Application of Potentials in the Description of Transport Processes

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The most important equations of motion in physics are summarized in differential equations. Variational calculus is suitable to unify the different disciplines of physics; it is even classical mechanics, electrodynamics or modern field theories. The basic equations of the disciplines can be deduced from the least action principle, the Hamilton's principle. It is shown that the Lagrange function can be formulated for dissipative processes, in systems with infinite degree of freedom, thus the Hamilton's principle can be considered as a basis of the theory. The Lagrange function can be constructed by an introduced scalar (potential) field that defines the measurable physical quantities.

In the present paper we will construct a Lagrangian density function in such a way that the field equations (equations of motion) are known, but these equations contain non-selfadjoint operators. For this, it is necessary to introduce potentials. We suggest what possible directions are open in the study of the system, through the elaboration of the mathematical model.

Keywords: Hamilton's principle; dissipation; potential; adjoint operator; canonical formalism

1 Introduction

When Lagrange showed Euler his work, in which he deduced the principles of mechanics, based on the variational calculus, he did not think that it would spread to all disciplines of physics or the presented method might become a pillar of modern physics.

It is known that the equations for motion in physics can be formulated by differential equations. Most of them can be deduced from the least action principle, the Hamilton's principle. Experience shows that for those theories, where the Hamilton's principle can be applied and the related Hamilton-Lagrange formulas can be elaborated not only the aesthetics" of the theory are impressive, but often, further improvements and discoveries develop.

The degrees of freedom of continuous media (physical fields) are infinite. Their descriptions change from place to place and moment to moment. We assign mathematical variables (field quantities) to individual points of geometric fields at each moment. The time evolution of these variables can be described by the field equation (equations of motion). In general, there are two basic steps to construct the actions for systems with infinite degrees of freedom: taking into account the properties of the system the Lagrange density function should be formulated by the field variables; the action can be obtained by the spatial and time integration of the Lagrange density function. If we know the action, we accept the Hamilton's principle, as an axiom (basic principle), then the complete Hamilton-Lagrange formalism can be built up and applied. It took a long time to recognize just how to establish this description for dissipative systems. It can be shown that the Lagrange function of a dissipative process, with an infinite degree of freedom, can be formulated by introducing a relevant physical-mathematical additional field, thus, Hamilton's principle gives the foundation of the theory [1, 2, 3]. The Lagrange function itself can be formulated with the help of this scalar field, which has a consistent mathematical relation, with measurable physical fields. Since the Hamilton principle is not sensitive as to how the Lagrange function is created, we can exploit the possibilities of variational calculus, the elaboration the complete canonical formalism and we can explore the various related research directions, based on the developed theory.

2 Construction of Lagrange Functions

2.1 Hamilton's Principle

In order to consider the Hamilton's principle, as a base of the theory, we need to formulate the Lagrange density function *L*, which the time integral is the action *S*.

$$S = \int L \, \mathrm{d}V \mathrm{d}t \tag{1}$$

The Lagrange density function for a Ψ scalar field is written by its first order derivatives as:

$$L = L\big(\Psi, \dot{\Psi}, \nabla\Psi\big) \tag{2}$$

In the sense of the Hamilton's principle, the variation of action is:

$$\delta S = \delta \int_{t_1}^{t_2} L \, \mathrm{d}V \mathrm{d}t = 0 \tag{3}$$

This means that for a realistic process of nature, the action is an extremum, i.e., the variation of action is zero. If the Lagrange function depends on the physical field Ψ and its derivatives then after the variation of action the Euler-Lagrange differential equation can be obtained. The following describes the time and spatial evolution of the field:

$$\frac{\partial L}{\partial \Psi} - \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{\Psi}} - \nabla \cdot \frac{\partial L}{\partial \nabla \Psi} = 0 \tag{4}$$

Naturally, the Lagrange function may include more variables and higher order derivatives.

