

# Structure of variational principles in nonequilibrium thermodynamics

Péter Ván

*Department of Chemical Physics, Technical University of Budapest, Budapest, Hungary*

Wolfgang Muschik

*Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany*

(Received 20 March 1995)

There are a lot of different methods to construct variational principles in physics. In this paper we investigate and classify some of the known methods, focusing our treatment mainly on the variational principles in nonequilibrium thermodynamics. This area of physics is remarkably rich in different variational methods, because here we cannot obtain a classical, Hamiltonian variational principle for the transport equations, as far as if we consider them in their original form and with their original variables.

PACS number(s): 05.70.Ln

## I. INTRODUCTION

In physics, dynamic behavior is usually described by a dynamical law, i.e., by an ordinary or partial system of differential equations governing the evolution of the considered system in space and time. By help of an extremum principle we can construct the governing differential equations. Such an extremum principle represents an alternative description of the dynamics, also suggesting a tool for generalizations and offering methods to solve the differential equations. These are the reasons why we think that extremum principles are important both from theoretical and practical points of view [1,2].

The relationship between these alternative descriptions is one of the basic questions of the calculus of variations. We can distinguish between differential and integral principles and a lot of different variational prescriptions. This variety of the extremum principles and methods sometimes makes it possible to give alternate variational formulations for the same differential equation. A good example is classical mechanics of mass-points where a great collection of integral and differential principles exists. However, usually we are looking for a so-called “Hamiltonian” variational formulation [3], that is, we prefer a given type of integral principle with well defined variational prescriptions. There are well known methods as to how we can get the differential equations from an extremum principle, moreover we know well defined conditions on the solution of the inverse problem, the possibility for constructing a Hamiltonian variational principle belonging to a given differential equation [4,5]. On the basis of these conditions we can conclude that for many dynamical laws in physics there definitely does not exist an appropriate Lagrange function or Lagrange density (variational potential) that would satisfy the requirements of such a formulation. But the question is believed to be such an important one that several attempts exist to circumvent the mentioned classical conditions. In con-

tinuum physics and nonequilibrium thermodynamics the transport equations (heat conduction equation, Navier-Stokes equation) have been challenging the researchers for more than a century. After the development of Onsager’s irreversible thermodynamics, the attempts of constructing a variational principle renewed [6–11] and inspired new ideas. Thus a lot of “variational principles” appeared in this field. Recently dynamic equations of extended irreversible thermodynamics have been the parade ground of old and more modern methods.

Knowing the strict conditions for the existence of a Hamiltonian principle we can state that the transport equations do not have a variational potential. This can be connected in some sense to their basic structure, for example the presence of a first time derivative in them. If we want to construct variational methods for these equations we must go beyond the Hamiltonian formulation. Therefore there are a lot of new ideas and unusual prescriptions in the new suggestions. The developers of these principles usually generalize some elements of the formalism of the classical variational calculus, mostly without a careful examination of the mathematical meaning of the constructed algorithms. Under these circumstances some new methods do not deserve the name “variational principle” as far as we understand it in a mathematical sense. However, even in this case these unconventional methods can be the root of better understanding and of developing new numerical methods.

In this paper we will examine some variational methods and principles of physics, focusing our treatment on the basic structure of the construction and on a classification of the existing methods. Most of our examples are from nonequilibrium thermodynamics, but there are important tricks in this field that were not often applied yet.

The paper contains three sections. In Sec. II we formulate the conditions of the existence of a variational potential (action functional) for a given differential equation. Section III gives the classification and at the end there is a discussion.

## II. THE INVERSE PROBLEM OF THE CALCULUS OF VARIATIONS

In this section we summarize some results on the conditions of how a differential equation can be the Euler-Lagrange equation of a variational potential. We have to introduce some notions and notations to be able to formulate the variational methods of nonequilibrium thermodynamics in a sufficiently exact manner. Here we try to reduce the used mathematics to a minimum, considering the structural questions only. In the following,  $\mathbf{V}$  and  $\mathbf{W}$  are normed spaces,  $\text{Lin}(\mathbf{V}, \mathbf{W})$  denotes the vector space of  $\mathbf{V} \rightarrow \mathbf{W}$  (not necessarily continuous) linear functions, and  $U$  is an open subset of  $\mathbf{V}$ .

*Definition II.1.* A function  $f : U \rightarrow \mathbf{V}^*$  is called *potent* on  $U$ , if a function  $F : U \rightarrow \mathbb{R}$  exists, so that  $DF(x) = f(x)$  for every  $x \in U$ . Then  $F$  is called the *potential* of  $f$ .

