Quantum mechanics of higher derivative systems and total derivative terms

1996 J. Phys. A: Math. Gen. 29 5049

(http://iopscience.iop.org/0305-4470/29/16/025)

J. Phys. A: Math. Gen. **29** (1996) 5049–5058. Printed in the UK

Quantum mechanics of higher derivative systems and total derivative terms

Yasuhito Kaminaga†

Department of Physics, Toho University, Miyama 2-2-1, Funabashi 274, Japan

Received 4 December 1995, in final form 20 May 1996

Abstract. A general theory is presented of the classical and quantum mechanics of singular, non-autonomous, higher derivative systems. It is shown that adding a total derivative to a Lagrangian does not materially affect either, (a) the canonical analysis of the system, or (b) its quantum mechanics.

1. Introduction

Higher derivative theories occur in various aspects of modern physics—gravity, strings, particle phenomenology, and so on. It is of importance to clarify general properties of such theories.

The main purpose of this paper is to prove a very simple, but important, theorem for the quantum mechanics of higher derivative theories. *Total derivative terms in a Lagrangian never affect the quantum mechanics.* The theorem is proven within the most general, i.e. singular and non-autonomous (explicitly time-dependent), situation. Needless to say, the classical version of the theorem is well known and is trivial. And the classical result often plays an important role in various theories. Surprisingly enough, the quantum version, despite its importance, has not been proven, up to now, except special cases. It is in fact non-trivial and requires a proof. On the way to the final goal, we will show that total derivative terms do not change the constraint structures in a essential respect.

The paper is laid out as follows: in section 2, the canonical theory, now known as the Ostrogradski formalism [1], is reviewed and the canonical quantization according to Dirac is performed. Section 3 is devoted to the canonical analysis of the system and the proof of the theorem.

2. General theory of higher derivative systems

2.1. The Ostrogradski formalism

Let us consider a Lagrangian which depends on the coordinates q^i's and their time derivatives up to the Nth order,

$$L(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(1)}, \ldots, \boldsymbol{q}^{(N)}, t) \tag{2.1}$$

† E-mail address: kaminaga@toho-u.ac.jp

where $\boldsymbol{q}^{(I)}$'s are abbreviations for $q^{(I)i} := \mathrm{d}^I q^i/\mathrm{d}t^I$, $I = 0, 1, \ldots, N$. The Euler–Lagrange equations for (2.1) are given by

$$\sum_{I=0}^{N} \left(-\frac{\mathrm{d}}{\mathrm{d}t}\right)^I \frac{\partial L}{\partial q^{(I)i}} = 0. \tag{2.2}$$

We introduce canonical variables,

$$q^{Ii} := q^{(I)i} \tag{2.3a}$$

$$p_{Ii} := \sum_{K=I+1}^{N} \left(-\frac{\mathrm{d}}{\mathrm{d}t}\right)^{K-I-1} \frac{\partial L}{\partial q^{(K)i}} \tag{2.3b}$$

to parametrize the $2N$ dimensional (for each i) phase space of (2.2). Throughout the present paper, we take the convention that I, J, and K run from 0 to $N-1$, unless otherwise stated. We have relations as follows

$$\frac{\partial L}{\partial q^{(0)i}} = \frac{\mathrm{d}p_{0i}}{\mathrm{d}t} \tag{2.4a}$$

$$p_{N-1,i} = \frac{\partial L}{\partial q^{(N)i}} \tag{2.4b}$$

$$p_{Ai} = \frac{\partial L}{\partial q^{(A+1)i}} - \frac{\mathrm{d}}{\mathrm{d}t} p_{A+1,i} \tag{2.4c}$$

with $A = 0, 1, \ldots, N-2$. Equation (2.4*a*) is the Euler–Lagrange equation (2.2).

When $\det(\partial^2 L/\partial q^{(N)i}\partial q^{(N)j}) = 0$ the Lagrangian (2.1) is singular, which means there exist primary constraints

$$\phi_m(\boldsymbol{q}, \boldsymbol{p}, t) \approx 0 \tag{2.5}$$

where $\boldsymbol{q}$ and $\boldsymbol{p}$ are abbreviations for q^{Ii}'s and p_{Ii}'s. The number of primary constraints is *larger than* or equal to the nullity of the Hessian matrix $\|\partial^2 L/\partial q^{(N)i}\partial q^{(N)j}\|$; the larger case may occur when $N \geqslant 2$.

