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DOCTORAL THESIS

On

well-posed variational principle

and

degrees of freedom counting of

geometrical trinity of gravity

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Abstract

This thesis is devoted to searching for fundamental issues of constraint systems, aiming for applications to theories of gravity. Theories of constraint systems play a crucial role in constructing theories of gravity since these theories are constraint systems, and theories of gravity provide the fundamentals of cosmology. Hence, it would be no exaggeration to say that theories of constraint systems are a fundamental ground of cosmology.

A wide range of theories of modern physics is constructed upon the variational principle, and so are the theories of gravity. The variational principle requires appropriate boundary conditions to derive the equations of motion of a given theory. For non-degenerate systems, the Dirichlet boundary conditions are imposed as usual. For degenerate systems, however, the existence of constraints generically disturbs the consistency of the boundary conditions with the possible dynamics. This means that an inappropriate choice of boundary conditions is prone to restrict the possible solutions to a narrow region. Therefore, the well-posed variational principle demands a methodology to compose valid boundary conditions without such restriction to the solutions. In particular, since the theories of gravity have the property of higher-order derivative degenerate systems, the identification of such boundary conditions is important for introducing counter-terms like the Gibbons-York-Hawking counter-terms. The first topic of this thesis is the study of establishing the methodology.

Metric-affine gauge theories of gravity are one of the modified/extended theories of general relativity in a geometric and the most generic manner and describe gravity by using curvature, torsion, and non-metricity, and it is expected to give perspectives into problems such as the late-time accelerated expansion of the universe (, or equivalently, dark energy problem, cosmological constant problem), the origin of inflation from the viewpoint of low-energy effective theories of quantum gravity based on the UV-competition, H_0- and/or

σ_8-tension problems. These theories are classified into eight subclasses from viewpoints of gauge structures in the internal space based on the Möbius representations. In particular, the three subclasses of the so-called geometrical trinity of gravity, which is composed of General Relativity (GR), Teleparallel Equivalent to GR (TEGR), and Symmetric TEGR (STEGR), have gathered attention in recent days since the non-linear extensions of these subclasses have the potential for explaining problems given in above. However, the propagating Degrees of Freedom (pDoF) of those subclasses has not been unveiled yet, and the study of investigating these numbers is the second topic of this thesis.

One of the methods to identify the pDoF of a given theory is the use of the so-called Dirac-Bergmann analysis. The heart of this analysis is very simple; the time evolution of a given system is described by the so-called total Hamiltonian, which is composed of the Legendre transformation of the Lagrangian of the given system such that it is compatible with the existence of the primary constraints, and all constraints satisfy the so-called consistency conditions, which demands all constraints to be static. For point particle systems, this analysis is mathematically well-formulated, meaning that the Poisson brackets are always well-defined. For field theories, which include, of course, theories of gravity, however, the well-definedness should be reconsidered since the existence of the Dirac delta function causes problematic situations when determining the Lagrange multipliers such as contradictions in the consistency conditions to the properties of the given system that are derived from its action functional. In this thesis, the issues of the Dirac-Bergmann analysis in field theories are scrutinized and clarified, and a prescription to make the pathological situation easier is proposed. This prescription may restrict the solution space to a narrow region but makes it possible to give a reliable result to each analysis. Then, based on the prescription, the analysis is performed for each subclass in the geometrical trinity of gravity and its non-linear extension.

Finally, the uncompleted works and future directions of this thesis are discussed.

Impact statement

The new results of this thesis are based on two published papers and two peer-reviewing papers when this thesis was submitted but confirmed their validity by the committee of doctoral thesis. This thesis is devoted to providing new perspectives for the following two problems: the well-posedness of the variational principle in degenerate systems and the degrees of freedom counting in the use of the Dirac-Bergmann analysis of the modified/extended theories of gravity, in particular, the so-called geometrical trinity of gravity and its non-linear extension.

There are three impacts of this thesis. The first impact is that a methodology for setting appropriate boundary conditions for the well-posed variational principle in degenerate systems is established. Before the methodology appeared, boundary conditions of constraint systems were naively determined as the apparent variables in the first-order variation of the action functional, and there generically were incompatibilities with constraints of the given system on the boundaries. This methodology would also provide the fundamentals of deriving the counter-terms in the action functionals of theories of gravity since a counter-term is derived only after appropriate boundary conditions are determined for the given theory.

The second impact is that the geometric quantities, *i.e.*, curvature, torsion, and non-metricity, are formulated in a unified manner based on the Möbius representation. Before this approach appeared, these geometric quantities were separately introduced in each own and ad hoc way. This unified perspective would provide a more comprehensive understanding of geometric quantities and gauge theories of gravity constructed by such geometric quantities, and it might bring a discovery of new geometric quantities. If it is realized, the construction of a new theory of gravity by using the new geometric quantity could be possible.

The third impact is that the issues of the Dirac-Bergmann analysis in field theories are revealed and a prescription to make the analysis valid is established. Before the issues were clarified and the prescription appeared, the result of the analysis of a given theory was based on a set of PDEs with respect to the Lagrange multipliers which is not guaranteed whether or not it is solvable, therefore, the degrees of freedom derived by the method was always nothing more than a speculation. The prescription provides a reliable result of the analysis and a set of concrete conditions to guarantee it.

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To all my loving things...

Contents

Chapter 1

Introduction

The quest for the universe has fascinated mankind over the ages. In modern physics, this quest is positioned as cosmology, and researchers have continued to devote all their efforts to unveiling the mysteries of the universe from both theoretical and phenomenological points of view. The beginning of cosmology dates back to the era of A. Einstein, who established the general theory of relativity. This theory is the most successful classical theory of gravity and describes how the universe evolves together with matter. Hence, combining the standard model of particle physics, cosmology has challenged to unveil the history of the universe.

ΛCDM model is the standard model of cosmology based on FLRW spacetime with cosmological parameters that are determined by observations. (Stage 1 in Figure 1.1.) This model became the standard model of cosmology around the beginning of twenty-first century based on the observations of the cosmic microwave background [Spergel et al. (2003)], the large-scale structure [Tegmark et al. (2004)], and the late-time accelerated expansion of the universe [Riess et al. (1998); Perlmutter et al. (1999)]. The most recent observation at the moment writing this thesis is provided in *Planck 18* [Aghanim et al. (2020a,b)]. These observations further indicated that the universe is anisotropic and inhomogeneous in the distribution of photons and matter, respectively. In order to understand these observational facts, it is mandatory to take the cosmological perturbation into account of the standard model of cosmology together with the Big Bang and inflation hypothesis. A series of Boltzmann equations with respect to the perturbations of cosmic ingredients and Einstein field equations describe how the ingredients develop with time under the influence of gravity. (Stage 3 in Figure 1.1.) Based on this system, the power spectrum of each ingredient is derived and compared to the observations. (Stages 4 and 5 in Figure 1.1.) This is the basic

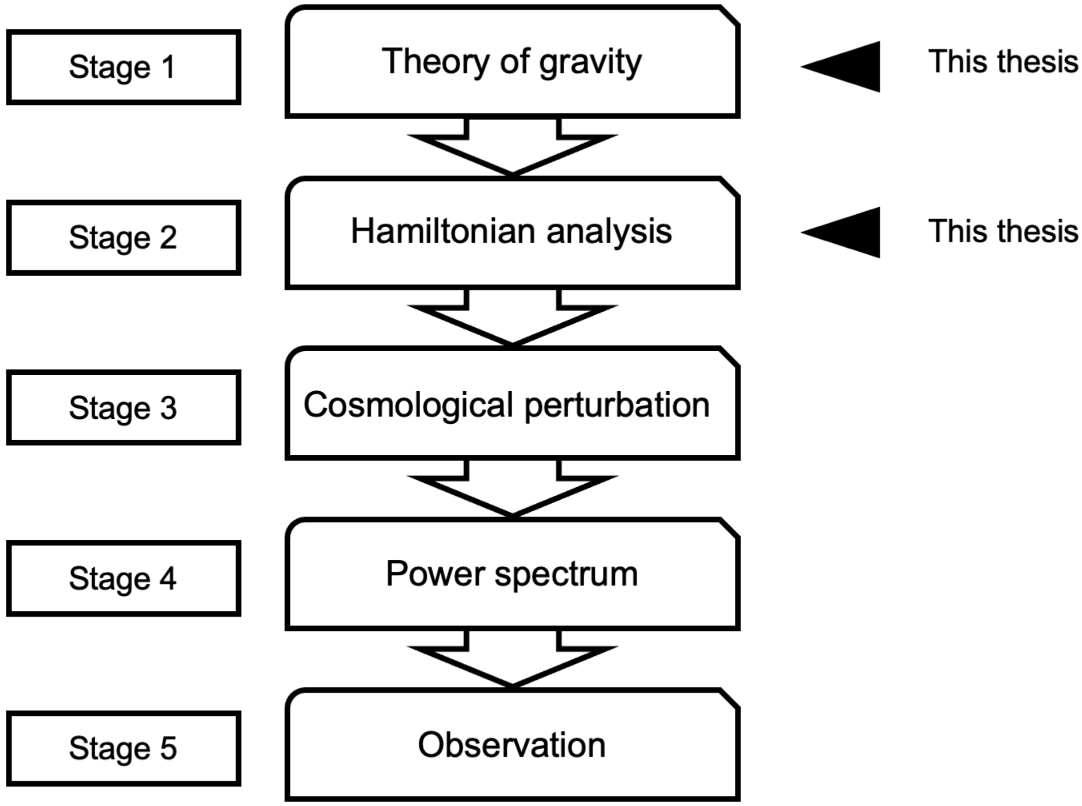

Figure 1.1: Modern framework for cosmology

formulation of the modern cosmology [Dodelson (2003); Mukhanov (2005); Weinberg (2008)].

The modern cosmology has also unveiled a series of new mysteries. The ingredients of the universe should contain the so-called dark energy and dark matter in the percentile of about 95% but the true identity and the origin of these ingredients have not been unveiled yet. So is the mechanism of how inflation occurs and its origin. Furthermore, the recent observations point out the so-called tension problem in the cosmological parameters of σ_8 and H_0 [Aghanim et al. (2020b)], which is the discrepancy of the estimated values of H_0 and σ_8 between the estimation based on the ΛCDM model and the model-independent observation. H_0- and σ_8-tensions are confirmed in about 5σ and 3σ confidence level, respectively [Wong et al. (2020); Nunes and Vagnozzi (2021)]. In particular, Figure 1.2 indicates that the discrepancies of H_0 between the value obtained from the CMB measurement (based

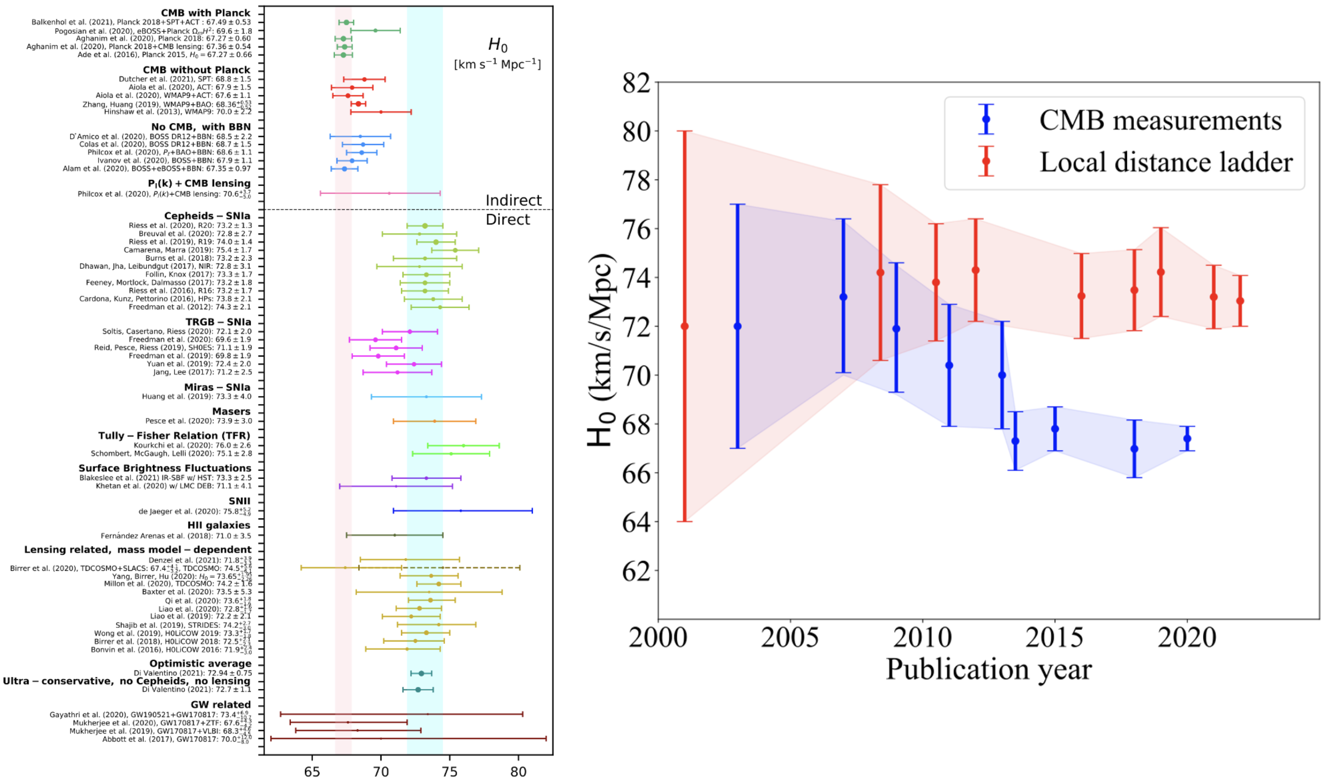

Figure 1.2: The recent observations of Hubble parameter H_0 and its discrepancy. The left- and right-panels are given in Ref [Di Valentino et al. (2021)] and Ref [Hu and Wang (2023)], respectively.

on the ΛCDM model) and the Type Ia Supernovae (model-independent) have not gradually been impossible to ignore. These problems may be related to the expansion of the universe, or equivalently, spacetime, and such phenomena could be ascribed to the nature of gravity. It would imply a possibility of the alternation of the basic theory of gravity: Stage 1 in Figure 1.1 should be scrutinized. Combined further with the recent development in the accuracy of the observation of gravitational waves, the elaboration of modified/extended theories of gravity is rapidly proceeding. This provides a natural motivation to investigate the modified/extended theories of gravity.

The current thesis treats three topics. Metric-affine gauge theories of gravity are one of the modified/extended theories of gravity, which describes gravity in terms of geometric quantities of curvature, torsion, and non-metricity [Blagojevic (2001)], and the Weitzenböch connection introduces the covariant derivatives [Weitzenboch (1923)]. Since the metric-affine gauge theory of gravity is the most generic extension of the general theory of relativity in a geometric manner, the extended theories have a possibility to explain gravitational phenomena that are hard to treat within the general theory of relativity. The beginning of the gauge approach to gravity dates back to the era of the birth of Yang-Mills gauge theory [Yang and Mills (1954)], which provides the foundation of modern particle physics. Inspired by this theory, R. Utiyama extended it into describing gravity in a unification manner under the concept of gauge invariant principle [Utiyama (1956)]. Combined the series of works by E. Cartan [Cartan (1924)] and H. Weyl [Weyl (1952); Hehl et al. (1986); Blagojevic (2001)], the fundamentals of the theories are formulated as the formulation in the current days. This is one of three topics of the present thesis.

A set of subclasses of the metric-affine gauge theories of gravity called the geometrical trinity of gravity is the most actively researched one on the purpose of the cosmological application for explaining the problems such as dark energy (the late-time accelerating expansion of the universe without the cosmological constant) and the origin of inflation [Beltrán Jiménez et al. (2019); Heisenberg (2023); Bahamonde et al. (2023a)]. This set includes the general theory of relativity as a special case and these subclasses are equivalent to one another up to boundary terms in action functional. The notable point is that this equivalence gets changed when some extension or modification is performed and it gives rise to the fertility for resolving the problems in cosmology. For instance, $f(\mathring{R})$-gravity is one of the non-linear extensions of the geometrical trinity of gravity, and it includes the most successful inflation model so-called Starobinsky R^2-inflation model (Figure 1.3). In addition, the non-linear extensions of the teleparallel and symmetric teleparallel gravity, which are also subclasses of the geometrical trinity of gravity, generically provide the so-called effective cosmological constant, and it can explain the late-time accelerated ex-

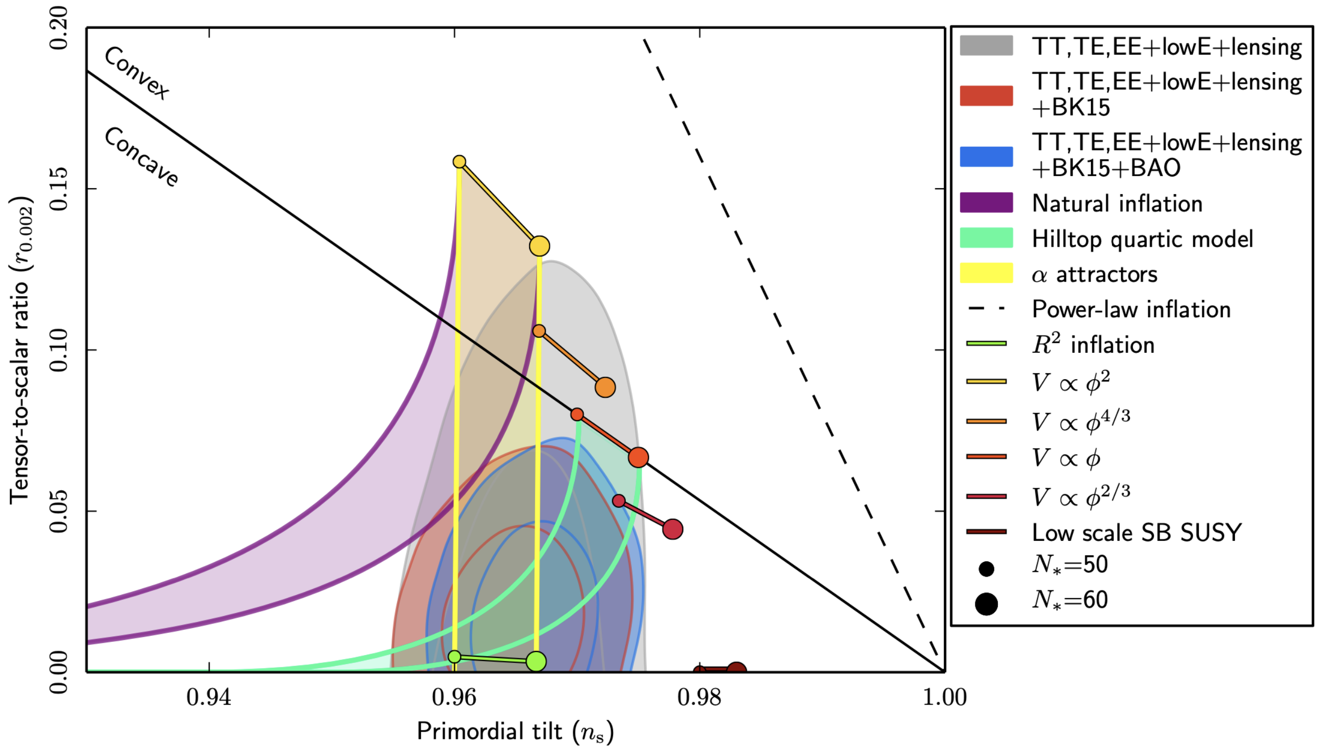

Figure 1.3: Tensor-to-scalar ratio [Aghanim et al. (2020a)].

pansion of the universe. Furthermore, those extensions in quadratic, non-linear, and non-local ways have also gathered attention as possible candidates for consistent low-energy effective theories of quantum gravity from the viewpoint of UV-completion [Stelle (1978); Starobinsky (1980); Koshelev et al. (2023)], which are ways to grasp a clue for understanding the mechanism of inflation [De Felice and Tsujikawa (2010); Capozziello and De Laurentis (2011); Donoghue and Menezes (2022)]. However, the cosmological application of the modified/extended theories of gravity demands unveiling such as the constraint structure of those theories such as gauge symmetry, propagating degrees of freedom, the existence of (Ostrogradski's) ghost modes. The Hamiltonian/Dirac-Bergmann analysis makes it possible to unveil such structures [Dirac (1950, 1958a,b); Anderson and Bergmann (1951); Bergmann et al. (1950); Bergmann (1949); Bergmann and Brunings (1949)]. (Stage 2 in Figure 1.1.) For instance, the analysis of $f(\mathring{R})$-gravity unveils that this theory has diffeomorphism and local

Lorentz invariance, three possible propagating degrees of freedom, and no ghost degrees of freedom. The first and third properties are completely the same as the general theory of relativity. The different property is the second one, and it is important since one of three propagating degrees of freedom can be used for generating inflation and the remaining two degrees of freedom are precisely the same modes in the general theory of relativity. The Dirac-Bergmann analyses of these theories are also one of three topics of the present thesis.

The last one of three topics of the present thesis is a consideration of the well-posedness of the variational principle. This topic is important in particular for the theories of gravity since these theories are degenerate systems and many of these theories include second-order or higher-order derivative terms in those action functionals. The former property (degenerate system), on one hand, implies that the variational principle requires appropriate boundary conditions that are consistent with the constraints of the theory. On the other hand, the latter property (higher-order derivative system) indicates that the action functional demands appropriate counter-terms under the imposition of the well-posed boundary conditions of the variational principle known as the Gibbons-York-Hawking counter-terms in the general theory of relativity [York (1972, 1986a); Gibbons and Hawking (1977); Hawking and Horowitz (1996)]. It is well known that this sort of counter-terms plays a crucial role in constructing theories of quantum gravity in the use of the path-integral formulation and blackhole thermodynamics [Gibbons and Hawking (1977); York (1986b); Braden et al. (1990); Brown and York (1993b,a)], which could contribute to understanding of the origin of inflation. In this thesis, the well-posedness provides the action functionals of the theories of gravity being suitable for the Dirac-Bergmann analysis, in which the absence of Ostrogradsky's ghost modes is guaranteed by virtue of the work of the Gibbons-York-Hawking counter-term.

Reassembling these three topics in theoretical order, the current thesis aims to give new perspectives for the following three problems:

1. Well-posedness of the variational principle
2. Classification of the metric-affine gauge theory of gravity
3. Degrees of freedom counting of the geometrical trinity of gravity and its non-linear extension with the Dirac-Bergmann analysis

Based on these problems, the current thesis is composed as follows:
The first two chapters are devoted to a review of degenerate systems and a method of making the variational principle well-posed, respectively.

In chapter 2, a theory of analytical mechanics for theories of gravity is provided in a self-contained manner. Theories of gravity have the properties of degenerate and higher-order derivative systems. Starting with reviewing the basic concepts of non-degenerate point particle systems, a theory of degenerate point particle systems is introduced. In particular, the Dirac-Bergmann analysis is reconstructed in detail. Based on these ingredients, the concepts of gauge symmetry/transformation, Dirac structure, propagating degrees of freedom, and gauge degrees of freedom are established. Finally, higher-order derivative point particle systems are introduced. The problematic situations caused by the Ostrogradsky instability/degrees of freedom are pointed out, and a methodology for removing these problematic degrees of freedom is provided.

In chapter 3, a methodology for making the variational principle in point particle systems well-posed is established. The extension to field theories has been developing, but some specific cases will be provided in the succeeding chapters of the present thesis. First of all, the problems of degenerate systems in the variational principle are explained. It is shown that the valid boundary conditions in a higher-order time derivative system but which has equations of motion up to second-order time derivative are restricted to position-fixing boundary conditions. Based on the Pons formulation, which is introduced in Section 2.5, Frobenius integrability conditions of first-order degenerate time derivative systems are investigated, and the concrete formulae of the conditions are derived. After these preparations, the well-posedness of the variational principle is reformulated. Introducing two types of embeddings of the symplectic manifold based on the Shanmugadhasan-Maskawa-Nakajima theorem, *i.e.,* quasi-canonical embeddings and canonical embeddings, the well-posedness is investigated. As a result, appropriate boundary conditions are specified. Finally, examples are given, and this chapter is summarized with the outlook for these works.

Chapter 2 is based on

- K. Tomonari, "On the well-posed variational principle in degenerate point particle systems using embeddings of the symplectic manifold", PTEP 2023 6 063A05.
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  Copyright (2023) by the Physical Society of Japan [Tomonari (2023b)].

- K. Izumi, K. Shimada, K. Tomonari, and M. Yamaguchi, "Boundary Conditions for Constraint Systems in Variational Principle", PTEP 2023 10 103E03.
  DOI: 10.1093/ptep/ptad122, arXiv:2303.03805 [hep-th].
  Copyright (2023) by the Physical Society of Japan [Izumi et al. (2023)].

The next two chapters provide a review of the general theory of relativity and bundle theory in a self-contained form. Many of the recent works of the metric-affine gauge theories of gravity are discussed just by imposing some conditions on three fundamental geometric quantities: curvature, torsion, and non-metricity, but, in the author's opinion, it is over-simplified. These geometric quantities and conditions are closely and precisely related to the gauge structures of internal space, and, in order to unveil the relations and structures, it is mandatory to discuss them based on bundle theories. Otherwise, the fertility of the metric-affine gauge theories of gravity would be lost.

In chapter 4, the general theory of relativity, which is the most successful classical theory of gravity in the modern physics, is established. First of all, the fundamental concepts of the theory such as spacetime, weak/Einstein/strong equivalence principles are introduced. Based on these concepts, the geodesic equations and the Einstein field equations are derived from both viewpoints of physical considerations (bottom-up approach) and the variational principle (top-down approach). As mentioned in Section 3.9, we assume that the well-posedness of the variational principle demands consistency with the primary constraint(s): $\mathfrak{C}^{(1)}$. In particular, before deriving the Einstein field equations by using the variational principle, the ADM-foliation/decomposition of the spacetime is introduced. This technique is mandatory not only to apply the variational principle in a well-posed manner being consistent with $\mathfrak{C}^{(1)}$ but also to perform the Dirac-Bergmann analysis. Finally, performing the Dirac-Bergmann analysis, the propagating and gauge degrees of freedom of the theory are clarified.

In chapter 5, a mathematical framework for gauge approach to gravity is constructed. First of all, three fundamental bundles, *i.e.,* fiber bundles, G-bundles, and principal G-bundles are defined. For principal G-bundles, the Ehresmann connection and its curvature are introduced. After that, vector bundles together with gauge fields and those curvature (field strengths) are derived. Internal space bundles, which play a crucial role in constructing the metric-affine gauge theories of gravity, are also derived, in particular, focusing on frame fields and Weitzenböch connection. Finally, a gauge-approach derivation of the Einstein field equations is described. This chapter gives mathematical basics for the succeeding chapters.

Based on the previous chapters, the final two chapters are devoted to formulating the metric-affine gauge theory of gravity, in particular, focusing on the geometrical trinity of gravity and those non-linear extension, and performing the Dirac-Bergmann analysis of these theories.