Here  $D$  denotes the strong or Fréchet derivative of the function. The notion *variational potential* is used for potentials in variational principles. In this case  $U$  and  $\mathbf{V}$  are function spaces; they are sets of functions furnished with topologies (norms).

*Definition II.2.* A function  $T \in \text{Lin}(\mathbf{V}, \mathbf{V}^*)$  is called *symmetric*, if  $\langle T\mathbf{x}, \mathbf{y} \rangle = \langle T\mathbf{y}, \mathbf{x} \rangle$  for every  $\mathbf{x}, \mathbf{y} \in \mathbf{V}$ .

Here  $\langle -, - \rangle$  denotes the effect of the elements of the dual space  $\mathbf{V}^*$  on the elements of  $\mathbf{V}$ , therefore  $\langle -, - \rangle : \mathbf{V}^* \times \mathbf{V} \rightarrow \mathbb{R}$ , so that  $(\mathbf{p}, \mathbf{x}) \mapsto \langle \mathbf{p}, \mathbf{x} \rangle$ , where  $\mathbf{x} \in \mathbf{V}, \mathbf{p} \in \mathbf{V}^*$ .

After these preparations the most important result about the existence of variational potentials can be formulated as follows.

*Theorem II.1.* If a function  $f : U \rightarrow \mathbf{V}^*$  is continuously differentiable for every  $x \in U$  and  $Df(x) \in \text{Lin}(\mathbf{V}, \mathbf{V}^*)$  is symmetric, then  $f$  is potent on  $U$ .

*Proof.* The theorem is a trivial modification of [5, p. 56] taking into account that if a function is weakly differentiable in a neighborhood of a point inside of its domain, and its weak derivative is continuous at the point, then the function is strongly differentiable and its strong and weak derivatives are equal at the given point.

The finite dimensional versions of this theorem are well known in physics. For example, we can find it if we investigate whether a force field is conservative (potent) or not. The vanishing of the curl of the force field is equivalent to the system being conservative. Moreover this statement is equivalent to the theorem mentioned above applied to this very special case.

There are some elements in the theorem which are worthwhile to remember for infinite dimensional applications.

*Remark 1.* The existence of the derivative of  $f : U \rightarrow \mathbf{V}^*$  depends on the norm given on  $\mathbf{V}$ . There may be norms for which  $f$  is differentiable and there are other norms for which  $f$  is not differentiable. In a finite dimensional vector space all norms are equivalent to each other (they define the same topology). Thus the existence of a potential for a given  $f$  does not depend on the norm in finite dimensional spaces.

*Remark 2.* The other important fact is that a poten-

tial exists only for functions mapping  $\mathbf{V} \rightarrow \mathbf{V}^*$  because a derivative of a function  $\mathbf{V} \rightarrow \mathbb{R}$  is necessarily the element of  $\mathbf{V} \rightarrow \mathbf{V}^*$ . With the help of a scalar product the elements of a vector space can be identified with the elements of its dual in a natural way. In the following we will suppose that the problems can be formulated in Hilbert spaces, so we do not need to deal with duals. In this case the duality mapping can be identified with the scalar product.

*Remark 3.* In the calculus of variation one usually deals with weak derivatives. In this case we cannot deal with norms on the domain of the given function which can be helpful in special problems. However the theorems and definitions are more simple with strong derivatives and some care makes the difficulties manageable.

*Remark 4.* In the following a mapping (or function) is called an *operator*, if its domain and its range are spaces of functions. A mapping is called a *functional*, if its domain is a function space and its range a linear space of real (or complex) numbers. In this sense we will speak of potent operators and variational functionals. Actually we should specify the domain and range of the corresponding operators properly. The correct specification of function spaces that is the consideration of the boundary and initial conditions is an essential part of the application of the following methods. We never want to find a *variational principle* for a given equation but for a given *problem*: an equation with the necessary boundary and initial conditions [12].

