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Poisson Bracket Filter for the Effective Lagrangians

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Abstract: One might think that a Lagrangian function of any form is suitable for a complete description of a process. Indeed, it does not matter in terms of the equations of motion, but it seems that this is not enough. Expressions with Poisson brackets are displayed as required fulfillment filters. In the case of the Schrödinger equation for a free particle, we show what we have to be careful about.

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1. Introduction

The least action principle has an efficiency that is difficult to overestimate in the study of physical processes. The principle is axiomatic. Mathematically it is based on the variational calculus that pertains to the extremal problems of motion integrals [1,2]. Lagrange original idea was to deduce the Newton's laws from a "higher principle". Today, we consider that these desciptions are equivalent. The first step is to find the Lagrange function, to which we obtain the equation of motion of the physical problem by applying the extremization procedure. However, over the equations of motion or field equations, the Lagrangian formulation involves more desired physical relations. We can explore inner symmetries, conserved quantities of the process, the energy expressions, canonical variables and conjugated pairs [3]. The identifiability of these relationships and quantities enables the theory to become the basis of modern physics. The motivation of the present article is the following. There are such opinions in the literature that all Lagrangians are equivalent, producing the correct equations of motion [4,5]. We show that a careful examination of the Poisson bracket formulation is required to be sure of the right choice because deriving the correct equations of motion is only part of the solution.

A system can be described by a Lagrange function L_V, by which the action S can be obtained

$$S = \int_{t_1}^{t_2} L_V dt, \tag{1}$$

and it is extremal for the real physical path during the time evolution ($t_1 \leq t \leq t_2$). Applying the calculus of variations we obtain the so-called Euler-Lagrange equations as equations of motions. If Lagrangian L_V depends on the coordinate q and its time derivative $\dot{q}$, i.e., $L_V = L_V(q, \dot{q})$, the Euler-Lagrange equation is

$$\frac{\partial L_V}{\partial q} - \frac{d}{dt}\frac{\partial L_V}{\partial \dot{q}} = 0, \tag{2}$$

which is a second order ordinary differential equation. In the case of the systems with infinite degree of freedom (continua), the principle can be expressed by

$$\delta S = \delta \int_{t_1}^{t_2} L dV dt = 0, \tag{3}$$

where L is the Lagrange density function. The Lagrangian L may depend on the field variable $\Psi = \Psi(r, t)$ as a generalized coordinate, and its time $\dot{\Psi}, \ddot{\Psi}$ and space $\nabla\Psi, \triangle\Psi$ derivatives (∇ is the gradient, $\triangle$ is the Laplace operator), i.e., $L = L(\Psi, \dot{\Psi}, \ddot{\Psi}, \nabla\Psi, \triangle\Psi)$. Then, the Euler-Lagrange equation is

$$\frac{\partial L}{\partial \Psi} - \frac{\partial}{\partial t}\frac{\partial L}{\partial \dot{\Psi}} - \nabla \frac{\partial L}{\partial \nabla \Psi} + \frac{\partial^2}{\partial t^2}\frac{\partial L}{\partial \ddot{\Psi}} + \triangle \frac{\partial L}{\partial \triangle \Psi} = 0. \tag{4}$$

As a general rule, if the Lagrangian L contains a linear operator A acting on Ψ, then the term

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

appears in the Euler-Lagrange equation, where $\tilde{A}$ is the adjoint operator to A. The $A = \tilde{A}$ means that the operator is self-adjoint. Here, we find the answer why it is impossible to calculate a Lagrangian for e.g., first time derivative of variables without any mathematical tricks. In general, we can say that for non-selfadjoint operators the Lagrangian can not be constructed directly. There are some useful ideas to override the difficulties: e.g., introducing the dissipation potential [6–13] in mechanical, and [14–21] in tranport problems. Many other modifications of variation methods exist to find relevant calculus to obtain the correct equations of motion [22–42]. The duplication of the variables—introduction the complex conjugted field variables—is also an applicable method in the case of Schrödinger field [43,44], other quantum fields [45], moreover the transport equations such as Fourier heat conduction [46–48]. A promising solution is usage of potential (generator) functions in different ways for electrodynamics [49,50], for the field theory of thermodynamics [51], or for dissipative mechanical systems [52]. In this method the potential functions generates the measurable fields. The potential based proceure is so effective that the canonical quantization of the dissipative harmonic oscillator becomes possible [53].

Regardless of the method used, it is true that not only the derived equations of motion (and their solutions) of the investigated system must be clear, but also that all related concepts must be part of the coherent description [54–57]. In this article, we present a well-known and interesting problem, which control points may be necessary for the correct construction of the theory.