In chapter 6, the metric-affine gauge theories of gravity are constructed. First, based on Sections 5.2 and 5.4, three fundamental geometric quantities, *i.e.,* curvature, torsion, and non-metricity are introduced. Second, using the so-called Möbius representation of a gauge group, the metric-affine geometries are classified into eight subclasses: Riemann-Cartan, teleparallel, Riemann, Minkowski, Weyl-Cartan, Weyl, metric-affine, and symmetric teleparallel geometries. In this formulation, each geometric quantity is given by the exterior covariant derivative of each corresponding potential. Third, The geometrical trinity of gravity, which is composed of the three subclasses: Riemann (general relativity), symmetric teleparallel, and torsion teleparallel, is established. These three subclasses are equivalent up to boundary terms in the meaning of action functional. Finally, two extensions of the geometrical trinity of gravity, that is, quadratic extension and non-linear extension, are introduced. The latter extension plays a main role in the next section.

In chapter 7, the Dirac-Bergmann analysis is performed for each subclass of the geometrical trinity of gravity and its non-linear extension. In order to apply the analysis, which was introduced in Section 2.2 but restricted to point particle systems, to field theories, three fundamental issues are clarified. These issues are commonly caused by the spatial derivatives of the Dirac delta function. And then a prescription that circumvents the issues is proposed. Based on the prescription, the analysis is performed for TEGR, CGR, a non-linear extension of GR, TEGR, and CGR, and the propagating degrees of freedom of each theory is unveiled. Throughout these analyses, the three issues in field theories of the Dirac-Bergmann analysis are concretely clarified for each subclass, and the reason why the prescription is valid for removing the issues is investigated. I emphasize that these analyses are not a complete manipulation of the issues; it is just a *prescription* to circumvent the issues and make it possible to perform the Dirac-Bergmann analysis. Therefore, the results could be valid only for some classes of solutions. Finally, this chapter is summarized with the outlook for these works.

Chapter 6 is based on

- K. Tomonari , "A unified description of curvature, torsion, and non-metricity of the metric-affine geometry with the Möbius representation", arXiv:2312.11558 [gr-qc]. [Tomonari (2023a)].

Chapter 7 is based on

- K. Tomonari and S. Bahamonde, "Dirac-Bergmann analysis and Degrees of Freedom of Coincident $f(Q)$-gravity", arXiv:2308.06469 [gr-qc]. [Tomonari and Bahamonde (2023)].

Finally, in Chapter 8, I summarize the conclusions of this thesis.

Chapter 2

Analytical mechanics on degenerate point particle systems

Chapter abstract

In this chapter, a theory of analytical mechanics for theories of gravity is provided in a self-contained manner. Theories of gravity have the properties of degenerate and higher-order derivative systems. Starting with reviewing the basic concepts of non-degenerate point particle systems, a theory of degenerate point particle systems is introduced. In particular, the Dirac-Bergmann analysis is reconstructed in detail. Based on these ingredients, the concepts of gauge symmetry/transformation, Dirac structure, propagating degrees of freedom, and gauge degrees of freedom are established. Finally, higher-order derivative point particle systems are introduced. The problematic situations caused by the Ostrogradsky instability/degrees of freedom are pointed out, and a methodology for removing these problematic degrees of freedom is provided.

2.1. Non-degenerate systems

In this section, the basics of the Lagrangian and Hamiltonian formalism of non-degenerate point particle systems are briefly reviewed. First of all, let us introduce the Lagrangian formalism.

The principle of least action/variational principle plays the most fundamental role in this formalism. This principle derives the equations of motion of a given system with respect to the generic variations: not only to the variations of the configuration variables and those velocity variables but also to the time variable. Assume that it exists that a system which is described by a Lagrangian $L = L(\dot{q}^i\,, q^i\,, t)$ ($i \in \{1\,, 2\,, \cdots\,, N\}$) defined on the velocity phase space $T\mathcal{Q} \times \mathbb{R}$ of a configuration space $\mathcal{Q}$. Here, $q^i = q^i(t)$ are a coordinate system for the configuration space. $\dot{q}^i = \dot{q}^i(t)$ are the velocity variables of $q^i(t)$, respectively, and then, $\dot{q}^i$ and q^i give a coordinate system for the velocity phase space. A non-degenerate system satisfies a condition that the rank of the kinetic (or Hessian) matrix, *i.e.*,

$$K_{ij} = \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \tag{2.1}$$

is full rank. Then the action functional is introduced as follows:

$$I[q^i\,, t] = \int_{t_1}^{t_2} L(\dot{q}^i\,, q^i\,, t)\ dt\,, \tag{2.2}$$

where " $[q^i\,, t]$ " denotes that the right-hand side of the equation is a functional defined on the configuration space $T\mathcal{Q} \times \mathbb{R}$. The principle of least action/variational principle, stating that the path in nature locally minimizes the value of the action functional, leads to a set of equations of motion. Consider the following variations:

$$\begin{aligned} &q^i(t) \to q'^i(t') = q^i(t) + \delta q^i(t)\,, \\ &t \to t' = t + \delta t(t). \end{aligned} \tag{2.3}$$

Since the time variable is also varied, the commutativity of the variational operation δ and the time derivative operation d/dt is lost; it indicates the necessity to reconsider the variation of the time variables. Introducing the equal-time variation, *i.e.*,

$$\bar{\delta} q^i = q'^i(t) - q^i(t)\,, \tag{2.4}$$

the following variation formula is derived:

$$\delta \dot{q}^i(t) = \bar{\delta}\dot{q}^i(t) + \ddot{q}^i(t)\delta t\,, \tag{2.5}$$

where second-order variational terms are neglected. In the same manner, the variation of the configurations are also calculated as follows:

$$\delta q^i(t) = \bar{\delta} q^i(t) + \dot{q}^i(t)\delta t. \tag{2.6}$$

Then the first variation of the action functional (2.2) is calculated as follows:

$$\delta I[q^i\,, t] = \int_{t_1}^{t_2} \left[\left\{ \frac{\partial L}{\partial q^i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i} \right) \right\} \bar{\delta} q^i + \frac{d}{dt} \left\{ \left(\frac{\partial L}{\partial \dot{q}^i} \right) \bar{\delta} q^i + L\delta t \right\} \right]\, dt\,. \tag{2.7}$$

Under the imposition of the Dirichlet boundary conditions, $i.e.$,

$$\bar{\delta} q^i(t_2) = \bar{\delta} q^i(t_1) = 0\,, \quad \delta t(t_2) = \delta t(t_1) = 0\,, \tag{2.8}$$

then the variational principle, $\delta I[q^i\,, t] = 0$, leads to the equations of motion, $i,e.$, Euler-Lagrange equations, as follows:

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i} \right) = 0\,. \tag{2.9}$$

The above derivation is based on the variational principle with respect to the generic variations Eq (2.5). Without the time variation, the boundary conditions $\delta t(t_2) = \delta t(t_1) = 0$ are satisfied by definition, and the derivation results back to the ordinary one in which the variations are taken only to the configuration and those velocity variables.

Second, assuming that the Euler-Lagrange equations hold, Noether's first theorem is derived. Then, using Eq (2.6), Eq (2.7) becomes as follows:

$$\begin{aligned}
\delta I[q^i\,,t] &= \int_{t_1}^{t_2} \frac{d}{dt}\Theta(\delta q^i(t)\,,\delta t(t)\,,t)\,,\\
\Theta(\delta q^i\,,\delta t\,,t) &= \left(\frac{\partial L}{\partial \dot{q}^i}\right)\delta q^i - \left\{\left(\frac{\partial L}{\partial \dot{q}^i}\right)\dot{q}^i - L\right\}\delta t\,.
\end{aligned} \tag{2.10}$$

Since boundary terms do not affect to the Euler-Lagrange equations, the Lagrangian has an arbitrariness of the boundary terms. That is,

$$L \to L' = L + \frac{d}{dt}W(q^i\,,t)\,, \tag{2.11}$$

and this symmetry is called quasi-invariance of the system. Therefore, the following formula holds:

$$\frac{d}{dt}\left\{\Theta(\delta q^i(t)\,,\delta t(t)\,,t) - W(q^i(t)\,,t)\right\} = 0\,. \tag{2.12}$$

This formula indicates that the quantity $\Theta - W$ is invariant with respect to the variation Eq (2.3) in the time evolution of the system; $\Theta - W$ is a conserved quantity of the system. This is a result of the quasi-invariance given in Eq (2.11).

Third, to exist a Lagrangian for given equations of motion, a set of relations have to be satisfied as necessary and sufficient conditions. This theorem is crucial to validate Noether's first theorem since it is meaningless without the existence of a Lagrangian for the equations of motion even if symmetries exist. All physics of a given system is engraved into a Lagrangian excepting initial conditions. Assume that a set of equations of motion is given such that these equations include up to second-order time derivative terms of the configurations as follows:

$$[\mathrm{EoM}]_i(\ddot{q}^k\,,\dot{q}^k\,,q^k\,,t) = K_{ij}(\dot{q}^k\,,q^k\,,t)\ddot{q}^j + A_i(\dot{q}^k\,,q^k\,,t) = 0\,, \tag{2.13}$$

where K_{ij} is the kinetic matrix defined in Eq (2.1) and A_i are arbitrary functions. The well-posedness of the variational principle under the imposition of the Dirichlet boundary conditions guarantees the validity of the generic expression of these equations of motion above. This point will be discussed in Section 3.2. The necessary conditions are nothing but the satisfaction of the following formula:

$$K_{ij}(\dot{q}^k\,,q^k\,,t)\ddot{q}^j + A_i(\dot{q}^k\,,q^k\,,t) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i}\,. \tag{2.14}$$

Comparing the coefficients of $\ddot{q}^i$, $\dot{q}^i$, q^i, and other terms, it leads to the following equivalent formulae:

$$\begin{aligned}
&K_{ij} = K_{ji}\,,\\
&\frac{\partial K_{jk}}{\partial \dot{q}^i} = \frac{\partial K_{ki}}{\partial \dot{q}^j}\,,\\
&\frac{\partial A_i}{\partial \dot{q}^j} + \frac{\partial A_j}{\partial \dot{q}^i} = 2\left(\dot{q}^k\frac{\partial}{\partial q^k} + \frac{\partial}{\partial t}\right)K_{ij}\,,\\
&2\left(\frac{\partial A_i}{\partial q^j} - \frac{\partial A_j}{\partial q^i}\right) = \left(\dot{q}^k\frac{\partial}{\partial q^k} + \frac{\partial}{\partial t}\right)\left(\frac{\partial A_i}{\partial \dot{q}^j} - \frac{\partial A_j}{\partial \dot{q}^i}\right)\,.
\end{aligned} \tag{2.15}$$

Therefore, for a set of the equations of motion (2.13), if a Lagrangian exists then the above relations have to be satisfied.

Conversely, if the above relations hold then the Lagrangian can be derived as follows:

$$L = K(\dot{q}^j\,,q^j\,,t) + D_i(q^j\,,t)\dot{q}^i + C(q^j\,,t)\,, \tag{2.16}$$

where K, D_i, and C are given as follows:

$$\begin{aligned}
K(\dot{q}^i\,,q^i\,,t) &= \int_0^1 \dot{q}^i H_i(\dot{q}^j\tau\,,q^j\,,t)\;d\tau + W_1(q^j,t)\,,\\
D_i(q^k,t) &= q^j\int_0^1 \tau Z_{[ij]}(q^k\tau,t)\;d\tau + W_2(\dot{q}^k,t)\,,\\
C(q^i\,,t) &= q^i\int_0^1 Y_i(q^j\tau\,,t)\;d\tau + W_3(\dot{q}^j\,,t)\,,
\end{aligned} \tag{2.17}$$

where W_1, W_2, and W_3 are arbitrary functions and H_i, $Z_{[ij]}$, and Y_i are defined as follows:

$$
\begin{aligned}
H_i &= \int_0^1 \dot{q}^j K_{ij}(\dot{q}^k \tau, q^k, t)\ d\tau\,, \\
Z_{[ij]} &= \frac{1}{2}\left(\frac{\partial A_i}{\partial \dot{q}^j} - \frac{\partial A_j}{\partial \dot{q}^i}\right) + \frac{\partial^2 K}{\partial q^i \partial \dot{q}^j} - \frac{\partial^2 K}{\partial q^j \partial \dot{q}^i}\,, \\
Y_i &= \left\{\frac{\partial^2 K}{\partial q^i \dot{q}^j} + \frac{1}{2}\left(\frac{\partial A_i}{\partial \dot{q}^j} - \frac{\partial A_j}{\partial \dot{q}^i}\right)\right\}\dot{q}^j - \frac{\partial K}{\partial q^i} - A_i + \frac{\partial^2 K}{\partial \dot{q}^i \partial t} + \frac{\partial D_i}{\partial t}\,.
\end{aligned}
\tag{2.18}
$$

These arbitrary functions can be neglected as total divergent terms. This statement is shown as follows: Without any loss of generality, these functions are encapsulated as $K' = K + U_i(q^j\,, t)\dot{q}^i + V(q^j\,, t)$ for appropriate functions U_i and V. Using K', Eq (2.16) is rewritten as $L' = K' + D'_i\dot{q}^i + C' = L + \bar{D}_i\dot{q}^i + \bar{C}$, where $\bar{D}_i = D'_i + U_i - D_i$ and $\bar{C} = C' + V - C$. Since Eq (2.14) leads to $\partial\bar{D}_i/\partial q^j - \partial\bar{D}_j/\partial q^i = 0$ and $\partial\bar{C}/\partial q^i - \partial\bar{D}_i/\partial t = 0$, it exists a function $W = W(q^i, t)$ such that $\bar{D}_i = \partial W/\partial q^i$ and $\bar{C} = \partial W/\partial t$, and these conditions indicate that $L' = L + dW/dt$.

There is a remark; Eq (2.13) has an arbitrariness of the multiplication of a non-singular matrix $X_i{}^j$: $[\mathrm{EoM}]'_i = X_i{}^j[\mathrm{EoM}]_j = 0$. It indicates that the correspondence between a Lagrangian and a set of the equations of motion, Eq (2.13), is not generically determined uniquely and also implies that there is a possibility for the existence of a Lagrangian even though once the initial set of Eq (2.13) does not satisfy the necessary and sufficient conditions given in Eq (2.15). That is, it is enough to satisfy the conditions (2.15) up to this arbitrariness to exist a Lagrangian for Eq (2.13).

Finally, Hamiltonian formalism is introduced. The second equation in Eq (2.10) introduces canonical momentum variables as follows:

$$
p_i = \frac{\partial L}{\partial \dot{q}^i}\,. \tag{2.19}
$$

Then q^i and p_i span a coordinate system for the phase space $T^*\mathcal{Q} \times \mathbb{R}$ by virtue of the implicit function theorem since the system is non-degenerate. For the coordinate system, the Hamiltonian is introduced as follows:

$$H(q^j\,, p_j\,, t) = p_i\dot{q}^i - \left. L(\dot{q}^j\,, q^j\,, t)\right|_{\dot{q}^j = F^j(q^k\,, p_k\,, t)}\,, \tag{2.20}$$

where $F^i(q^j\,, p_j\,, t)$ are a set of functions that are determined by the implicit function theorem. This is nothing but the Legendre transformation of the Lagrangian $L = L(\dot{q}^i\,, q^i\,, t)$. The variation of the Hamiltonian under the Euler-Lagrange equations leads to $\delta H = F^i(q^j\,, p_j\,, t)\delta p_i - p_i \delta q^i$, and it guarantees that the Hamiltonian formalism is described in the phase space $T^*\mathcal{Q} \times \mathbb{R}$ in a well-defined manner. The action functional in the phase space is given as follows:

$${}_*I[q^i\,, p_i\,, t] = \int_{t_1}^{t_2} \left(p_i\dot{q}^i - H(q^j\,, p_j\,, t)\right)\, dt\,, \tag{2.21}$$

where the left under " ${}_*$ " of ${}_*I[q^i\,, p_i\,, t]$ denotes a quantity in the phase space. The variational principle under the Dirichlet boundary conditions, $\delta q^i(t_2) = \delta q^i(t_1) = 0$, leads to the Hamilton equations as follows:

$$\dot{q}^i = \frac{\partial H}{\partial p_i}\,, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}\,. \tag{2.22}$$

Under the satisfaction of the Legendre transformation Eq (2.20) and its inverse transformation, the first equations reproduce the relations $\dot{q}^j = F^j(q^k\,, p_k\,, t)$ and the second equations are equivalent to the Euler-Lagrange equations given in Eq (2.9). This derivation is valid only in the case that δq^i and δp_i are independent. If a set of constraints to the phase space exist then the derivation has to be reconsidered. We need a theory on constraint/degenerate systems. The derivation of the Hamilton equations under the existence of constraints will be discussed in Sections 3.6 and 3.7.

2.2. Degenerate systems and Dirac-Bergmann analysis

In this section, degenerate systems are defined, and a methodology to determine the time evolution of a given system, *i.e.*, the Dirac-Bergmann analysis [Dirac (1950, 1958a,b); Bergmann (1949); Bergmann and Brunings (1949); Bergmann et al. (1950); Anderson and Bergmann (1951)], is introduced. First of all, let us introduce the Hamiltonian formulation of degenerate systems.

The rank of the kinetic matrix of the system, *i.e.*, Eq (2.1), discriminates the degeneracy/singularity of a given system from the non-degenerate systems. Assume that the rank of the kinematic matrix is $N-R$: $\operatorname{rank} K = N-R$ $(R \geq 1)$. Then the number of R primary constraints exist, and such system is defined as a degenerate/singular system. Let us denote these primary constraints as ${}_*\phi^{(1)}_\alpha(q^i\,, p_i) := 0$ $(\alpha \in \{1\,, 2\,, \cdots\,, R\})$ and the phase subspace which is restricted by the constraints as $\mathfrak{C}^{(1)}(t) = \{P \in T^*\mathcal{Q} \times \{t\} |_* \phi^{(1)}_\alpha(q^i(t)\,, p_i(t)) := 0\}$ $(t \in \mathbb{R})$, where P is a point in $T^*\mathcal{Q} \times \mathbb{R}$ at a time t; P is coordinated by q^i and p_i under the satisfaction of ${}_*\phi^{(1)}_\alpha(q^i\,, p_i) := 0$, and " $:=$ " denotes the imposition as a condition. The degeneracy also implies the existence of the number of r zero-eigenvalue vectors of the kinetic matrix. Based on this, taking into account that the number of $N-R$ velocity variables $\dot{q}^a$ $(a \in \{1\,, 2\,, \cdots\,, N-R\})$ can be expressed as $\dot{q}^a = F^a(q^i\,, p_b\,; \dot{q}^\alpha)$ $(b \in \{1\,, 2\,, \cdots\,, N-R\}$ $\alpha \in \{N-R+1, N-R+2, \cdots\,, N\})$ by virtue of the implicit function theorem, it is shown that the Lagrangian depends linearly on the velocity variables $\dot{q}^\alpha$ $(\alpha \in \{N-R+1\,, N-R+2\,, \cdots\,, N\})$ [Saito et al. (1989, 1993)]

$$\frac{\partial}{\partial \dot{q}^\alpha} \frac{\partial L}{\partial \dot{q}^\beta}\bigg|_{\dot{q}^a = F^a(q^i\,, p_b; \dot{q}^\alpha)} = 0\,. \tag{2.23}$$

Therefore, the Legendre transformation of the Lagrangian becomes as follows:

$$H = H_0 + \dot{q}^\alpha {}_*\phi^{(1)}_\alpha\,, \quad H_0 = \left[p_a \dot{q}^a + p_\alpha \dot{q}^\alpha - L(q^i\,, F^a(q^i\,, p_a; \dot{q}^\alpha); \dot{q}^\alpha)\right]_{\dot{q}^\alpha := 0} \tag{2.24}$$

under the imposition of $\dot{q}^\alpha := 0$, where ${}_*\phi^{(1)}_\alpha = p_\alpha - f_\alpha(q^i \, , p_i) := 0$ for some functions $f_\alpha(q^i \, , p_i)$ which are determined by the given Lagrangian. If the Legendre transformation is restricted to the subspace $\mathfrak{C}^{(1)}(t)$ then $H \approx H_0$, where " $\approx$ " denotes the weak equality: equality under the imposition of all the constraints. It indicates that $\dot{q}^\alpha$ can be expressed by the phase space variables of a neighbor region of $\mathfrak{C}^{(1)}(t)$ in $T^*\mathcal{Q} \times \mathbb{R}$, denoted by $\mathcal{O}(\mathfrak{C}^{(1)}(t))$, and therefore $\dot{q}^\alpha$ in Eq (2.24) can be replaced as a set of Lagrange multipliers, denoted by $\lambda^\alpha = \lambda^\alpha(q^i, p_i)$, as follows:

$$H_T = H_0 + \lambda^\alpha {}_*\phi^{(1)}_\alpha \, . \tag{2.25}$$

This quantity is noting but the so-called total Hamiltonian of the system, and this quantity governs the time evolution of the system. H_0 is called as the kernel Hamiltonian of the system. Remark that the total Hamiltonian is defined in $\mathcal{O}(\mathfrak{C}^{(1)}(t))$, which is a *region* of $T^*\mathcal{Q} \times \mathbb{R}$, not in the *subspace* $\mathfrak{C}^{(1)}(t)$ of $T^*\mathcal{Q} \times \mathbb{R}$.

In order to reveal the dynamics of the system, it is necessary to determine the multipliers. For this purpose, let us introduce the Dirac-Bergmann analysis. A natural way to resolve this problem is that, since the constraints restrict the phase space to a possible subspace in which the dynamics live, the constraints should not develop according to passing time. Expressing in a formula, denoting " $\overset{\mathfrak{C}^{(1)}}{\approx}$ " as the weak equality under the imposition of the primary constraints, it becomes as follows:

$${}_*\dot{\phi}^{(1)}_\alpha = \{ {}_*\phi^{(1)}_\alpha \, , H_T \}_{P.b.} \overset{\mathfrak{C}^{(1)}}{\approx} \{ {}_*\phi^{(1)}_\alpha \, , H_0 \}_{P.b.} + \lambda^\beta D_{\alpha\beta} := 0 \, , \tag{2.26}$$

these equations are called consistency conditions, where " $\{ \cdot \, , \cdot \}_{P.b.}$ " denotes the Poisson bracket and $D_{\alpha\beta}$ is called as Dirac matrix which is defined as follows:

$$D_{\alpha\beta} = \{ {}_*\phi^{(1)}_\alpha \, , {}_*\phi^{(1)}_\beta \}_{P.b.} \, . \tag{2.27}$$

Therefore, the consistency conditions determine the multipliers depending on the number of the rank of the Dirac matrix. Assume that the rank of the Dirac matrix is $R-R_1$ ($R_1 \geq 1$). Then the number of $R-R_1$ multipliers are determined but that of R_1 multipliers remain arbitrary. It indicates that the same number of new constraints, higher-order constraints, appear. The fundamental matrix transformations can split out the higher-order constraints from the consistency conditions. This manipulation is allowed since the constraints can be reorganized up to linear combinations. Applying this manipulation, the Dirac matrix is transformed as follows: $D'^{(1)}_{\alpha\beta} = P^{(1)}D^{(1)}Q^{(1)}$ for appropriate non-degenerate matrices $P^{(1)}$ and $Q^{(1)}$. The shape of the transformed matrix $D'^{(1)}_{\alpha\beta}$ is free to choose for the purpose of the analysis. In this section, let us choose the shape as $D'^{(1)}_{\alpha\beta} = \mathrm{diag}(\tau^{(1)}_1\,, \tau^{(1)}_2\,, \cdots\,, \tau^{(1)}_{R-R_1}\,, 0\,, 0\,, \cdots\,, 0)$. Using these ingredients, the consistency conditions are transformed as follows:

$$P^{(1)}{}_\alpha{}^\beta\{{}_*\phi^{(1)}_\beta, H_0\}_{P.b.} + D'^{(1)}_{\alpha\beta}\lambda'^{(1)^\beta} := 0\,, \tag{2.28}$$

where $\lambda'^{(1)^\alpha} = Q^{(1)^{-1}}{}^\alpha{}_\beta\lambda^\beta$. Eq (2.26) is equivalent to Eq (2.28) by virtue of the regularity of the matrices $P^{(1)}$ and $Q^{(1)}$. For the indices $a^{(1)} \in \{1\,, 2\,, \cdots\,, R-R_1\}$, on one hand, the multipliers are determined as $\lambda'_{a^{(1)}} = -\tau^{(1)}{}_{a^{(1)}}P^{(1)}{}^\beta_{a^{(1)}}\{{}_*\phi^{(1)}_\beta, H_0\}$. Remark that we do not sum over with respect to $a^{(1)}$. On the other hand, for the indices $\alpha^{(1)} \in \{R-R_1+1\,, R-R_1+2\,, \cdots\,, R\}$, new constraints, *i. e.*, secondary constraints, have to be imposed as follows:

$${}_*\phi^{(2)}_{\alpha^{(1)}} = P^{(1)}{}^\beta_{\alpha^{(1)}}\{{}_*\phi^{(1)}_\beta\,, H_0\}_{P.b.} := 0\,. \tag{2.29}$$

In addition, there is a case that, in Eq (2.28), removing some multipliers from an equation using other equations, a new constraint appears. In such cases, these constrains include in ${}_*\phi^{(2)}_{\alpha^{(1)}}$ extending the range of the index $\alpha^{(1)}$. Then the total Hamiltonian can be reassembled as follows:

$$H^{(1)}_T = H^{(1)}_0 + \lambda^{\alpha^{(1)}}{}_*\Phi^{(1)}_{\alpha^{(1)}}\,, \tag{2.30}$$

where $H_0^{(1)}$ and ${}_*\Phi^{(1)}_{\alpha^{(1)}}$ are defined as follows:

$$H_0^{(1)} = H_0 + \lambda^{a^{(1)}} {}_*\phi^{(1)}_{a^{(1)}} , \quad {}_*\Phi^{(1)}_{\alpha^{(1)}} = {}_*\phi^{(1)}_\beta {Q^{(1)}}^\beta{}_{\alpha^{(1)}} . \tag{2.31}$$

That is, the determined terms are encapsulated as the first term $H_0^{(1)}$ in the reassembled-total Hamiltonian $H_T^{(1)}$. The second term in $H_T^{(1)}$ still has arbitrariness.