*Example.* With help of *theorem II.1* the general structure of the "Hamiltonian" variational principles is well understandable. Let  $\hat{L}$  denote a continuous linear operator from a Hilbert space to another one. Suppose that this operator is symmetric. Then the self-adjointness of the operator follows from the continuity. In this case the generally used variational potential is  $\hat{S}(\varphi) = \frac{1}{2} \langle \varphi, \hat{L}\varphi \rangle$ , where  $\varphi$  is an element of the Hilbert space. It is easy to calculate the strong derivative of  $\hat{S}$ :

$$\begin{aligned} D\hat{S}(\varphi)\delta\varphi &= \delta\hat{S}(\varphi) = \delta\frac{1}{2}\langle\varphi, \hat{L}\varphi\rangle \\ &= \frac{1}{2}\langle\delta\varphi, \hat{L}\varphi\rangle + \frac{1}{2}\langle\varphi, \hat{L}\delta\varphi\rangle \\ &= \left\langle\delta\varphi, \frac{\hat{L} + \hat{L}^*}{2}\varphi\right\rangle = \langle\delta\varphi, \hat{L}\varphi\rangle = 0, \end{aligned}$$

where  $\hat{L}^*$  denotes the adjoint of  $\hat{L}$ . Here we denoted two different things with the same letter, the strong (or weak) derivation with  $\delta$  ("the variation of  $S$ ") and the elements of the domain of the derivative with  $\delta\varphi$  ("the variation of  $\varphi$ "). This notation is well accepted and used in physics, and the classical literature of the calculus of variation. Here the different meanings of  $\delta$  can be grasped with the use of affine spaces. If the scalar product is represented by a Lebesgue integral, the equality above is equivalent to  $\hat{L}\varphi = 0$ , as is expected (Lagrange lemma).

### III. CLASSIFICATION

Generally, most of the differential equations cannot be derived as a Euler-Lagrange equation of a variational potential because their derivatives are not symmetric. The importance and the need of extremum principles for these problems resulted in a lot of methods for constructing potentials for nonpotent operators as well. In the following a classification of the most important ideas is given. Some other aspects of this classification can be found in [8, pp. 307–312], [13,14], and especially in [15].

$\hat{\Theta}$  denotes a nonpotent operator and  $\hat{L}$  a (not necessarily symmetric) linear operator on a Hilbert space  $\mathbf{H}$ . A variational principle shall be formulated for the equation  $\hat{\Theta}(\varphi) = 0$  or  $\hat{L}\varphi = 0$ . Usually in nonequilibrium thermodynamics  $\hat{\Theta}$  and  $\hat{L}$  are differential operators.

#### A. Method of additional variables or dual principles

The essence of this trick is that more variables (and more equations) are introduced into the problem, thus extending the corresponding function space in such a way that the original operator will be a part of a potent operator. The most important problem of this method is always the “physical meaning” of the new variables and equations.

A variational potential is sought for the equation  $\hat{L}\varphi = 0$ , where  $\varphi \in \mathbf{H}$ . According to this method we take the adjoint  $\hat{L}^*$  of  $\hat{L}$ , and we exploit that the composite operator

$$\begin{pmatrix} 0 & \hat{L}^* \\ \hat{L} & 0 \end{pmatrix}$$

is symmetric on the extended  $\mathbf{H} \times \mathbf{H}^*$  Hilbert space. Really, a corresponding variational potential can be constructed for the equations  $\hat{L}\varphi = 0$  and  $\hat{L}^*\varphi^* = 0$ :

$$\hat{S}(\varphi, \varphi^*) = \frac{1}{2} [\langle \varphi^*, \hat{L}\varphi \rangle + \langle \hat{L}^*\varphi^*, \varphi \rangle],$$

where  $\varphi^* \in \mathbf{H}^*$ .

*Example.* A well known example is the variational principle for the  $(\hat{H} + E)\phi = 0$  Schrödinger equation, where the wave function  $\phi$  is an element of the function space of square integrable functions, and  $\hat{H}$  is a Hamilton operator. Here a formal variational potential is [16]

$$\hat{S}(\phi^*, \phi) = \int \phi^*(\hat{H} + E)\phi dq.$$

*References.* Another nomination of the method of dual principles is the “method of mirror equations” in Morse and Feshbach [16, pp. 314–316 and 335–337]. The extension of this method for nonlinear operators was formally a “multiplication” of the equation with the new variable, like the example of the Schrödinger equation, or can be considered as an “extension” of the concept of the adjoint to nonlinear operators [7,8]. However it has a clear and well discussed mathematical formulation

(see, for example, [17]). Direct methods coming from this kind of principle are equivalent with the Galerkin method applied for the operator (differential equation) directly. These extensions are sometimes called “complementary principles” in [18–20] or “composite principles” [13,21]. Examples for the application of this method in continuum physics is given by Collins [22].