2. Lagrange Density Functions for the Schrödinger Field of Free Particles

We show some examples for the possible Lagrange density functions in the classical quantum mechanics. It can be easily seen that the choice is not unique. The question is, are they all suitable for further description? We will use the physically-mathematically simplest example, the free quantum particle, to point out the background of the problem. It is enough because, from a logical point of view, even one case is enough to reveal a faulty construction. We can formulate different Lagrangians of a free quantum particle [4], e.g.,

$$L_1 = -\frac{\hbar^2}{2m}\nabla\Psi^*\nabla\Psi + \frac{i\hbar}{2}(\Psi^*\dot{\Psi} - \dot{\Psi}^*\Psi), \tag{6}$$

$$L_2 = -\frac{\hbar^2}{2m}\nabla\Psi^*\nabla\Psi - i\hbar\dot{\Psi}^*\Psi, \tag{7}$$

$$L_3 = \frac{\hbar^2}{2m}\Psi\triangle\Psi^* + \frac{i\hbar}{2}(\Psi^*\dot{\Psi} - \dot{\Psi}^*\Psi), \tag{8}$$

$$L_4 = \frac{\hbar^2}{2m}\Psi\triangle\Psi^* - i\hbar\dot{\Psi}^*\Psi. \tag{9}$$

Here, Ψ^* is the complex conjugated variable to Ψ, and these are considered as independent of each other. All of these give the same two Euler-Lagrange equations

$$i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\triangle\Psi \tag{10}$$

$$i\hbar\dot{\Psi}^* = \frac{\hbar^2}{2m}\triangle\Psi^*, \tag{11}$$

which are the Schrödinger equations. The real question is, are these Lagrangian functions equivalent? We show that it seems somehow contradictory to specify with Equations (6) and (8). It is enough to restrict our examination for the free particle because, in the case of any conservative potential of V, the required $V\Psi\Psi^*$ does not influence the exposition below.

3. Canonical Momenta, Hamiltonian, and Poisson Bracket Expressions

To develop the description of behavior of the Schrödinger field, we shortly discuss the canonical formalism and the Poisson brackets. In general, the canonical momentum is

$$p = \frac{\partial L}{\partial \dot{q}}, \tag{12}$$

when the Lagrangian is $L(q, \dot{q})$, it does not contain higher order time derivatives. In the case of fields when $L(\Psi, \dot{\Psi}, \nabla\Psi, \triangle\Psi)$ is without higher order time derivatives, the momentum can be similarly written by

$$p = \frac{\partial L}{\partial \dot{\Psi}}. \tag{13}$$

When the Lagrangian depends on two independent variables (Ψ and Ψ^* in Equations (10) and (11)), there are two momenta

$$p = \frac{\partial L}{\partial \dot{\Psi}}, \quad \text{and} \quad p^* = \frac{\partial L}{\partial \dot{\Psi}^*}. \tag{14}$$

The Hamilton density function will be as it is usual

$$H = p\dot{\Psi} + p^*\dot{\Psi}^* - L. \tag{15}$$

The time evolution of a physical quantity F can be obtained by the Poisson bracket expression, which means

$$\dot{F} = [F, H], \tag{16}$$

where F and H may depend on $\varphi_i, \varphi_i^*, \nabla\varphi_i, \nabla\varphi_i^*, \triangle\varphi_i, \triangle\varphi_i^*, p_i$ and p_i^*. Here, Ψ, p, Ψ^* and p^* are considered independent variables. The Poisson bracket is

$$[F, H] = \frac{\delta F}{\delta\varphi_i}\frac{\delta H}{\delta p_i} - \frac{\delta F}{\delta p_i}\frac{\delta H}{\delta\varphi_i}, \tag{17}$$

where we apply the notations $\varphi_1 = \Psi$, $\varphi_2 = \Psi^*$, $p_1 = p$ and $p_2 = p^*$, and

$$\frac{\delta}{\delta\varphi_i} = \frac{\partial}{\partial\varphi_i} - \nabla\frac{\partial}{\partial(\nabla\varphi_i)} + \triangle\frac{\partial}{\partial(\triangle\varphi_i)}, \quad \text{and} \quad \frac{\delta}{\delta p_i} = \frac{\partial}{\partial p_i} \tag{18}$$

are the functional derivatives. In our cases we may expect that

$$\dot{\Psi} = [\Psi, H], \quad \dot{p} = [p, H], \tag{19}$$

and

$$\dot{\Psi}^* = [\Psi^*, H], \quad \dot{p}^* = [p^*, H] \tag{20}$$

are completed.