The canonical Hamiltonian is defined by

$$H(\boldsymbol{q}, \boldsymbol{p}, t) := \sum_{A=0}^{N-2} p_{Ai} q^{A+1,i} + p_{N-1,i}\dot{q}^{N-1,i} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}^{N-1}, t) \tag{2.6}$$

which is conserved if the system is autonomous

$$\frac{\mathrm{d}H}{\mathrm{d}t} + \frac{\partial L}{\partial t} = 0. \tag{2.7}$$

The quantities $\dot{q}^{N-1,i}$'s appearing in the right-hand side of (2.6) indicate that they should be replaced by $p_{N-1,i}$ in the final expression. We avoid the use of such a symbol as $q^{N,i}$ for $\dot{q}^{N-1,i}$. This is because $q^{N,i}$ looks as if it is an independent variable, and hence it may cause confusion in the following discussion.

Once we reach here, higher derivative theories do not differ much from usual theories with first-order derivatives. The well known Dirac procedure [1, 2] for singular Lagrangians is applied to higher derivative systems without any modification.

All the constraints (the primary and the secondary ones) are classified into first class, $\gamma_a \approx 0$, and second class, $\chi_\alpha \approx 0$. The Poisson bracket is defined by

$$\{F, G\} := \frac{\partial F}{\partial q^{Ii}}\frac{\partial G}{\partial p_{Ii}} - \frac{\partial F}{\partial p_{Ii}}\frac{\partial G}{\partial q^{Ii}} \tag{2.8}$$

with which the equations of motion for an arbitrary quantity $F(\boldsymbol{q}, \boldsymbol{p}, t)$ is

$$\dot{F} \approx \{F, H_{\mathrm{T}}\} + \frac{\partial F}{\partial t}. \tag{2.9}$$

The total Hamiltonian H_{T} is defined as

$$H_{\mathrm{T}} := H + u^{\alpha_1}\chi_{\alpha_1} + \lambda^{a_1}\gamma_{a_1} \tag{2.10}$$

where H is the canonical Hamiltonian (2.6), u^{α_1}'s are functions of $\boldsymbol{q}, \boldsymbol{p}$, and t determined by consistency, and λ^{a_1}'s are the arbitrary Lagrange multipliers. The indices α_1 and a_1 run only on the primary constraints. The second-class constraints $\chi_\alpha \approx 0$ become strong equations $\chi_\alpha = 0$ in terms of the Dirac bracket

$$\{F, G\}^* := \{F, G\} - \{F, \chi_\alpha\}C^{-1\,\alpha\beta}\{\chi_\beta, G\} \tag{2.11}$$

with $C_{\alpha\beta} := \{\chi_\alpha, \chi_\beta\}$.

2.2. *Quantum mechanics*

The quantization is formally performed by replacing the Dirac bracket $\{\ ,\ \}^*$ by the quantum commutator $(\mathrm{i}\hbar)^{-1}[\ ,\ ]$. Unfortunately, it is incredibly difficult to find out the operator representation of the Dirac bracket. In order to proceed further, it is desirable to circumvent the Dirac bracket. Here let us remember a general result [2] that second-class constraints can always be turned into first-class constraints, if necessary, by adding extra variables. Without losing generality, therefore, we assume there are no second-class constraints. Then we have only to consider the Poisson bracket. Quantization is performed by replacing the Poisson bracket by the commutator, and the first-class constraints by the subsidiary conditions on the wave function.

Let us take the Schrödinger picture with coordinate representation. The commutator algebra is represented by $\hat{q}^{Ii} = q^{Ii}$, and $\hat{p}_{Ii} = -\mathrm{i}\hbar\partial/\partial q^{Ii}$. One obtains the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{q}, t)}{\partial t} = \hat{H}\left(\boldsymbol{q}, -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{q}}, t\right)\psi(\boldsymbol{q}, t) \tag{2.12}$$

and the subsidiary conditions

$$\hat{\gamma}_a\left(\boldsymbol{q}, -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{q}}, t\right)\psi(\boldsymbol{q}, t) = 0 \tag{2.13}$$

in which $\boldsymbol{q}$ and $\partial/\partial\boldsymbol{q}$ are abbreviations for q^{Ii}'s and $\partial/\partial q^{Ii}$'s.

This section is concluded by emphasizing a peculiarity of the quantum mechanics of higher derivative systems. The quantities q^i's, $\dot{q}^i$'s, ..., and $q^{(N-1)i}$'s are indeed all treated as coordinates, so there are no uncertainty relations between them, but there will be uncertainty relations between q^i's and $q^{(2N-1)i}$'s, between $\dot{q}^i$'s and $q^{(2N-2)i}$'s, ..., and between $q^{(N-1)i}$'s and $q^{(N)i}$'s.