A hardly discussed but important problem in connection with this method is its formal character: the resulting dual equations usually lack any physical meaning. In the case of the Schrödinger equation this fact is well known, because here the multiplication of the wave function with its conjugate results in the probability density. But, for example, in Anthony’s method [23,24], which introduced a variational formalism for the heat conduction equation by quantum mechanical analogies, the interpretation is difficult. Of course, there are examples for which the introduced new variables are physical quantities [25,26]. Another important example for the application of physically meaningful additional variables is the governing principle of dissipative processes. Here the thermodynamical currents are the new variables and the constitutive functions defining them are the additional equations [27,9].

#### B. Method of integrating operator

In this and in the following method we do not refer to a particular operator, but only to its kernel. We denote two operators as equivalent if their homogeneous equations have the same solutions, that is, the kernels of the two operators are the same. This is a well acceptable agreement from a physical point of view.

The essence of the method of an integrating operator consists in considering instead of the operator  $\hat{\Theta}$  a composite operator  $\hat{\Lambda} \circ \hat{\Theta}$  in a special way: (i) The composition should be meaningful ( $\text{Dom}\hat{\Lambda} \subset \text{Ran}\hat{\Theta}$ ); (ii) the corresponding equations should have the same solutions [ $\text{Ker}(\hat{\Lambda} \circ \hat{\Theta}) = \text{Ker}\hat{\Theta}$ ], (iii) the composite operator ( $\hat{\Lambda} \circ \hat{\Theta}$ ) is a potent one.  $\hat{\Lambda}$  is called an *integrating operator*.

There are two important special applications of this method:

(i) *Method of least squares.* For continuous linear operators ( $\hat{L}$ ) the integrating operator can be the adjoint of the original one ( $\hat{\Lambda} = \hat{L}^*$ ). In this case a variational potential is

$$\hat{S}(\varphi) = \frac{1}{2} \langle \hat{L}\varphi, \hat{L}\varphi \rangle.$$

Here the Euler-Lagrange equation is  $\hat{L}^*\hat{L}\varphi = 0$ , which has the same solutions as  $\hat{L}\varphi = 0$  if  $\hat{L}^*$  is invertible. A well known example is the Gauss principle of “least constraint” in mechanics [1,2]. A direct application to nonlinear heat conduction is [28].

(ii) *Integrating multipliers.* In this case  $\hat{\Lambda}$  is restricted to a function of the variables [ $\hat{\Lambda} = l(\varphi)$ ] and is called an *integrating multiplier*.

*Example.* An important special example is when  $\varphi \in$

$C^2(\mathbb{R})$  and the nonpotent operator is  $\hat{L} = (\tau \frac{d^2}{dt^2} + \frac{d}{dt})$ ,  $\tau \in \mathbb{R}$ . In this case  $e^{t/\tau} \hat{L}$  is potent and a variational potential is  $\hat{S}(\varphi) = \frac{\tau}{2} e^{t/\tau} (\frac{d\varphi}{dt})^2$ .

The special trick showed in the example is applied to the equations of extended irreversible thermodynamics by Vujanovic and Sieniutycz [29–33] and others. A more systematic treatment of the method of integrating multipliers in field theories can be found in [34].

A general formulation of this method is due to Tonti [12], who showed that an integrating operator can be constructed for every nonlinear operator in a way very similar to the least squares, although this construction is not unique. He obtains the “integrated equation” in the following form:

$$\delta^* \hat{\Theta}(\varphi) \cdot \hat{K} \cdot \hat{\Theta}(\varphi) = 0,$$

where  $\hat{K}$  is introduced to give compatibility between the corresponding spaces, and it is a linear, symmetric, invertible operator from  $\text{Ran}(\hat{\Theta})$  to  $\text{Dom}[\delta^* \hat{\Theta}(\varphi)]$ . In this case under some more conditions on  $\hat{\Theta}$  this is the Euler-Lagrange equation of the variational potential

$$\hat{S}(\varphi) = \frac{1}{2} \langle \hat{\Theta}(\varphi), \hat{K} \cdot \hat{\Theta}(\varphi) \rangle.$$

There are several possibilities for the construction of  $\hat{K}$ .

Of course there is only one possibility for the construction of an integrating operator. Another way of the construction is used by Gerjuoy and co-workers [35–40] and is denoted as the method of “Lagrange multipliers.” This method is not as elaborated mathematically as the one before, but it is often applied.