In general, if a linear operator O acts on the function Ψ in the Lagrange function then an expression

$$\tilde{O}\frac{\partial L}{\partial (O\Psi)} \tag{5}$$

appears in the Euler-Lagrange equation where $\tilde{O}$ is the adjoint operator of operator O. The most frequent operator – adjoint operator pairs in physics are:

$$O = \frac{\partial}{\partial t} \rightarrow \tilde{O} = -\frac{\partial}{\partial t} \tag{6}$$

$$O = \mathrm{grad}(= \nabla) \ \rightarrow \ \tilde{O} = -\mathrm{div}(= \nabla \cdot) \tag{7}$$

$$O = \mathrm{rot}(= \nabla \times) \rightarrow \ \tilde{O} = \mathrm{rot}(= \nabla \times) \tag{8}$$

$$O = \mathrm{div}(= \nabla \cdot) \rightarrow \tilde{O} = -\mathrm{grad}(= \nabla) \tag{9}$$

$$O = \frac{\partial^2}{\partial t^2} \rightarrow \tilde{O} = \frac{\partial^2}{\partial t^2} \tag{10}$$

$$O = \Delta \rightarrow \tilde{O} = \Delta \tag{11}$$

If the equality $O = \tilde{O}$ is completed then we speak about a self-adjoint operator. The Lagrange function can easily be constructed if equation of motion of a variable is known.

2.2 The Example of Electrodynamics

In the knowledge base for electric charges and currents, using the Maxwell equations, an electromagnetic field can be formulated in a simpler form, introducing the scalar and vector potentials. These define the measurable field variables as [4]:

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} - \mathrm{grad}\varphi \tag{12}$$

$$\vec{B} = \mathrm{rot}\vec{A} \tag{13}$$

In order to simplify the equations the potentials can be modified as:

$$\overrightarrow{A'} = \vec{A} + \mathrm{grad}\psi \tag{14}$$

$$\varphi' = \varphi - \frac{\partial \psi}{\partial t} \tag{15}$$

i.e., the definition of potentials are free from a gradient or time derivative, of an arbitrary scalar field. This means a free choice of potentials, suitably, e.g. it can be (Lorenz measure):

$$\mathrm{div}\vec{A} = -\varepsilon_o \mu_o \frac{\partial \varphi}{\partial t} \tag{16}$$

In that part of space where the charge density and the currents are zero, the Lagrange density function for the Maxwell equations can be expressed by the potentials:

$$\mathcal{L} = \frac{1}{2}\varepsilon_o \left(\frac{\partial \vec{A}}{\partial t} + \mathrm{grad}\varphi\right)^2 - \frac{1}{2\mu_o}\left(\mathrm{rot}\vec{A}\right)^2 \tag{17}$$

The Euler-Lagrange differential equations can be obtained by the variation of $\vec{A}$:

$$\mathrm{rot}\,\mathrm{rot}\frac{\vec{A}}{\mu_o} - \varepsilon_o \frac{\partial}{\partial t}\left(-\frac{\partial \vec{A}}{\partial t} - \mathrm{grad}\varphi\right) = 0 \tag{18}$$

which results the Euler-Lagrange differential equations. By the application of definition equation (13) the well-known Maxwell equations are obtained:

$$\mathrm{rot}\vec{B} = \varepsilon_o \mu_o \frac{\partial \vec{E}}{\partial t} \tag{19}$$

After the variation by φ the equation

$$\mathrm{div}\left(\frac{\partial \vec{A}}{\partial t} + \mathrm{grad}\varphi\right) = 0 \tag{20}$$

can be deduced. Applying equation (12), we get

$$\mathrm{div}\vec{E} = 0 \tag{21}$$

formulating the next Maxwell equation. The equations

$$\mathrm{div}\vec{B} = 0 \tag{22}$$

$$\mathrm{rot}\vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{23}$$

are completed automatically by the application of definition equations (12) and (13).

Considering the $\vec{A}$ dependence in the Lagrange density function, the operators $O_1 = \frac{\partial}{\partial t}$ and $O_2 = rot$ appear. According to the previous mathematical list in equations (6) – (11) the terms $-\frac{\partial}{\partial t}\frac{\partial L}{\partial(\frac{\partial \vec{A}}{\partial t})}$ and $\mathrm{rot}\frac{\partial L}{\partial(\mathrm{rot}\vec{A})}$ appear in the Euler-Lagrange equation. The validity can be easily checked, since

$$-\frac{\partial}{\partial t}\frac{\partial L}{\partial\left(\frac{\partial \vec{A}}{\partial t}\right)} = -\varepsilon_o \frac{\partial}{\partial t}\left(\frac{\partial \vec{A}}{\partial t} + \mathrm{grad}\varphi\right) \tag{24}$$

and

$$\mathrm{rot}\frac{\partial L}{\partial(\mathrm{rot}\vec{A})} = -\frac{1}{\mu_o}\mathrm{rot}\,\mathrm{rot}\vec{A} \tag{25}$$

from which

$$\frac{1}{\mu_o}\mathrm{rot}\,\mathrm{rot}\vec{A} = \frac{1}{\mu_o}\mathrm{rot}\vec{B} = \varepsilon_o\frac{\partial}{\partial t}\left(\frac{\partial\vec{A}}{\partial t} + \mathrm{grad}\varphi\right) = \varepsilon_o\frac{\partial\vec{E}}{\partial t} \tag{26}$$