Repeating the same procedure for the secondary constraints under the reassembled-total Hamiltonian Eq (2.30), and if it gives rise to new constraints then repeat over the same process until all the multipliers are determined or the new constraint does not appear up to linear combinations. Let us assume the process stops by S-steps. Then we obtain the final results; the constraints ${}_*\phi^{(1)}_\alpha := 0$, ${}_*\phi^{(2)}_{\alpha^{(1)}} := 0, \cdots$, ${}_*\phi^{(S)}_{\alpha^{(S-1)}} := 0$ appear, the multipliers $\lambda^{a^{(1)}}$, $\lambda^{a^{(2)}}, \cdots$, $\lambda^{a^{(S)}}$ are determined, the reassembled-total Hamiltonian

$$H_T^{(S)} = H_0^{(S)} + \lambda^{\alpha^{(S)}} {}_*\Phi^{(S)}_{\alpha^{(S)}} , \tag{2.32}$$

where

$$H_0^{(S)} = H_0^{(S-1)} + \lambda^{\alpha^{(S)}} {}_*\phi^{(1)}_{\alpha^{(S)}} , \quad {}_*\Phi^{(S)}_{\alpha^{(S)}} = {}_*\phi^{(S)}_\beta {Q^{(S)}}^\beta{}_{\alpha^{(S)}} \tag{2.33}$$

is derived, and the dynamics of the system is restricted to the phase subspace $\mathfrak{C}^{(S)}(t) = \{P \in T^*\mathcal{Q} \times \{t\} |{}_*\phi^{(1)}_\alpha := 0, {}_*\phi^{(2)}_{\alpha^{(1)}} := 0, \cdots , {}_*\phi^{(S)}_{\alpha^{(S-1)}} := 0\}$. The multipliers $\lambda^{\alpha^{(S)}}$ remain arbitrary and the existence of such multipliers then implies that this system has gauge symmetry. This point will be discussed in detail in the next Section 2.3. There is a remark; as long as all the consistency conditions for up to sth-order constraints hold, where $s \in \{1, 2, \cdots , S\}$, the argument " (t) " can be removed from the subspaces $\mathfrak{C}^{(1)}(t), \mathfrak{C}^{(2)}(t), \cdots , \mathfrak{C}^{(s)}(t)$ since all the constraints up to sth-order are static.

The Dirac-Bergmann analysis reveals all the constraints of the system. These constraints are classified into two classes: first-class and second-class. The former is defined as a set of constraints that are commutative with all other constraints in the phase subspace $\mathfrak{C}^{(S)}$ with respect to the Poisson bracket. The number of the set of first-class constraints has to be taken into the maximum number. Otherwise, the constraints are classified into second-class and the total number of second-class constraints is always even as long as the first-class constraints are taken in the maximum number [Castellani (1982)]. The constraints satisfy the following propositions; (i) A Poisson bracket between two first-class constraints is also classified into first-class constraint; (ii) The product of two constraints is classified into first-class constraint. For a function f in $T^*\mathcal{Q} \times \mathbb{R}$ such that $f = 0$ in $\mathfrak{C}^{(S)}$, (iii) f is expressed in a neighbor $\mathcal{O}(\mathfrak{C}^{(S)})$ as a linear combination of the constraints with appropriate coefficient functions: $f = g_{(s)}^{\alpha^{(s-1)}}\, {}_*\phi^{(s)}_{\alpha^{(s-1)}}$, where $\alpha_0 = \alpha$. In more detail, for first-class constraints ${}_*\chi_v \overset{\mathfrak{C}^{(S)}}{\approx} 0$ ($v \in \{1\,, 2\,, \cdots\,, V\}$) and second-class constraints ${}_*\theta_w \overset{\mathfrak{C}^{(S)}}{\approx} 0$ ($w \in \{1\,, 2\,, \cdots\,, 2W\}$), (iv) A first-class function f is expressed in a neighbor $\mathcal{O}(\mathfrak{C}^{(S)})$ as a linear combination of the first-class constraints with appropriate coefficient functions: $f = g^v{}_*\chi_v$; (v) A second-class function f is expressed in a neighbor $\mathcal{O}(\mathfrak{C}^{(S)})$ as a linear combination of both the first-class and second-class constraints with appropriate coefficient functions: $f = g^v{}_*\chi_v + h^w{}_*\theta_w$. In particular, Proposition (ii) indicates that the first-class constraints ${}_*\phi^{(S+1)}_{\alpha^{(S)}} = \{{}_*\phi^{(S)}_{\alpha^{(S-1)}}\,, H_T\}_{P.b.}$ can be expressed as a linear combination of the first-class constraints ${}_*\phi^{(s)}_{\alpha^{(s-1)}}$ ($s \in \{1\,, 2\,, \cdots\,, S\}$, $\alpha^{(0)} = \alpha$) with appropriate coefficient functions: ${}_*\phi^{(S+1)}_{\alpha^{(S)}} = C^{\alpha^{(s-1)}}{}_{\alpha^{(S)}(s)}\ {}_*\phi^{(s)}_{\alpha^{(s-1)}} \overset{\mathfrak{C}^{(S)}}{\approx} 0$.

Based on the above manipulations for the system, the time evolution of a quantity, denoted by f, of the system is described by the reassembled-total Hamiltonian $H_T^{(S)}$ as follows: $\dot{f} = \{f\,, H_T^{(S)}\}_{P.b.} = X_T^{(S)} f = \mathcal{L}_{X_T^{(S)}} f$, where $X_T^{(S)}$ and $\mathcal{L}_{X_T^{(S)}}$ denote the Hamiltonian vector field with respect to $H_T^{(S)}$, which is defined by

$$X_T^{(S)} = \frac{\partial H_T^{(S)}}{\partial q^i}\frac{\partial}{\partial p_i} - \frac{\partial H_T^{(S)}}{\partial p_i}\frac{\partial}{\partial q^i} + \frac{\partial}{\partial t}\,, \tag{2.34}$$

and the Lie derivative with respect to $X_T^{(S)}$, respectively. The remarkable point here is that, in the cases that the Dirac-Bergmann analysis does not determine all the multipliers, the time evolution of quantities of the system cannot be uniquely determined, and it is caused by the existence of first-class constraints. Therefore, it needs to construct a theory to resolve this situation and to identify the unique time evolution.

2.3. Gauge symmetries and Dirac structures

In this section, based on the properties of constraints of a given degenerate system, gauge symmetry is formulated [Sugano and Kimura (1983); Sugano et al. (1986); Sugano and Kimura (1990a,b); Sugano and Kagraoka (1991a,b)]. Then, the Dirac structure [Dirac (1950, 1958b)], which identifies the time evolution of dynamical/physical quantities of the system, is introduced. First of all, let us formulate the gauge symmetry.

In order to formulate the change of quantities of a given system, let us introduce the concept of infinitesimal canonical transformation. For a canonical coordinate system q^i and p_i, denoted by $\{q^i\,, p_i\}$, consider a canonical transformation from $\{q^i\,, p_i\}$ to $\{Q^i, P_i\}$ which is generated by a generator: $W = -p_i Q^i + \epsilon G(Q^j\,, P_j\,, t)$, where ϵ and G are an infinitesimal parameter and an arbitrary function of Q^i, P_i, and t, respectively. Then, taking into account up to first-order terms of ϵ, q^i and p_i are transformed as follows:

$$q^i \to Q^i = q^i + \epsilon \frac{\partial G(q^j\,, p_j\,, t)}{\partial p_i}\,, \quad p_i \to P_i = p_i - \epsilon \frac{\partial G(q^j\,, p_j\,, t)}{\partial q^i}\,. \tag{2.35}$$

Remark that, in Eq (2.35), G becomes a function of q^i, p_i, and t in the first-order approximation with respect to ϵ due to the existence of ϵ in the front of the partial derivatives. For this infinitesimal canonical transformation, a quantity of the system, denoted by $f = f(q^i\,, p_i\,, t)$, is transformed into as follows:

$$\delta_G f = \{f\,, G\}_{P.b.} = X_G f = \mathcal{L}_{X_G} f\,. \tag{2.36}$$

In the above manipulation, G governs the transformation; G can be regarded as the generator of the transformation rather than W. Replacing the generator G by the total Hamiltonian H_T, the Hamilton equations are derived; the time evolution of the system is nothing but the sequences of the infinitesimal canonical transformations that are generated by the total Hamiltonian.

The perspective described above for the change of quantities of the system reveals the relation between first-class constraints and gauge transformations. For simplicity, assume that a degenerate system has only first-class constraints: ${}_*\Psi^{(s)}_{\alpha^{(s-1)}} \overset{\mathfrak{C}^{(s)}}{\approx} 0$ ($s \in \{1\,,2\,,\cdots\,,S\}$, $\alpha^{(0)} = \alpha \in \{1\,,2\,,\cdots\,,N - \mathrm{rank}\,K\}$). Then the total Hamiltonian is given by $H_T = H_0 + \lambda^\alpha{}_*\Psi^{(1)}_\alpha$. Since the multipliers λ^α can be arbitrarily determined, for the transformation of a generator G and a quantity f, it is possible to impose the following relation:

$$\mathcal{L}_{X_G}(X_T f) := X_{\lambda^\alpha{}_*\Psi^{(1)}_\alpha} f\,, \tag{2.37}$$

or equivalently, it is calculated as follows:

$$\{G\,,H_T\}_{P.b.} + \frac{\partial G}{\partial t} := -\lambda^\alpha{}_*\Psi^{(1)}_\alpha \overset{\mathfrak{C}^{(1)}}{\approx} 0\,. \tag{2.38}$$

That is, the generator G is static under the imposition of the primary constraints; it indicates that $\delta_G f = \mathcal{L}_{X_G} f$ is nothing but a gauge transformation of the quantity f and G is the generator of the gauge transformation, and the system is, of course, invariant under the satisfaction of the relation Eq (2.38). That is, using the Hamilton equations and the relations from the Legendre transformation, the variation of the Lagrangian L with respect to the gauge transformation in the phase subspace $\mathfrak{C}^{(1)}$, *i.e.*, ${}_*\delta_G L$, is calculated as ${}_*\delta_G L = d(p_i\delta_G q^i - G)/dt - \lambda^\alpha{}_*\Psi^{(1)}_\alpha \overset{\mathfrak{C}^{(1)}}{\approx} d(p_i\delta_G q^i - G)/dt$, and it varies up to a total divergent term: ${}_*\delta_G L = dF/dt$. Therefore, the following relation is derived:

$$F \overset{\mathfrak{C}^{(1)}}{\approx} p_i \frac{\partial G}{\partial p_i} - G\,. \tag{2.39}$$

This relation implies a possible explicit form of the generator G.

In order to derive a concrete form of the generator G, let us consider an infinitesimal transformation for the Lagrangian formulation which includes a set of arbitrary functions:

$$\delta_\epsilon q^i = (D^{l_\alpha}\epsilon^\alpha(t)) g^i{}_{\alpha,l_\alpha}(\dot{q}^j\,, q^j)\,, \tag{2.40}$$

where $D^{l_\alpha} = d^{l_\alpha}/dt^{l_\alpha}$, $\epsilon^\alpha(t)$ are arbitrary functions of time, $g^i{}_{\alpha,l_\alpha}(\dot{q}^j\,, q^j)$ are determined by the Lagrangian, and $l_\alpha \in \{0\,, 1\,, \cdots\,, M_\alpha - 1\}$. $D^{l_\alpha}\epsilon^\alpha(t)$ are independent functions with respect to l_α and α. The invariance of the system to the above transformation indicates that the Lagrangian varies up to a total divergent term: $\delta_\epsilon L = DF$, where F is defined by

$$F = D^{l_\alpha}\epsilon^\alpha(t) f_{\alpha,l_\alpha}(\dot{q}^j\,, q^j)\,. \tag{2.41}$$

The functions $f_{\alpha,l_\alpha}(\dot{q}^j\,, q^j)$ are also determined by the Lagrangian. Since $\delta_\epsilon L = [\mathrm{EoM}]_i \delta_\epsilon q^i + D(p_i \delta_\epsilon q^i) = DF$, the following identity is derived:

$$\begin{aligned} &[\mathrm{EoM}]_i (D^{l_\alpha}\epsilon^\alpha) g^i{}_{\alpha,l_\alpha} + D\{(D^{l_\alpha}\epsilon^\alpha)\Delta_{\alpha,l_\alpha}\} = 0\,, \\ &\Delta_{\alpha,l_\alpha} = p_i g^i{}_{\alpha,l_\alpha} - f_{\alpha,l_\alpha}\,, \end{aligned} \tag{2.42}$$

where $[\mathrm{EoM}]_i$ denote the equations of motion in Lagrange formulation. Integrating by parts in the range of $(t_1\,, t_2)$ under the imposition of the boundary conditions $D^{l_\alpha}\epsilon^\alpha(t_2) = D^{l_\alpha}\epsilon^\alpha(t_1) =$

0, the following identities are derived:

$$\sum_{l_\alpha=0}^{M_\alpha-1}(-1)^{l_\alpha}D^{l_\alpha}([\mathrm{EoM}]_i g^i{}_{\alpha,l_\alpha}) = 0\,, \tag{2.43}$$

and

$$\begin{aligned}
&\Delta_{\alpha,M_\alpha-1} = 0\,,\\
&\Delta_{\alpha,l_\alpha} + D\Delta_{\alpha,l_\alpha+1} + [\mathrm{EoM}]_i g^i{}_{\alpha,l_\alpha+1} = 0\,, \quad (l_\alpha \in \{1\,,2\,,\cdots\,,M_\alpha-2\})\\
&D\Delta_{\alpha 0} - \sum_{l_\alpha=1}^{M_\alpha-1}(-1)^{l_\alpha}D^{l_\alpha}([\mathrm{EoM}]_i g^i{}_{\alpha,l_\alpha}]) = 0\,.
\end{aligned} \tag{2.44}$$

Eq (2.43) and the third identity of Eq (2.44) lead to the following identity:

$$D\Delta_{\alpha 0} + [\mathrm{EoM}]_i g^i{}_{\alpha,l_\alpha-1} = 0\,. \tag{2.45}$$

The first identity of Eq (2.44) is nothing but the primary constraints in the Lagrangian formulation: ${}_*\Psi_\alpha^{(1)} = \Delta_{\alpha,M_\alpha-1} = 0$. The second identity of Eq (2.44) leads to higher-order constraints in the Lagrangian formulation under the imposition of the Euler-Lagrange equations: ${}_*\Psi_\alpha^{(M_\alpha-l_\alpha)} = \Delta_{\alpha,l_\alpha} = -D\Delta_{\alpha,l_\alpha+1} - [\mathrm{EoM}]_i g^i{}_{\alpha,l_\alpha+1} = -D{}_*\Psi_\alpha^{(M_\alpha-l_\alpha-1)} = 0$, applying sequentially in the order of $l_\alpha = M_\alpha-2, M_\alpha-3,\cdots,0$. This sequence implies that

$${}_*\Psi_\alpha^{(l_\alpha)} = \Delta_{\alpha,M_\alpha-l_\alpha} = 0\,, \quad (l_\alpha \in \{1,2,\cdots,M_\alpha\})\,. \tag{2.46}$$

In the Hamiltonian formulation, using the Hamilton equations, these constraints are converted into

$${}_*\Psi_\alpha^{(l_\alpha+1)} = \Delta_{\alpha,M_\alpha-l_\alpha-1} = \{{}_*\Psi_\alpha^{(l_\alpha)}, H_T\}_{P.b.} \overset{\mathfrak{C}^{(l_\alpha)}}{\approx} 0\,. \tag{2.47}$$

This indicates $M_\alpha = S_\alpha$. Based on these ingredients, Eq (2.40), Eq (2.41), the definition of

Δ_{α,l_α} given in Eq (2.42), and Eq (2.47) derive the following expression of the generator G:

$$G = \sum_{l_\alpha=0}^{M_\alpha-1} (D^{l_\alpha}\epsilon^\alpha)\Delta_{\alpha,l_\alpha} \overset{\mathfrak{C}^{(1)}}{\approx} \sum_{l_\alpha=0}^{M_\alpha-1} (D^{I_\alpha}\epsilon^\alpha)_*\Psi_\alpha^{(M_\alpha-l_\alpha)} = p_i\delta_\epsilon q^i - F \tag{2.48}$$

in a consistent manner with Eq (2.39). Therefore, since $D^{l_\alpha}\epsilon^\alpha$ can be regarded as independent functions $\epsilon^\alpha_{l_\alpha}$, a possible expression of the generator G is nothing but a linear combination of the first-class constraints ${}_*\Psi_\alpha^{(s)}$ with coefficient functions $\epsilon^\alpha_{l_\alpha}(t)$

$$G = \epsilon^\alpha_{l_\alpha}(t)_*\Psi_\alpha^{(l_\alpha)}\,. \tag{2.49}$$

That is, the first-class constraints dominate gauge transformations under the satisfaction of the condition of Eq (2.38).

The coefficient functions $\epsilon^\alpha_{l_\alpha}(t)$ are restricted from the conditions of Eq (2.38) as follows:

$$\begin{aligned} &\{G\,,H_0\}_{P.b.} + \frac{\partial G}{\partial t} = -\lambda^\alpha{}_*\Psi_\alpha^{(1)} \overset{\mathfrak{C}^{(1)}}{\approx} 0\,, \\ &\{G\,,{}_*\Psi_\alpha^{(1)}\}_{P.b.} \overset{\mathfrak{C}^{(1)}}{\approx} 0\,. \end{aligned} \tag{2.50}$$

Taking into account Eq (2.49), the first relations above lead to

$$\sum_{l_\alpha=1}^{S_\alpha} \dot{\epsilon}^\alpha_{l_\alpha *}\Psi_\alpha^{(l_\alpha)} + \sum_{l_\alpha=1}^{S_\alpha-1} \epsilon^\alpha_{l_\alpha *}\Psi_\alpha^{(l_\alpha+1)} + \sum_{l_\alpha=1}^{S_\alpha} \epsilon^\alpha_{S_\alpha} C^\beta{}_{\alpha,l_\alpha *}\Psi_\beta^{(l_\alpha)} \overset{\mathfrak{C}^{(1)}}{\approx} 0\,, \tag{2.51}$$

where the Greek letters run from 1 to the total number of the primary first-class constraints. Therefore, a set of recurrence relations hold as follow:

$$\dot{\epsilon}^\alpha_{l_\alpha} + \epsilon^\alpha_{l_\alpha-1} + \epsilon^\beta_{S_\alpha} C^\alpha{}_{\beta,l_\alpha} = 0\,, \tag{2.52}$$

where $l_\alpha \in \{2\,,3\,,\cdots\,,S_\alpha\}$. The recurrence relations indicate that, providing the number of the primary first-class constraints functions $\epsilon^{\beta}_{S_\alpha}$ under the satisfaction of the conditions in Eq (2.50), all the remaining functions $\epsilon^{\beta}_{l_\alpha}$ are sequentially determined. That is, the generator of a gauge transformation in Eq (2.49) is determined from the recurrence relations Eq (2.52) under the satisfaction of the second conditions in Eq (2.50), and for this transformation, the system is invariant; gauge symmetries are now formulated. The Poisson bracket algebra of the first-class constraints, $\{{}_*\Psi_\alpha\,, {}_*\Psi_\beta\}_{P.b.} = C^{\gamma}{}_{\alpha\beta *}\Psi_\gamma$, characterise the symmetries. In the existence of second-class constraints, the above construction is valid for the reassembled-total Hamiltonian $H_T^{(S)} = H_0^{(S)} + \lambda^{\alpha^{(S)}}{}_*\Psi^{(S)}_{\alpha^{(S)}}$, recomposing the first-class constraints ${}_*\Psi^{(S)}_{\alpha^{(S)}}$ into the form ${}_*\Psi^{(l_\alpha)}_\alpha$ up to linear combinations.

There is a remark on Eq (2.44); if $S_\alpha = 2$, the identities becomes as follows:

$$\begin{aligned} &\Delta_{\alpha,1} = 0\,, \\ &\Delta_{\alpha,0} + D\Delta_{\alpha,1} + [\mathrm{EoM}]_i g^i{}_{\alpha,1} = \Delta_{\alpha,0} + [\mathrm{EoM}]_i g^i{}_{\alpha,1} = 0\,. \end{aligned} \tag{2.53}$$

These identities are noting but Noether's second theorem with no time variation. Considering time variation, $\delta_\epsilon t = \epsilon^\alpha(t)\tau_\alpha(\dot{q}^i, q^i, t)$, the second identity becomes as follows:

$$\begin{aligned} &\Delta_{\alpha,0} - E\tau_\alpha + [\mathrm{EoM}]_i g^i{}_{\alpha,1} = 0\,, \\ &E = p_i\dot{q}^i - L(\dot{q}^i, q^i, t)\,. \end{aligned} \tag{2.54}$$

The first identity in Eq (2.53) and Eq (2.54) are nothing but Noether's second theorem in the most general form.

So far all the quantities of the system are arbitrary functions that are defined in the phase space $T^*\mathcal{Q} \times \mathbb{R}$. A dynamical/physical quantity, denoted by f, is restricted to a gauge invariant quantity: $\delta_G f = \mathcal{L}_{X_G} f = \{f\,, G\}_{P.b.} \overset{\text{1st}}{\approx} 0$, or equivalently, $\{f\,, {}_*\Psi_\alpha\}_{P.b.} \overset{\text{1st}}{\approx} 0$ for all the first-class constraints ${}_*\Psi_\alpha \overset{\text{1st}}{\approx} 0$ ($\alpha \in \{1\,, 2\,, \cdots, U\}$), where " $\overset{\text{1st}}{\approx}$ " denotes the equality under the satisfaction of all the first-class constraints. In addition to the first-class constraints, hereinafter in the rest of the section, assume that second-class constraints exist: ${}_*\Theta_a \overset{\text{2nd}}{\approx} 0$ ($a \in \{1\,, 2\,, \cdots\,, 2V\}$), where " $\overset{\text{2nd}}{\approx}$ " denotes the equality under the imposition of all the second-class constraints. The Poisson brackets among f and ${}_*\Psi_\alpha \overset{\text{1st}}{\approx} 0$ are already weak equal to zero by its definition, but that among f and ${}_*\Theta_a \overset{\text{2nd}}{\approx} 0$ do generically not vanish in the weak equality even under the imposition of all the constraints. The Dirac bracket realizes the weak equal vanishing not only for the first-class constraints but also for the second-class constraints. Let us consider the following quantity:

$$f^* = f - \sum_{a=1,b=1}^{2V} \{f\,, {}_*\Theta_a\}_{P.b.} (D^{-1})_{ab}\, {}_*\Theta_b + \sum_{\alpha=1}^{U} A^\alpha\, {}_*\Psi_\alpha\,, \tag{2.55}$$

where A^α are arbitrary functions. This quantity satisfies not only $\{f^*\,, {}_*\Psi_\alpha\}_{P.b.} \approx \{f\,, {}_*\Psi_\alpha\}_{P.b.} \approx 0$ but also $\{f^*\,, {}_*\Theta_a\}_{P.b.} \approx 0$. Since $f^{**} \overset{\text{1st}}{\approx} f$, the map $f \mapsto f^*$ is interpreted as a projection map under the imposition of all the first-class constraints. Considering another physical quantity g, the Dirac bracket, denoted by " $\{\,\cdot\,,\cdot\,\}_{D.b.}$ ", between f and g is introduced as follows:

$$\{f\,, g\}_{D.b.} = \{f^*\,, g^*\}_{P.b.} \approx \{f\,, g\}_{P.b.} - \sum_{a=1,b=1}^{2v} \{f\,, {}_*\Theta_a\}_{P.b.} (D^{-1})_{ab} \{{}_*\Theta_b\,, g\}_{P.b}\,. \tag{2.56}$$

The Dirac bracket inherits all algebraic properties of the Poisson bracket and satisfies the following properties: $\{f\,, g\}_{D.b.} \approx \{f^*\,, g\}_{P.b.} \approx \{f\,, g^*\}_{P.b.}$. Then the Dirac structure is introduced as follows: For the linear transformation of the constraints

$${}_*\Psi_\alpha \to {}_*\Psi'_\alpha = X^\alpha\, {}_*\Psi_\alpha\,, \quad {}_*\Theta_a \to {}_*\Theta'_a = Y^a\, {}_*\Theta_a + Z^\alpha\, {}_*\Psi_\alpha\,, \tag{2.57}$$

where X^α, Y^a, and Z^α are arbitrary functions, the Dirac bracket is invariant

$$\{f\,, g\}'_{D.b.} \approx \{f\,, g\}_{D.b.}\,. \tag{2.58}$$

Using the Dirac bracket, the time evolution of the physical quantity f is described as follows

$$\dot{f} = \{f\,, H_T\}_{D.b} \approx \{f\,, H_0^{(S)}\}_{D.b}\,, \tag{2.59}$$

where $H_0^{(S)}$ is the determined part of the reassembled-total Hamiltonian $H_T = H_T^{(S)} = H_0^{(S)} + \lambda^{\alpha^{(S)}}{}_*\Phi^{(S)}_{\alpha^{(S)}}$. That is, for a gauge invariant quantity, *i.e.*, a physical quantity, the time evolution is given by Eq (2.59). The Dirac structure introduces the dynamical/propagating degrees of freedom and the gauge degrees of freedom.

2.4. Propagating and gauge degrees of freedom

In this section, the concepts of dynamical/propagating and gauge degrees of freedom are introduced. The gauge Degrees of Freedom (gDoF) of a given system, on one hand, is already implied in Section 2.3; the number of the undetermined multipliers $\lambda^{\alpha^{(S)}}$ (*c.f.* Eq (2.32) and Eq (2.33) in Section 2.2), or equivalently, that of the functions $\epsilon^{\alpha} = \epsilon^{\alpha}_{S_\alpha}$ (*c.f.* Eqs (2.52) in Section 2.3) is nothing but the gDoF. On the other hand, the propagating Degrees of Freedom (pDoF) can be introduced in two different ways: based either on the Dirac structure or a theorem known as the Shanmugadhasan-Maskawa-Nakajima theorem [Shanmugadhasan (1973); Dominici and Gomis (1980, 1982); Maskawa and Nakajima (1976); Tomonari (2023b)]. First of all, let us consider the first case.

Assume that only second-class constraints, ${}_*\Theta_a \approx 0$, exist. Then the Dirac structure holds for any quantities of the system, and then the time evolutions of these quantities are uniquely determined by Eq (2.59). Since the second-class constraints are static for the *unique* time evolution, the number of possible canonical coordinate variables to describe the system, *i.e.*, propagating Degrees of Freedom (pDoF), is counted out as follows: pDoF $= (2N - 2V)/2 = N - V$. In the case of existing first-class constraints, ${}_*\Psi_\alpha \approx 0$, the situation is different; the time evolution is no longer uniquely determined until the gauge degrees of freedom are removed. One of the methods to realize this removal is the gauge fixing method.

This method turns the first-class constraints into second-class constraints by imposing a set of additional constraints.