Now we introduce an unknown operator  $\hat{u}$  so that  $\text{Dom}(\hat{u}) \subseteq \text{Dom}(\hat{\Theta})$ , and we look for a variational potential of the shape  $\hat{S}(\varphi) = \hat{S}(\varphi, \hat{u}(\varphi))$ . If we require the following conditions:

$$\partial_1 \hat{S}(\varphi, \hat{u}(\varphi)) = 0, \quad (1)$$

$$\partial_2 \hat{S}(\varphi, \hat{u}(\varphi)) = \hat{\Theta}(\varphi), \quad (2)$$

the general solution of the second simple partial differential equation is

$$\hat{S}(\varphi, u) = \langle \hat{\Theta}(\varphi), u \rangle + \hat{w}(\varphi).$$

Here  $\hat{w}$  is an arbitrary function or functional. In this case Eq. (1) gives a condition to determine  $\hat{u}(\varphi)$ :

$$\partial_1 \hat{S}(\varphi, \hat{u}(\varphi)) \delta \varphi = \langle \delta \hat{\Theta}(\varphi) \delta \varphi, u \rangle + \delta \hat{w}(\varphi) \delta \varphi = 0.$$

In particular cases we can determine  $\hat{u}$  relatively easily and write down the particular form of the variational potential  $\hat{S}(\varphi)$ . The resulting Euler-Lagrange equation is

$$\delta^* \hat{u}(\varphi) \hat{\Theta}(\varphi) = 0,$$

and this is equivalent to  $\hat{\Theta}(\varphi) = 0$ , if  $\delta^* \hat{u}(\varphi)$  is invertible. Technically the determination of  $\hat{w}$  so that  $\delta^* \hat{u}(\varphi)$  is invertible represents the crucial point of this method.

These examples show that there is a great flexibility in

constructing an integrating operator and consequently in obtaining variational potentials. Generally the application of *theorem II.1* allows us to write down a functional differential equation for the operator  $\hat{\Lambda}$ :

$$\delta \hat{\Lambda} \circ \hat{\Theta}(\varphi) \cdot \delta \hat{\Theta}(\varphi) = \delta^* \hat{\Theta}(\varphi) \cdot \delta^* \hat{\Lambda} \circ \hat{\Theta}(\varphi).$$

Determining the explicit solution of this equation seems hopeless, but some special assumptions and the investigation of particular examples may simplify the procedure and can lead to new results.

### C. Method of transformation of variables

The essence of this method is that we change the independent variable into an operator, more precisely, instead of the operator  $\hat{\Theta}$  we consider a composite operator  $\hat{\Theta} \circ \hat{\varphi}$  in a special way: (i) The composition should be meaningful ( $\text{Ran} \hat{\varphi} \subseteq \text{Dom} \hat{\Theta}$ ); (ii) the corresponding equations should have the same solutions:

$$\bigwedge x, x \in \text{Ker}(\hat{\Theta} \circ \hat{\varphi}) \leftrightarrow y := \varphi(x) \in \text{Ker} \hat{\Theta},$$

which results in

$$\hat{\varphi}(\text{Ker}(\hat{\Theta} \circ \hat{\varphi})) = \text{Ker} \hat{\Theta};$$

(iii) the composite operator ( $\hat{\Theta} \circ \hat{\varphi}$ ) is a potent one. We can see that this method represents the counterpart of the method of integrating operators.

*Example.* The best known example is the variational principle for the Maxwell equations in vacuum. These equations are nonpotent in their original variables ( $\mathbf{E}, \mathbf{B}$ ), but introducing the scalar and the vector potential ( $\mathbf{A}, \Phi$ ) the resulting wave equations are potent ones.

This special example motivated us to introduce new variables  $\xi$  which should be called *potentials*. If  $\hat{\varphi}$  is a composition operator (a composition with a simple function)  $\text{Dom} \varphi = \text{Ran} \xi$  and  $\hat{\varphi}(\xi) = \varphi \circ \xi$ , the transformation is called an *algebraic* one.

These algebraic transformations are widely used for constructing variational principles for perfect fluids [41]. A more general formulation of this method for special nonlinear operators (and some applications) is given by Nyíri [42]. He constructs a variational potential for operators in the form  $\hat{\Theta}(\varphi) = \hat{L} \cdot f(\varphi)$ , where  $\hat{L}$  is a linear operator and  $f(\varphi)$  is a composition of functions. The essence of his method shows similarities with that of Gerjuoy *et al.* An application in nonequilibrium thermodynamics and the search for some physical consequences is due to Gambár and Márkus [43–46].

