generator (3.166). It is called *entropy balance*. Formally it is preferred above the other observables of the second kind by two facts:

1. The gauge-induced generator together with the central balance of perturbation space results in a balance in state space operating on the same level as the balances of the observables of the first kind, especially as the first law. There are involved the field variables and their derivatives up to the second-order, only.
2. The underlying central balance (3.135) is basic and universal in LF. In contrast to the symmetry-induced balances (3.120) it never gets obsolete! Breaking symmetries destroys Noether balances. The central balance, however, is due to an algebraic structure.

The denomination “entropy” for this distinguished observable of the second kind is chosen because of its final agreement with the traditional entropy concept in special cases. Thus, by means of a straightforward procedure Lagrange formalism results in the *second law of thermodynamics (first part)* [16]:

(from Eq. (3.135))

$$\partial_t s + \nabla \cdot \vec{J}_{(s)} = \sigma_{(s)}, \quad (3.175)$$

(from Eqs. (3.136) and (3.166))

$$\text{entropy density: } s = s(\psi, \partial\psi) = \left(\sum_{j=1}^{f/2} \frac{\partial \Omega(\psi, \partial\psi|\eta, \partial\eta)}{\partial(\partial_t \eta_j)} \eta_j + \text{c.c.} \right) \Big|_{\eta \Rightarrow i\psi, \eta^* \Rightarrow -i\psi^*}, \quad (3.176)$$

(from Eqs. (3.137) and (3.166))

$$\text{entropy flux density: } \vec{J}_{(s)} = \vec{J}_{(s)}(\psi, \partial\psi) = \left(\sum_{j=1}^{f/2} \frac{\partial \Omega(\psi, \partial\psi|\eta, \partial\eta)}{\partial(\nabla \eta_j)} \eta_j + \text{c.c.} \right) \Big|_{\eta \Rightarrow i\psi, \eta^* \Rightarrow -i\psi^*}, \quad (3.177)$$

(from Eqs. (3.138) and (3.166))

$$\text{entropy production rate density: } \sigma_{(s)} = \sigma_{(s)}(\psi, \partial\psi) = 2\Omega(\psi, \partial\psi|\eta, \partial\eta) \Big|_{\eta \Rightarrow i\psi, \eta^* \Rightarrow -i\psi^*}. \quad (3.178)$$

For these formulae the complex and conjugate complex field variables are ordered as in Eq. (3.102).

The *second part of the second law* [16],

$$\sigma_{(s)} \geq 0, \quad (3.179)$$

is no straightforward, universal outcome of LF. It is an individual structure of the particular system, i.e. it depends on the particular form of the Lagrangian. According to the stability theory reported in Section 3.9 *it is supposed that dynamically stable systems give necessarily rise to entropy production*. This statement is supported by special examples, e.g. by the heat conduction process within the frame of the PLE. (See the arguments for Eq. (3.159) and the subsequent formulae in the present chapter.) However, a general proof for the statement is still missing. One final remark supporting the statement: *an asymptotically stable system, i.e. a system, all processes of which are stable, is necessarily irreversible!* The formulae (3.175)–(3.178) will now be exemplified.

Example I (The reversible flow of an ideal fluid). We have to calculate the kernel Ω depending on the fundamental complex field variables $\psi = \{\Psi, \Psi, Z, Z\}$. However, the calculations based on the Lagrangian (3.10) get extremely lengthy and boring. So, we turn over to the equivalent set of field variables $\psi' = \{\rho, \Phi, \Lambda, M\}$ in order to determine Ω on the detour (3.114). Now, one easily sees, that $\Omega' = \Omega'(\psi', \partial\psi'|\eta', \partial\eta')$ calculated from the Lagrangian (3.11) and evaluated for the gauge-induced generator $|\eta'\rangle_{(\text{gauge})} = \{\eta_\rho, \eta_\Phi, \eta_\Lambda, \eta_M\} = \{0, 1, 0, 1\}$ vanishes. Also the four-divergence in Eq. (3.114) vanishes.³⁶ Thus, for the reversible flow of an ideal fluid the entropy concept is completely empty!

$$s = 0, \quad \vec{J}_{(s)} = 0, \quad \sigma_{(s)} = 0. \quad (3.180)$$

For the pure mechanical system this situation is quite satisfactory.