Assume that the gDoF is T and ${}_*\Psi^{(1)}_\alpha \approx 0\,,\ {}_*\Psi^{(2)}_\alpha = \{{}_*\Psi^{(1)}_\alpha\,, H_T\}_{P.b.} \approx 0\,, \cdots, {}_*\Psi^{(S)}_\alpha = \{{}_*\Psi^{(S-1)}_\alpha\,, H_T\}_{P.b.} \approx 0$ $(\alpha = 1\,, 2\,, \cdots, T)$ are first-class constraints. Since the total Hamiltonian contains the number of T undetermined multipliers, only the number of T additional constraints can be imposed. Let us denote these T additional constraints as ${}_*\Xi^{(1)}_\alpha := 0$. Then a gauge fixing condition is given as follows [Sugano et al. (1992)]:

$$\begin{aligned}
&\{{}_*\Psi^{(k)}_\alpha\,, {}_*\Xi^{(1)}_\beta\}_{P.b.} \overset{\text{1st;1}}{\approx} 0\,,\\
&\det\left(\{{}_*\Psi^{(K)}_\alpha\,, {}_*\Xi^{(1)}_\beta\}_{P.b.}\right) \overset{\text{NOT:1st;1}}{\approx} 0\,,\\
&\{{}_*\Xi^{(1)}_\beta\,, H_0\}_{P.b.} \overset{\text{NOT:1st;1}}{\approx} 0\,,
\end{aligned} \tag{2.60}$$

where "$\overset{\text{1st;1}}{\approx}$" and "$\overset{\text{NOT:1st;1}}{\approx}$" denote the weak equality and the weak *not* equality, respectively, under the imposition of all the first-class constraints and ${}_*\Xi^{(1)}_\alpha := 0$. The remaining $T \times (S-1)$ additional constraints are automatically derived as ${}_*\Xi^{(s+1)}_\alpha = \{{}_*\Xi^{(s)}_\alpha, H_T\}_{P.b.} \overset{\text{1st;1}\,,2\,,\cdots\,,s}{\approx} \{{}_*\Xi^{(s)}_\alpha, H_0\}_{P.b.}$. Then, impose: ${}_*\Xi^{(s)}_\alpha := 0$ $(s \in \{1\,, 2\,, \cdots, S\})$. Using the Jacobi identity, it is shown that ${}_*\Psi^{(s)}_\alpha \approx 0$ and ${}_*\Xi^{(s)}_\alpha \approx 0$ satisfy the following relation:

$$\det\left(\{{}_*\Psi^{(s)}_\alpha, {}_*\Xi^{(S-s+1)}_\alpha\}_{P.b.}\right) \overset{\text{NOT:1st;1}\,,2\,,\cdots\,,S}{\approx} 0\,, \tag{2.61}$$

otherwise the determinant among ${}_*\Psi^{(s)}_\alpha$ and ${}_*\Xi^{(s)}_\alpha$ are weak equal to zero under the imposition of all the first-class constraints and all the additional constraints, as desired; This relation indicates that ${}_*\Psi^{(s)}_\alpha \approx 0$ and ${}_*\Xi^{(s)}_\alpha \approx 0$ are now classified into second-class constraint. The third conditions in Eq (2.60) determine the multipliers λ^α.

The pDoF in the case of existing the first-class constraints, $i.e.$, ${}_*\Psi^{(1)}_\alpha \approx 0\,,\ {}_*\Psi^{(2)}_\alpha = \{{}_*\Psi^{(1)}_\alpha\,, H_T\}_{P.b.} \approx 0\,, \cdots, {}_*\Psi^{(S)}_\alpha = \{{}_*\Psi^{(S-1)}_\alpha\,, H_T\}_{P.b.} \approx 0$ $(\alpha = 1\,, 2\,, \cdots, T)$, or equivalently, gathering these into ${}_*\Psi_\alpha \approx 0$ ($\alpha \in \{1, 2, \cdots, V = T \times S\}$), is now obvious by applying the pDoF in the case of existing only second-class constraints: pDoF $= (2N - (V + V))/2 = N - V$. In addition, in the case of existing the second-class constraints ${}_*\Theta_a \approx 0$, the pDoF is $(2N - 2U - 2V)/2 = N - U - V$.

Finally, let us introduce the pDoF in a direct way based on the Shanmugadhasan-Maskawa-Nakajima theorem. The statement of the theorem is expressed as follows:

Theorem 1.

For a symplectic 2-form of the given system: $\Omega = dq^i \wedge dp_i$ ($i \in \{1\,, 2\,, \cdots\,, N\}$)*, it exists a canonical coordinate system such that* $\Omega = dQ^I \wedge dP_I + d_*\Theta^a \wedge d_*\Theta_a + d_*\Xi^\alpha \wedge d_*\Psi_\alpha$ *(*$I \in \{1\,, 2\,, \cdots\,, N - V - U\}$*;* $a \in \{1\,, 2\,, \cdots\,, V\}$*;* $\alpha \in \{1\,, 2\,, \cdots\,, U\}$*), where* ${}_*\Theta^a \approx 0$ *and* ${}_*\Theta_a \approx 0$ *are composed only of all the* $2V$ *second-class constraints,* ${}_*\Psi_a \approx 0$ *are composed only of all the* U *first-class constraints.*

■

Applying this theorem, the pDoF and gDoF of a given system are counted out. A point which should be careful is that the conjugate pairs of the second-class constraints, *i.e.*, ${}_*\Theta^a \approx 0$ and ${}_*\Theta_a \approx 0$, are static in the time evolution, but so are not the configuration variables for the first-class constraints, *i.e.*, ${}_*\Xi^\alpha$, unless appropriate gauge fixing conditions are imposed. Therefore, on one hand, if the system has only second-class constraints then the counting is performed in the same manner as the previous paragraph. On the other hand, if the system has first-class constraints then the counting for pDoF *in the phase space* turns out to be ${}_*$pDoF $= 2N - 2V - U$. In order to convert ${}_*$pDoF into that of the velocity-phase space, *i.e.*, pDoF, *speculating the possibility of gauge fixing*, pDoF should be counted out as follows: pDoF $= ({}_*pDoF - U)/2 = N - V - U$. This means that, when counting out pDoF based on the above theorem, the resulting number of pDoF is generically different from the number of actual propagating modes since the set of degrees of freedom which evolves in time, *i.e,.*, ${}_*\Xi^\alpha$, is removed out. That is, there may occur a situation such that the pDoF counted out based on the above theorem is less than the number of actual propagating modes. If encountering such a situation, we should perform gauge fixing and check whether this discrepancy is reconciled or not.

There is a remark; Taking into account the rank of the kinetic matrix Eq (2.1), it gives the upper limit of the pDoF of the given system. That is, let us assume rank $K = N - R$. If R is an even number then the theorem indicates that the upper limit becomes $(2N - R)/2$: pDoF $\leq N - R/2$. If R is an odd number then the theorem implies that the limit becomes $(2N - R - 1) = (2N - 2R' - 2)/2$: pDoF $\leq N - R' - 1$, where $R = 2R' + 1$. The pDoF counted out by the Dirac-Bergmann analysis has to satisfy this upper limit as consistency with existing constraints.

2.5. Higher-order derivative systems and Ostrogradsky ghost degrees of freedom

In this section, higher-order derivative systems, of which Lagrangian contains higher-order time derivatives, are introduced. Such systems generically have the so-called Ostrogradsky instability. There are two ways to formulate such systems: Ostrogradsky's original formulation [Ostrogradsky (1850); Woodard (2015); Saito et al. (1989, 1993)] and Pons' modified formulation [Pons (1989)]. First of all, let us introduce Ostrogradsky's formulation.

Assume that a Lagrangian $L = L(q^i, Dq^i, \cdots, D^M q^i)$ $(i \in \{1\,, 2\,, \cdots\,, N\}\,, D = d/dt)$ exists. Then the kinetic matrix of the system is given as follows:

$$K^{(M)}_{ij} = \frac{\partial^2 L}{\partial(DQ^i_{(M)})\partial(DQ^j_{(M)})}\,, \tag{2.62}$$

and the action functional is introduced as follows:

$$I[Q^i_{(1)}, Q^i_{(2)}, \cdots, Q^i_{(M)}] = \int_{t_1}^{t_2} L(Q^i_{(1)}, Q^i_{(2)}, \cdots, Q^i_{(M)}, DQ^i_{(M)})\, dt\,, \tag{2.63}$$

where

$$Q^i_{(s)} = D^{s-1} q^i \,, \quad DQ^i_{(M)} = D^M q^i \quad (s \in \{1\,, 2\,, \cdots\,, M\})\,. \tag{2.64}$$

First, let us consider the non-degenerate case: $\det K^{(M)} \neq 0$.

The variational principle is applied under the imposition of the Dirichlet boundary conditions, $Q^i_{(s)}(t_2) = Q^i_{(s)}(t_1) = 0$; the variation of the action functional with respect to the configurations $Q^i_{(s)} = D^{s-1}q^i$ is computed as follows:

$$\delta I = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial Q^i} - \dot{P}^{(1)}_i \right) \delta\, Q^i \, dt + \left[P^{(s)}_i \, \delta\, Q^i_{(s)} \right]_{t_1}^{t_2} \,, \tag{2.65}$$

where $P^{(s)}_i$, canonical momentum variables with respect to $Q^i_{(s)}$, are defined as follows:

$$P^{(s)}_i = \sum_{r=s}^{M} (-1)^{r-s} D^{r-s} \left(\frac{\partial L}{\partial DQ^i_{(r)}} \right) \,. \tag{2.66}$$

These definitions can be reassembled as a reccurence relation, the so-called Ostogradsky transformation, as follows:

$$P^{(M)}_i = \frac{\partial L}{\partial (DQ^i_{(M)})} \,, \quad P^{(s-1)}_i = \frac{\partial L}{\partial DQ^i_{(s-1)}} - \dot{P}^{(s)}_i \,, \tag{2.67}$$

together with Eq (2.64), where $s \in \{2\,, 3\,, \cdots\,, M\}$. Therefore, the variational principle, $\delta I := 0$, the Euler-Lagrange equations are derived as follows:

$$\frac{\partial L}{\partial Q^i} - \dot{P}^{(1)}_i = 0\,. \tag{2.68}$$

Remark that the second equations in Eq (2.67) do not describe the time evolution of the system, although each equation contains the time derivative of the canonical momentum variable. From the viewpoint of the variational principle, the equations of motion are given only as Eq (2.68).

In order to introduce the Hamiltonian formalism, let us consider the canonical variables $\{Q^i_{(s)}, P^{(s)}_i\}$ ($s \in \{1\,, 2\,, \cdots, M\}$) and the Legendre transformation, the so-called Ostrogradsky Hamiltonian, given as follows:

$$H(Q^i_{(s)}, P^{(s)}_i) = \sum_{s=1}^{M-1} P^{(s)}_i DQ^i_{(s)} + P^{(M)}_i F^i - L(Q^i_{(1)}, Q^i_{(2)}, \cdots, Q^i_{(M)}; F^i)\,, \tag{2.69}$$

where

$$F^i = DQ^i_{(M)} = F^i(Q^i_{(1)}, Q^i_{(2)}, \cdots, Q^i_{(M)}; P^{(M)}_i) \tag{2.70}$$

is determined by the implicit function theorem for Eq (2.62). Notice that all the velocity variables are removed from the theory. The first term depends linearly on $P^{(s)}_i$. Since $P^{(s)}_i$ ($s \in \{1\,, 2\,, \cdots, M-1\}$) can take the range of arbitrary value, on one hand, H would not be bounded from below; the system may have an instability. If this is the case, it is nothing but the Ostrogradsky instability and the corresponding degrees of freedom is called Ostrogradsky ghosts, the total number of them is $N \times (M-1)$ in this case. On the other hand, since the canonical momentum variables $P^{(M)}_i$ can be bounded from below via the relation (2.70), therefore, if the first terms are absent, H is bounded from below. The variational principle of the Ostrogradsky Hamiltonian derives the equations of motion as follows:

$$\dot{Q}^i_{(s)} = \frac{\partial H}{\partial P^{(s)}_i}\,, \quad \dot{P}^{(s)}_i = -\frac{\partial H}{\partial Q^i_{(s)}}\,. \tag{2.71}$$

The first equations for $s \in \{1\,, 2\,, \cdots, M-1\}$ and the second equations for $s \in \{2\,, 3\,, \cdots, M\}$ reproduce the Ostrogradski transformation. The first equations for $s = M$ lead to the relations in Eq (2.70). The second equations for $s = 1$ derive the Euler-Lagrange equations (2.68).

The next stage is the degenerate cases but it is easy to describe from the knowledge in Section 2.2. Let us assume that the rank of the kinetic matrix is $N-R$: $\operatorname{rank} K^{(M)} = N-R$.

In the same manner as Section 2.2, the total Hamiltonian can be introduced as follows:

$$H_T = H_0 + \lambda^\alpha {}_*\phi^{(1)}_\alpha \,, \tag{2.72}$$

where ${}_*\phi^{(1)}_\alpha = {}_*\phi^{(1)}_\alpha(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}; P^{(M)}_i)$ $(\alpha \in \{1\,, 2\,, \cdots\,, R\})$. The Dirac-Bergmann analysis is also applied in the same manner as Section 2.2. The time evolution of the canonical variables is calculated as follows:

$$\begin{aligned}
&DQ^i_{(s)} = \{Q^i_{(s)}\,, H_T\}_{P.b.} \approx Q^i_{(s+1)} \quad s \in \{1\,, 2\,, \cdots\,, M-1\}\,,\\
&DQ^a_{(M)} \approx F^a(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}; P^{(M)}_b; \lambda^\alpha)\,,\\
&DQ^\alpha_{(M)} \approx \lambda^\alpha\,,\\
&DP^{(1)}_i \approx \frac{\partial L}{\partial Q^i_{(1)}}\,,\\
&DP^{(s)}_i \approx -P^{(s-1)}_i + \frac{\partial L}{\partial DQ^i_{(s-1)}} \quad s \in \{2\,, 3\,, \cdots\,, M\}\,.
\end{aligned} \tag{2.73}$$

The fourth equations describe the time evolution of the system. The others reproduce the Ostrogradsky transformation.

Finally, let us introduce Pons' formulation; a method to decompose a higher-order derivative system into a first-order system with the corresponding second-class constraints using a set of auxiliary variables. This formulation is frequently used in the studies of modified/extended theories of gravity. Assume that a Lagrangian $L = L(q^i, Dq^i, \cdots, D^M q^i)$ $(i \in \{1\,, 2\,, \cdots\,, N\}\,, D = d/dt)$ exists. Then let us require the first relations of the Ostrogradsky transformation Eq (2.64) as a set of constraints:

$$DQ^i_{(s)} - Q^i_{(s+1)} := 0\,, \quad (s \in \{1\,, 2\,, \cdots\,, M-1\})\,. \tag{2.74}$$

These constraints decompose the Lagrangian into

$$L \to L' = L'(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}\,, DQ^i_{(M)}) + \sum_{i=1}^{N}\sum_{s=1}^{M-1} \lambda^i_{(s)}(DQ^i_{(s)} - Q^i_{(s+1)})\,, \tag{2.75}$$

or schematically,

$$L \to L' = L'(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}\,; DQ^i_{(1)}\,, DQ^i_{(2)}\,, \cdots\,, DQ^i_{(M)}\,; D\lambda^i_{(s)}, \lambda^i_{(s)})\,. \tag{2.76}$$

That is, the original system is decomposed into the first-order derivative system with a set of auxiliary variables. Remark that, in the Ostrogradsky formulation, Eq (2.74) is not a set of constraints but just that of replacement Eq (2.64); the given system remains Mth-order derivative system. First, let us consider the case: $\det K^{(M)} \neq 0$ for the kernel kinetic matrix

$$K^{(M)} = \frac{\partial^2 L'}{\partial(DQ^i_{(M)})\partial(DQ^j_{(M)})}\,, \tag{2.77}$$

but $\det \tilde{K}^{(M)} = 0$ for the entire kinetic matrix

$$\tilde{K}^{(M)} = \frac{\partial^2 L'}{\partial(DX^{i'})\partial(DX^{j'})}\,, \tag{2.78}$$

where $X^{i'} = \{Q^i_{(M)}, \lambda^i_{(s)}\}$; the sector for the configurations $Q^i_{(M)}$ is non-degenerate but the whole sector for $X^{i'}$ is degenerate due to the existence of the configurations $\lambda^i_{(s)}$. It indicates that there is a set of primary constraints as follows:

$${}_*\theta^{(1)}{}^s_i = \pi^{(s)}_i := 0\,, \quad {}_*\theta^{(1)}{}^{M-1+s}_i = P^{(s)}_i - \lambda^{(s)}_i := 0\,, \tag{2.79}$$

where $\pi_i^{(s)}$ and $P_i^{(s)}$ are canonical momentum variables

$$\pi_i^{(s)} = \frac{\partial L'}{\partial D\lambda^i_{(s)}} = 0\,, \quad P_i^{(s)} = \frac{\partial L'}{\partial DQ^i_{(s)}} = \lambda_i^{(s)}\,. \tag{2.80}$$

Since the sector for the configurations $Q^i_{(M)}$ is non-degenerate, the system does not give rise to another primary constraint. The Poisson brackets among ${}_*\theta^{(1)}{}^s_i$ and ${}_*\theta^{(1)}{}^{M-1+s}_i$ are $\{{}_*\theta^{(1)}{}^u_i\,, {}_*\theta^{(1)}{}^{M-1+v}_j\}_{P.b.} = \delta_{ij}\delta^{uv}$; these constraints are classified into second class constraint. The total Hamiltonian is derived as follows:

$$\begin{aligned} H'_T =& P_i^{(s)} DQ^i_{(s)} + P_i^{(M)} F^i - L'(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}\,, F^i) \\ & - \sum_{i=1}^{N} \sum_{s=1}^{M-1} \lambda^i_{(s)}(DQ^i_{(s)} - Q^i_{(s+1)}) + \sigma^i_s\, {}_*\theta^{(1)}{}^s_i + \tau^i_s\, {}_*\theta^{(1)}{}^{M-1+s}_i\,, \end{aligned} \tag{2.81}$$

where σ^i_s and τ^i_s are multipliers, F^i are implied from the implicit functions theorem for $\tilde{K}^{(M)}$ as follows:

$$F^i = DQ^i_{(M)} = F^i(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots\,, Q^i_{(M)}\,, P_i^{(M)})\,, \tag{2.82}$$

and $P_i^{(M)}$ are canonical momentum variables as follows:

$$P_i^{(M)} = \frac{\partial L'}{\partial DQ^i_{(M)}}\,. \tag{2.83}$$

The linear dependence on $P_i^{(s)}$ that is not bounded from below gives rise to the Ostrogradsky instability. Since the first three terms in Eq (2.81) do not contain $\pi_i^{(s)}$ and $\lambda_i^{(s)}$, the consistency conditions determine all multipliers as

$$\sigma^i_s \overset{\mathfrak{C}^{(1)}}{\approx} -P_i^{(s-1)} + \frac{\partial L'}{\partial DQ^i_{(s-1)}}\,, \quad \tau^i_s \overset{\mathfrak{C}^{(1)}}{\approx} DQ^i_{(s)} - Q^i_{(s+1)}\,. \tag{2.84}$$

Therefore, the Pons formulation is completely equivalent to the Ostrogradsky formulation in terms of *Dirac brackets*. In particular, applying the equations of motion with respect to $\lambda_i^{(s)}$, *i.e.*, $DQ^i_{(s)} - Q^i_{(s+1)} \approx 0$, then $\tau_s^i \overset{\mathfrak{C}^{(1)}}{\approx} 0$.

The next consideration is a degenerate case for the configurations $Q^i_{(M)}$; assume that $\operatorname{rank} \tilde{K}^{(M)} = N - R$. Then the number of R primary constraints

$$
{}_*\phi^{(1)}_\alpha = {}_*\phi^{(1)}_\alpha(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots, Q^i_{(M)}\,, P_i^{(M)}) := 0 \quad \alpha \in \{1\,, 2\,, \cdots, R\} \tag{2.85}
$$

are added to the above consideration. Then the total Hamiltonian (2.81) becomes as follows:

$$
\begin{aligned}
H'_T &= H_0 + P_i^{(s)} DQ^i_{(s)} - \sum_{i=1}^{N}\sum_{s=1}^{M-1} \lambda^i_{(s)}(DQ^i_{(s)} - Q^i_{(s+1)}) + \sigma^i_s\, {}_*\theta^{(1)}{}^s_i + \tau^i_s\, {}_*\theta^{(1)}{}^{M-1+s}_i + \kappa^\alpha\, {}_*\phi^{(1)}_\alpha\,, \\
H'_0 &= P_a^{(M)} F^a - L'(Q^i_{(1)}\,, Q^i_{(2)}\,, \cdots, Q^i_{(M)}\,, F^b)\,,
\end{aligned} \tag{2.86}
$$

where $a \in \{N - R + 1\,, N - R + 2\,, \cdots, N\}$. The linear dependence on $P_i^{(s)}$ that is not bounded from below gives rise to the Ostrogradsky instability also in the degenerate case. The consistency conditions for ${}_*\theta^{(1)}{}^s_i \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and ${}_*\theta^{(1)}{}^{M-1+s}_i \overset{\mathfrak{C}^{(1)}}{\approx} 0$ determine the multipliers τ^i_s and σ^i_s as follows:

$$
\sigma^i_s \overset{\mathfrak{C}^{(1)}}{\approx} -P_i^{(s-1)} + \frac{\partial L'}{\partial DQ^i_{(s-1)}} - \kappa^\alpha \frac{\partial \phi^{(1)}_\alpha}{\partial Q^i_{(s)}}\,, \quad \tau^i_s \overset{\mathfrak{C}^{(1)}}{\approx} DQ^i_{(s)} - Q^i_{(s+1)}\,. \tag{2.87}
$$

In particular, the second equations turn into being weak equal zero under the equations of motion with respect to $\lambda^i_{(s)}$. This situation is different from the non-degenerate case; the multipliers σ^i_s are not determined until the multipliers κ^α are fixed. It indicates that the constraint structure, which is given by the primary constraints ${}_*\phi^{(1)}_\alpha \approx 0$ and those consistency conditions, dominates all physics of the system. Notice that if it exists first-class constraints then the equivalence in terms of Dirac brackets between the Pons and

Ostrogradsky formulation only holds for physical quantities (gauge invariant quantities). Only the cases of existing second-class constraints hold the complete equivalence.

2.6. Ostrogradsky ghost-free theories

In this section, a set of conditions to remove the Ostrogradsky instability is introduced. The most general theorem is very complicated, therefore, let us first discuss two simple cases: $L = L(\ddot{\phi}\,, \dot{\phi}\,, \phi; \dot{q}, q)$ and $L = L(\ddot{\phi}^a\,, \dot{\phi}^a\,, \phi^a; \dot{q}^i\,, q^i)$ ($a \in \{1\,, 2\,, \cdots\,, A\}$; $i \in \{1\,, 2\,, \cdots\,, N\}$) to understand the essential points. After that, the general statement is just given without proof. The detailed considerations including the explicit proofs are given in Refs [Motohashi et al. (2016, 2018a,b)].

The first case is $L = L(\ddot{\phi}\,, \dot{\phi}\,, \phi; \dot{q}\,, q)$; the Lagrangian contains at most second-order time derivative and first-order time derivative of $\phi = \phi(t)$ and $q = q(t)$, respectively. The Ostrogradsky instability is generated by the variable ϕ. In Pons' formulation given in Section 2.5, the Lagrangian is decomposed by using an auxiliary variable as follows:

$$L \to L' = L'(\dot{Q}\,, Q\,, \phi; \dot{q}\,, q) + \lambda(\dot{\phi} - Q)\,, \tag{2.88}$$

where Q is an auxiliary variable, λ is a multiplier. The total Hamiltonian is derived as follows:

$$H'_T = H'_0 + \lambda Q + \mu_* \Phi + \nu_* \Psi\,, \quad H'_0 = PF + pf - L'(F\,, Q\,, \phi; f\,, q)\,, \tag{2.89}$$

where P, p, π, and ρ are canonical momentum variables with respect to Q, q, ϕ, and λ, respectively. μ and ν are multipliers. ${}_*\Phi = \pi - \lambda \approx 0$ and ${}_*\Psi = \rho \approx 0$ are primary second-class constraints. Remark that the multiplier λ is regarded as a configuration variable. $F = F(Q\,, P; q\,, p)|_{\phi,\pi,\lambda,\rho}$ and $f = f(q\,, p; Q\,, P)|_{\phi,\pi,\lambda,\rho}$ are functions that are determined from the implicit function theorem under arbitrarily fixing values of ϕ, π, λ, ρ for the kernel kinetic matrix given by

$$K^{(2)} = \begin{bmatrix} L_{\dot{Q}\dot{Q}} & L_{\dot{q}\dot{Q}} \\ L_{\dot{Q}\dot{q}} & L_{\dot{q}\dot{q}} \end{bmatrix}, \quad L_{XY} = \frac{\partial^2 L}{\partial X \partial Y}. \tag{2.90}$$

Here, the kernel kinetic matrix is assumed as non-degenerate. The entire kinetic matrix $\tilde{K}^{(2)} = L_{XY}$, where $X, Y \in \{\dot{Q}\,, \dot{q}\,, \dot{\phi}\,, \dot{\lambda}\}$, has its rank of $4-2=2$; this is consistent with the existence of the two primary constraints. Then the consistency conditions for ${}_*\Phi \approx 0$ and ${}_*\Psi \approx 0$ determine all the multipliers μ and ν as follows: $\mu \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and $\nu \overset{\mathfrak{C}^{(1)}}{\approx} \{{}_*\Phi\,, H_0'\}_{P.b.}$. That is, there is no secondary constraint. Therefore, the degrees of freedom of the system is $(4\times 2-2)/2 = 2+1$. The extra degrees of freedom is caused by the term λQ in Eq (2.89) since $\lambda \overset{\mathfrak{C}^{(1)}}{\approx} \pi$ is unbounded from below; this is nothing but an Ostrogradsky ghost degrees of freedom.

In order to remove this difficulty, an extra condition has to be imposed as follows:

$$R(P\,, p\,;\, Q\,, \phi, q) = 0\,. \tag{2.91}$$

In a local region, this additional condition leads to the following conditions by virtue of the implicit function theorem: either $P = G_1(p\,;\, Q\,, \phi\,, q)$ or $p = G_2(P\,;\, Q\,, \phi\,, q)$. Therefore, the following additional primary constraint can be imposed; either

$${}_*\Xi = P - G_1(p\,;\, Q\,, \phi\,, q) := 0 \tag{2.92}$$

or

$${}_*\Pi = p - G_2(P\,;\, Q\,, \phi\,, q) := 0\,. \tag{2.93}$$

Let us consider the first condition (2.92). The total Hamiltonian of the system is modified as follows:

$$H_T'' = H_0' + \lambda Q + \mu\, {}_*\Phi + \nu\, {}_*\Psi + \xi\, {}_*\Xi\,, \tag{2.94}$$

where H'_0 is given in Eq (2.89). The consistency conditions for these primary constraints, ${}_*\Phi := 0$, ${}_*\Psi := 0$, and ${}_*\Xi := 0$, determine the two multipliers μ and ν as $\mu \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and $\nu \overset{\mathfrak{C}^{(1)}}{\approx} \{{}_*\Phi\,, H'_0\}_{P.b.} + \xi(\partial G_1/\partial\phi)$, respectively, and give rise to a secondary constraint

$$ {}_*\Theta = \{{}_*\Xi\,, H''_T\}_{P.b.} = -\pi + \{{}_*\Xi\,, H'_0\}_{P.b.} - Q\frac{\partial G_1}{\partial\phi} := 0\,. \tag{2.95} $$

Notice that the momentum variable $\pi \overset{\mathfrak{C}^{(1)}}{\approx} \lambda$ is now related to other phase space variables by virtue of Eq (2.95). Furthermore, since all constraints that appeared here are classified into second-class constraints, therefore, the degrees of freedom is at least $(4\times 2-4)/2 = 2$. Taking into account the fact that $\pi \overset{\mathfrak{C}^{(1)}}{\approx} \lambda$ is bounded with other phase space variables, the Ostrogradsky instability is now removed from the system. Remark that the second condition (2.93) concludes the same result.