Using Nyíri’s method we look for a variational potential in the form  $\hat{S}(\xi) = \hat{S}(\xi, \hat{\varphi}(\xi))$ . If we require the following conditions:

$$\partial_1 \hat{S}(\xi, \hat{\varphi}(\xi)) = \hat{\Theta}(\hat{\varphi}(\xi)), \quad (3)$$

$$\partial_2 \hat{S}(\xi, \hat{\varphi}(\xi)) = 0, \quad (4)$$

the general solution of the first partial differential equation is

$$\hat{S}(\xi, \varphi) = \langle \hat{\Theta}(\varphi), \xi \rangle + \hat{w}(\varphi).$$

Here  $\hat{w}$  is an arbitrary function or functional. In this case Eq. (4) is a condition to determine  $\hat{\varphi}(\xi)$ :

$$\partial_2 \hat{S}(\xi, \varphi) \delta \varphi = \langle \delta \hat{\Theta}(\varphi) \delta \varphi, \xi \rangle + \delta \hat{w}(\varphi) \delta \varphi = 0.$$

Now the explicit determination of  $\hat{\varphi}$  can be technically more difficult than in the case of Gerjuoy *et al.*, because it requires the determination of the inverse of a nonlinear operator. In the special case treated by Nyíri we need to invert a function only. Now the full form of the variational potential is as follows:

$$\hat{S}(\xi) = \langle \hat{\Theta}(\hat{\varphi}(\xi)), \xi \rangle + \hat{w}(\hat{\varphi}(\xi)).$$

The resulting Euler-Lagrange equation is the original one (in contrast to the method of Gerjuoy *et al.*), with the introduced new variables

$$\hat{\Theta}(\hat{\varphi}(\xi)) = 0.$$

Now we can choose  $\hat{w}$  to make the computation simple.

If we try to apply *theorem II.1*, we can get a condition for the determination of  $\hat{\varphi}$ , like in the method of integrating operators. Only a detailed investigation of this functional differential equation can show whether another constructive method exists or not.

#### D. Method of modifications

These methods are sometimes referred to as quasivariational principles, or “restricted” variational principles [6,8,11]. Two types of them can be distinguished.

##### 1. Modified operators

By this method the operator  $\hat{\Theta}$  is modified in such a way that the transformed operator  $\hat{\Theta}_m$  will be potent. The domain of the modified operator is the same as the original one. Of course, in this case variational potentials exist only for the modified operator, not for the original one.

“Variational principles” coming from the method of modified operators are usually believed to be valid in a more general sense than they really are. For instance, the resulting Euler-Lagrange equations are transformed to get back the original operator. Sometimes the method is interpreted as the application of a “restriction” because the modification is usually a restriction of the original operator, as it is shown in the following example. However, well applicable numerical methods can be elaborated with the help of this procedure to solve the original equation.

*Example.* The typical example is the stationary heat conduction equation with a temperature-dependent heat conduction coefficient:  $\hat{\Theta}(T) = \nabla(\lambda(T)\nabla T)$ . The usual modification is the following  $\hat{\Theta}_m(T) = \nabla(\lambda(T_0)\nabla T)$ . Here  $T_0$  is a given arbitrary temperature. If we write

down a variational principle for the modified equation [where  $\lambda(T)$  is a given function which has to be taken at  $T = T_0$ ], then we can get information for solutions of the original equation, too. The numerical method is a special fix point iteration. According to the iteration scheme the solution of the equation  $\hat{\Theta}_n(T) = \nabla(\lambda(T_n)\nabla T)$  (generated by a direct method from the variational principle) gives  $T_{n+1}$ .

*References.* This method was originally invented by Rosen [47], applied among others by Glandsdorff and Prigogine and his co-workers in the method of local potentials [48,49], and by Lambermont and Lebon [50] in their variational method.

##### 2. Modified function spaces

In this case the domain of the original operator is restricted, so that the originally nonpotent operator becomes potent on the restricted domain. With other words the operator is modified by restricting its domain and not its “shape.”

The modification of function spaces leads to well defined extremum problems on an appropriate “restricted” function space for a differential equation. Moreover, in the case of usual initial-boundary value problems this procedure can lead to well manageable numerical methods for the *original* equation too [52,49]. Thus Finlayson is wrong in declaring that this method is out of the framework of the calculus of variation [8, pp. 342 and 343].

*References.* A classical example of application of this method is Gauss’ principle of “least constraint” in mechanics [1,2]. In practice this method is often applied to get variational principles for differential equations containing first order time derivatives. This is the case in nonequilibrium thermodynamics where it was introduced by Rosen [51], using the method of potentials [48,49] or in different forms of the Gyarmati principle [27].