4. Discussion of Lagrangians

Now, let us examine the different versions of Lagrangians given by Equations (6)–(9) from the viewpoint of the canonical formalism. We would expect that canonical variables ensures the same correct Hamiltonians. This is a strong requirement since the Hamiltonian relates to the energy of the system.
In the case of L_1 the momenta are

$$p_1 = \frac{i\hbar}{2}\Psi^*, \quad \text{and} \quad p_1^* = -\frac{i\hbar}{2}\Psi. \tag{21}$$

Applying Equation (15) the deduced Hamilton density is

$$H_1 = \frac{\hbar^2}{2m}\nabla\Psi^*\nabla\Psi, \tag{22}$$

by which we obtain the equation

$$\dot{\Psi} = [\Psi, H_1] = \frac{\delta\Psi}{\delta\Psi}\frac{\delta H_1}{\delta p_1} - \frac{\delta\Psi}{\delta p_1}\frac{\delta H_1}{\delta\Psi} + \frac{\delta\Psi}{\delta\Psi^*}\frac{\delta H_1}{\delta p_1^*} - \frac{\delta\Psi}{\delta p_1^*}\frac{\delta H_1}{\delta\Psi^*} = -\frac{\hbar}{im}\triangle\Psi. \tag{23}$$

It can be seen that the result is not the Schrödinger equation, i.e., Equation (10) is not equal to Equation (23). Similarly,

$$\dot{\Psi}^* = [\Psi^*, H_1] = \frac{\hbar}{im}\triangle\Psi^*. \tag{24}$$

We can try it in another way. Substituting Ψ^* from Equation (21)

$$\Psi^* = \frac{2}{i\hbar}p_1$$

into the Hamilton density (22), so we get

$$H_1 = \frac{\hbar}{im}\nabla p_1\nabla\Psi. \tag{25}$$

Then we obtain

$$\dot{\Psi} = [\Psi, H_1] = \frac{\delta\Psi}{\delta\Psi}\frac{\delta H_1}{\delta p_1} - \frac{\delta\Psi}{\delta p_1}\frac{\delta H_1}{\delta\Psi} + \frac{\delta\Psi}{\delta\Psi^*}\frac{\delta H_1}{\delta p_1^*} - \frac{\delta\Psi}{\delta p_1^*}\frac{\delta H_1}{\delta\Psi^*} = -\frac{\hbar}{im}\triangle\Psi, \tag{26}$$

which is also incorrect, and of course this is the same as in Equation (23). The number 2 is missing from the denominator. It seems to us that there is no way to find the correct Schrödinger equation. Calculating the time evolution of p we obtain

$$\dot{p}_1 = [p_1, H_1] = \frac{\delta p_1}{\delta\Psi}\frac{\delta H_1}{\delta p_1} - \frac{\delta p_1}{\delta p_1}\frac{\delta H_1}{\delta\Psi} = \frac{\hbar}{im}\triangle p_1, \tag{27}$$

and using the form of p by Equation (21) we can write

$$\dot{\Psi}^* = \frac{\hbar}{im}\triangle\Psi^* \tag{28}$$

Here, the number 2 is similarly missing from the denominator. This discrepancy is the previously mentioned motivation of the work.

In the case of L_2 the momenta are asymmetric

$$p_2 = 0, \quad \text{and} \quad p_2^* = -i\hbar\Psi, \tag{29}$$

the total momentum is in one of the canonical variable. The Hamiltonian is

$$H_2 = \frac{\hbar^2}{2m} \nabla \Psi^* \nabla \Psi, \tag{30}$$

which is equal to H_1. Learning from the previous example, it is obvious to eliminate one of the variables, e.g., Ψ, by which we get

$$H_2 = -\frac{\hbar}{2im} \nabla p_2^* \nabla \Psi^*. \tag{31}$$

At this point we should calculate $\dot{\Psi}^*$

$$\dot{\Psi}^* = [\Psi^*, H_2] = \frac{\delta \Psi^*}{\delta \Psi^*} \frac{\delta H_2}{\delta p_2^*} - \frac{\delta \Psi^*}{\delta p_2^*} \frac{\delta H_2}{\delta \Psi^*} = \frac{\hbar}{2im} \triangle \Psi^*, \tag{32}$$

which is exactly the Schrödinger equation for Ψ^*

$$i\hbar \dot{\Psi}^* = \frac{\hbar^2}{2m} \triangle \Psi^*. \tag{33}$$

Let us calculate $\dot{p}_2^*$

$$\dot{p}_2^* = [p^*, H_2] = -\frac{\hbar}{2im} \triangle p_2^*. \tag{34}$$

Using the form of p_2^* from Equation (29) we obtain

$$i\hbar \dot{\Psi} = -\frac{\hbar^2}{2m} \triangle \Psi, \tag{35}$$

which is also correct. It seems that the only non-zero momentum resolves the problem.