There is an important theorem that relates either the additional condition (2.92) or (2.93) to the degeneracy of the system and vice versa, stated as Condition (2.92) is equivalent to

$$ \det K^{(2)} = L_{\dot{Q}\dot{Q}}L_{\dot{q}\dot{q}} - (L_{\dot{Q}\dot{q}})^2 = 0 \tag{2.96} $$

under the imposition of $L_{\dot{q}\dot{q}} \neq 0$. The same statement holds for Condition (2.93) under the imposition of $L_{\dot{Q}\dot{Q}} \neq 0$. If $L_{\dot{q}\dot{q}} = L_{\dot{q}\dot{q}} = 0$ then the dependence on p and P is eliminated from both the conditions and these coincide one another. This theorem can be shown by using the implicit function theorem. Using this theorem and the fact that the degeneracy of the kinetic matrix $K^{(2)}$ leads to the existence of its null-eigenvalue vector, it is shown that the Euler-Lagrange equations of the system contain at most second-order time derivative not only for q but also for ϕ. This is another signal for removing the Ostrogradsky instability from the system.

The above arguments can be generalized into the case of existing multiple variables: $L =$

$L(\ddot{\phi}^a\,,\dot{\phi}^a\,,\phi^a;\dot{q}^i\,,q^i)$ $(a\in\{1\,,2\,,\cdots\,,A\geq 2\};\, i\in\{1\,,2\,,\cdots\,,N\})$. The original Lagrangian is decomposed as follows:

$$L\rightarrow L'=L'(\dot{Q}^a\,,Q^a;\dot{\phi}^a\,,\phi^a;\dot{q}^i\,,q^i\,,\lambda_a)+\lambda_a(\dot{\phi}^a-Q^a)\,, \tag{2.97}$$

where Q^a are auxiliary variables and λ_a are multipliers. The total Hamiltonian is derived as follows:

$$H_T''=H_0'+\lambda_a Q^a+\mu^a\,{}_*\Phi_a+\nu^a\,{}_*\Psi_a+\xi^a\,{}_*\Xi_a\,,\quad H_0'=P_aF^a+p_if^i-L'(F^a,Q^a,\phi^a;f^i,q^i)\,, \tag{2.98}$$

where P_a, p_i, π^a, and ρ_a are canonical momentum variables with respect to Q^a, q^i, ϕ_a, and λ_a, respectively. $F^a=F(Q^a,P_a;q^i,p_i)|_{\phi^a,\pi^a,\lambda_a,\rho_a}$ and $f^a=f(q^i,p_i;Q^a,P_a)|_{\phi^a,\pi^a,\lambda_a,\rho_a}$ are functions that are determined from the implicit function theorem. ${}_*\Phi_a=\pi_a-\lambda_a:=0$ and ${}_*\Psi_a=\rho_a:=0$ are primary constraints, and

$${}_*\Xi_a=P_a-G_a(p_i\,,q^i\,,Q^b\,,\phi^b):=0 \tag{2.99}$$

are additional primary constraints that need to remove the Ostrogradsky instability, and that are equivalent to the following condition:

$$\det K^{(2)}=L_{ab}-L_{ai}L^{ij}L_{jb}=0\,, \tag{2.100}$$

where $K^{(2)}$ is defined as follows:

$$K^{(2)}=\begin{bmatrix} L_{ab} & L_{aj} \\ L_{ib} & L_{ij}\end{bmatrix}\,, \tag{2.101}$$

where $L_{ab}=\partial^2L/\partial\dot{Q}^a\partial\dot{Q}^b$, $L_{aj}=\partial^2L/\partial\dot{Q}^a\partial\dot{q}^j$, and $L_{ij}=\partial^2L/\partial\dot{q}^i\partial\dot{q}^j$. Then the consistency conditions for ${}_*\Phi_a := 0$, ${}_*\Psi_a := 0$, and ${}_*\Xi_a := 0$ determine the multipliers μ^a and ν^a as $\mu^a \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and $\nu^a \overset{\mathfrak{C}^{(1)}}{\approx} \{{}_*\Phi_a\,, H_0'\}_{P.b.} + \xi^a(\partial G/\partial\phi^a)$, respectively, and give rise to secondary constraints as follows:

$$
{}_*\dot{\Xi}_a = -\pi_a + \{{}_*\Xi_a\,, H_0'\}_{P.b.} - Q^b\frac{\partial G_a}{\partial\phi^b} + \xi^b\{{}_*\Xi_a\,, {}_*\Xi_b\}_{P.b.} := 0\,. \tag{2.102}
$$

Here, a departure from the single variable case appears; the rank of the matrix $\Delta_{ab} = \{{}_*\Xi_a\,, {}_*\Xi_b\}_{P.b.}$ in the last terms dominates whether or not the above conditions derive secondary constraints. To remove the Ostrigradsky instabilities, it is necessary and sufficient conditions to impose the rank of Δ_{ab} is zero, or equivalently,

$$
\Delta_{ab} = \{{}_*\Xi_a\,, {}_*\Xi_b\}_{P.b.} := 0\,. \tag{2.103}
$$

These conditions are new additional conditions when existing multiple second-order time derivative variables. Then the number of A secondary constraints appear, that is

$$
{}_*\Phi_a = -\pi_a + \{{}_*\Xi_a\,, H_0'\}_{P.b.} - Q^b\frac{\partial G_a}{\partial\phi^b} := 0\,, \tag{2.104}
$$

and the degrees of freedom are now $(6A+2N-2A-2A)/2 = A+N$. Taking into account that Eq (2.102) under Eq (2.103) relate π_a to the other phase space variables, the Ostrogradsky instability is now removed from the system. Then the additional constraints ${}_*\Xi^a := 0$ and the degeneracy of $K^{(2)}$ lead to the fact that the Euler-Lagrange equations contain at most second-order time derivative terms.

Finally, let us state a most general case: $L = L(\phi^{i_0}\,, D\phi^{i_0};\ \phi^{i_1}\,, D\phi^{i_1}\,, D^2\phi^{i_1};\ \cdots;\ \phi^{i_d}\,, D\phi^{i_d}\,, D^2\phi^{i_d}\,, \cdots, D^{d+1}\phi^{i_d})$. That is, a system which includes at most $(d+1)$-order time derivative terms. Here, the indices i_k $(k \in \{0\,,1\,,2\,,\cdots,d\})$ run the range of as follows: $i_0 = 1\,,2\,,\cdots,n_0$ and $i_k = \sum_{l=0}^{d-1}(n_l+1)\,,\sum_{l=0}^{d-1}(n_l+2)\,,\cdots,\sum_{l=0}^{d-1}(n_l+n_k)\quad(k\geq 1)$. In order to apply Pons' formulation in Section 2.5, the following configurations are introduced:

$$Q_{00}^{i_0} = \phi^{i_0}\,, \quad Q_{10}^{i_1} = \phi^{i_1}\,, \quad \cdots \quad Q_{d0}^{i_d} = \phi^{i_d}\,. \tag{2.105}$$

Then the original Lagrangian is decomposed as follows:

$$\begin{aligned}
L' = {} & L(Q_{00}^{i_0}\,, \dot{Q}_{00}^{i_0};\, Q_{10}^{i_1}\,, Q_{11}^{i_1}\,, \dot{Q}_{11}^{i_1};\, Q_{20}^{i_2}\,, Q_{21}^{i_2}\,, Q_{22}^{i_2}\,, \dot{Q}_{22}^{i_2};\, \cdots;\, Q_{d0}^{i_d}\,, Q_{d1}^{i_d}\,, \cdots, Q_{dd}^{i_d}\,, \dot{Q}_{dd}^{i_d}) \\
& + \lambda_{10}^{i_1}(\dot{Q}_{10}^{i_1} - Q_{11}^{i_1}) \\
& + \lambda_{20}^{i_2}(\dot{Q}_{20}^{i_2} - Q_{21}^{i_2}) + \lambda_{21}^{i_2}(\dot{Q}_{21}^{i_2} - Q_{22}^{i_2}) \\
& + \cdots \\
& + \lambda_{d0}^{i_d}(\dot{Q}_{d0}^{i_d} - Q_{d1}^{i_d}) + \lambda_{d1}^{i_d}(\dot{Q}_{d1}^{i_d} - Q_{d2}^{i_d}) + \cdots + \lambda_{d,d-1}^{i_d}(\dot{Q}_{d,d-1}^{i_d} - Q_{dd}^{i_d})\,.
\end{aligned}$$

The configurations of the system, *i.e.*, $Q_{kl}^{i_k}$, $\lambda_{kl}^{i_k}$ lead to the corresponding canonical momentum variables; let us denote them as $P_{kl}^{i_k}$, $\rho_{kl}^{i_k}$. In particular, $q^i \in \{Q_{00}^{i_0}\}$, $p_i \in \{P_{00}^{i_0}\} = \{L_i\}$, $\tilde{Q}_{I_1}^{(0)} \in \{Q_{11}^{i_1}\,, Q_{22}^{i_2}\,, \cdots, Q_{dd}^{i_d}\}$, and $\tilde{P}_{I_1}^{(0)} \in \{P_{11}^{i_1}\,, P_{22}^{i_2}\,, \cdots, P_{dd}^{i_d}\} = \{L_{I_1}\}$, where $I_1 \in \{i_1\,, i_2\,, \cdots, i_d\}$. Then the following notations are introduced: $\mathbf{Q} \in \{Q_{kl}^{i_k}\} \setminus \{\tilde{Q}_{I_1}^{(0)}\}$, $\boldsymbol{\lambda} \in \{\lambda_{kl}^{i_k}\} \setminus \{\lambda_{kl}^{i_0}\}$, $\mathbf{P} = \{P_{kl}^{i_k}\} \setminus \{\tilde{P}_{I_1}^{(0)}\} = \boldsymbol{\lambda}$, and $\boldsymbol{\rho} \in \{\rho_{kl}^{i_k}\} \setminus \{\rho_{kl}^{i_0}\} = \mathbf{0}$. Therefore, the dimension of the entire phase space is $N_{\text{total}} = 2\sum_{k=0}^{d} n_k + 4\sum_{k=1}^{d} k n_k$. Assembling further notations as $\tilde{Q}_{I_1}^{(1)} \in \{(Q_{10}^{i_1}\,, Q_{21}^{i_2}\,, Q_{32}^{i_3}\,, \cdots, Q_{d,d-1}^{i_d}\}$, $\tilde{Q}_{I_2}^{(2)} \in \{Q_{20}^{i_2}\,, Q_{31}^{i_3}\,, \cdots, Q_{d,d-2}^{i_d}\}$, $\tilde{Q}_{I_{d-1}}^{(d-1)} \in \{Q_{d-1,0}^{i_{d-1}}\,, Q_{d1}^{i_d}\}$, and $\tilde{Q}_{I_d}^{(d)} \in \{Q_{d0}^{i_d}\}$, where $I_k \in \{i_k\,, \cdots, i_d\}$, and then $\tilde{Q}_{I_k}^{(k)} \in \{Q_{k0}^{i_k}\,, \tilde{Q}_{I_{k+1}}^{(k)}\}$,
$\tilde{Q}_{I_{k+1}}^{(k)} \in \{Q_{k+1,1}^{i_{k+1}}\,, Q_{k+2,2}^{i_{k+2}}\,, \cdots, Q_{d,d-k}^{i_d}\}$, and $\tilde{P}_{I_k}^{(k)} \in \{P_{k0}^{i_k}\,, P_{k+1,1}^{i_{k+1}}\,, \cdots, P_{d,d-k}^{i_d}\}$, the above Lagrangian is arranged as follows:

$$L'' = L(q^i\,, \dot{q}^i;\, \tilde{Q}_{I_1}^{(0)}\,, \dot{\tilde{Q}}_{I_1}^{(0)};\, \tilde{Q}_{I_1}^{(1)}\,, \tilde{Q}_{I_2}^{(2)}\,, \cdots, \tilde{Q}_{I_d}^{(d)}) + \sum_{k=1}^{d} \tilde{\lambda}_{I_k}^{(k)}(\dot{\tilde{Q}}_{I_k}^{(k)} - \tilde{Q}_{I_k}^{(k-1)})\,. \tag{2.106}$$

Therefore, the total Hamiltonian is derived as follows:

$$
\begin{aligned}
H''_T &= H'' + \mu_\alpha\, {}_*\Phi_\alpha + \bar{\mu}_\alpha\, {}_*\bar{\Phi}_\alpha + \tilde{\nu}^{(0)}_{I_1}\, {}_*\tilde{\Psi}^{(0)}_{I_1}\,,\\
H'' &= H''_0 + \tilde{Q}^{(0)}_{I_1}\tilde{P}^{(1)}_{I_1} + \tilde{Q}^{(1)}_{I_2}\tilde{P}^{(2)}_{I_2} + \cdots + \tilde{Q}^{(d-1)}_{I_d}\tilde{P}^{(d)}_{I_d}\,,\\
H''_0 &= \dot{\tilde{Q}}^{(0)}_{I_1}\tilde{P}^{(0)}_{I_1} + \dot{q}^i p_i - L''\,,
\end{aligned}
\tag{2.107}
$$

where ${}_*\Phi_\alpha \in \{\boldsymbol{P} - \boldsymbol{\lambda}\} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and ${}_*\bar{\Phi}_\alpha \in \{\boldsymbol{\rho}\} \overset{\mathfrak{C}^{(1)}}{\approx} 0$. μ_α and $\bar{\mu}_\alpha$ are Lagrange multipliers. Notice that the linear terms $\tilde{Q}^{(k-1)}_{I_k}\tilde{P}^{(k)}_{I_k}$ cause the Ostrogradsky instability.

The degeneracy conditions that have to be imposed to eliminate the Ostrogradsky instabilities are derived by performing the Dirac-Bergmann analysis. The same considerations of the case as $L = L(\ddot{\phi}^a, \dot{\phi}^a, \phi^a; \dot{q}^i, q^i)$ ($a \in \{1\,, 2\,, \cdots\,, A \geq 2\}$; $i \in \{1\,, 2\,, \cdots\,, N\}$) leads to the following degeneracy conditions:

$$
\begin{aligned}
&L_{I_1 J_1} - L_{I_1 i} L^{ij} L_{j J_1} := 0\,,\\
&\{{}_*\tilde{\Psi}^{(0)}_{I_1}\,, {}_*\tilde{\Psi}^{(0)}_{J_1}\}_{P.b.} := 0\,,
\end{aligned}
\tag{2.108}
$$

where ${}_*\tilde{\Psi}^{(0)}_{I_1} \in \{{}_*\Psi^{i_1}_{11}\,, {}_*\Psi^{i_2}_{22}\,, \cdots\,, {}_*\Psi^{i_d}_{dd}\}$ are defined as follows:

$$
{}_*\tilde{\Psi}^{(0)}_{I_1} = \tilde{P}^{(0)}_{I_1} - \tilde{F}^{(0)}_{I_1}(p_i\,, q^i\,, \tilde{Q}^{(0)}_{I_1}\,, \mathbf{Q}) \overset{\mathfrak{C}^{(1)}}{\approx} 0\,. \tag{2.109}
$$

The higher-order structure which is more than third-order requires further degeneracy conditions to remove the Ostrogradsky instability. The consistency conditions for the secondary constraints, ${}_*\tilde{\Upsilon}^{(1)}_{I_1} \in \{{}_*\Upsilon^{i_1}_{10}\,, {}_*\Upsilon^{i_2}_{21}\,, \cdots\,, {}_*\Upsilon^{i_d}_{d,d-1}\}$, that is,

$$
{}_*\tilde{\Upsilon}^{(1)}_{I_1} = -\{{}_*\tilde{\Psi}^{(0)}_{I_1}\,, H''\}_{P.b.} = \tilde{P}^{(1)}_{I_1} - G^{(1)}_{I_1}(p^i\,, q^i\,, \tilde{Q}^{(0)}_{I_1}\,, \mathbf{Q}) \overset{\mathfrak{C}^{(2)}}{\approx} 0 \tag{2.110}
$$

demand the following degeneracy conditions:

$$\{{}_*\boldsymbol{\Upsilon}\,,{}_*\tilde{\Psi}^{(0)}_{J_1}\}_{P.b.} := 0 \quad \text{except} \quad {}_*\Upsilon^{i_1}_{10} \tag{2.111}$$

where ${}_*\boldsymbol{\Upsilon}$ is defined as follows:

$${}_*\tilde{\Upsilon}^{(k)}_{I_k} \equiv -\{{}_*\tilde{\Upsilon}^{(k-1)}_{I_k}\,,H''\}_{P.b.} = \tilde{P}^{(k)}_{I_k} - \tilde{G}^{(k)}_{I_k}(p^i\,,q^i\,,\tilde{Q}^{(0)}_{I_1}\,,\mathbf{Q}) \overset{\mathfrak{C}^{(k)}}{\approx} 0 \tag{2.112}$$

for $k \in \{1\,,2\,,\cdots\,,d\}$. $\{{}_*\Upsilon^{i_k}_{k0}\,,{}_*\tilde{\Psi}^{(0)}_{I_1}\}_{P.b.} \overset{\mathfrak{C}^{(k)}}{\approx} 0 \quad (k \in \{2\,,3\,,\cdots\,,d\})$ are included since these conditions will be required below. Notice that ${}_*\boldsymbol{\Upsilon} \overset{\mathfrak{C}^{(k)}}{\approx} 0$ fix the linear dependence of the canonical momentum in Eq (2.107). The counterpart of the consistency conditions are given as follows:

$$\{{}_*\Upsilon^{i_k}_{k0}\,,H''\}_{P.b.} + \tilde{\nu}^{(0)}_{I_1}\{{}_*\Upsilon^{i_k}_{k0}\,,{}_*\tilde{\Psi}^{(0)}_{I_1}\}_{P.b.} \overset{\mathfrak{C}^{(k)}}{\approx} 0 \quad (k \in \{1\,,2\,,\cdots\,,d\}) \tag{2.113}$$

Imposing $\{{}_*\Upsilon^{i_k}_{k0}\,,{}_*\tilde{\Psi}^{(0)}_{I_1}\}_{P.b.} \overset{\mathfrak{C}^{(k)}}{\approx} 0 \quad (k \in \{2\,,3\,,\cdots\,,d\})$, these conditions yield the following additional constraints:

$${}_*\Omega^{i_k}_{k0} = -\{{}_*\Upsilon^{i_k}_{k0}\,,H''\}_{P.b.} \overset{\mathfrak{C}^{(k)}}{\approx} 0 \quad (k \in \{2\,,3\,,\cdots\,,d\})\,, \tag{2.114}$$

and the consistency conditions for ${}_*\Omega^{i_k}_{k0} \overset{\mathfrak{C}^{(k)}}{\approx} 0$ demand the following degeneracy conditions

$$\{{}_*\boldsymbol{\Omega}\,,{}_*\tilde{\Psi}^{(0)}_{J_1}\}_{P.b.} := 0 \quad \text{except} \quad {}_*\tilde{\Omega}^{(2)}_{I_2}\,, \tag{2.115}$$

where ${}_*\boldsymbol{\Omega} \in \{-\{{}_*\Omega^{i_k}_{k,l-1}\,,H''\}_{P.b.} \overset{\mathfrak{C}^{(k)}}{\approx} 0\} \quad (k \in \{l+1\,,l+2\,,\cdots\,,d\};\, l \in \{2\,,3\,,\cdots\,,d-3\})$. Then, since all the constraints are classified into second-class constraints, therefore, the number of degrees of freedom is $N'_{\text{total}} = \sum_{k=0}^{d} n_k$; the number of the Ostrogradsky ghost degrees of freedom is now removed out.

These conditions correspond to Eq (2.96) in the single second-order time derivative systems, or Eq (2.100) in the multiple second-order time derivative systems, and Eq (2.103), respectively. The existence of the higher-order time derivative terms that are more than third-order requires the additional degeneracy conditions, that is, the third and the fourth conditions, Eq (2.111) and Eq (2.115), to remove the Ostrogradsky instability. Furthermore, under these conditions, it is shown that the Euler-Lagrange equations of the system include the time derivative terms up to second-order by applying the implicit function theorem.

2.7. Summary

In this chapter, a theory of analytical mechanics for theories of gravity, focusing on degenerate and higher-order derivative point particle systems, was established. The Dirac-Bergmann analysis reveals the constraint structure of a given system. It also provides a set of fundamental concepts that play the main role of the present thesis: the propagating degrees of freedom, the gauge degrees of freedom, and the methodology of removing the Ostrogradsky degrees of freedom. Since theories of gravity have the properties of degenerate and higher-order derivative systems, therefore, a theory established in this chapter provides fundamental tools for treating theories of gravity.

Chapter 3

The well-posed variational principle in degenerate point particle systems

Chapter abstract

In this chapter, a methodology for making the variational principle in point particle systems well-posed is established. The extension to field theories has been developing, but some specific cases will be provided in the succeeding chapters of the present thesis. First of all, the problems of degenerate systems in the variational principle are explained. It is shown that the valid boundary conditions in a higher-order time derivative system but which has equations of motion up to second-order time derivative are restricted to position-fixing boundary conditions. Based on the Pons formulation, which is introduced in Section 2.5, Frobenius integrability conditions of first-order degenerate time derivative systems are investigated, and the concrete formulae of the conditions are derived. After these preparations, the well-posedness of the variational principle is reformulated. Introducing two types of embeddings of the symplectic manifold based on the Shanmugadhasan-Maskawa-Nakajima theorem, *i.e.,* quasi-canonical embeddings and canonical embeddings, the well-posedness is investigated. As a result, appropriate boundary conditions are specified. Finally, examples are given, and this chapter is summarized with the outlook for these works.

3.1. Cumbersome situations of the variational principle in degenerate systems

In this section, the difficulties of applying the variational principle to degenerate point particle systems are clarified. Let us start with considering four examples

$$
\begin{aligned}
L_1 &= \frac{1}{2}\dot{x}^2 + \frac{1}{2}\dot{y}^2 + \lambda(x+y)\,, \\
L_2 &= \dot{q}^1\dot{q}^3 + \frac{1}{2}q^2(q^3)^2\,, \\
L_3 &= q^1\dot{q}^2 - q^2\dot{q}^1 - (q^1)^2 - (q^2)^2\,, \\
L_4 &= -\frac{1}{2}q\ddot{q} - \frac{1}{2}q^2\,.
\end{aligned} \tag{3.1}
$$

The first system is a textbook example of existing an exterior constraint that is taken into account by a Lagrange multiplier. The second and third ones are systems only with first-class constraints and only with second-class constraints, respectively [Cawley (1979); Dirac (1928)]. The last one is an example of existing with a second-order time derivative term [Dyer and Hinterbichler (2009); Izumi et al. (2023)].

The first-order variation of these systems are computed as follows:

$$
\begin{aligned}
\delta L_1 &= \left\{\lambda - \ddot{q}^1\right\}\delta q^1 + \left\{\lambda - \ddot{q}^2\right\}\delta q^2 + (q^1+q^2)\delta\lambda + \frac{d}{dt}\left[\dot{q}^1\delta q^1 + \dot{q}^2\delta q^2\right]\,, \\
\delta L_2 &= \left\{-\ddot{q}^3\right\}\delta q^1 + \left\{\frac{1}{2}(q^3)^2\right\}\delta q^2 + \left\{-\ddot{q}^1 + q^2q^3\right\}\delta q^3 + \frac{d}{dt}\left[\dot{q}^3\delta q^1 + \dot{q}^1\delta q^3\right]\,, \\
\delta L_3 &= \left\{2\dot{q}^2 - 2q^1\right\}\delta q^1 + \left\{-2\dot{q}^1 - 2q^2\right\}\delta q^2 + \frac{d}{dt}\left[(-q^2)\delta q^1 + q^1\delta q^2\right]\,, \\
\delta L_4 &= \left\{-\ddot{q} - q\right\}\delta q + \frac{d}{dt}\left[\frac{1}{2}\dot{q}\delta q - \frac{1}{2}q\delta\dot{q}\right]\,,
\end{aligned} \tag{3.2}
$$

where in the first system the multiplier is regarded as a configuration. Integrating these over an open interval $(t_1\,, t_2)$, and imposing appropriate boundary conditions at each end-point t_1 and t_2, the variational principle leads to the Euler-Lagrange equations for each system are obtained. It is easy to confirm that the naive imposition of Dirichlet boundary conditions for all the configuration variables in the boundary term does not work well; For the first system, the boundary conditions $\delta q^1(t_2) = \delta q^1(t_1) := 0$ and $\delta q^2(t_2) = \delta q^2(t_1) := 0$ are equivalent to $q^1(t_\tau) := a^1_\tau$ and $q^2(t_\tau) := a^2_\tau$ $(\tau = 1\,, 2)$, where a^1_τ and a^2_τ are arbitrary constants. Then the variational principle leads to the Euler-Lagrange equations of motion but one of the equations, *i.e.*, $q^1 + q^2 = 0$, it is nothing but an exterior constraint, is generically inconsistent with the boundary conditions at each end-point t_1 and t_2; For the second system, in the same manner as the first case, it is shown that the naive boundary conditions $\delta q^1(t_2) = \delta q^1(t_1) := 0$ and $\delta q^3(t_2) = \delta q^3(t_1) := 0$ are inconsistent at least with the constraint $q^3 = 0$; For the third system, the system has only one propagating degrees of freedom since the equations of motion are either $\ddot{q}^1 + q^1 = 0$ or $\ddot{q}^2 + q^2 = 0$. Therefore, the naive boundary conditions $\delta q^1(t_2) = \delta q^1(t_1) = 0$ and $\delta q^2(t_2) = \delta q^2(t_1) = 0$ become over-imposing, and these boundary conditions cannot uniquely determine the two initial conditions in the solution; the dynamics of the system cannot be determined uniquely; For the last system, the naive boundary conditions $\delta q(t_2) = \delta q(t_1) = 0$ and $\delta \dot{q}(t_2) = \delta \dot{q}(t_1) = 0$ are themselves inconsistent in general since there is one equation of motion and therefore the velocities at the boundaries are of course determined by the derivative of the solution $q = q(t)$; it is impossible to fix the configuration and its velocity variable at the boundaries in an independent and arbitrary manner. These cumbersome situations are caused by the constraint structure of each system. That is, in order to make the variational principle well-posed in degenerate systems, a methodology for taking appropriate boundary conditions is mandatory.

A clue to formulating the well-posed variational principle is the coincidence between the number of boundary conditions and that of initial conditions, and the half numbers of them are also equivalent to the propagating degrees of freedom. Therefore, in order to approach the problem, the following guiding principle is assumed, stated as "*as many inte-*

gral constants (/initial conditions) in the solutions of a given system as possible should be uniquely determined through the boundary conditions". While, as mentioned in Section 2.4, the Shanmugadhasan-Maskawa-Nakajima theorem decomposes the entire phase space into a physical subspace and a constraint subspace, and it indicates that the existence of a canonical coordinate system that spans each subspace and that the original canonical coordinate system can be transformed into the new canonical coordinate system by performing the corresponding canonical transformation. Therefore, it would be expected that fixing the configurations for the physical space is a possible candidate for appropriate boundary conditions that are to make the variational principle well-posed from the viewpoints of the coincidence of the numbers. In fact, this insight gives a correct way, although the cases of existing first-class constraints need more careful considerations. In order to proceed with this strategy, the Dirac-Bergmann analysis has to be valid without depending on the well-posedness of the variational principle. Finally, let us confirm this statement.