*Remark.* If we use the hint “the time derivative must be held fixed during the variation,” then such a modified function space is introduced for the variation.

Finally we remark that the different methods mentioned here can be mixed for constructing variational principles. For example, this is the case in the method of local potentials [48,49] in which both types of modifications of this section are used. If we apply this method to the full heat conduction equation, we have to modify the function space to overcome the nonpotentness of the first time derivative and we have to modify the operator as well to solve the problem of the quasilinear term. The other example is the variational principle of Anthony [23,24], where we can find a mixing of the method of additional variables and variable transformations. The last and perhaps the most complex example is the governing principle of dissipative processes of Gyarmati. This principle exploits the special structure of the transport equations of Onsager’s irreversible thermodynamics and does the following: introduces the thermodynamical currents as *additional variables* (here the additional variables have a physical meaning); has a Gaussian form resembling the method of least squares [9,53]; modifies the original func-

tion space; and possesses some other peculiarities too. A detailed investigation of the structure of the governing principle of dissipative processes according to the points mentioned above is given in [54].

#### IV. DISCUSSION

Here we did not make any efforts to give a complete reference list of the flood of literature on variational principles of nonequilibrium thermodynamics, but the references mentioned characterize typical examples. However, we truly hope that the presented classification covers all logical possibilities and that our references typify the existing methods.

After having discussed these methods, it seems to be more plausible than before that potent differential equations (or operators) can be constructed by help of these different methods. Another remark is that we cannot

hope to construct a *single* variational principle for entire nonequilibrium thermodynamics, or for any other branch of physics. There are always possibilities to construct several principles being equal or more or less acceptable. Of course there are always physical constraints, but the remaining freedom is still enormous.

As a conclusion we want to remark that this accumulated knowledge of different possibilities of constructing variational principles can change today the *art of searching and finding* such variational principles to a more systematic procedure. For discussing variational principles of irreversible processes beyond nonequilibrium thermodynamics we want to refer to Ichiyanagi's detailed paper [55].

#### ACKNOWLEDGMENTS

Financial support by the DAAD sponsoring the cooperation between both our departments is gratefully acknowledged.