It is easy to check by a short calculation that the case of L_3 is similar to the (L_1). The momenta are

$$p_3 = \frac{i\hbar}{2} \Psi^*, \quad \text{and} \quad p_3^* = -\frac{i\hbar}{2} \Psi. \tag{36}$$

The Hamilton density is

$$H_3 = -\frac{\hbar^2}{2m} \Psi \triangle \Psi^*, \tag{37}$$

by which we obtain

$$\dot{\Psi} = [\Psi, H_3] = \frac{\delta \Psi}{\delta \Psi} \frac{\delta H_3}{\delta p_3} - \frac{\delta \Psi}{\delta p_3} \frac{\delta H_3}{\delta \Psi} + \frac{\delta \Psi}{\delta \Psi^*} \frac{\delta H_3}{\delta p_3^*} - \frac{\delta \Psi}{\delta p_3^*} \frac{\delta H_3}{\delta \Psi^*} = -\frac{\hbar}{im} \triangle \Psi. \tag{38}$$

One can recognize that the term

$$\frac{i\hbar}{2} (\Psi^* \dot{\Psi} - \dot{\Psi}^* \Psi) \tag{39}$$

causes the problem in both cases, because it results the devided momenta.

In the last case, L_4, the canonical momenta are asymmetric

$$p_4 = 0, \quad \text{and} \quad p_4^* = -i\hbar \Psi. \tag{40}$$

The Hamiltonian density is

$$H_4 = -\frac{\hbar^2}{2m} \Psi \triangle \Psi^* = H_4 = \frac{\hbar}{2im} p_4^* \triangle \Psi^*. \tag{41}$$

Now, we can calculate the Poisson bracket

$$\dot{\Psi}^* = [\Psi^*, H_4] = \frac{\hbar}{2im} \triangle \Psi^*, \tag{42}$$

which results the Schrödinger equation. Moreover, we obtain $\dot{p_4}^*$

$$\dot{p}_4^* = [p_4^*, H_4] = -\frac{\hbar}{2im} \triangle p_4^*, \tag{43}$$

which gives the Schrödinger equation for Ψ

$$\dot{\Psi} = -\frac{\hbar}{2im} \triangle \Psi. \tag{44}$$

That is correct, i.e., the there must be only one non-zero canonical momentum. The space derivative terms keep intact the description.

5. Resolution of the Problem

As we see, the problem is with the "symmetric" cases, with the time derivatives in the Lagrange term in Equations (6), (8) and (39). In contrast, the Poisson bracket of the "asymmetric" Lagrangian term results the correct equations of motion. It is because one of the canonically conjugate momenta, e.g., p, is zero, so the entire pulse of the space is in the other momentum p^*. This total pulse takes part in the generation of the time evolution of the relevant fields. From the point of view of the variational problem, the spaces Ψ and Ψ^* are considered independent. However, physically they are not. Similarly, the momenta p and p^*. They share the total impulse. On the other hand, it is also necessary to remember that Hamilton means total energy. Thus, when we calculate the Poisson brackets, the effect of Hamilton appears with a double weight. That is why division by two disappears. The solution is to enter only half of the Hamiltonian in the Poisson bracketed expression. We have shown this problem in a simple case. For complex tasks, the calculation of the Poisson brackets can ensure the selection of the correct Lagrange function.

6. Conclusions

We can deduce the equations of motion from different Lagrangian functions. In general, the canonical formulation and the construction of Hamiltonian allow a free choice since the Poisson brackets result from the correct equations of motion. In the present article, we point out a particular trap. We show the case of the free particle quantum motion, the Schrödinger equation, in which we must restrict the construction. The wave function, its complex conjugate, and derivatives formulate the time-dependent part. If both the canonical conjugated momenta (pulses) are non-zero, the Poisson brackets do not serve the required Scröndinger equations. If one of the momenta is zero, we obtain the correct Scrödinger equation. The reason for the faulty solution is the physical situation that the wave function and its complex conjugate are not independent fields. However, in the calculus of variation, we consider these fields independent. The requirement of physical independence is fulfilled if one of the momenta is zero. It means that the contradiction disappears by the asymmetric choice in the time-dependent term of the Lagrangian. The conclusion is that the Poisson brackets give a filter to get the correct Lagrangians.

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