Example II (The irreversible heat conduction). The quantities (3.176)–(3.178) have to be calculated from the Lagrangian (3.12) based on the fundamental set $\psi = (\chi, \chi^*)$ field variables. Turning over to the equivalent set $\psi' = \{T, \xi\}$ and taking the same detour as before we find on the basis of the Lagrangian (3.13), that the kernel Ω' evaluated for the gauge-induced generator $|\eta'\rangle = \{\eta'_T, \eta'_\xi\} = \{0, 1\}$ again vanishes. The four-divergence in Eq. (3.114), however, does not vanish. For the quantity (3.176) we get

$$s = \frac{1}{\omega} \left(cT_0 + 2T \frac{dg(T)}{dT} \right), \quad (3.181)$$

which together with Eq. (3.15) results in

$$s = \frac{T_0}{\omega} \frac{cT + p(T)}{T}. \quad (3.182)$$

Deleting (T_0/ω) , which appears as common factor in all three terms of the entropy balance, and substituting the energy density from Eq. (3.95) we finally get the

$$\text{entropy density : } s = \frac{u + p}{T}. \quad (3.183)$$

Similarly from Eqs. (3.177) and (3.178) and using Eq. (3.96) we get the

$$\text{entropy flux density : } \vec{J}_{(s)} = \frac{-\lambda \cdot \nabla T}{T} = \frac{\vec{J}_{(u)}}{T}, \quad (3.184)$$

and the

$$\text{entropy production rate density : } \sigma_{(s)} = \frac{\nabla T \cdot \lambda \cdot \nabla T}{T^2} = \vec{J}_{(u)} \cdot \nabla \left(\frac{1}{T} \right) \geq 0. \quad (3.185)$$

All these expressions are well-known in traditional TIP for linear heat conduction theory [22]. Obviously Eq. (3.183) coincides with the PLE (3.16)₂. The yet undetermined quantity $p(T)$ finds its interpretation as *hydroelastic pressure* which, however, has to be interpreted in the present situation as a rigid body reaction

³⁶ A few hints for those who wish to do the calculations: Φ and M do not enter into the Lagrangian (3.11). So, all derivatives of Ω' with respect to Φ and M vanish. On the other hand all components of the gauge-induced generator $|\eta'\rangle$ are constant and especially η_ρ and η_Λ vanish. As a result all terms in Ω' vanish. The gauge transformation $\{\Psi \Rightarrow \Psi \exp(i\varepsilon), \Psi^* \Rightarrow \Psi^* \exp(-i\varepsilon)\}$ or equivalently $\{\rho \Rightarrow \rho, \Phi \Rightarrow \Phi + \varepsilon\}$ gives rise to the components $\{\eta_\psi = i\Psi, \eta_{\psi^*} = -i\Psi\}$ of the generator $|\eta\rangle_{(\text{gauge})}$ or to the components $\{\eta_\rho = 0, \eta_\Phi = 1\}$ of the generator $|\eta'\rangle_{(\text{gauge})}$.

of the rigid material background. So, at the very end the Lagrangian (3.12) and (3.13) is completely fitted to the traditional theory of heat conduction. From Eqs. (3.95) and (3.16)₁ we get

$$s = c \ln \frac{T}{T_0}, \quad (3.186)$$

and from Eqs. (3.15), (3.95), (3.183) and (3.186)

$$p(T) = cT \left(\ln \left(\frac{T}{T_0} \right) - 1 \right), \quad \partial_t g(T) = \frac{cT_0}{2T} \left(\ln \left(\frac{T}{T_0} \right) - 1 \right) \partial_t T. \quad (3.187)$$

The undetermined function $\partial_t g(T)$ in the Lagrangian (3.12) and (3.13) is thus determined. Of course, starting with Eq. (3.187) in the Lagrangian the formalism will finally end with the expression (3.186) for the entropy density.

Example III (Irreversible process heat conduction + diffusion + chemical reaction). The calculations follow the same line as those for Example II. From the Lagrangian (3.17) we finally get the

$$\text{entropy density : } s = \frac{1}{T} \left(u + p - \sum_{j=1}^N \mu_j n_j \right), \quad (3.188)$$

$$\text{entropy flux density : } \vec{J}_{(s)} = \frac{1}{T} \left(\vec{J} - \sum_{j=1}^N \mu_j \vec{J}_j \right) = \frac{\vec{J}_{(Q)}}{T}, \quad (3.189)$$

$$\begin{aligned} \text{entropy production rate density : } \sigma_{(s)} &= \vec{J} \cdot \nabla \left(\frac{1}{T} \right) + \sum_{j=1}^N \vec{J}_j \cdot \nabla \left(-\frac{\mu_j}{T} \right) + \sum_{j=1}^N \sigma_j \left(-\frac{\mu_j}{T} \right) \\ &= \vec{J}_{(Q)} \cdot \nabla \left(\frac{1}{T} \right) + \sum_{j=1}^N \vec{J}_j \cdot \frac{\nabla(-\mu_j)}{T} + \sum_{j=1}^N \sigma_j \left(-\frac{\mu_j}{T} \right). \end{aligned} \quad (3.190)$$