Taking the φ dependence of the Lagrange density function, the operator $O_3 =$ grad stands, thus the term $-\mathrm{div}\frac{\partial L}{\partial(\mathrm{grad}\varphi)}$ appears in the second Euler-Lagrange equation. After these, as an Euler-Lagrange equation we arrive at a Maxwell equation with zero charge

$$0 = \mathrm{div}\left(\frac{\partial\vec{A}}{\partial t} + \mathrm{grad}\varphi\right) = \mathrm{div}\vec{E} \tag{27}$$

In general, the Hamilton density function of the field can be introduced as

$$\mathcal{H} = \mathcal{P}\frac{\partial\overrightarrow{A^{\blacksquare}}}{\partial t} - \mathcal{L} \tag{28}$$

where

$$\overrightarrow{A^{\blacksquare}} = \left(A_x, A_y, A_z, \frac{i}{c}\varphi\right) \tag{29}$$

is the four-potential, and $\mathcal{P}$ is the canonically conjugated variable (four-mometum) to $\overrightarrow{A^{\blacksquare}}$:

$$\mathcal{P} = \frac{\partial\mathcal{L}}{\partial\frac{\partial\overrightarrow{A^{\blacksquare}}}{\partial t}} = -\varepsilon_o\left(-\frac{\partial\vec{A}}{\partial t} - \mathrm{grad}\varphi\right) \tag{30}$$

After all, after using the Lagrange density function in equation (17) the Hamilton density function can be written for pure radiation field:

$$\mathcal{H} = \frac{\mathcal{P}^2}{2\varepsilon_o} - \mathcal{P}\mathrm{grad}\varphi + \frac{1}{2\mu_o}\left(\mathrm{rot}\vec{A}\right)^2 \tag{31}$$

The application of scalar and vector potentials is not the only choice to describe the electromagnetic field. Another representation also exist which is especially suitable to solve certain problems (e.g. dipol radiation) [4, 5].

The so-called Hertz vector $\overrightarrow{\Pi}$ can be introduced to the vector potential as:

$$\vec{A} = \varepsilon_o\mu_o\frac{\partial\overrightarrow{\Pi}}{\partial t} \tag{32}$$

It can be seen that the relation

$$\mathrm{div}\vec{A} = -\varepsilon_o\mu_o\frac{\partial\varphi}{\partial t} = \varepsilon_o\mu_o\frac{\partial}{\partial t}\mathrm{div}\overrightarrow{\Pi} \tag{33}$$

is completed, in which the Lorenz condition can be recognized. As direct consequence of this that the scalar field φ can be deduced by $\overrightarrow{\Pi}$:

$$\varphi = -\mathrm{div}\overrightarrow{\Pi} \tag{34}$$

Then the measurable field variables can be given by this only one potential field:

$$\vec{B} = \varepsilon_o \mu_o \frac{\partial}{\partial t} \mathrm{rot}\overrightarrow{\Pi} \tag{35}$$

$$\vec{E} = -\varepsilon_o \mu_o \frac{\partial^2 \overrightarrow{\Pi}}{\partial t^2} + \mathrm{grad}\ \mathrm{div}\overrightarrow{\Pi} \tag{36}$$

It can be checked by a short calculation that the Hertz vector $\overrightarrow{\Pi}$ completes the wave equation:

$$\frac{\partial}{\partial t}\left(\Delta\overrightarrow{\Pi} - \varepsilon_o \mu_o \frac{\partial^2 \overrightarrow{\Pi}}{\partial t^2}\right) = 0 \tag{37}$$

3 Hamilton-Lagrange Formalism for Dissipative Processes

3.1 The Simplest Transport Process: Linear Heat Conduction

The simplest pure dissipative process is the Fourier heat conduction, which is described by a parabolic differential equation. This differential equation is formulated for the classic temperature, applying the local equilibrium hypothesis. This can be done – and it gives a good description – if the energy transport is rather slow [1, 2, 3, 6, 7, 8].