- 
- [1] W. Yourgrau and S. Mandelstam, *Variational Principles in Dynamics and Quantum Mechanics* (Pitman, London, 1956).
- [2] C. L nczos, *The Variational Principles of Mechanics* (University of Toronto Press, Toronto, 1949).
- [3] L. D. Landau, and E. M. Lifshitz, *Mechanics/Course of Theoretical Physics* (Pergamon Press, Oxford, 1960), Vol. 1.
- [4] P. Havas, *Nuovo Cimento* **1**, 363 (1957).
- [5] M. M. Vainberg, *Variational Methods for the Study of Nonlinear Operators* (Holden-Day, San Francisco, 1964).
- [6] B. A. Finlayson and L. E. Scriven, *Int. J. Heat Mass Transfer* **10**, 799 (1967).
- [7] B. A. Finlayson, *Phys. Fluids* **15**, 963 (1972).
- [8] B. A. Finlayson, *The Method of Weighted Residuals and Variational Principles (With Application in Fluid Mechanics, Heat and Mass Transfer)*, Mathematics in Science and Engineering Vol. 87 (Academic Press, New York, 1972).
- [9] I. Gyarmati, *Non-equilibrium Thermodynamics (Field Theory and Variational Principles)* (Springer Verlag, Berlin, 1970).
- [10] J. Verh s, *Thermodynamics and Rheology* [M szaki K nyvkiad  (Technical Publishers), Budapest, 1985] (in Hungarian).
- [11] G. Lebon, in *Recent Developments in Thermomechanics of Solids*, edited by G. Lebon and P. Perzyna (Springer Verlag, Wien, 1980), p. 221.
- [12] E. Tonti, *Int. J. Eng. Sci.* **22**, 1343 (1984).
- [13] R. W. Atherton and G. M. Homsy, *Stud. Appl. Math.* **54**, 31 (1975).
- [14] W. Muschik and R. Trostel, *ZAMM* **63**, T190 (1983).
- [15] P. V n and W. Muschik, *Periodica Polytech.* (to be published).
- [16] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1.
- [17] P. Blanchard and E. Br ning, *Variational Methods in Mathematical Physics* (Springer Verlag, Berlin, 1992).
- [18] A. N. Arthus, *Complementary Variational Principles* (Oxford University Press, Oxford, 1970).
- [19] J. T. Oden and J. N. Reddy, *Variational Methods in Theoretical Mechanics* (Springer Verlag, Berlin, 1976).
- [20] A. M. de Oliveira and W. A. Boruszewski, *Int. J. Non-Linear Mech.* **27**, 1015 (1992).
- [21] S. Sieniutycz, *Conservation Laws in Variational Thermohydrodynamics* (Kluwer Academic, Dordrecht, 1994).
- [22] W. D. Collins, *Proc. R. Soc. Edinburgh, Sect. A* **77**, 273 (1977).
- [23] K. H. Anthony, in *Continuum Models of Discrete Systems 4*, edited by O. Brulin and R. K. Hsieh (North-Holland, Amsterdam, 1981), p. 481.
- [24] K. H. Anthony, *Acta Phys. Hung.* **67**, 321 (1990).
- [25] I. Kirschner, *Acta Phys. Hung.* **30**, 61 (1971).
- [26] I. Kirschner and R. T r s, *J. Non-Equilib. Thermodyn.* **9**, 165 (1984).
- [27] I. Gyarmati, *Ann. Phys.* **23**, 353 (1969).
- [28] B. Vujanovic and B. Baelic, *Int. J. Heat Mass Transfer* **19**, 721 (1976).
- [29] B. Vujanovic and D. Djukic, *Int. J. Heat Mass Transfer* **15**, 1111 (1972).
- [30] B. D. Vujanovic and S. E. Jones, *Variational Methods in Nonconservative Phenomena* (Academic Press, Boston, 1989).
- [31] S. Sieniutycz, *Int. J. Heat Mass Transfer* **22**, 585 (1979).
- [32] S. Sieniutycz, *J. Non-Equilib. Thermodyn.* **9**, 61 (1984).
- [33] S. Sieniutycz, *Appl. Sci. Res.* **42**, 211 (1985).
- [34] R. M. Santilli, *Ann. Phys.* **103**, 354 (1977); **103**, 409 (1977); **105**, 227 (1977).
- [35] E. Gerjuoy, A. R. P. Rau, and L. Spruch, *Rev. Mod. Phys.* **55**, 725 (1983).
- [36] E. Gerjuoy, A. R. P. Rau, and L. Spruch, *J. Math. Phys.* **13**, 1797 (1972).
- [37] E. Gerjuoy, A. R. P. Rau, and L. Spruch, *Phys. Rev. A* **8**, 662 (1973).
- [38] E. Gerjuoy, A. R. P. Rau, L. Rosenberg, and L. Spruch, *Phys. Rev. A* **9**, 108 (1974).
- [39] E. Gerjuoy, A. R. P. Rau, L. Rosenberg, and L. Spruch, *J. Math. Phys.* **16**, 1104 (1975).
- [40] E. Gerjuoy, L. Rosenberg, and L. Spruch, *J. Math. Phys.* **16**, 455 (1975).
- [41] S. D. Mobbis, *Proc. R. Soc. London, Sect. A* **381**, 457 (1982).

- [42] B. Nyíri J. Non-Equilib. Thermodyn. **16**, 39 (1991).
- [43] F. Márkus and K. Gambár, J. Non-Equilib. Thermodyn. **16**, 27 (1991).
- [44] K. Gambár, F. Márkus, and B. Nyíri, J. Non-Equilib. Thermodyn. **16**, 217 (1991).
- [45] K. Gambár and F. Márkus, J. Non-Equilib. Thermodyn. **18**, 51 (1993).
- [46] K. Gambár and F. Márkus, Phys. Rev. E **50**, 1227 (1994).
- [47] P. Rosen, J. Appl. Phys. **25**, 336 (1954).
- [48] P. Glansdorff and I. Prigogine, *Thermodynamic Theory of Structure, Stability and Fluctuations* (Wiley-Interscience, London, 1971).
- [49] R. S. Schechter, *The Variational Method in Engineering* (McGraw-Hill, New York, 1967).
- [50] J. Lambermont and G. Lebon, Ann. Phys. **28**, 15 (1972).
- [51] P. Rosen, J. Chem. Phys. **21**, 1220 (1953).
- [52] A. Stark, Ann. Phys. **31**, 53 (1974).
- [53] B. Nyíri, Acta Phys. Hung. **66**, 19 (1989).
- [54] P. Ván, J. Non-Equilib. Thermodyn. (to be published).
- [55] M. Ichiyangi, Phys. Rep. **243**, 125 (1994).