Again these expressions are well-known in traditional TIP [22]. We have used Eqs. (3.55) and (3.69). Especially, Eq. (3.188) coincides with the PLE (3.23)₂. Specifying the energy density $u(\dots)$ and the chemical potentials $\mu_j(\dots)$ the hydroelastic pressure $p(\dots)$ and thus the term $\partial_t g(\dots)$ in the Lagrangian (3.17) can finally be determined.

4. Supplementary remarks and perspectives

The theory presented here is quite general. It has been shown, that by means of LF reversible and irreversible processes can be described in a methodically unified way. However, so far the Lagrangians (3.12), (3.13) and (3.17) for the respective irreversible processes are associated with dynamics in the framework of the PLE. The solutions have been constraint by the particular solutions (3.41) and (3.59), and (3.60) of the thermal phase and material phase functions.

$$\xi - \xi^0(t, T) = 0, \quad \varphi_k - \varphi_k^0(t, T, n_k) = 0, \quad k = 1, \dots, f. \quad (3.191)$$

Furthermore, it has been shortly reported that these solutions are dynamically unstable if the manifold of solutions is allowed to extend towards

$$\xi - \xi^0(t, T) \neq 0, \quad \varphi_k - \varphi_k^0(t, T, n_k) \neq 0, \quad k = 1, \dots, f. \quad (3.192)$$

These extensions are associated with deviations of the processes from local equilibrium, i.e. they are no more constrained by the PLE. How to liberate these solutions from dynamical instability?

Let us discuss the heat conduction problem (Example II) representatively also for other cases. It is a well-known fact that the traditional Fourier's law of heat conduction (3.38), being a parabolic equation, involves an infinite speed of heat propagation. This physically quite unsatisfactory feature is due to the absence of a thermal inertia term in the heat conduction equation. Looking at the Lagrangian (3.13) one observes that terms $\partial(\xi - \xi_j^0(\dots))$ appear linearly. Thus, one may consider this Lagrangian as *a truncated form of a more general Lagrangian*, the Taylor expansion of which with respect to $\partial(\xi - \xi_j^0(\dots))$ is broken after the linear terms.³⁷ It is immediately evident that one can present generalized Lagrangians which allow of thermal inertia effects and which are not charged with dynamical instabilities. This generalization can be done in quite a systematic way by extending the Taylor expansion (3.13) to higher orders with respect to $\partial(\xi - \xi_j^0(\dots))$ [19,25,26].

Irrespective of these generalizations a comparison of the Examples II and III shows that the LF allows to involve traditional non-linear as well as linear TIP. Furthermore, the formalisms is open to take account of hidden internal variables. So, traditional linear TIP as well as rational thermodynamics may be included into LF.

Reversible material flow (Example I) and irreversible thermodynamical processes (Examples II and III) have been described as *pure phenomena* without mutual coupling. In reality, however, thermodynamical processes are embedded into material, deformable bodies, especially in a material flow giving rise to thermo-mechanical coupling effects. The problem arises, how to couple the mechanical and thermal dynamics. LF is particularly distinguished to do such a job within a methodically unified theory. I refer, e.g. to the method of “minimal coupling” associated with breaking of Lie symmetries.³⁸ The coupling problem is also intimately related with the various inverse problems in LF.³⁹ It has to be elaborated on the basis of pure phenomena like the Examples I–III presented in this paper.

The Examples II and III are concerned with irreversible processes heat conduction and diffusion but not yet with *dissipative processes*. The chemical reactions involved in Example III are even reversible. Dissipation of chemical energy is involved only indirectly in so far, as the locally produced reaction heat is irreversibly spread out by heat conduction. Dissipation in its proper sense is phenomenologically associated with *friction*, especially with *internal friction*. Physically it is due to a hidden dynamics on a particular microscale of the system. It is intended to take explicitly into account these processes in LF by means of additional field variables, which will be called *transfer variables* [11]: From the phenomenological point of view *dissipation is an irreversible energy transfer from mechanical (and other non-thermal) variables to thermal variables*, i.e. to the thermion field. Traditionally

³⁷ The term $(\xi - \xi_j^0(\dots))$ may not appear because of gauge invariance. Higher order derivatives are excluded because of the Lagrange formalism of the first order.