Let us consider the linear Fourier heat conduction as the simplest dissipative process which can be written by the equation

$$\frac{\partial T}{\partial t} - \frac{\lambda}{c_v}\frac{\partial^2 T}{\partial x^2} = 0 \tag{38}$$

The process is described by parabolic partial differential equation in general where $T(x,t)$ means the local equilibrium temperature. The Lagrange density function cannot be directly formulated by temperature T, since the time derivative is not self-adjoint operator. This difficulty can be resolved with the introduction of four times differentiable scalar field $\varphi(x,t)$ that generates the measurable field:

$$T = -\frac{\partial \varphi}{\partial t} - \frac{\lambda}{c_v}\Delta\varphi \tag{39}$$

Then by the potential φ the Lagrange density function of Fourier heat conduction can be expressed:

$$L = \frac{1}{2}\left(\frac{\partial \varphi}{\partial t}\right)^2 + \frac{1}{2}\frac{\lambda^2}{c_v^2}(\Delta\varphi)^2 \tag{40}$$

In the sense of Hamilton's principle the action has an extremum during the motion

$$S = \int L\ \mathrm{d}V\mathrm{d}t = \text{extremum} \tag{41}$$

i.e., the variation of action is zero:

$$\delta S = \int \left(\frac{1}{2} \left(\frac{\partial \varphi}{\partial t} \right)^2 + \frac{1}{2} \frac{\lambda^2}{c_v^2} (\Delta \varphi)^2 \right) \mathrm{d}V \mathrm{d}t = 0 \tag{42}$$

The resulting Euler-Lagrange differential equation gives the equation of motion (field equation) for the problem. The Euler-Lagrange equation for the Lagrange density function given by equation (40) is:

$$\frac{\partial^2 \varphi}{\partial t^2} + \frac{\lambda^2}{c_v^2} \Delta \Delta \varphi = 0 \tag{43}$$

which yields the heat equation (38), taking into account the definition equation (39) we use:

$$\frac{\partial T}{\partial t} - \frac{\lambda}{c_v} \Delta T = 0 \tag{44}$$

This equation describes slow energy transport, however, the finite speed of propagation of action is not required.

3.1.1 Poisson Bracket, Hamilton Equations

It is worth to define the Poisson bracket expression of variables, since it can be proved that the Poisson bracket of the Hamilton density function with a certain variable gives its time derivative [9]:

$$[F, \mathcal{H}] = \frac{\delta F}{\delta \varphi} \frac{\delta \mathcal{H}}{\delta p} - \frac{\delta F}{\delta p} \frac{\delta \mathcal{H}}{\delta \varphi} \tag{45}$$

$$\dot{F} = [F, \mathcal{H}] \tag{46}$$

As a consequence, the Euler-Lagrange equation can be substituted by these two Hamilton equations:

$$\frac{\partial \varphi}{\partial t} = [\varphi, \mathcal{H}] \tag{47}$$

$$\frac{\partial P}{\partial t} = [P, \mathcal{H}] \tag{48}$$

The advantage of this description is the appearance of the lower order differential equation rather than the more complex Euler-Lagrange equation; the solutions may thus, be easier. At the same time, the introduction of the canonical variables gives the chance to construct the phase field.

For a compete and consistent theory, not all of the Lagrange functions are suitable for a developed equation of motion, that can be deduced using variations. Thus, the necessary condition for the suitable Lagrange density function, is to ensure the Euler-Lagrange equation, as the equation of motion, deduced from the Hamilton's principle, but this is not enough for a complete and consistent theory. The necessary condition and the relevant choice of the Lagrange density function is required so that the canonical equations meet the equations of motion of the problem. Thus, the canonical equations are essential for the consistent elaboration of the formulization.

3.1.2 Canonically Conjugated Momentum and Hamilton Function

If we know the Lagrange density function, the canonically conjugated momentum to the field variable can be introduced which can be obtained after the general variation:

$$P = \frac{\partial L}{\partial \dot{\varphi}} = \dot{\varphi} = \frac{\partial \varphi}{\partial t} \tag{49}$$

After then the Hamilton function (the Legendre transformed of the Lagrange function) can be written [9]:

$$\mathcal{H}(P, \varphi) = \dot{\varphi} P - \mathcal{L} = \frac{1}{2}\left(\frac{\partial \varphi}{\partial t}\right)^2 - \frac{1}{2}\frac{\lambda^2}{c_v^2}(\Delta\varphi)^2 = \frac{1}{2}P^2 - \frac{1}{2}\frac{\lambda^2}{c_v^2}(\Delta\varphi)^2 \tag{50}$$

The fulfillment of the canonical equations can be easily checked by a short calculation:

$$\frac{\partial \mathcal{H}}{\partial P} = \frac{\partial \varphi}{\partial t} \tag{51}$$

$$-\Delta \frac{\partial \mathcal{H}}{\partial \Delta\varphi} = \frac{\partial P}{\partial t} \tag{52}$$

4 Elaboration of Formalism and the Directions of Applications

Considering the Lagrange density function can be formulated by non-exclusive self-adjoint operators, suddenly, more directions open in relation to the study of such processes, which were not possible with the Hamiltonian method. Previously, this effective theory and the related methods cannot be part of the developments and deep understanding of various physical processes.