This statement can be proved by noticing that the well-posedness relates only to the symplectic potential $\omega = p_i dq^i$; this quantity is nothing but the boundary term of the first variation of a Lagrangian with $p_i = \partial L/\partial \dot{q}^i$. That is, after performing the appropriate canonical transformation, when varying, the well-posed variational principle should give rise to a symplectic potential schematically such that $\omega' = P_I dQ^I + \textit{Constraint Structure in 1-form} + \delta W$ as its boundary term up to some total divergent term W. While this transformation does not affect the symplectic structure since $\Omega = \delta\omega = \delta q^i \wedge \delta p_i \overset{\text{C.T.}}{=} \delta\omega' = \delta Q^I \wedge \delta P_I + \textit{Constraint Structure in 2-form} = \Omega'$, where " $\overset{\text{C.T.}}{=}$ " denotes the equality under a canonical transformation; canonical transformations never change the symptectic structure, or equivalently, the symplectic 2-form. Therefore, taking into account the following two facts; (i) The definition of the Poisson bracket: $\{f\,, g\}_{P.b.} = \Omega(X_f\,, X_g)$, where X_f and X_g are the Hamiltonian vector fields with respect to some functions f and g, respectively; (ii) The time development of a quantity f of the system is given as $\dot{f} = \{f\,, H_T\}_{P.b.}$, where H_T is the total

Hamiltonian of the given system, it shows that the statement holds.

3.2. Dirichlet boundary conditions and second-order derivative equations of motions

In this section, the meaning of Dirichlet/position-fixing boundary conditions is clarified in the variational principle [Tomonari (2023b)]. In higher-order derivative systems, the first-order variation of the Lagrangian of a given system gives generically rise not only to the first-order variation of position variables but also to that of the derivatives of these variables at the boundaries. In such theories, the Euler-Lagrange equations generically include higher-order derivative terms that are more than second-order. However, in order to make sense of the equations as physical meanings, these equations have to be at most second-order differential equations. This ansatz restricts the boundary conditions in the variational principle.

Let us first consider a second-order derivative system given as follows:

$$I^{(2)}[q^i\,,\dot{q}^i\,,t] = \int_{t_1}^{t_2} L(\ddot{q}^i\,,\dot{q}^i\,,q^i\,,t)\,dt\,, \tag{3.3}$$

where $i \in \{1\,,2\,,\cdots\,,N\}$. This is a special case of Eq (2.63) with $M = 2$. The first-order variation is given as follows:

$$\begin{aligned}\delta I^{(2)} = &\int_{t_1}^{t_2} \sum_{i=1}^{N} \left[\frac{\partial L^{(2)}}{\partial q^i} - \frac{d}{dt}\left(\frac{\partial L^{(2)}}{\partial \dot{q}^i}\right) + \frac{d^2}{dt^2}\left(\frac{\partial L^{(2)}}{\partial \ddot{q}^i}\right)\right]\delta q^i dt \\ &+ \left[\sum_{i=1}^{N}\left\{\frac{\partial L^{(2)}}{\partial \dot{q}^i} - \frac{d}{dt}\left(\frac{\partial L^{(2)}}{\partial \ddot{q}^i}\right)\right\}\delta q^i + \sum_{i=1}^{N}\left(\frac{\partial L^{(2)}}{\partial \ddot{q}^i}\right)\delta \dot{q}^i\right]_{t_1}^{t_2}\,,\end{aligned} \tag{3.4}$$

check also Eq (2.65). The variational principle leads to the following Euler-Lagrange equations (check also Eq (2.66) and Eq (2.68)):

$$\frac{\partial L^{(2)}}{\partial q^i} - \frac{d}{dt}\left(\frac{\partial L^{(2)}}{\partial \dot{q}^i}\right) + \frac{d^2}{dt^2}\left(\frac{\partial L^{(2)}}{\partial \ddot{q}^i}\right) = 0 \tag{3.5}$$

under fixing both the position and velocity coordinates as follows:

$$\begin{aligned}\delta q^i(t_1) =&\delta q^i(t_2) = 0,\\ \delta \dot{q}^i(t_1) =&\delta \dot{q}^i(t_2) = 0\end{aligned} \tag{3.6}$$

if the system is non-degenerate, *i.e.*, $K^{(2)} = \partial^2 L^{(2)}/\partial \ddot{q}^i \partial \ddot{q}^j$ is full rank, but this condition is not satisfied due to the ansatz; the order of the Euler-Lagrange equations has to be at most second-order in time derivative. That is, the Euler-Lagrange equations (3.5) are rewritten as follows:

$$K^{(2)}_{ij}\ddddot{q}^j + E^{(2)}_{ij}\dddot{q}^j + (\text{up to 2nd-order terms}) = 0 \tag{3.7}$$

where we defined

$$K^{(2)}_{ij} = \frac{\partial^2 L^{(2)}}{\partial \ddot{q}^i \partial \ddot{q}^j}\,, \quad E^{(2)}_{ij} = \frac{\partial^2 L^{(2)}}{\partial \ddot{q}^i \partial \dot{q}^j} - \frac{\partial^2 L^{(2)}}{\partial \ddot{q}^j \partial \dot{q}^i}. \tag{3.8}$$

To turn the equations into at most second-order time differential equations, the matrices $K^{(2)}$ and $E^{(2)}$ have to be zero-matrices:

$$K^{(2)} = 0\,, \quad E^{(2)} = 0. \tag{3.9}$$

Then the Euler-Lagrange equations have at most second-order time derivative. The first condition in (3.9) indicates that this system has to be degenerate as the second-order derivative theory. Notice also that Condition (3.9) are noting but the Ostrogradsky ghost-free conditions given in Section 2.6.

In addition, on one hand, the first condition of Eq (3.9) leads to a specific form of Lagrangian [Motohashi and Suyama (2015); Motohashi et al. (2016)]:

$$L^{(2)} = \sum_{i=1}^{N} f_i(\dot{q}^j\,, q^j)\ddot{q}^i + g(\dot{q}^j\,, q^j). \tag{3.10}$$

On the other hand, this second-order time derivative system should be equivalent to a first-order time derivative system discussed in Section 2.1. It indicates that the Lagrangian of the system should be equivalent up to surface terms. That is,

$$L^{(2)} \to L'^{(1)} = L^{(2)} + \frac{dW}{dt}, \tag{3.11}$$

where $W = W(\dot{q}^i\,, q^i)$. If W satisfies the following conditions:

$$f_i + \frac{\partial W}{\partial \dot{q}^i} = 0 \tag{3.12}$$

or equivalently,

$$W = -\sum_{i=1}^{N} \int f_i d\dot{q}^i + C(q^j), \tag{3.13}$$

where C is an arbitrary function of position coordinates, the first terms in the Lagrangian (3.10) vanish, and the system turns into a first-order time derivative system. Note, here, that Eq (3.13) is nothing but a counter-term in the second-order time derivative system. Furthermore, the first-order variation of the action functional of $L'^{(1)}$ becomes as follows:

$$\delta I'^{(1)} = \text{ the same terms to } \delta I^{(2)} + \left[\sum_{i=1}^{N} \left\{ \frac{\partial L^{(2)}}{\partial \dot{q}^i} - \frac{d}{dt}\left(\frac{\partial L^{(2)}}{\partial \ddot{q}^i} \right) + \frac{\partial W}{\partial q^i} \right\} \delta q^i \right]_{t_1}^{t_2} \tag{3.14}$$

Therefore, the boundary condition (3.6) for the variational principle now turns into position-fixing boundary conditions:

$$\delta q^i(t_1) = \delta q^i(t_2) = 0 \tag{3.15}$$

if the kinetic matrix $K_{ij}^{(1)} = \partial^2 L'^{(1)}/\partial \dot{q}^i \partial \dot{q}^j$ is non-degenerate. This coincides with the boundary conditions for the first-order time derivative systems: Eq (2.8) with no time variation. It makes sense since boundary conditions should uniquely determine the dynamics. From these considerations, the ansatz reveals that appropriate boundary conditions for the variational principle in second-order time derivative theories are position-fixing boundary conditions.

In general, the action functional for the systems is given as follows:

$$I^{(M)} = \int_{t_1}^{t_2} L^{(M)} \left(D^M q^i \,, \cdots , Dq^i \,, q^i \,, t\right) dt \,, \tag{3.16}$$

this is nothing but Eq (2.63). The first-order variation of the action functional is given as follows (check Eq (2.65)):

$$\delta I^{(M)} = \int_{t_1}^{t_2} \sum_{i=1}^{N} \left[\sum_{r=0}^{M} (-1)^r D^r \frac{\partial L^{(M)}}{\partial (D^r q^i)}\right] \delta q^i \, dt + \left[\sum_{i=1}^{N} \sum_{r=s\geq 1}^{M} (-1)^{r-s} D^{r-s} \frac{\partial L^{(M)}}{\partial (D^r q^i)} \delta(D^{s-1} q^i)\right]_{t_1}^{t_2} . \tag{3.17}$$

If the following differential equations for $W = W(q^i \,, Dq^i \,, \cdots , D^{M-1} q^i)$:

$$\sum_{r=s\geq 2}^{M} \left[(-1)^{r-s} D^{r-s} \frac{\partial L^{(M)}}{\partial (D^r q^i)} + \frac{\partial W}{\partial (D^{s-1} q^i)}\right] = 0 \,, \tag{3.18}$$

are solvable, the Euler-Lagrange equations are derived as follows (check also Eq (2.66) and Eq (2.68)):

$$\sum_{r=0}^{M} (-1)^r D^r \frac{\partial L^{(1)}}{\partial (D^r q^i)} = \frac{\partial L^{(1)}}{\partial q^i} - \frac{d}{dt} \frac{\partial L^{(1)}}{\partial \dot{q}^i} = 0 \,, \tag{3.19}$$

where $L^{(1)} = L^{(d)} + dW/dt$, under position-fixing boundary conditions:

$$\delta q^i(t_1) = \delta q^i(t_2) = 0 \,, \tag{3.20}$$

if the kinetic matrix $K^{(1)}_{ij} = \partial^2 L'^{(1)} / \partial \dot{q}^i \partial \dot{q}^j$ is non-degenerate. Therefore, the ansatz indicates that appropriate boundary conditions for the variational principle in Mth-order derivative theories are nothing but position-fixing boundary conditions. Remark, finally, that the Ostrogradsky ghost-free conditions given in Section 2.6 are also verified by a straightforward computation although it is so tedious.

Based on the above considerations, as long as the ansatz, stated as *the order of the Euler-Lagrange equations has to be at most second-order in time derivative*, is assumed, the higher-order time derivative systems need the position-fixing boundary conditions when applying the variational principle. Therefore, the problem is a methodology to identify a set of position variables that should be fixed on the boundaries when the variational principle applies in the first-order time derivative degenerate systems under the addition of an appropriate counter-term if needed.

3.3. Frobenius integrability of first-order time derivative systems

In this section, based on the Frobenius theorem, the existence of solutions in both non-degenerate and degenerate systems is considered [Sugano and Kamo (1982)]. This existence also means that a set of integral constants is derived, and these play a crucial role in formulating the well-posed variational principle [Tomonari (2023b)]; it relates to the realization of the guiding principle, stated as "*as many integral constants (/initial conditions) in the solutions of a given system as possible should be uniquely determined through the boundary conditions*". From the previous section 3.2, introducing appropriate counter-terms, it revealed that the Lagrangian describing a system of which equations of motion contain at most second-order time derivative terms becomes first-order. This indicates that it is enough to investigate the cases that Lagrangians contain at most first-order time derivative terms. Let us start with introducing the Pfaffian system of the Lagrangian formulation in a non-degenerate system and investigating its Frobenius integrability.

The Euler-Lagrange equations, Eq (2.9), are given as follows:

$$\frac{\partial L}{\partial q^i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) = 0\,. \tag{3.21}$$

Pfaffian system is introduced by splitting the equations into 1-forms as follows:

$$\begin{aligned} \rho^i &= dq^i - v^i dt = 0\,, \\ \theta_i &= K_{ij} dv^i - S_i dt = 0\,, \end{aligned} \tag{3.22}$$

where K_{ij} and S_i are defined as follows:

$$K_{ij} = \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}\,, \quad S_i = -v^i \frac{\partial^2 L}{\partial q^i \partial v^i} - \frac{\partial^2 L}{\partial t \partial v^i} + \frac{\partial L}{\partial q^i}\,. \tag{3.23}$$

Remark that the 1-forms in Eq (3.22) can be derived by calculating the exterior derivative of the second equation in Eq (2.10). It implies another viewpoint from the Lagrangian formulation for the validity of the Dirac-Bergmann analysis without depending on the well-posedness of the variational principle as mentioned in Section 3.1. The Frobenius theorem states that the Pfaffian system is Frobenius integrable, or equivalently, the system described by Eq (2.9) has solutions, *if and only if a system of generators for the Pfaffian system, that is, a closed algebra in the Lie bracket composed of vector fields that are orthogonal to the Pfaffian system, exists.* Since the Pfaffian system spans $2N$-dimensional subspace of $T^*(T\mathcal{Q} \times \mathbb{R})$, the system of generators is 1-dimensional subspace of $T(T\mathcal{Q} \times \mathbb{R})$ as follows:

$$\begin{aligned} X_t &= a^i \frac{\partial}{\partial v^i} + b^i \frac{\partial}{\partial q^i} + \frac{\partial}{\partial t}\,, \\ a^i &= (K^{-1})^{ij} S_j\,, \quad b^i = v^i\,. \end{aligned} \tag{3.24}$$

Then the Frobenius theorem indicates the existence of the number of $2n$ functions f^I and integral constants c^I such that

$$f^I(q^i\,, v^i\,, t) = c^I, \tag{3.25}$$

where $I \in \{1\,, 2\,, \cdots\,, 2N\}$. Therefore, the implicit function theorem leads to the solutions as follows:

$$q^i = q^i(t\,, c^I)\,, \quad v^i = v^i(t\,, c^I). \tag{3.26}$$

Under the solutions of the first equation in Eq (3.22), the second solutions above can be rewritten as $\dot{q}^i = \dot{q}^i(t\,, c^I)$.

In the Hamiltonian formulation, the Hamilton equations, Eq (2.22), are given as follows:

$$\dot{q}^i = \frac{\partial H}{\partial p_i}\,, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i} \tag{3.27}$$

and expressed as the following Pfaffian system:

$$\begin{aligned} {}_*\rho^i &= dq^i - \frac{\partial H}{\partial p_i} dt = 0\,, \\ {}_*\theta_i &= dp_i + \frac{\partial H}{\partial q^i} dt = 0\,. \end{aligned} \tag{3.28}$$

The same considerations as the Lagrangian formulations but in the phase space $T^*\mathcal{Q} \times \mathbb{R}$ lead to the following generator:

$$\begin{aligned} {}_*X_t &= {}_*a^i \frac{\partial}{\partial q^i} + {}_*b_i \frac{\partial}{\partial p_i} + \frac{\partial}{\partial t}\,, \\ {}_*a^i &= \frac{\partial H}{\partial p_i}\,, \quad {}_*b_i = -\frac{\partial H}{\partial q^i}\,. \end{aligned} \tag{3.29}$$

Then the Frobenius theorem leads to the following relations:

$${}_*f^I(q^i\,, p_i\,, t) = {}_*c^I\,, \tag{3.30}$$

where I runs from 1 to $2N$, ${}_*f^I$ and ${}_*c^I$ are functions and integral constants, respectively, which are implied from this theorem. Therefore, the implicit function theorem gives the solutions:

$$q^i = {}_*q^i(t\,, {}_*c^I)\,, \quad p_i = p_i(t\,, {}_*c^I)\,. \tag{3.31}$$

Since the configurations are given by the first formulae in Eq (3.26) and both the formulations have a common configuration space, ${}_*q^i(t\,,{}_*c^I)$ should exactly be the same as $q^i(t\,,c^I)$. Therefore, ${}_*c^I = c^I$ are concluded, and the solutions become

$$q^i = q^i(t\,,c^I)\,,\quad p_i = p_i(t\,,c^I)\,. \tag{3.32}$$

The non-degeneracy, $\det K \neq 0$, implies the equivalence between the solution (3.26) and (3.32) by virtue of the implicit function theorem. This is also a conclusion from the following one-to-one correspondences:

$$\begin{aligned} &\frac{\partial}{\partial q^i} \leftrightarrow \frac{\partial}{\partial q^i} + \frac{\partial p_j}{\partial q^i}\frac{\partial}{\partial p_j}\,, \\ &\frac{\partial}{\partial v^i} \leftrightarrow \frac{\partial p_j}{\partial v^i}\frac{\partial}{\partial p_j} = K_{ij}\frac{\partial}{\partial p_j}\,, \\ &\frac{\partial}{\partial t} \leftrightarrow \frac{\partial p_i}{\partial t}\frac{\partial}{\partial p_i} + \frac{\partial}{\partial t}\,, \end{aligned} \tag{3.33}$$

where the left-hand side and the right-hand side are composed of the coordinate basis of $T(T\mathcal{Q}\times\mathbb{R})$ and $T(T^*\mathcal{Q}\times\mathbb{R})$, respectively.

Next, let us consider the Frobenius integrability of the given degenerate system in the Lagrangian formulation, *i.e.*, in the velocity phase space $T\mathcal{Q}\times\mathbb{R}$. Assume that the degeneracy condition $\operatorname{rank} K = R(< N)$, or equivalently, the following condition:

$$K_{ij}\tau^j_\alpha = 0\,, \tag{3.34}$$

is taken into account, where $\alpha \in \{1\,,2\,,\cdots\,,N-R\}$ and τ^i_α are zero-eigenvalue vectors. The given system has the number of R primary constraints: $\phi^{(1)}_\alpha = 0$, and these are satisfied as identity. This property and the second equation in Eq (3.22) lead to the following secondary constraints:

$$\phi^{(2)}_\alpha = \tau^i_\alpha S_i := 0\,. \tag{3.35}$$

The completeness of the zero-eigenvalue vectors implies the existence of a set of vectors, η^i, such that

$$S_i \overset{\mathfrak{C}^{(2)}}{\approx} K_{ij}\eta^j\,. \tag{3.36}$$

The generator of the Pfaffian system (3.22) are derived as follows:

$$X_T = X_t + \zeta^\alpha Y_\alpha + \xi^\alpha Z_\alpha\,, \tag{3.37}$$

where ζ^α and ξ^α are multipliers, X_t, Z_α, and Y_α are defined as follows:

$$X_t = \eta^i\frac{\partial}{\partial v^i} + v^i\frac{\partial}{\partial q^i} + \frac{\partial}{\partial t}\,, \quad Z_\alpha = -\tau^i_\alpha\frac{\partial}{\partial v^i}\,, \quad Y_\alpha = [X_t\,, Z_\alpha] = \tau^i_\alpha\frac{\partial}{\partial q^i} + \left(-Z_\alpha\eta^i - X_t\tau^i_\alpha\right)\frac{\partial}{\partial v^i}\,. \tag{3.38}$$

In the presence of the constraints, $\phi^{(s)}_\alpha \approx 0$ ($s \in \{1\,,2\}$), the space in where the dynamics processes is restricted into a subspace of the entire phase space, $T^*\mathcal{Q}\times\mathbb{R}$. It implies that the generators of the Pfaffian system have to be formed with respect not to the entire phase space but to the constraint subspace that is restricted by all the constraints. In order to find all other constraints, the following condition has to be imposed:

$$d\phi^{(2)}_\alpha(X_T) := 0\,. \tag{3.39}$$

If $d\phi^{(2)}_\alpha(Y^{(1)}_\beta) \neq 0$ hold for a β then this condition determines a multiplier ζ^α. Otherwise it gives rise to a new constraint: $\phi^{(3)}_\alpha = d\phi^{(2)}_\alpha(X_T) := 0$. Remark that $d\phi^{(2)}_\alpha(Z_\beta) = 0$ are automatically satisfied therefore the multipliers ξ^α remain arbitrary. Repeating this procedure, all constraints are derived as follows:

$$\begin{aligned}
&\phi^{(s+1)}_\alpha = d\phi^{(s)}_\alpha(X_T) := 0 \quad (s = 2, 3, \cdots, S_\alpha - 1),\\
&\phi^{(S_\alpha+1)}_\alpha = d\phi^{(S_\alpha)}_\alpha(X_T) = C^\beta_{\alpha s}\phi^{(s)}_\beta \overset{\mathfrak{C}^{(S_\alpha)}}{\approx} 0\,,
\end{aligned} \tag{3.40}$$

where $C^{\beta}_{\alpha s}$ are some coefficients functions. The above conditions are called consistency conditions *in the Lagrangian formulation*. Under these constraints, if the following conditions are satisfied then the system is Frobenius integrable:

$$\theta_i(X_T) = -\zeta^{\alpha} K_{ij}(Z_{\alpha}\eta^j + X_t \tau^j_{\alpha}) \overset{\mathfrak{C}^{(S_\alpha)}}{\approx} 0\,. \tag{3.41}$$

$\rho_i(X_T) \overset{\mathfrak{C}^{(S_\alpha)}}{\approx} 0$ are automatically satisfied by virtue of $\rho_i := K_{ij}\rho^j$. Then the number of $(2N - \textit{all constraints})$ functions and integral constraints exist, and the implicit function theorem derives the solution of the Euler-Lagrange equations (3.22) of the system, in the same manner as the non-degenerate case, under the imposition of the Frobenius integrablity condition (3.41).

Finally, let us consider the Frobenius integrability of the given system in the Hamiltonian formulation. Under the degeneracy condition $\operatorname{rank} K = R(< N)$, the Dirac-Bergmann analysis in Section 2.2 leads to all constraints from the primary constraints ${}_*\phi^{(1)}_{\alpha} := 0$ as follows:

$$\begin{aligned} {}_*\phi^{(s'+1)}_{\alpha} &= \{{}_*\phi^{(s')}_{\alpha}, H_T\}_{P.b.} + \frac{\partial {}_*\phi^{(s')}_{\alpha}}{\partial t} := 0\,, \\ {}_*\phi^{(S'_\alpha+1)}_{\alpha} &= {}_*X_{H_T}{}_*\phi^{(S'_\alpha)}_{\alpha} = {}_*C^{\beta}_{\alpha s'}{}_*\Phi^{(s')}_{\beta} \overset{\mathfrak{C}^{(S'_\alpha)}}{\approx} 0\,, \end{aligned} \tag{3.42}$$

where $s' \in \{1\,, 2\,, \cdots, S'_\alpha - 1\}$ and the total Hamiltonian H_T is given by $H_T = H_0 + \zeta^{\alpha}{}_*\phi^{(1)}_{\alpha}$. Remark that all indices are primed since the equivalence of constraints between the Lagrangian and Hamiltonian formulations is not proved yet (it will be proved later). Under these constraints, for the Pfaffian system of Eq (3.28), if the following conditions are satisfied then the system is Frobenius integrable:

$${}_*\theta_i({}_*X_T) = -\zeta^{\alpha}\frac{\partial {}_*\phi^{(1)}_{\alpha}}{\partial q^i} \overset{\mathfrak{C}^{(S'_\alpha)}}{\approx} 0\,, \tag{3.43}$$

${}_*\rho_i({}_*X_T) \overset{\mathfrak{C}^{(S'_\alpha)}}{\approx} 0$ are automatically satisfied, where ${}_*\rho_i = K_{ij*}\rho^j$. Then the number of $(2N - \textit{all constraints})$ functions and integral constraints exist, and the implicit function theorem derives the solution of the Hamilton equations (3.28) of the system, in the same manner as the non-degenerate case, under the imposition of the Frobenius integrability conditions (3.43).

In a non-degenearate case, a one-to-one correspondence of vector fields between $T(T\mathcal{Q}\times\mathbb{R})$ and $T(T^*\mathcal{Q}\times\mathbb{R})$ given as Eq (3.33) exists, but in a degenerate case such correspondence is violated due to the degeneracy of the kinetic matrix K_{ij}:

$$\frac{\partial}{\partial v^i} \to \frac{\partial p_j}{\partial v^i}\frac{\partial}{\partial p_j} = K_{ij}\frac{\partial}{\partial p_j}\,. \tag{3.44}$$

Therefore, the Hamiltonian formulation cannot be transformed into the Lagrangian formulation but the opposite is possible as follows:

$$\begin{aligned}
&X_t \to {}_*X_t = \frac{\partial H_0}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H_0}{\partial q^i}\frac{\partial}{\partial p_i} + \frac{\partial}{\partial t} = X_{H_0} + \frac{\partial}{\partial t},\\
&Z_\alpha \to {}_*Z_\alpha = 0,\\
&Y_\alpha \to {}_*Y_\alpha = \frac{\partial_*\phi^{(1)}_\alpha}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial_*\phi^{(1)}_\alpha}{\partial q^i}\frac{\partial}{\partial p_i} = X_{{}_*\phi^{(1)}_\alpha}.
\end{aligned} \tag{3.45}$$

Therefore, $X_{H_T} \to {}_*X_{H_T}$ becomes

$$X_T \to {}_*X_{H_T} = {}_*X_{H_0} + \zeta^\alpha{}_*X_{{}_*\phi^{(1)}_\alpha} + \frac{\partial}{\partial t} = {}_*X_{H_T} + \frac{\partial}{\partial t}, \tag{3.46}$$

where $H_T = H_0 + \zeta^\alpha{}_*\phi^{(1)}_\alpha$ is nothing but the total Hamiltonian of the system. Therefore, the indices s and s' are identified and so are S_α and S'_α; $\phi^{(s)}_\alpha$ and ${}_*\phi^{(s')}_\alpha$ have a one-to-one correspondence, respectively.

3.4. Reformulation of the well-posed variational principle

In this section, introducing three fundamental maps that are correspondences between integral constants from the Frobenius integrability and position-fixing boundary conditions in the variational principle, velocity variables and momentum variables, and the Hamiltonian vector fields in the Lagrangian and Hamiltonian formulations, respectively, the well-posedness of the variational principle is reformulated [Tomonari (2023b)]. First of all, let us start by introducing the three fundamental maps scrutinizing a non-degenerate system.

Based on the considerations in the previous section, a non-degenerate system is Frobenius integrable and has the solutions Eq (3.26) in the Lagrangian formulation, or equivalently Eq (3.32) in the Hamiltonian formulation, and vice versa. The solutions of configurations are common in both the formulations as follows: $q^A = q^A(t\,, c^B)$ $(A, B \in \{1\,, 2\,, \cdots\,, 2N\})$. In a local open region U of the configuration space $\mathcal{Q}$, regarding the integral constants, c^I, as continuous parameters and assuming $\partial q^A/\partial c^B \neq 0$ on U, the implicit function theorem becomes applicable. This leads to a map ι that maps the configurations at times t_1 and t_2 to a $2N$-dimensional parameter space $\mathcal{C}$ which is spanned by all the integral constants:

$$\iota :\ \mathcal{Q}[t_1]\times\mathcal{Q}[t_2] \to \mathcal{C};\ (q^1(t_1)\,, q^2(t_1)\,, \cdots\,, q^N(t_1)\,, q^1(t_2)\,, q^2(t_2)\,, \cdots\,, q^N(t_2)) \mapsto (c^1\,, c^2\,, \cdots\,, c^{2N})\,, \tag{3.47}$$

where $\mathcal{Q}[t]$ is the space spanned by the configurations at a time t and $q^i(t_1)$ are the values of configuration coordinates at the time t_1. $q^i(t_2)$ are defined in the same manner. The space $\mathcal{Q}[t]$ is usually a local region since the variational principle leads to a local minimum of the action functional. The important point is that map ι is invertible by virtue of the implicit function theorem. In other words, the position-fixing boundary conditions can be replaced by the integral constants in the solutions and determine the dynamics uniquely when the propagating degrees of freedom matches the number of the independent integral constants.