3. The reduction theorem

3.1. *Problem setting*

Consider an $(N-1)$th order Lagrangian $L^\sharp$ that may be singular. We define an Nth order Lagrangian L as follows

$$L(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(1)}, \ldots, \boldsymbol{q}^{(N)}, t) := L^\sharp(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(1)}, \ldots, \boldsymbol{q}^{(N-1)}, t) + \frac{\mathrm{d}}{\mathrm{d}t}W(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(1)}, \ldots, \boldsymbol{q}^{(N-1)}, t) \tag{3.1}$$

where W is an arbitrary function of $q^{(I)i}$'s and t. Needless to say, L and $L^\sharp$ are classically equivalent because the total derivative term is turned, in the action integral, into a surface term, which does not affect the classical equations of motion. Nevertheless, their quantum equivalence is non-trivial. Note that L and $L^\sharp$ are different-order Lagrangians. As is stated in section 2, different-order Lagrangians lead to different conjugate pairs, which means different uncertainty relations. The canonical variables (2.3) for the Lagrangian (3.1) are given as

$$q^{Ii} = q^{(I)i} \tag{3.2a}$$

$$p_{N-1,i} = \frac{\partial W}{\partial q^{(N-1)i}} \tag{3.2b}$$

$$p_{Ai} = p^\sharp_{Ai} + \frac{\partial W}{\partial q^{(A)i}}. \tag{3.2c}$$

We take the convention that I, J, K run from 0 to $N-1$, and A, B, C run from 0 to $N-2$, unless otherwise stated. Here $p^\sharp_{Ai}$'s are the canonical momentum in the $L^\sharp$-theory,

$$p^\sharp_{N-2,i} := \frac{\partial L^\sharp}{\partial q^{(N-1)i}} \tag{3.3a}$$

$$p^\sharp_{Ai} := \frac{\partial L^\sharp}{\partial q^{(A+1)i}} - \frac{\mathrm{d}}{\mathrm{d}t} p^\sharp_{A+1,i} \tag{3.3b}$$

with $A = 0, 1, \ldots, N-3$. The canonical Hamiltonian (2.6) becomes

$$\begin{aligned} H(\boldsymbol{q}, \boldsymbol{p}, t) &= p_{Ai} q^{A+1,i} + p_{N-1,i}\dot{q}^{N-1,i} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}^{N-1}, t) \\ &= H^\sharp(\boldsymbol{q}, \boldsymbol{p}^\sharp, t) - \frac{\partial W(\boldsymbol{q}, t)}{\partial t} \end{aligned} \tag{3.4}$$

with

$$H^\sharp(\boldsymbol{q}, \boldsymbol{p}^\sharp, t) := p^\sharp_{Ai} q^{A+1,i} - L^\sharp(\boldsymbol{q}, t). \tag{3.5}$$

We should distinguish $H^\sharp(\boldsymbol{q}, \boldsymbol{p}^\sharp, t)$ defined here from the canonical Hamiltonian in the $L^\sharp$ theory

$$H^\sharp(\boldsymbol{q}_\sharp, \boldsymbol{p}^\sharp, t) := \sum_{A=0}^{N-3} p^\sharp_{Ai} q^{A+1,i} + p^\sharp_{N-2,i}\dot{q}^{N-2,i} - L^\sharp(\boldsymbol{q}_\sharp, \dot{\boldsymbol{q}}^{N-2}, t) \tag{3.6}$$

where $\boldsymbol{q}_\sharp$ is an abbreviation for q^{Ai}'s, while $\boldsymbol{q}$ without $\sharp$ is the abbreviation for q^{Ii}'s. Note that there is a relation as $\boldsymbol{q} = (\boldsymbol{q}_\sharp, q^{N-1,i})$.

These two $H^\sharp$'s, (3.5) and (3.6), are the same in their value but different as functions of canonical variables (see appendix). This implies the following: while the equation (3.4) with (3.5) defines a Hamiltonian system equivalent to the original Lagrangian system (3.1), the use of (3.6) instead of (3.5) results in another Hamiltonian system *not* equivalent to the original Lagrangian system. In other words, equation (3.6) has forgotten the relations

$$\dot{q}^{N-2,i} = q^{N-1,i}. \tag{3.7}$$

Equation (3.5), on the other hand, remembers them as canonical equations, $\dot{q}^{N-2,i} = \partial H(\boldsymbol{q}, \boldsymbol{p}, t)/\partial p_{N-2,i}$. Thus (3.6) defines a larger theory, in which the original one is contained as a special case. If we impose, by hand, the relation (3.7) on the larger theory, then it reduces to the original one.

Since the larger theory is quite useful for our purposes, we use, in the following, (3.6) instead of (3.5). As will be stated in section 3.3, the larger theory is a kind of gauge theory and we can impose (3.7) as a gauge-fixing condition to it.