³⁸ “Localization” of Lie-groups.

³⁹ For the LF for thermo-mechanical processes I refer to [10].

used friction coefficients are seemingly too poor representatives in order to incorporate friction into LF.⁴⁰

5. Realizations

In future the Lagrangian field theory presented in this paper is expected to apply to each particular field of thermodynamics of irreversible processes (TIP), i.e. we believe in the methodical universality of Lagrange formalism. So far we succeeded in the following topics:

1. Linear theory of heat conduction in a rigid body at rest (Example II [11,12]).
2. Generalization of (1) for the non-linear theory of heat conduction (reduce Example III to pure heat conduction [15]).
3. Diffusion in a rigid body (reduce Example III to pure diffusion [15]).
4. Chemical reactions (reduce Example III to pure chemical reactions [15]).
5. The general diffusion-reaction dynamics of arbitrary many chemical constituents including the chemical reaction heat and heat conduction in a system at rest (Example III [15]).
6. Generalization of (1) and (2) taking into account thermal inertia in heat conduction [25] (The paradox of infinite velocity of heat propagation of traditional heat conduction theory can quite naturally be overcome in various ways).
7. Defect dynamics in a crystal. (Topological defects such as lattice vacancies and interstitial atoms or dislocations and its respective dynamics are analogous to diffusion-reaction dynamics of chemical constituents [4,18]. The same holds for electronically excited atoms in a crystal.)
8. Flow of an ideal fluid (Example I [10], pure mechanics).
9. Thermomechanics of a flowing ideal fluid (coupling of (1) and (8), local compression gives rise to local heating of the fluid and thus to heat conduction in the flowing material [10,28]).
10. Newtonian mechanics with friction within Lagrange formalism. (Friction gives rise to an irreversible energy transfer from mechanical to thermal degrees of freedom. For the sake of Lagrange formalism a characterization of friction by means of friction coefficients is too poor. “Transfer variables” as a kind of internal variables are associated with the friction [11].)
11. Lagrange formalism allows for internal friction in a non-ideal fluid (a Lagrangian is presented whose processes after a relaxation time join solutions of the Navier–Stokes equations [10]).
12. Plastic deformation of a crystal is microscopically due to the dynamics of dislocations. (So far only pure mechanics without dissipation has been considered [4]. In Lagrange formalism the system is formally regarded as a fluid with elastic (solid) stiffness (Cosserat-continuum). The correlations within the dislocation network are taken into account by means of a set of complex “dislocation fields”. Plastic yield is associated with material flow as in the problem 8.)
13. The Lagrange formalism presented in this paper has been analogously transposed to the six-dimensional μ -space dynamics of gases [29]. (The Boltzmann and Fokker–Planck equations are embedded into this formalism. The entropy concept presented in the present paper results in μ -space in Boltzmann’s entropy formula.)

⁴⁰ Attempts to involve Coulomb’s and Stokes’ friction by means of transfer variables into LF have already been partially successful [11]. Slightly modified Navier–Stokes equations have been involved into LF [10]. These equations are regarded as Noether’s momentum balance, as it should be according to the universal definition of linear momentum.