This is the first correspondence and nothing but the realization of the guiding principle, that is, "*as many integral constants (/initial conditions) in the solutions of a given system as possible should be uniquely determined through the boundary conditions*".

The second correspondence is introduced by a map as follows:

$$\kappa : T\mathcal{Q} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R}; \dot{q}^i(t) \mapsto p_i(t) = \frac{\partial L}{\partial \dot{q}^i}\,. \tag{3.48}$$

In the non-degenerate system, that is, $\det K \neq 0$ implies that map κ is invertible by virtue of the implicity function theorem:

$$\kappa^{-1} : T^*\mathcal{Q} \times \mathbb{R} \to T\mathcal{Q} \times \mathbb{R}; p_i(t) \mapsto \dot{q}^i(t) = v^i(q^j\,, p_j\,, t)\,. \tag{3.49}$$

This property is of course satisfied in a local region.

The final correspondence is expressed in a map as follows:

$$\mathfrak{O} : \mathfrak{G}[T(T\mathcal{Q} \times \mathbb{R})] \to \mathfrak{G}[T(T^*\mathcal{Q} \times \mathbb{R})]; X_T \mapsto {}_*X_{H_T}\,, \tag{3.50}$$

where $\mathfrak{G}[T(T\mathcal{Q} \times \mathbb{R})]$ and $\mathfrak{G}[T^*(T\mathcal{Q} \times \mathbb{R})]$ denote spaces of the system of generator for the Pfaffian systems (3.22) and (3.28), respectively. The Hamiltonian vector fields X_t and ${}_*X_t$ are defined in Eq (3.37) and Eq (3.46), respectively. Note that Eq (3.46) is directly indicates the existence of the above map $\mathfrak{O}$ and its well-definedness. The existence of its inverse map is guranteed from Eq (3.33).

Finally, let us define the well-posedness of the variational principle as follows:

Definition 1.

The variational principle is well-posed if and only if the three fundamental maps ι, κ, and $\mathfrak{O}$ are well-defined and invertible on a phase (sub)space in which the physical phase space exists.

$\blacksquare$

In a degenerate system, the degeneracy makes it generically impossible to introduce map ι in a well-defined manner. Furthermore, maps κ and $\mathfrak{O}$ are always introduced in a well-defined manner, but their inverses generically do not exist. Therefore, in order to establish a well-posed variational principle in the degenerate system, we have to remove these incompatibilities from the theory. The strategy to tackle this problem is that we restrict the entire phase space to a subspace such that each invertible map for κ and $\mathfrak{O}$ exists, and then we construct a well-defined map ι in the subspace of which the inverse map exists. The construction of subspaces of phase space, however, differs from the cases of ordinary differential manifolds. That is, arbitrary restrictions, or strictly speaking, embeddings, are not allowed, unlike ordinary differential manifolds.

3.5. Embeddings of Symplectic manifolds

In this section, based on the Shanmugadhasan-Maskawa-Nakajima theorem, which is already stated in Section 2.4, the embeddings of a symplectic manifold are introduced [Tomonari (2023b)]. The embeddings are classified into two types, "*canonical*" or "*quasi-canonical*" embeddings, according to the existence of first-class constraints. In order to formulate the embeddings, a method of fixing coordinate functions is applied. This method introduces an embedding and a submanifold simultaneously. Let us start by reviewing this method in ordinary differential manifolds by using examples.

Assume that an *abstract* embedding "ψ" : "$\mathcal{S}$" $\to \mathbb{R}^3$ for some differential submanifold $\mathcal{S}$ of $\mathbb{R}^3$ exists. The submanifold "$\mathcal{S}$" is also *abstract* one; it symbolically denotes all possible submanifolds of $\mathbb{R}^3$. That is, any concrete embedding and submanifold are determined yet; there is only a structure ("ψ" , "$\mathcal{S}$"). Now, let us equip $\mathbb{R}^3$ with a coordinate system. For instance, assume that $\mathbb{R}^3$ is equipped with polar-coordinates $(r\,,\theta\,,\varphi)$. Then the abstract embedding becomes ψ : "$\mathcal{S}$" $\to \mathbb{R}^3; (\psi^* r\,,\psi^*\theta\,,\psi^*\varphi) \mapsto (r\,,\theta\,,\varphi)$, where ψ^* is the pullback operator of ψ; the structure can be identified by fixing a set of pullback of the coordinate functions by ψ. If $\psi^* r$ is fixed as 1 then the abstract embedding turns into $\psi : \mathcal{S} \to \mathbb{R}^3 ; (\psi^* r := 1 \,, \psi^* \theta \,, \psi^* \varphi) \mapsto (r \,, \theta \,, \varphi)$; this is nothing but the embedding of the unit sphere. Similarly, fixing either $\psi^* \theta$ or $\psi^* \varphi$ leads to an embedding of a 2-dimensional plane, respectively, fixing both $\psi^* \theta$ and $\psi^* \varphi$ derives an embedding of a line. In general, for a differential manifold, $\mathcal{M}$ and a possible submanifold "$\mathcal{S}$", an abstract embedding "ψ" : "$\mathcal{S}$" $\to \mathcal{M}$ can be introduced, and it forms a structure ("ψ" , "$\mathcal{S}$"). Then, equipping a coordinate system with $\mathcal{M}$ and fixing a set of the pullbacks of the coordinate functions, the structure is identified: $(\psi \,, \mathcal{S})$.

In the case of phase space, however, embeddings by fixing coordinate functions are generically restricted. For instance, any odd-number dimensional subspaces cannot be embedded into the entire phase space. Therefore, *this restriction has to be realized as an embedding into the entire phase space such that the canonical structure holds at least for the subspace in which the dynamics lives.* Let us call such embedding "*canonical*" if it exists. To consider canonical embeddings, we need to introduce the concept of symplectic manifolds.

At each time $t \in I$, where $I \subset \mathbb{R}$ is an open interval of the time variable, a space $T^*\mathcal{Q} \times \mathbb{R}$ is equivalent to $T^*\mathcal{Q}$. Then a symplectic manifold of $T^*\mathcal{Q}$ is defined as the structure $(T^*\mathcal{Q} \,, \Omega)$ equipped with a 2-form Ω on $T^*\mathcal{Q}$ represented by

$$\Omega := \frac{1}{2} \Omega_{AB} dz^A \wedge dz^B \tag{3.51}$$

satisfying the following three conditions:

$$\begin{aligned} &\text{(i). } \Omega_{AB} = -\Omega_{BA} \\ &\text{(ii). } \det \Omega_{AB} \neq 0 \\ &\text{(iii). } d\Omega = 0 \,, \end{aligned} \tag{3.52}$$

where $A, B \in \{1, 2, \cdots, 2N\}$. The Darboux theorem under the conditions in Eq (3.52) leads to the canonical structure:

$$\Omega := \frac{1}{2} J_{AB} dz^A \wedge dz^B = dq^i \wedge dp_i \tag{3.53}$$

at least in a local region on the symplectic manifold $(T^*\mathcal{Q}, \Omega)$, where $(z^i, z^{N+i}) = (q^i, p_i)$ and

$$J = \begin{bmatrix} 0 & I_{N\times N} \\ -I_{N\times N} & 0 \end{bmatrix}. \tag{3.54}$$

$I_{N\times N}$ is an $N \times N$ unit matrix. Then the Poisson bracket is defined as follows:

$$\{f, g\}_{P.b.} := \Omega(X_f, X_g), \tag{3.55}$$

where X_f and X_g are the Hamiltonian vector fields of f and g, respectively. Using these concepts, we can define a canonical transformation as a coordinate transformation $\phi : T^*\mathcal{Q} \to T^*\mathcal{Q}; (q^i, p_i) \mapsto (Q^i, P_i)$ such that the symplectic 2-form is invariant under the pullback operation ϕ^*:

$$\phi^* \Omega_{Q,P} = \Omega_{q,p} \tag{3.56}$$

where

$$\begin{aligned} \Omega_{q,p} &:= dq^i \wedge dp_i = \frac{1}{2} J_{AB} dz^A \wedge dz^B, \\ \Omega_{Q,P} &:= dQ^i \wedge dP_i = \frac{1}{2} J_{AB} dZ^A \wedge dZ^B, \end{aligned} \tag{3.57}$$

and $(Z^i, Z^{N+i}) = (Q^i, P_i)$. The condition (3.56) is equivalent to

$$S^T J S = J, \tag{3.58}$$

where S^T is the transpose of S, and S is given as follows:

$$\phi^* dZ^A = S^A{}_B dz^B, \tag{3.59}$$

or more concretely,

$$S^A{}_B := \frac{\partial Z^A}{\partial z^B} \tag{3.60}$$

for $Z^A = (\phi^{-1})^* z^A$. The definition of Poisson bracket given in Eq (3.55) implies that a canonical transformation does not change the Poisson bracket. That is, the equations of motion are invariant; the dynamics remains unchanged before and after the transformation. Conversely, since the time evolution is decomposed into a series of infinitesimal canonical transformations, the symplectic 2-form in Eq (3.52), or more general form Eq (3.51), is invariant under the time evolution. Note that when we consider a subspace as an embedding into the symplectic manifold $(T^*\mathcal{Q}\,,\Omega)$ by fixing some coordinates, a set of conjugate variables, $i.e.$ pairs: q^i and p_i, have to be fixed simultaneously. Fixing either q^i or p_i would destroy the symplectic structure of the phase space. That is, the first and/or second conditions in the definition (3.52) would be violated. This is the peculiar property of symplectic manifolds differing from ordinary differential manifolds.

Now, let us introduce embeddings of a given symplectic manifold. The method needs to introduce an abstract embedding "σ" : "$\mathcal{S}$" $\times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R}$ and a coordinate system for the entire phase space $T^*\mathcal{Q} \times \mathbb{R}$. The required coordinate system is of course provided by the Shanmugadhasan-Maskawa-Nakajima theorem. Therefore, the abstract embedding turns into $\sigma(t)$: "$\mathcal{S}$" $\times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R}$; $(\sigma^*(t)Q^I\,, \sigma^*(t)P_I\,, \sigma^*(t)\,{}_*\Theta^a\,, \sigma^*(t)\,{}_*\Theta_a\,, \sigma^*(t)\,{}_*\Xi^\alpha\,, \sigma^*(t)\,{}_*\Psi_\alpha,$ $\sigma^*(t)u = t) \mapsto (Q^I\,, P_I\,, {}_*\Theta^a\,, {}_*\Theta_a\,, {}_*\Xi^\alpha\,, {}_*\Psi_\alpha, u)$, where $I \in \{1\,, 2\,, \cdots\,, N - V - U\}$; $a \in \{1\,, 2\,, \cdots\,, V\}$; $\alpha \in \{1, 2, \cdots\,, U\}$. Hereinafter, we abbreviate the notation of "${}_*$" for the phase space variables if it is apparent. The possible set of pullback of the coordinate functions is only constraint coordinate functions, $i.e.$, Θ^a, Θ_a, and Ψ_α, since other coordinate functions evolve in time passing. In other words, the consistency conditions for Θ^a, Θ_a, and Ψ_α make it possible to fix for incarnating the abstract embedding. In addition, fixing Ξ^α is also possible since this manipulation corresponds to gauge fixing. Therefore, there are eight possibilities to incarnate the abstract embedding; (i) Fix Θ^a and Θ_a when Ψ_α do not exist; (ii) Impose gauge fixing conditions to Ξ^α, and fix Ξ^α and Ψ_α when Θ^a and Θ_a do not exist; (iii) Impose gauge fixing conditions to Ξ^α, and fix Θ^a, Θ_a, Ξ^α, and Ψ_α; (iv) Fix Ψ_α when Θ^a and Θ_a do not exist; (v) Fix Θ^a, Θ_a, and Ψ_α; (i)' Fix only Θ^a and Θ_a when Ψ_α do exist; (ii)' Impose gauge fixing conditions to Ξ^α, and fix only Ξ^α and Ψ_α when Θ^a and Θ_a do exist; (iv)' Fix only Ψ_α when Θ^a and Θ_a do exist; (vi) Impose gauge fixing conditions to Ξ^α, and fix only Θ^a and Θ_a. Here, the prime " ' " of (i)' denotes the existence of Ψ_α. If this is not the case then we remove the prime " ' " from it. So are for the prime " ' " of (ii)' and (iv)' with respect to Θ_a and Θ^a. Remark that imposing gauge fixing conditions to Ξ^α means that these variables turn into a set of constraints and satisfy those consistency conditions: $\dot{\Xi}^\alpha \overset{\text{all constraints}}{\approx} 0$, where " $\overset{\text{all constraints}}{\approx}$ " denotes the weak equality under the imposition of all the constraints including the gauge fixing conditions.

First, let us consider Cases (i), (ii), and (iii). Case (i) leads to the following embedding:

$$\begin{aligned}&\sigma_2(t) : T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R} \\ &\qquad ; (\sigma_2^*(t)Q^I \,, \sigma_2^*(t)P_I \,, \sigma_2^*(t)\Theta^a := \epsilon^a \,, \sigma_2^*(t)\Theta_a := \epsilon_a \,, \sigma_2^*(t)u = t) \mapsto (Q^I \,, P_I \,, \Theta^a \,, \Theta_a \,, u) \,,\end{aligned} \tag{3.61}$$

where ϵ^a and ϵ_a are constant parameters, and $T^*\mathcal{Q}|_{Q,P}$ denotes that the phase subspace coordinated by Q^I and P_I. This embedding pulls back the entire symplectic manifold, $(T^*\mathcal{Q} \times \mathbb{R} \,, \Omega = dq^i(u) \wedge dp_i(u))$, to the submanifold, $(T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \,, \Omega_{Q,P} = d\sigma_2^*(t)Q^I \wedge d\sigma_2^*(t)P_I)$: $\sigma_2^*(t)(T^*\mathcal{Q}\times\mathbb{R} \,, \Omega = dq^i(u)\wedge dp_i(u)) = (T^*\mathcal{Q}|_{Q,P}\times\mathbb{R} \,, \Omega_{Q,P} = d\sigma_2^*(t)Q^I\wedge d\sigma_2^*(t)P_I)$. $\Omega_\Theta(t) = d\sigma_2^*(t)\Theta^a \wedge d\sigma_2^*(t)\Theta_a = 0$ on $T^*\mathcal{Q}|_\Theta \times \mathbb{R}$ throughout all time implies that it does not relate to the dynamics, but $\Omega_{Q,P}(t) \neq 0$ on $T^*M|_{Q,P} \times \mathbb{R}$ with the symplectic structure describes the dynamics, and this subspace is nothing but the physical one. Notice that taking limits of $\epsilon^a \to 0$ and $\epsilon_a \to 0$, $\sigma_2(t)$ restores the constraint space. Therefore, Case (i) leads to a canonical embedding: $\sigma_2(t)$. $\sigma_2(t)$ occupies $2V$ integral constants that are indicated by the Frobenius integrability in Section 3.3.

In the same manner, Cases (ii) and (iii) lead to the following embeddings:

$$\begin{aligned}
\sigma_1(t) : & T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R} \\
& ; (\sigma_1^*(t)Q^I , \sigma_1^*(t)P_I , \sigma_1^*(t)\Xi^\alpha := \epsilon^\alpha , \sigma_1^*(t)\Psi_\alpha := \epsilon_\alpha , \sigma_1^*(t)u = t) \mapsto (Q^I , P_I , \Xi^\alpha , \Psi_\alpha , u) ,
\end{aligned} \tag{3.62}$$

and

$$\begin{aligned}
\sigma_3(t) : & T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R} \\
& ; (\sigma_3^*(t)Q^I , \sigma_3^*(t)P_I , \sigma_3^*(t)\Xi^\alpha := \epsilon^\alpha , \sigma_3^*(t)\Psi_\alpha := \epsilon_\alpha , \sigma_3^*(t)\Theta^a := \epsilon^a , \sigma_3^*(t)\Theta_a := \epsilon_a , \sigma_3^*(t)u = t) \\
& \quad \mapsto (Q^I , P_I , \Xi^\alpha , \Psi_\alpha , \Theta^a , \Theta_a , u) .
\end{aligned} \tag{3.63}$$

In the both cases, $\sigma_1(t)$ and $\sigma_3(t)$, the original symplectic structure, $(T^*\mathcal{Q} \times \mathbb{R} , \Omega = dq^i(u) \wedge dp_i(u))$, is pulled back to $(T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} , \Omega_{Q,P} = d\sigma_2^*(t)Q^I \wedge d\sigma_2^*(t)P_I)$; it is the same conclusion as $\sigma_2(t)$. Therefore, Cases (ii) and (iii) also lead to the canonical embeddings: $\sigma_\tau(t)$ ($\tau \in \{1 , 2 , 3\}$), and occupy $2V$ integral constants that are indicated by the Frobenius integrability in Section 3.3.

Second, let us consider Cases (iv) and (v). Case (iv) leads to the following embedding:

$$\begin{aligned}&\tilde{\sigma}_1(t) : T^*\mathcal{Q} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R} \\ &\qquad ; (\sigma_1^*(t)Q^I\,, \sigma_1^*(t)P_I\,, \sigma_1^*(t)\Xi^\alpha\,, \sigma_1^*(t)\Psi_\alpha := \epsilon_\alpha\,, \sigma_1^*(t)u = t) \mapsto (Q^I\,, P_I\,, \Xi^\alpha\,, \Psi_\alpha\,, u)\,.\end{aligned} \tag{3.64}$$

Remark that $\sigma_1^*(t)\Xi^\alpha$ cannot be fixed since the corresponding variables Ξ^α evolve in time unless gauge fixing conditions, or equivalently, a set of consistency conditions, are imposed. In the case of the above embedding, the symplectic 2-form is pulled back as follows:

$$\tilde{\sigma}_1^*(t)\Omega = d\tilde{\sigma}_1^*(t)Q^I \wedge d\tilde{\sigma}_1^*(t)P_I + d\tilde{\sigma}_1^*(t)\Xi^\alpha \wedge 0\,. \tag{3.65}$$

This result indicates that the case without the consistency conditions for Ξ^α does not reduce the phase space into the physical space. In addition, since the first and/or the second condition of the definition for symplectic 2-form in Eq (3.52) would be violated, this embedding is not canonical as it is. However, we will confirm that this embedding can be canonical as we impose gauge fixing conditions. This is a peculiar feature of systems existing of first-class constraints. Let us call this sort of embeddings being "*quasi-canonical*". Notice that if we take the limit of $\epsilon_\alpha \to 0$, then $\tilde{\sigma}_1(t)$ restores the constraint space wherein all the constraints are satisfied; this is another reason why $\sigma_1^*(t)\Xi^\alpha$ cannot be fixed in $\sigma_1^*(t)$. Ξ^α do not restrict the constraint space at all. Notice also that $\tilde{\sigma}_1(t)$ occupies U integral constants that are indicated by the Frobenius integrability given in Section 3.3.

In the same manner, Case (v) leads to the following embedding:

$$\begin{aligned}\tilde{\sigma}_3(t) :& T^*\mathcal{Q}|_{\Xi\,,\Psi} \times T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R} \to T^*\mathcal{Q} \times \mathbb{R} \\ &; (\tilde{\sigma}_3^*(t)Q^I\,, \tilde{\sigma}_3^*(t)P_I\,, \tilde{\sigma}_3^*(t)\Xi^\alpha\,, \tilde{\sigma}_3^*(t)\Psi_\alpha := \epsilon_\alpha\,, \tilde{\sigma}_3^*(t)\Theta^a := \epsilon^a\,, \tilde{\sigma}_3^*(t)\Theta_a := \epsilon_a\,, \tilde{\sigma}_3^*(t)u = t) \\ &\mapsto (Q^I\,, P_I\,, \Xi^\alpha\,, \Psi_\alpha\,, \Theta^a\,, \Theta_a\,, u)\,.\end{aligned} \tag{3.66}$$

This embedding is also quasi-canonical and occupies $2V + U$ integral constants that are indicated by the Frobenius integrability given in Section 3.3.

Finally, let us consider Cases (i)', (ii)', (iv)', and (vi). Considering in the same manner as above, it is shown that (i)', (ii)', and (vi) become canonical embeddings, and (iv)' becomes a quasi-canonical embedding. Cases (i)', (ii)', (iv)', and (vi) occupy $2U$, $2V$, V, $2U$ integral constants that are indicated by the Frobenius integrability in Section 3.3. However, it is also shown that these embeddings cannot introduce the well-posed variational principle [Tomonari (2023b)], although these embeddings are also well-defined ones as embeddings of the symplectic manifold. A way to grasp this point is that if all the parameters are taken as the limit vanishing, the embeddings have to restore the original constraint subspace; However, the embeddings above cannot realize this specific case. Therefore, as the results, only the embeddings $\sigma_\tau(t)$ ($\tau \in \{1\,,2\,,3\}$), $\tilde{\sigma}_1(t)$, and $\tilde{\sigma}_3(t)$ are valid to formulate the well-posed variational principle.

3.6. Well-posed variational principle 1: Cases of canonical embeddings

In this section, based on Definition 1 and the canonical embeddings, $\sigma_\tau(t)$ ($\tau \in \{1, 2, 3\}$), which are introduced in the previous section 3.5, the well-posed variational principle for a system that includes second-class constraints or first-class constraints under the imposition of gauge fixing conditions is formulated [Tomonari (2023b)]. Hereinafter, we abbreviate the notation of " $_*$ " for the phase space variables if it is apparent. First of all, let us show that, in the pullback of the entire symplectic manifold $(T^*\mathcal{Q}\,,\Omega)$ by $\sigma_\tau(t)$, $\sigma^*_\tau(t)(T^*\mathcal{Q}\times\mathbb{R}\,,\Omega) = (T\mathcal{Q}|_{Q\,,P}\times\mathbb{R}\,,\Omega_{Q,P}(t) = dQ^I(t)\wedge dP_I(t))$, it restores the existence of the inverse of κ and $\mathfrak{O}$, respectively.

The dual bundle of $T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R} = \sigma^*_\tau(t)(T^*\mathcal{Q}\times\mathbb{R})$ is determined as $T\mathcal{Q}|_{Q\,,R}\times\mathbb{R}$ up to isomorphism, where $R^I(t)$ are a set of contra-variant vector components on $\mathcal{Q}|_Q$, where $|_Q$ denotes the configuration space $\mathcal{Q}$ equipped with the coordinates Q^I. Then assume that there is a function $L = L(Q^I(t)\,,R^I(t)\,,t)$ defined on $T\mathcal{Q}|_{Q\,,R}\times\mathbb{R}$ such that the following conditions are satisfied:

$$P_I(t) = \frac{\partial L}{\partial R^I(t)}\,,\quad \det\left(\frac{\partial P_I(t)}{\partial R^J(t)}\right)\neq 0\,. \tag{3.67}$$

Using the implicit function theorem, we get a set of functions: $R^I = R^I(Q^I(t)\,,P^I(t)\,,t)$. Since $\dot{Q}^I(t)$ are contra-variant vector components on $\mathcal{Q}|_Q$ as well, without any loss of generality, R^I can be identified as $\dot{Q}^I(t)$. Therefore, we acquire a coordinate system for the velocity phase space $T\mathcal{Q}$: $Q^I(t)$ and $\dot{Q}^I(t)$. This construction leads to a one-to-one correspondence between $P_I(t)$ and $\dot{Q}^I(t)$. That is, the following map is a well-defined and invertible map:

$$\kappa|_{\sigma_\tau(t)}:\ T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R}\to T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R};\ \dot{Q}^I(t)\mapsto P_I(t)\,, \tag{3.68}$$

which restricts the domain $T\mathcal{Q}\times\mathbb{R}$ and the range $T^*\mathcal{Q}\times\mathbb{R}$ of κ to $\sigma^*_\tau(t)(T\mathcal{Q}\times\mathbb{R}) = T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R}$ and $\sigma^*_\tau(t)(T^*\mathcal{Q}\times\mathbb{R}) = T^*\mathcal{Q}|_{Q,P}\times\mathbb{R}$, respectively. Of course, there is a relation: $T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R}\simeq T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R}$, and it implies that $T\mathcal{Q}|_{Q\,,\dot{Q}}\times T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R}$ is equivalent to $T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R}$ and $T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R}$.

Second, we define a Lagrangian in the space $T\mathcal{Q}|_{Q\,,\dot{Q}}\times T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R}$, denoted by L_T, which corresponds to the total Hamiltonian H_T, as follows:

$$\begin{aligned} L_T &:= \sigma_\tau^*(t)\left[P_I\dot{Q}^I + \Theta_a\dot{\Theta}^a - H_T(\Theta^a\,,\Theta_a\,,Q^I\,,P_I)\right] \\ &= P_I(t)\dot{Q}^I(t) - H_T(\Theta^a(t)=\epsilon^a\,,\Theta_a(t)=\epsilon_a\,,Q^I(t)\,,P_I(t))\,. \end{aligned} \tag{3.69}$$

That is, $L = L_T$ and $P_I(t)$ are introduced by Eq (3.67). Here, $\sigma_\tau^*(t)(dX/ds) = d(\sigma_\tau^*(t)X)/d(\sigma_\tau^*(t)s) = dX(t)/dt$ is applied, replacing X by Q^I and Θ^a. This leads to $\sigma_\tau^*(t)\dot{\Theta}^a = \sigma_\tau^*(t)\{\Theta^a\,,H_T\}_{P.b.} = \sigma_\tau^*(t)F^a(\Theta) = F^a(\sigma_\tau^*(t)\Theta) = constant$, where $F^a(\Theta)$ denote a function depending only on the constraint coordinates: Θ^a and Θ_a. It is used also that, for $\tau\in\{1\,,3\}$, all of Ξ^α and Ψ_α in the Shanmugadhasan-Maskawa-Nakajima theorem turn into second-class by virtue of the gauge fixing conditions. Based on this, these variables are gathered together into Θ^a and Θ_a. The Lagrangian L_T is uniquely determined by its construction up to surface terms. Let us define the pullback of "*total Lagrangian*" by $\sigma_\tau^*(t)$ as in the above. Taking into account the $\kappa|_{\sigma_\tau(t)}$, it suggests that the following map is a well-defined and invertible map:

$$\mathfrak{O}|_{\sigma_\tau(t)}:\ \mathfrak{G}[T(T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R})]\to\mathfrak{G}[T(T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R})];\ X_t|_{Q\,,\dot{Q}}\mapsto{}_*X_t|_{Q\,,P} \tag{3.70}$$

where $X_t|_{Q\,,\dot{Q}}$ and ${}_*X_t|_{Q\,,P}$ are Hamiltonian vector fields restricted to $T(T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R})$ and $T(T^*\mathcal{Q}|_{Q\,,P}\times\mathbb{R})$, respectively, and these corresponds in a one-to-one manner.