3.2. Constraint analysis

Equation (3.2*b*) does not involve $q^{(K)i}$'s for $K \geqslant N$. This implies that they are primary constraints

$$\gamma_i(\boldsymbol{q}, \boldsymbol{p}, t) := p_{N-1,i} - \frac{\partial W}{\partial q^{N-1,i}} \approx 0. \tag{3.8}$$

When $L^\sharp$ is singular, i.e. $\det(\partial^2 L^\sharp/\partial q^{(N-1)i} q^{(N-1)j}) = 0$, there are other primary constraints in addition to γ_i's

$$\gamma_a^\sharp(\boldsymbol{q}_\sharp, \boldsymbol{p}^\sharp, t) \approx 0 \tag{3.9}$$

which stems from (3.2*c*) together with (3.3). It is not a hard task to show

$$\begin{aligned}\{\gamma_i, \gamma_j\} &= -\left\{p_{N-1,i}, \frac{\partial W}{\partial q^{N-1,j}}\right\} - \left\{\frac{\partial W}{\partial q^{N-1,i}}, p_{N-1,j}\right\} \\ &= \frac{\partial^2 W}{\partial q^{N-1,i}\partial q^{N-1,j}} - \frac{\partial^2 W}{\partial q^{N-1,j}\partial q^{N-1,i}} \\ &= 0 \end{aligned} \tag{3.10a}$$

$$\begin{aligned}\{\gamma_i, \gamma_a^\sharp\} &= \{p_{N-1,i}, \gamma_a^\sharp\} - \left\{\frac{\partial W}{\partial q^{N-1,i}}, \gamma_a^\sharp\right\} \\ &= \{p_{N-1,i}, q^{N-1,k}\}\frac{\partial \gamma_a^\sharp}{\partial p_{Aj}^\sharp}\frac{\partial p_{Aj}^\sharp}{\partial q^{N-1,k}} - \left\{\frac{\partial W}{\partial q^{N-1,i}}, p_{Bk}\right\}\frac{\partial \gamma_a^\sharp}{\partial p_{Aj}^\sharp}\frac{\partial p_{Aj}^\sharp}{\partial p_{Bk}} \\ &= \frac{\partial \gamma_a^\sharp}{\partial p_{Aj}^\sharp}\frac{\partial^2 W}{\partial q^{N-1,i}\partial q^{Aj}} - \frac{\partial^2 W}{\partial q^{A,j}\partial q^{N-1,i}}\frac{\partial \gamma_a^\sharp}{\partial p_{Aj}^\sharp} \\ &= 0. \end{aligned} \tag{3.10b}$$

The total Hamiltonian is given by

$$H_T = H + \lambda^a \gamma_a^\sharp + \lambda^i \gamma_i \tag{3.11}$$

where λ^a's and λ^i's are the Lagrange multipliers. Straightforward calculation shows that γ_i's do not produce secondary constraints

$$\begin{aligned}\dot{\gamma}_i &\approx \{\gamma_i, H_T\} + \frac{\partial \gamma_i}{\partial t} \\ &\approx \left\{\gamma_i, H^\sharp - \frac{\partial W}{\partial t}\right\} + \frac{\partial \gamma_i}{\partial t} \\ &= \frac{\partial H^\sharp}{\partial p_{Aj}^\sharp}\frac{\partial^2 W}{\partial q^{N-1,i}\partial q^{Aj}} + \frac{\partial^2 W}{\partial q^{N-1,i}\partial t} - \frac{\partial^2 W}{\partial q^{Aj}\partial q^{N-1,i}}\frac{\partial H^\sharp}{\partial p_{Aj}^\sharp} - \frac{\partial^2 W}{\partial t\, \partial q^{N-1,i}} \\ &= 0. \end{aligned} \tag{3.12}$$

This conclusion would not be obtained if we adopted (3.5) in (3.4). As for $\gamma_a^\sharp$'s, one obtains

$$\begin{aligned}\dot{\gamma}_a^\sharp &\approx \{\gamma_a^\sharp, H_T\} + \frac{\partial \gamma_a^\sharp}{\partial t} \\ &\approx \{\gamma_a^\sharp, H^\sharp\} + \frac{\partial \gamma_a^\sharp}{\partial p_{Ai}^\sharp}\frac{\partial^2 W}{\partial q^{Ai}\partial t} + \lambda^b\{\gamma_a^\sharp, \gamma_b^\sharp\} - \frac{\partial \gamma_a^\sharp}{\partial p_{Ai}^\sharp}\frac{\partial^2 W}{\partial t\, \partial q^{Ai}} + \left(\frac{\partial \gamma_a^\sharp}{\partial t}\right)_\sharp \\ &\approx \{\gamma_a^\sharp, H_T^\sharp\} + \left(\frac{\partial \gamma_a^\sharp}{\partial t}\right)_\sharp \end{aligned} \tag{3.13}$$