References

- [1] H. Goldstein, *Klassische Mechanik*, Aula-Verlag, Wiesbaden, 1989.
- [2] G. Hamel, *Theoretische Mechanik*, Springer, Berlin, 1949.
- [3] E.M. Corson, *Introduction to Tensors, Spinors and Relativistic Wave-Equations*, Blackie, London, 1953.
- [4] K.-H. Anthony, Lagrangian field theory of plasticity and dislocation dynamic-Attempts towards a unification with thermodynamics of irreversible processes, *Arch. Mech. (Warsaw)* 50 (1997) 345–365.
- [5] C. Truesdell, W. Noll, *The Non-linear Field Theories of Mechanics*, *Handbuch der Physik (Flügge)*, Bd. III/3, Springer, Berlin, 1965.
- [6] R.M. Santilli, *Foundations of Theoretical Mechanics I — The Inverse Problem in Newtonian Mechanics*, Springer, New York, 1978.
- [7] R.M. Santilli, Necessary and sufficient conditions for the existence of a Lagrangian in field theory I, *Ann. Phys.* 103 (1977) 354–408.
- [8] R.M. Santilli, Necessary and sufficient conditions for the existence of a Lagrangian in field theory II, *Ann. Phys.* 103 (1977) 409–468.
- [9] R.M. Santilli, Necessary and sufficient conditions for the existence of a Lagrangian in field theory III, *Ann. Phys.* 105 (1977) 227–258.
- [10] M. Scholle, *Das Hamilton'sche Prinzip in der Kontinuumsmechanik nichtdissipativer und dissipativer Systeme*, Dissertation Universität Paderborn, Paderborn, 1999.
- [11] K.-H. Anthony, Remarks on dissipation in Lagrange formalism and attempts to overcome the difficulties, in: A. Radowicz (Ed.), *Dissipation in Physical Systems*, Politechnika Świętokrzyska Kielce, 1998, pp. 55–77.
- [12] I. Gyarmati, *Non-equilibrium Thermodynamics, Field Theory and Variational Principles*, Springer, Berlin, 1970.
- [13] K.-H. Anthony, A new approach describing irreversible processes, in: O. Brulin, R.T.K. Hsieh (Eds.), *Continuum Models of Discrete Systems 4*, North Holland Publ. Comp., Amsterdam, 1981, pp. 481–494.
- [14] K.-H. Anthony, A new approach to thermodynamics of irreversible processes by means of Lagrange formalism, in: C.W. Kilmister (Ed.), *Disequilibrium and Self-Organization*, Reidel Publishing Company, Dordrecht, 1986, pp. 75–92.
- [15] K.-H. Anthony, Phenomenological thermodynamics of irreversible processes within Lagrange formalism, *Acta Physica Hungarica* 67 (1990) 321–340.
- [16] K.-H. Anthony, Entropy and dynamical stability — a method due to Lagrange formalism as applied to thermodynamics of irreversible processes, in: J.F. Besseling, W. Eckhaus (Eds.), *Trends in Applications of Mathematics to Mechanics*, Springer, Berlin, 1988, pp. 297–320.
- [17] K.-H. Anthony, Unification of continuum mechanics and thermodynamics by means of Lagrange formalism — present status of the theory and presumable applications, *Arch. Mech. (Warsaw)* 41 (1989) 511–534.
- [18] K.-H. Anthony, Defect dynamics and Lagrangian thermodynamics of irreversible processes, in: G.A. Maugin (Ed.), *Continuum Models and Discrete Systems 6*, Vol. 2, Longman, New York, 1991, pp. 231–242.
- [19] A. Azirhi, *Thermodynamik und Quantenfeldtheorie — Ein quantenfeldtheoretisches Modell der Wärmeleitung*, Diploma-thesis, Universität Paderborn, 1993.
- [20] E. Schmutzer, *Symmetrien und Erhaltungssätze der Physik*, Akademie-Verlag, Berlin, 1972.
- [21] V.I. Zubov, *Methods of A.M. Lyapunov and their Application*, Verlag Noordhoff, Groningen, 1964.
- [22] S.R. de Groot, P. Mazur, *Non-equilibrium Thermodynamics*, North-Holland, Amsterdam, 1969.
- [23] R.L. Seliger, G.B. Whitham, Variational principles in continuum mechanics, *Proc. R. Soc. London, Ser. A* 305 (1968) 1–25.
- [24] R. Klötzler, *Mehrdimensionale Variationsrechnung*, Birkhäuser-Verlag, Basel, 1970.
- [25] K.-H. Anthony, H. Knoppe, Phenomenological thermodynamics of irreversible processes and Lagrange formalism — hyperbolic equations for heat transport, in: I. Müller, T. Ruggeri (Eds.), *Kinetic Theory and Extended Thermodynamics*, Pitagora Editrice, Bologna, 1987, pp. 15–30.
- [26] M. Schargott, *Trägheitseffekte in der Wärmeleitung — Beiträge zur Wärmeleitungstheorie im Thermionenformalismus*, Diploma-thesis Universität Paderborn, 1997.
- [27] H.-J. Wagner, *Das inverse Problem der Lagrangeschen Feldtheorie in Hydrodynamik, Plasmadynamik und hydrodynamischem Bild der Quantenmechanik*, Habilitationstheise Universität Paderborn, 1997.
- [28] M. Scholle, K.-H. Anthony, Heat conduction in an ideal fluid — a phenomenological approach by means of Lagrange formalism, submitted for publication.
- [29] B. Sievers, K.-H. Anthony, Non-local Lagrange formalism in the thermodynamics of irreversible processes: variational procedures for kinetic equations, *Phys. A* 225 (1996) 89–128.