The study of certain nonlinear processes can be part of the themes for potential Lagrangian theories. Such an example, for this description, is the Fourier heat conduction, with space, time and temperature – dependent conducting coefficients [10, 11]. Since the Lagrange formalism means a unified frame, there is the possibility to couple the different processes in a natural way. Here, not exclusively, the classic transports can be coupled with other areas of physics. This may have a special importance, because the concept of dissipation will be an integral part of the formulation. The coupling of the thermal and the cosmologic expanding field, the inflation field is a good example for this, in which, the expanding process is thermodynamically interpretable [12, 13]. The greatest challenge is also the most exciting field, the realization of coupling with the quantized processes.

One of the methods to involve the finite action speed in the theory, is to write the process with a telegrapher hyperbolic equation. Such equations are formulated for transport processes given by linear differential equations. The consistent general canonical theory has been elaborated in [6, 14]. This also means that the same type of equations can be coupled.

An older tough problem was on how to formulate the transport equations in a Lorentz invariant form, in order to embed them in the theory of special relativity. The general solution is not known at the time of this writing. We can conclude that there is a successful description for the thermal energy propagation with the help of the potential theory [15, 16]. Accordingly, this means that the laws of thermodynamics are completed in the Lorentz invariant formulation [17, 18]. Naturally, the developed method involves the classical heat propagation as a limit.

The examination of general variations of action reveals the geometric – time and space shift, spatial rotation – and the dynamic symmetries of the studied theory. Each geometric invariance, leads to a conservation law, namely, energy, momentum and angular momentum. The dynamic invariances express a special, property dependent conservation (e.g. electric but in general any charges, lepton and barion number). The symmetry of the Lagrange density function of coupled linear transports, verify the validity of the Onsager's reciprocity relations [8, 11, 19, 20]. This poof is important because it is based on field theoretical considerations.

An essential result of the described formalism for the dissipative processes is that the concept of phase space can be constructed; the Liouville equation can be expanded for telegrapher equations. As a consequence of this, it can be shown that the Chapman-Kolgomorov equation is fulfilled, the Onsager's regression hypothesis is valid and the system fluctuations can be handled [21].

The introduction of the constructed canonically conjugated quantities of thermal energy propagation opens the way towards the adoption and application of quantum theoretical methods for the case of dissipative processes. In this way, a kind of excitation of thermal processes (hotons) can be understood. These excitations are particularly interesting since these are deduced from a real thermodynamic background [22, 23, 24, 25]. If this field can be successfully coupled with other fields in a consistent frame, then it is expected that the required criteria of thermodynamics – especially the second law of thermodynamics – will be the part of the description. This may clearly mean that the concepts of dissipation and irreversibility become directly interpretable, in cases of open quantum systems.

An interesting quantum thermodynamic application is the study the quantum properties; the examination of non-extensive interacting boson systems, and the treatment of Bose condensation. During the examination a relation can be recognized between the non-extensive nature and the interaction parameter. Furthermore, it can be shown how the commutation relation is modified, due to the internal interaction of the system [26, 27].

The existence of a description for the dissipative processes has a possible significance to retrieve the dissipation free case, as a limit. It involves and operates two kinds of propagation mechanisms at the same time. Thus, if the process dynamics change, e.g. the wave-like or ballistic propagation turns into diffusive, then, this transition can be correctly discussed. This may yield remarkable progress, mainly in the interpretation of complex processes [14, 28].

Summary

We have shown how to construct a Lagrange density function for those processes which are described by differential equations involving non-selfadjoint operators. Potentials (scalar and vector fields) can be introduced to the measurable physical fields, by which, a complete description and solution of the processes is possible. We have shown this method on a well-known example in electrodynamics. Then, we applied the theory to a simple dissipative process, the Fourier heat conduction. The advantage of theory is that the canonical formalism yields further directions in the study. Finally, we described more possibilities for further research areas. Until now, there are very promising results in these themes, but further studies are needed.

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