where

$$H_T^\sharp := H^\sharp + \lambda^a \gamma_a^\sharp \tag{3.14}$$

is the total Hamiltonian in the $L^\sharp$-theory. The symbol $(\partial/\partial t)_\sharp$ represents partial derivative by t with $\boldsymbol{q}_\sharp$ and $\boldsymbol{p}^\sharp$ fixed. One can prove

$$\{q^{Ai}, p^\sharp_{Bj}\} = \delta^A_B \delta^i_j \tag{3.15a}$$

$$\{q^{Ai}, q^{Bj}\} = \{p^\sharp_{Ai}, p^\sharp_{Bj}\} = 0 \tag{3.15b}$$

which means

$$\{F^\sharp, G^\sharp\} = \{F^\sharp, G^\sharp\}_\sharp \tag{3.16}$$

where $F^\sharp$ and $G^\sharp$ are arbitrary functions of $\boldsymbol{q}_\sharp$, $\boldsymbol{p}^\sharp$, and t. The symbol $\{\ ,\ \}_\sharp$ is the Poisson bracket in the $L^\sharp$-theory. Using (3.16), one can rewrite (3.13) as

$$\dot{\gamma}^\sharp_a \approx \{\gamma^\sharp_a, H^\sharp_T\}_\sharp + \left(\frac{\partial \gamma^\sharp_a}{\partial t}\right)_\sharp . \tag{3.17}$$

Note that the only property we assumed in deriving (3.10*b*) and (3.17) is that $\gamma^\sharp_a$'s are functions of $\boldsymbol{q}_\sharp$, $\boldsymbol{p}^\sharp$, and t. Thus these equations remain valid even if secondary constraints are substituted for $\gamma^\sharp_a$'s. Therefore we have proven that *all the secondary constraints emerging from $\gamma^\sharp_a$'s are just the same as the ones derived in the $L^\sharp$-theory*. Furthermore one concludes, from (3.10*b*) and (3.12), that γ_i's are first class.

In the above discussion, $\gamma^\sharp_a$'s may be a mixture of the first-class and the second-class constraints. As is stated in section 2.2, in the following we assume that $\gamma^\sharp_a$'s and the secondary constraints derived from them are all first class. Let us write them again as $\gamma^\sharp_a \approx 0$. Then all the constraints in our Lagrangian (3.1) are exhausted by (3.8) and (3.9). The final form of the total Hamiltonian is (3.11), in which the summation on a should be taken only on the primary constraints. (The summation on all the first-class constraints defines the extended Hamiltonian formalism [2]; our discussion in what follows remains valid even if we take the extended formalism.)

3.3. Gauge transformations

In this subsection we investigate the gauge transformation generated by γ_i's. For an arbitrary quantity $F(\boldsymbol{q}, \boldsymbol{p}, t)$, the gauge transformation is defined as

$$\delta F := \varepsilon^i \{F, \gamma_i\} \tag{3.18}$$

where ε^i's are arbitrary functions of t, but are independent of the canonical variables. As is well known, physical quantities must be gauge invariant.

One can show that quantities related to the $L^\sharp$-theory, for example q^{Ai}, $p^\sharp_{Ai}$, and $H^\sharp$, are all gauge invariant. Whereas quantities proper to the L-theory are, in general, non-invariant. For example, one obtains

$$\delta p_{Ii} = \varepsilon^j \frac{\partial^2 W}{\partial q^{Ii} \partial q^{N-1,j}} \tag{3.19a}$$

$$\delta q^{N-1,i} = \varepsilon^i \tag{3.19b}$$

$$\delta W = \varepsilon^i \frac{\partial W}{\partial q^{N-1,i}} \tag{3.19c}$$

$$\delta H_{\mathrm{T}} = \delta H = -\varepsilon^i \frac{\partial^2 W}{\partial t\, \partial q^{N-1,i}} \tag{3.19d}$$

which show that p_{Ii}'s, $q^{N-1,i}$'s, W, H_{T}, and H are all non-invariant and unphysical.

Needless to say, true physical quantities must be gauge invariant under the gauge transformations generated by $\gamma_a^\sharp$'s as well. Further investigation of them requires the specification of $L^\sharp$'s concrete form. So we do not pursue it any more.

Note, remember that our theory is equivalent to the original Lagrangian system (3.1) when we impose (3.7) in addition. Since (3.7) is not gauge invariant, it works as a gauge-fixing condition. The gauge transformations generated by γ_i's are the symmetry of the larger theory but not the symmetry of the original Lagrangian (3.1). Nevertheless they are important; gauge invariance of our theory makes it clear that the condition (3.7) is in fact unessential and does not affect the physics.

3.4. *Proof of the theorem*

We now turn our attention to the quantum mechanics. The Schrödinger equation is given by (2.12) with the Hamiltonian operator

$$\hat{H}\left(\boldsymbol{q}, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}}, t\right) = \hat{H}^\sharp\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp} - \frac{\partial W}{\partial \boldsymbol{q}_\sharp}, t\right) - \frac{\partial W}{\partial t} \tag{3.20}$$

derived from (3.4) with (3.6) and (3.2*c*). The subsidiary conditions (2.13) are given by

$$\hat{\gamma}_i\psi(\boldsymbol{q}, t) = \left(-\mathrm{i}\hbar\frac{\partial}{\partial q^{N-1,i}} - \frac{\partial W}{\partial q^{N-1,i}}\right)\psi(\boldsymbol{q}, t) = 0 \tag{3.21}$$

$$\hat{\gamma}_a^\sharp\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp} - \frac{\partial W}{\partial \boldsymbol{q}_\sharp}, t\right)\psi(\boldsymbol{q}, t) = 0. \tag{3.22}$$

Equations (3.21) are solved as follows

$$\psi(\boldsymbol{q}, t) = \psi^\sharp(\boldsymbol{q}_\sharp, t)\exp\frac{\mathrm{i}W(\boldsymbol{q}, t)}{\hbar} \tag{3.23}$$

where $\psi^\sharp$ is an arbitrary function of q^{Ai}'s and t. The equation (3.23) gives the general form of the physical state. Note that $\psi^\sharp(\boldsymbol{q}_\sharp, t)$ is gauge invariant, while $\psi(\boldsymbol{q}, t)$ is not.

It is not hard to verify the identities

$$\left(-\mathrm{i}\hbar\frac{\partial}{\partial q^{Ai}} - \frac{\partial W}{\partial q^{Ai}}\right)^n\psi = \left[\left(-\mathrm{i}\hbar\frac{\partial}{\partial q^{Ai}}\right)^n\psi^\sharp\right]\exp\frac{\mathrm{i}W}{\hbar} \tag{3.24}$$

on the physical state (3.23). Here n is a non-negative integer. These identities imply the following identity

$$\hat{F}\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp} - \frac{\partial W}{\partial q^{Ai}}, t\right)\psi = \left[\hat{F}\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp}, t\right)\psi^\sharp\right]\exp\frac{\mathrm{i}W}{\hbar}. \tag{3.25}$$

Here $F(\boldsymbol{q}_\sharp, \boldsymbol{p}^\sharp, t)$ is an arbitrary quantity which is a polynomial with respect to $p^\sharp_{Ai}$'s. Assuming that $H^\sharp(\boldsymbol{q}_\sharp, \boldsymbol{p}^\sharp, t)$ and $\gamma_a^\sharp(\boldsymbol{q}_\sharp, \boldsymbol{p}^\sharp, t)$'s are polynomials with respect to $p^\sharp_{Ai}$'s, we apply (3.25) for them.

Inserting (3.23) into the Schrödinger equation (2.12) with (3.20), and using (3.25), we finally obtain

$$\mathrm{i}\hbar\frac{\partial\psi^\sharp(\boldsymbol{q}_\sharp, t)}{\partial t} = \hat{H}^\sharp\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp}, t\right)\psi^\sharp(\boldsymbol{q}_\sharp, t). \tag{3.26}$$

This is nothing but the Schrödinger equation in the $L^\sharp$-theory. As for the condition (3.22), it simply becomes

$$\hat{\gamma}_a^\sharp\left(\boldsymbol{q}_\sharp, -\mathrm{i}\hbar\frac{\partial}{\partial \boldsymbol{q}_\sharp}, t\right)\psi^\sharp(\boldsymbol{q}_\sharp, t) = 0. \tag{3.27}$$

Equation (3.26) together with (3.27) constitutes the full quantum mechanics for the $L^\sharp$-theory. Here $\psi^\sharp(\boldsymbol{q}_\sharp, t)$ is identified as the wave function of the $L^\sharp$-theory. Therefore we have proven the following proposition.

Proposition. nth order and $(n-1)$th order Lagrangians, which may be singular and non-autonomous, lead to the same quantum mechanics if their difference is a total time derivative.

The proposition implies the following theorem.

Theorem. nth order and mth order Lagrangians, which may be singular and non-autonomous, lead to the same quantum mechanics if their difference is a total time derivative.

Proof. Let us assume $n \geqslant m$, and put

$$L_n = L_m^\sharp + \frac{\mathrm{d}}{\mathrm{d}t} W_{n-1}. \tag{3.28}$$

Here, the subscript of L, $L^\sharp$, and W denote the order of highest derivatives contained. We use the same notation for $\mathcal{L}$ and $\mathcal{W}$, which appear in what follows, as well.

(i) $n = m$ case. Let us introduce an arbitrary function $\mathcal{W}_n$, and define a new Lagrangian $\mathcal{L}_{n+1}$ as follows

$$\mathcal{L}_{n+1} := L_n + \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{W}_n. \tag{3.29}$$

Then (3.28) is rewritten as

$$\mathcal{L}_{n+1} = L_n^\sharp + \frac{\mathrm{d}}{\mathrm{d}t}(W_{n-1} + \mathcal{W}_n). \tag{3.30}$$

These equations together with the proposition say

$$L_n \sim \mathcal{L}_{n+1} \sim L_n^\sharp \tag{3.31}$$

where $\sim$ means quantum mechanically equivalent.

(ii) $n = m+1$ case. This case is just the same as the proposition.

(iii) $n \geqslant m+2$ case. Let us introduce $n-m-1$ arbitrary functions $\mathcal{W}_i$, $i = m, m+1, \ldots, n-2$, and define the same number of new Lagrangians $\mathcal{L}_i$, $i = m+1, m+2, \ldots, n-1$, as follows

$$\begin{aligned}
\mathcal{L}_{m+1} &:= L_m^\sharp + \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{W}_m \\
\mathcal{L}_{m+2} &:= \mathcal{L}_{m+1} + \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{W}_{m+1} - \mathcal{W}_m) \\
&\vdots \\
\mathcal{L}_{n-1} &:= \mathcal{L}_{n-2} + \frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{W}_{n-2} - \mathcal{W}_{n-3}).
\end{aligned} \tag{3.32}$$

Consistency between these equations and (3.28) requires

$$L_n = \mathcal{L}_{n-1} + \frac{\mathrm{d}}{\mathrm{d}t}(W_{n-1} - \mathcal{W}_{n-2}). \tag{3.33}$$

Therefore we have proven

$$L_m^\sharp \sim \mathcal{L}_{m+1} \sim \mathcal{L}_{m+2} \sim \cdots \sim \mathcal{L}_{n-2} \sim \mathcal{L}_{n-1} \sim L_n. \tag{3.34}$$

This completes the proof. □

The autonomous case with $n = m = 1$ of the theorem has been proven by Kugo [3].

Corollary (Grosse-Knetter). An mth order Lagrangian, and the same Lagrangian formally treated as if it were an $n(\geqslant m)$th order Lagrangian lead to the same quantum mechanics.

Proof. This is the special case of the theorem with the vanishing total derivative term. □

The corollary has been proven by Grosse-Knetter [4] for the special case of autonomous Lagrangians. His proof is based on path integrals. Our corollary is the generalization of his result to non-autonomous Lagrangians.

Acknowledgments

The author thanks K Kamimura (Toho University) and J Gomis (Universitat de Barcelona) for discussions.

Appendix: A pedagogical example

In this appendix we want to clarify the difference between two $H^\sharp$'s, (3.5) and (3.6), using a simple example. The example we consider is

$$L(q,\dot q,\ddot q) = \tfrac{1}{2}(\dot q)^2 + \ddot q. \tag{A1}$$

This, of course, means $L^\sharp(q,\dot q) = (\dot q)^2/2$ and $W(q,\dot q) = \dot q$. For the $L^\sharp$-theory, we obtain $q^0 := q$ and $p_0^\sharp := \partial L^\sharp/\partial \dot q$ as the canonical variables, and

$$H^\sharp(q^0, p_0^\sharp) := p_0^\sharp \dot q^0 - L^\sharp(q^0, \dot q^0) = \tfrac{1}{2}(p_0^\sharp)^2 \tag{A2}$$

as the canonical Hamiltonian (3.6).

Now consider the L-theory (A1). The canonical variables (2.3) are $q^0 := q$, $q^1 := \dot q$, and

$$p_1 := \frac{\partial L}{\partial \ddot q} = 1 \tag{A3a}$$

$$p_0 := \frac{\partial L}{\partial \dot q} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \ddot q}\right) = \dot q. \tag{A3b}$$

From (A3a) we obtain a primary constraint

$$\gamma(q^0, q^1, p_0, p_1) := p_1 - 1 \approx 0 \tag{A4}$$

which corresponds to (3.8). The canonical Hamiltonian (3.4) becomes

$$\begin{aligned} H(q^0, q^1, p_0, p_1) &:= p_0 q^1 + p_1 \dot q^1 - L(q^0, q^1, \dot q^1) \\ &= p_0 q^1 - \tfrac{1}{2}(q^1)^2 \\ &= H^\sharp(q^0, q^1, p_0^\sharp). \end{aligned} \tag{A5}$$

Here

$$H^\sharp(q^0, q^1, p_0^\sharp) := p_0^\sharp q^1 - \tfrac{1}{2}(q^1)^2 \tag{A6}$$

is the concrete form of (3.5). In the above formulae, all the arguments have been written down explicitly without using the abbreviations, $\boldsymbol{q} := (q^0, q^1)$, $\boldsymbol{p} := (p_0, p_1)$, $\boldsymbol{q}_\sharp := (q^0)$, and $\boldsymbol{p}^\sharp := (p_0^\sharp)$.

Obviously (A6) and (A2) are different as a function of the canonical variables. For the sake of simplicity, let us refer to (A5) with (A6) as the 'true Hamiltonian',

$$H^{\mathrm{TRUE}}(q^0, q^1, p_0, p_1) = p_0^\sharp q^1 - \tfrac{1}{2}(q^1)^2. \tag{A7}$$

On the other hand, using (A2) instead of (A6), we obtain another Hamiltonian

$$H^{\mathrm{GAUGED}}(q^0, q^1, p_0, p_1) = \tfrac{1}{2}(p_0^\sharp)^2 \tag{A8}$$

which we call the 'gauged Hamiltonian'.

The true Hamiltonian (A7) is equivalent to the original Lagrangian (A8) in the sense that the canonical equations for (A7) reproduce the Euler–Lagrange equation for (A1). Unfortunately the true Hamiltonian is not suitable for our purposes. In fact we obtain

$$H_{\mathrm{T}}^{\mathrm{TRUE}} := p_0 q^1 - \tfrac{1}{2}(q^1)^2 + \lambda(p_1 - 1) \tag{A9a}$$

$$\dot{\gamma} \approx \{\gamma, H_{\mathrm{T}}^{\mathrm{TRUE}}\} = q^1 - p_0 =: \gamma' \approx 0 \tag{A9b}$$

$$\dot{\gamma}' \approx \{\gamma', H_{\mathrm{T}}^{\mathrm{TRUE}}\} = \lambda \approx 0 \tag{A9c}$$

$$\{\gamma, \gamma'\} = -1. \tag{A9d}$$

Equation (A9*d*) shows that the primary constraint $\gamma := p_1 - 1 \approx 0$ and the secondary constraint $\gamma' := q^1 - p_0 \approx 0$ are second class. This reflects the fact that the original Lagrangian (A1) has no gauge symmetry.

We now concentrate on the gauged Hamiltonian (A8). As is easily confirmed, the canonical equation for the gauged Hamiltonian does not contain the information

$$q^1 = \dot{q}^0 \tag{A10}$$

which corresponds to (3.7). The relation (A10) is indispensable for the equivalence to the original Lagrangian (A1). We can show that the gauged Hamiltonian, in fact, is equivalent to the 'gauged Lagrangian'

$$L^{\mathrm{GAUGED}}(q^0, q^1, \dot{q}^0, \dot{q}^1) := \tfrac{1}{2}(\dot{q}^0)^2 + \dot{q}^1, \tag{A11}$$

where q^0 and q^1 are *independent* variables. If we put the relation (A10) by hand, the gauged Lagrangian (A11) reduces to the original Lagrangian (A1). Thanks to the lack of (A10), (A11) becomes a gauge theory. That is, as shown in the text, there occurs no secondary constraint (3.12), and the only constraint (A5) is first class. The corresponding gauge transformation (3.19*a*) is given as

$$\delta q^1 = \varepsilon \tag{A12a}$$

$$\delta q^0 = \delta p_0^\sharp = \delta p_1^\sharp = 0 \tag{A12b}$$

under which the gauged Lagrangian (A11) is invariant up to a total derivative. We can impose the lost relation (A10) as a gauge-fixing condition for the gauged model (A11) or (A8).

References

[1] For a review, see e.g. Gitman D M and Tyutin I V 1990 *Quantization of Fields with Constraints* (Berlin: Springer)

[2] Henneaux M and Teitelboim C 1992 *Quantization of Gauge Systems* (Princeton: Princeton University Press)

[3] Kugo T 1985 *Soryushiron Kenkyu* (Kyoto) **71** 49 (in Japanese)

[4] Grosse-Knetter C 1994 *Phys. Rev.* D **49** 6709