Finally, let us consider the map ι. When varied, Eq (3.69) becomes as follows;

$$\delta L_T = \left[\dot{Q}^I - \frac{\partial H_T}{\partial P_I}\right]\delta P_I + \left[-\dot{P}_I - \frac{\partial H_T}{\partial Q^I}\right]\delta Q^I + \frac{d}{dt}\left[P_I\delta Q^I\right] \tag{3.71}$$

where the argument t in $Q^I(t)$ and $P_I(t)$ are abbreviated. In the form of action functional, it can be written as follows:

$$\delta\left(\sigma_\tau^*(t)I\right) = \int_{t_1}^{t_2}\left[\dot{Q}^I - \frac{\partial H_T}{\partial P_I}\right]\delta P_I dt + \left[-\dot{P}_I - \frac{\partial H_T}{\partial Q^I}\right]\delta Q^I dt + \left[P_I\delta Q^I\right]_{t_1}^{t_2}\,. \tag{3.72}$$

In the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}$, the formulas in Eq (3.67) or the invertible map $\kappa|_{\sigma_\tau(t)}$ can be used. Therefore, the above formula becomes as follows:

$$\delta\left(\sigma_\tau^*(t)I\right) = \int_{t_1}^{t_2} \left[\dot{Q}^I - \frac{\partial H_T}{\partial P_I}\right] \delta P_I dt + \left[-\frac{d}{dt}\left(\frac{\partial L_T}{\partial \dot{Q}^I}\right) - \frac{\partial H_T}{\partial Q^I}\right] \delta Q^I dt + \left[\frac{\partial L_T}{\partial \dot{Q}^I}\delta Q^I\right]_{t_1}^{t_2} . \tag{3.73}$$

The one-to-one correspondence between $\sigma_\tau^*(t)H_T$ and L_T indicates that

$$\sigma_\tau^*(t)H_T := P_I\dot{Q}^I - L_T(Q^I, \dot{Q}^I) \tag{3.74}$$

in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}$ under Eq (3.67). Therefore, Eq (3.73) becomes as follows:

$$\delta\left(\sigma_\tau^*(t)I\right) = \int_{t_1}^{t_2} \left[-\frac{d}{dt}\left(\frac{\partial L_T}{\partial \dot{Q}^I}\right) + \frac{\partial L_T}{\partial Q^I}\right] \delta Q^I dt + \left[\frac{\partial L_T}{\partial \dot{Q}^I}\delta Q^I\right]_{t_1}^{t_2} , \tag{3.75}$$

which is now defined in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R}$. The second condition of Eq (3.67) implies that L_T is non-degenerate. Therefore, the boundary conditions are given as follows:

$$\delta Q^I(t_1) = \delta Q^I(t_2) = 0 . \tag{3.76}$$

Here, notice that in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R}$ this system always holds the Frobenius integrability based on the consideration given in Section 3.3. In this formulation, map ι can be introduced in a well-defined manner as an invertible map automatically:

$$\iota|_{\sigma_\tau} : \mathcal{Q}|_Q[t_1] \times \mathcal{Q}|_Q[t_2] \to \mathcal{C}|_{\sigma_\tau};\ (Q^I(t_1), Q^I(t_2)) \mapsto c^{A'} , \tag{3.77}$$

where $\mathcal{Q}|_Q[t]$ is the configuration subspace restricted by the canonical embedding σ_τ and $\mathcal{C}|_{\sigma_\tau}$ is a parameter space spanned by the independent integral constants restricted by all the constraints. A' runs from 1 to the twice number of Q^I. Therefore, based on Definition 1, $\delta\left(\sigma_\tau^*(t)I\right) := 0$ is the well-posed variational principle.

Summarising, the well-posed variational principle is

$$\delta\left(\sigma_{\tau}^{*}(t)I\right) := 0 \tag{3.78}$$

under the boundary condition (3.76).

3.7. Well-posed variational principle 2: Cases of quasi-canonical embeddings

In this section, based on Definition 1 and the quasi-canonical embeddings, $\tilde{\sigma}_1(t)$ and $\tilde{\sigma}_3(t)$, which are introduced in the previous section 3.5, the well-posed variational principle for a system that includes first-class constraints without any gauge fixing conditions is formulated [Tomonari (2023b)]. Hereinafter, we abbreviate the notation of " $_*$ " for the phase space variables if it is apparent. First of all, let us consider the case of $\tilde{\sigma}_3(t)$. The same considerations are applicable to $\tilde{\sigma}_1(t)$.

The quasi-canonical embedding $\tilde{\sigma}_3(t)$ leads to $\tilde{\sigma}_3^{*}(t)(T^{*}\mathcal{Q}\times\mathbb{R}\,,\Omega) = (T^{*}\mathcal{Q}|_{\Xi\,,\Psi}\times T^{*}\mathcal{Q}|_{Q\,,P}\times\mathbb{R}\,,\Omega_{Q\,,P}(t)+\Omega_{\Psi\,,\Xi}(t) = dQ^{I}(t)\wedge dP_{I}(t) + d\Xi^{\alpha}(t)\wedge d\Psi_{\alpha}(t))$. For $T^{*}\mathcal{Q}|_{\Xi\,,\Psi}\times T^{*}\mathcal{Q}|_{Q\,,P}\times\mathbb{R}$, a function $L = L(\Xi^{\alpha}(t)\,,R^{\alpha}(t)\,,Q^{I}(t)\,,\dot{Q}^{I}(t)\,,t)$ defined in $T\mathcal{Q}|_{\Xi\,,R}\times T\mathcal{Q}|_{Q\,,\dot{Q}}\times\mathbb{R}$ such that

$$\frac{\partial L}{\partial R^{\alpha}(t)} = \Psi_{\alpha}(t) = constant \tag{3.79}$$

can be introduced, but, of course,

$$\frac{\partial \Psi_{\alpha}(t)}{\partial R^{\beta}(t)} = 0\,. \tag{3.80}$$

This indicates that invertible map κ does not exist even if the entire phase space $T^{*}\mathcal{Q}\times\mathbb{R}$ is restricted to the subspace $\tilde{\sigma}_3^{*}(t)(T^{*}\mathcal{Q}\times\mathbb{R})$. However, if $T^{*}\mathcal{Q}\times\mathbb{R}$ is restricted to $T^{*}\mathcal{Q}|_{Q,P}\times\mathbb{R}$, then P_I and $\dot{Q}^{I}$ correspond to one another in a one-to-one manner. Then an invertible map

$\kappa|_{\tilde{\sigma}_3(t)}$ between $T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R}$ and $T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}$ is introduced as follows:

$$\kappa|_{\tilde{\sigma}_3(t)} : T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R} \to T^*\mathcal{Q}|_{Q,P} \times \mathbb{R};\ \dot{Q}^I(t) \mapsto P_I(t) \tag{3.81}$$

in a well-defined manner. In addition, under the same restriction of the phase space $T^*\mathcal{Q}\times\mathbb{R}$, an invertible map $\mathfrak{O}|_{\tilde{\sigma}_3(t)} : \mathfrak{G}[T(T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R})] \to \mathfrak{G}[T(T^*\mathcal{Q}|_{Q,P} \times \mathbb{R})]$; $X_t|_{Q,\dot{Q}} \mapsto {}_*X_t|_{Q,P}$ is introduced in a well-defined manner.

Now, let us consider the map ι. The pullback of the total Lagrangian by $\tilde{\sigma}_3(t)$ corresponding to the total Hamiltonian H_T is defined as follows:

$$\begin{aligned} L_T =& P_I(t)\dot{Q}^I(t) + \Psi_\alpha(t)\dot{\Xi}^\alpha(t) + \Theta_a(t)\dot{\Theta}^a(t) \\ &- H_T(\Xi^\alpha(t)\,, \Psi_\alpha(t) = \epsilon_\alpha\,, \Theta^a(t) = \epsilon^a\,, \Theta_a(t) = \epsilon_a\,, \zeta^{\alpha_1}\,, Q^I(t)\,, P_I(t)) \\ =& P_I(t)\dot{Q}^I(t) - H_T(\Xi^\alpha(t)\,, \Psi_\alpha(t) = \epsilon_\alpha\,, \Theta^a(t) = \epsilon^a\,, \Theta_a(t) = \epsilon_a\,, \zeta^{\alpha_1}\,, Q^I(t)\,, P_I(t)) + \frac{d}{dt}\left[\Psi_\alpha(t)\Xi^\alpha(t)\right] \end{aligned} \tag{3.82}$$

in the space $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times T\mathcal{Q}|_{\Xi,\dot{\Xi}} \times T^*\mathcal{Q}|_{\Xi,\Psi} \times \mathbb{R}$, where α_1 denotes the indices that correspond to the *primary* first-class constraints. Remark that Condition (3.67) on Q^I and P_I holds in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}$ as well. ζ^α are Lagrange multipliers and α runs from 1 to the number of the *primary* first-class constraints. Hereinafter, the argument t in $Q^I(t)$, $P_I(t)$, $\Xi^\alpha(t)$ and $\Psi_\alpha(t)$ is abbreviated. Since P_I and $\dot{Q}^I$ have the one-to-one correspondence by virtue of $\det(\partial P_I/\partial \dot{Q}^J) \neq 0$ in Eq (3.67), when varying Eq (3.82) in the action functional form, it becomes as follows:

$$\begin{aligned} \delta\left(\tilde{\sigma}_3^*(t) I\right) = \int_{t_1}^{t_2} & \left[\dot{Q}^I - \frac{\partial H_T}{\partial P_I}\right]\delta P_I dt + \left[-\dot{P}_I - \frac{\partial H_T}{\partial Q^I}\right]\delta Q^I dt \\ & - \frac{\partial H_T}{\partial \Xi^\alpha}\delta\Xi^\alpha dt - \frac{\partial H_T}{\partial \zeta^{\alpha_1}}\delta\zeta^{\alpha_1} dt + \left[P_I\delta Q^I + \Psi_\alpha\delta\Xi^\alpha\right]_{t_1}^{t_2}. \end{aligned} \tag{3.83}$$

Note, here, that $\partial H_T/\partial\zeta^{\alpha_1}$ correspond to the pullback of the primary first-class constraints by $\tilde{\sigma}_3(t)$. Therefore, we get

$$
\begin{aligned}
\delta\left(\tilde{\sigma}_3^*(t)I\right) = &\int_{t_1}^{t_2}\left[-\frac{d}{dt}\left(\frac{\partial L_T}{\partial \dot{Q}^I}\right)+\frac{\partial L_T}{\partial Q^I}\right]\delta Q^I dt + \frac{\partial L_T}{\partial \Xi^{\alpha'}}\delta\Xi^{\alpha'}dt + \left[\frac{\partial L_T}{\partial \dot{Q}^I}\delta Q^I + \Psi_{\alpha'}\delta\Xi^{\alpha'}\right]_{t_1}^{t_2} \\
&+\int_{t_1}^{t_2}\frac{\partial L_T}{\partial \Xi^{\alpha_1}}\delta\Xi^{\alpha_1}dt + \frac{\partial L_T}{\partial \zeta^{\alpha_1}}\delta\zeta^{\alpha_1}dt + \left[\Psi_{\alpha_1}\delta\Xi^{\alpha_1}\right]_{t_1}^{t_2}
\end{aligned}
\tag{3.84}
$$

in the subspace $T\mathcal{Q}|_{Q,\dot{Q}}\times T\mathcal{Q}|_{\Xi,\dot{\Xi}}\times T^*\mathcal{Q}|_{\Xi,\Psi}\times\mathbb{R}$, where we used the one-to-one correspondence between $\dot{Q}^I$ and P_I which is described by $\kappa|_{\tilde{\sigma}_3(t)}$. α' denotes the indices that eliminate the range of α_1 form $\{1\,,2\,,\cdots\,,U\}$. Notice that in this subspace the symplectic structure breaks down: $\Omega_{Q\,,P}(t)$ satisfies the definition (3.52), but so is not $\Omega_{\Xi\,,\Psi}(t)$ as mention in Section 3.5. Here, let us define the "*effective first-order variation*" of the action functional as follows:

$$
\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t)I\right) := \int_{t_1}^{t_2}\left[-\frac{d}{dt}\left(\frac{\partial L_T}{\partial \dot{Q}^I}\right)+\frac{\partial L_T}{\partial Q^I}\right]\delta Q^I dt + \frac{\partial L_T}{\partial \Xi^{\alpha'}}\delta\Xi^{\alpha'}dt + \left[\frac{\partial L_T}{\partial \dot{Q}^I}\delta Q^I + \Psi_{\alpha'}\delta\Xi^{\alpha'}\right]_{t_1}^{t_2}. \tag{3.85}
$$

The coordinate variables Q^I and $\Xi^{\alpha'}$ are now independent. The reason why the terms concerning primary first-class constraints are split out will be revealed soon. Therefore, to vanish the effective first-order variation, all the position variables Q^I have to be fixed at both $t = t_1$ and $t = t_2$ as boundary conditions:

$$
\delta Q^I(t_2) = \delta Q^I(t_1) := 0 \tag{3.86}
$$

and, since $\Psi_{\alpha'}$ are constant, we have to impose

$$
\delta\Xi^{\alpha'}(t_2) = \delta\Xi^{\alpha'}(t_1)\,. \tag{3.87}
$$

Taking into account the equations of motion $\dot{\Xi}^{\alpha'} = \{\Xi^{\alpha'}\,,H_T\}_{P.b.}$, appropriate boundary conditions for these variables $\Xi^{\alpha'}$ have to be either

$$\delta\Xi^{\alpha'}(t_1) := 0\,, \tag{3.88}$$

then $\delta\Xi^{\alpha'}(t_2) = 0$ are automatically satisfied, or

$$\delta\Xi^{\alpha'}(t_2) := 0\,, \tag{3.89}$$

then $\delta\Xi^{\alpha'}(t_1) = 0$ are automatically satisfied, since each solution of $\dot{\Xi}^{\alpha'} = \{\Xi^{\alpha'}\,, H_T\}_{P.b.}$ has one integral constant, respectively. That is, each solution with a given integral constant on a boundary determines the value on the other boundary. Therefore, Eq (3.87) is satisfied and becomes zero if either Eq (3.88) or Eq (3.89) is imposed. In this work, we adopt the first choice; this choice is none other than setting initial conditions. Here, notice that for L_T on $T\mathcal{Q}|_{Q\,,\dot{Q}} \times T\mathcal{Q}|_{\Xi\,,\dot{\Xi}} \times \mathbb{R}$ the Frobenius integrability (3.43) has to be imposed. That is,

$$\theta_I(X_T) = \delta_I{}^i \zeta^{\alpha_1} \tau^{\alpha}_{\alpha_1} K_{ij} \frac{\partial \eta^j}{\partial \dot{\Xi}^{\alpha}} :\approx 0\,, \tag{3.90}$$

where I runs the range of indices eliminating the ones for the second-class constraint coordinates, τ^{α}_{β} are zero-eigenvalue vectors of the kinetic matrix, and $\eta^i \approx \left(K^{-1}\right)^{ij} S_j$. Remark that the $(I\,, J)$-block of the kinetic matrix is non-degenerate. In contrast, for $\tilde{\sigma}^*_3(t)H_T$ on $T^*\mathcal{Q}|_{Q\,,P} \times T^*\mathcal{Q}|_{\Xi\,,\Psi} \times \mathbb{R}$, the Frobenius integrability (3.43) is automatically satisfied as follows:

$${}_*\theta_I({}_*X_T) = -\delta_{I\alpha}\zeta^{\alpha_1}\frac{\partial \Psi_{\alpha_1}}{\partial \Xi^{\alpha}} - \delta_{IJ}\zeta^{\alpha_1}\frac{\partial \Psi_{\alpha_1}}{\partial Q^J} \approx 0\,, \tag{3.91}$$

since Ξ^{α} and Ψ_{α} form a part of the entire canonical coordinate system and all Ψ_{α} are canonical momentum variables with respect to Ξ^{α}, respectively.

In order to introduce the map ι in a well-defined manner, the following two conditions have to be taken into account; The first is that if gauge fixing conditions are imposed then $\tilde{\sigma}_3(t)$ turns into $\sigma_3(t)$; The second is that the dimension of a parameter space that is spanned by all independent integral constants is up to $2N-2V-U$. Then the map ι can be introduced as follows:

$$\iota|_{\tilde{\sigma}_3} : \mathcal{Q}|_{Q\,,\Xi}[t_1] \times \mathcal{Q}|_{Q}[t_2] \to \mathcal{C}|_{\tilde{\sigma}_3};\ (Q^I(t_1)\,, \Xi^{\alpha'}(t_1)\,, Q^I(t_2)) \mapsto c^{A'}\,, \tag{3.92}$$

$\delta\Xi^{\alpha'}(t_2) = 0$ are automatically satisfied, where $\mathcal{Q}|_Q$ and $\mathcal{Q}|_{Q\,,\Xi}$ are the configuration subspace of $T^*\mathcal{Q}|_{Q\,,P}$ and $T^*\mathcal{Q}|_{Q\,,P} \times T^*\mathcal{Q}|_{\Xi\,,\Psi}$, respectively, and $\mathcal{C}|_{\tilde{\sigma}_3}$ is the parameter space spanned by the independent integral constants restricted by all the constraints. A' runs from 1 to the sum of twice number of Q^I and $\Xi^{\alpha'}$. Then map ι is invertible. Therefore, based on Definition 1, $\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t)I\right) := 0$ is the well-posed variational principle.

Under the well-posed variational principle $\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t)I\right) := 0$ with the boundary conditions (3.86) and (3.88), the original first-order variation of the action functional (3.84) becomes as follows:

$$\delta\left(\tilde{\sigma}_3^*(t)I\right) = \int_{t_1}^{t_2} \frac{\partial L_T}{\partial \Xi^{\alpha_1}}\delta\Xi^{\alpha_1}dt + \frac{\partial L_T}{\partial \zeta^{\alpha_1}}\delta\zeta^{\alpha_1}dt + \left[\Psi_{\alpha_1}\delta\Xi^{\alpha_1}\right]_{t_1}^{t_2}\,. \tag{3.93}$$

Applying the variational principle: $\delta\left(\tilde{\sigma}_3^*(t)I\right) := 0$, we derive

$$\frac{\partial L_T}{\partial \Xi^{\alpha_1}} = -\frac{\partial H_T}{\partial \Xi^{\alpha_1}} = 0 \tag{3.94}$$

if the following equations are identically satisfied:

$$\frac{\partial L_T}{\partial \zeta^{\alpha_1}} = -\frac{\partial H_T}{\partial \zeta^{\alpha_1}} = \Psi_{\alpha_1}(t) = 0\,. \tag{3.95}$$

In fact, the boundary conditions $\delta\Xi^{\alpha_1}(t_2) = \delta\Xi^{\alpha_1}(t_1)$ are not satisfied since $\dot{\Xi}^{\alpha_1} = \{\Xi^{\alpha_1}\,, H_T\}_{P.b.} \approx$

$\zeta^{\alpha_1} + f(Q^I\,, P_I)$ leads to

$$\delta\Xi^{\alpha_1}(t_2) - \delta\Xi^{\alpha_1}(t_1) = \delta \int_{t_1}^{t_2} \left[\zeta^{\alpha_1} + f(Q^I, P_I)\right] dt = \delta \int_{t_1}^{t_2} \zeta^{\alpha_1} dt\,, \tag{3.96}$$

where f is the definite function determined by H_T and we used the fact that the integral on the interval $t_1 \leq t \leq t_2$ of f has a definite value since Q^I and P_I are propagating degrees of freedom and the equations of motion for these variables are already derived by virtue of the well-posed variational principle $\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t)I\right) := 0$. This result indicates that the configurations corresponding to the *primary* first-class constraints cannot be fixed on the boundaries. Therefore, we have to impose $\Psi_{\alpha_1}(t) = constant = 0$ in advance and this means that the existence of first-class constraints restricts the possible embedding $\tilde{\sigma}_3(t)$. Therefore, Eq (3.93) becomes as follows:

$$\delta\left(\tilde{\sigma}_3^*(t)I\right) = \int_{t_1}^{t_2} \frac{\partial L_T}{\partial \Xi^{\alpha_1}} \delta\Xi^{\alpha_1} dt\,. \tag{3.97}$$

The variational principle, $\delta\left(\tilde{\sigma}_3^*(t)I\right) := 0$, derives the equations of motion, $\partial L_T/\partial\Xi^{\alpha_1} = 0$, *without any boundary condition*. Under this assumption, if the effective first-order variation vanishes: $\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t)I\right) := 0$, the variational principle is applied to the entire phase space, and vice versa. As another aspect, it would be convenient to introduce the "*effective-total Hamiltonian*" as follows:

$$H_{\text{effective}} := H_T|_{\Psi_{\alpha_1} := 0}\,. \tag{3.98}$$

For this $H_{\text{effective}}$, repeating the same consideration going back to Eq (3.82), Eq (3.85) is directly derived. Of course, the appropriate boundary conditions are given by Eq (3.86) and Eq (3.88).

There is a remark. Eq (3.82) can be rewritten as follows:

$$L'_T(Q^I\,, P_I\,, \Xi^\alpha\,, \Psi_\alpha) := P_I\dot{Q}^I - \tilde{\sigma}_3^*(t) H_T \tag{3.99}$$

where

$$L'_T = L_T - \frac{d}{dt}\left[\Psi^\alpha \Xi_\alpha\right]\,, \tag{3.100}$$

and we abbreviatied Θ^a and Θ_a. L'_T in Eq (3.100) has the arbitrariness of continuous infinite since Ψ^α can be regarded as continuous parameters. In other words, L'_T is parametrized by Ψ^α. The arbitrariness is not the one deriving from a canonical transformation on $T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}$. That is, for a total Hamiltonian H_T, the corresponding Lagrangian is not uniquely determined, unlike the case of canonical embeddings. It is another aspect of the absence of the inverse map $\mathfrak{D}^{-1}$ in the entire space $T^*\mathcal{Q} \times \mathbb{R}$.

Summarising, the well-posed variational principle is

$$\delta_{\text{effective}}\left(\tilde{\sigma}_3^*(t) I\right) := 0 \tag{3.101}$$

under the boundary conditions (3.86) and (3.88). The important result is that the configurations corresponding to the *primary* first-class constraint coordinates never be fixed on the boundaries until some gauge fixing conditions are imposed.

3.8. Examples

In this section, the difficulties in the examples given in Section 3.1 are resolved by applying the theory that is established throughout this chapter [Izumi et al. (2023); Tomonari (2023b)]. Hereinafter, we abbreviate the notation of " $_*$ " for the phase space variables if it is apparent.

The first examples is the Lagrangian L_1 in Eq (3.1):

$$L_1 = \frac{1}{2}\dot{x}^2 + \frac{1}{2}\dot{y}^2 + \lambda(x+y)\,. \tag{3.102}$$

The kinetic matrix is

$$K = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\,, \tag{3.103}$$

where the following canonical momentum variables are used: $p_1 = \dot{x}$, $p_2 = \dot{y}$, $p_\lambda = 0$. Remark that the Lagrange multiplier λ is regarded as a configuration variable. Since the rank of the kinetic matrix is 2, there is a primary constraint as follows:

$$\phi^{(1)} = p_\lambda := 0\,. \tag{3.104}$$

The total Hamiltonian is given as follows:

$$H_T = H_0 + \zeta\phi^{(1)}\,, \quad H_0 = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 - \lambda(x+y)\,. \tag{3.105}$$

The Dirac-Bergmann procedure derives a secondary, a tertiary, and a quaternary constraint as follows:

$$\begin{aligned} \phi^{(2)} &= x + y := 0\,, \\ \phi^{(3)} &= \frac{1}{2}(p_x + p_y) := 0\,, \\ \phi^{(4)} &= \lambda := 0\,. \end{aligned} \tag{3.106}$$

The consistency for $\phi^{(4)}$ is automatically satisfied. Therefore, the procedure stops here. The Poisson brackets are $\{\phi^{(1)}\,, \phi^{(4)}\}_{P.b.} = 1$, $\{\phi^{(2)}\,, \phi^{(3)}\}_{P.b.} = 1$, otherwise vanish; all constraints are classified into second-class constraint and the propagating degrees of freedom of the system is $(3 \times 2 - 4)/2 = 1$. The Shanmugadhasan-Maskawa-Nakajima theorem indicates that the system has a canonical transformation from the original coordinates to the ones such that a part of the entire canonical coordinates are represented by the linear combination of the second-class constraints. In fact, the symplectic 2-form is computed as follows:

$$\Omega = dq^i \wedge dp_i = dQ \wedge dP + \Theta^a \wedge \Theta_a \,, \tag{3.107}$$

where Q, P, Θ^a, and Θ_a $(a \in \{1\,,2\})$ are defined as follows:

$$\begin{aligned} &Q = \frac{1}{2}(x - y)\,, \quad P = p_x - p_y \\ &\Theta^1 = \phi^{(4)}\,, \quad \Theta_1 = \phi^{(1)} \\ &\Theta^2 = \phi^{(2)}\,, \quad \Theta_2 = \phi^{(3)}\,. \end{aligned} \tag{3.108}$$

Notice that the second equality of Ω is the strong equality, not weak equality. In terms of these canonical variables, the total Hamiltonian is transformed as follows:

$$H_T = \frac{1}{4}P^2 + (\Theta_2)^2 - \Theta^1\Theta^2\,. \tag{3.109}$$

The pullback of total Lagrangian by the canonical embedding $\sigma_2(t)$ is derived as follows:

$$\begin{aligned} L_T &= \sigma_2^*(t)\left[P\dot{Q} + \Theta^a\dot{\Theta}_a - H_T\right] \\ &= P\dot{Q} - \frac{1}{4}P^2 - (\Theta_2)^2 - \Theta^1\Theta^2\,, \\ \therefore L_T &= P\dot{Q} - \frac{1}{4}P^2 + constant\,, \end{aligned} \tag{3.110}$$

which is defined in the subspace $T\mathcal{Q}|_{Q\,,\dot{Q}} \times T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}$. Here, we abbreviated the pullback operator $\sigma_2^*(t)$, which is defined in Section 3.5, in the second and the last line. Remark that the pullback of H_T by $\sigma_2(t)$ above is defined in the symplectic submanifold $(T^*\mathcal{Q}|_{Q\,,P} \times$

$\mathbb{R}\,, \Omega_{Q\,,P} = dQ \wedge dP$). This system is Frobenius integrable as mentioned in Section 3.6. In fact, it can be shown that this system has a unique solution.

The first-order variation of the action functional is calculated as follows:

$$\delta(\sigma_2^*(t)I) = \int_{t_1}^{t_2} \left[-\frac{1}{2}P + \dot{Q} \right] \delta P\, dt + \left[-\dot{P} \right] \delta Q\, dt + [P\delta Q]_{t_1}^{t_2} \, . \tag{3.111}$$

The appropriate boudnary conditions are set as follows:

$$\delta Q(t_2) = \delta Q(t_1) := 0 \tag{3.112}$$

Then the variational principle leads to the following equations:

$$-\frac{1}{2}P + \dot{Q} = 0\,, \quad -\dot{P} = 0\,. \tag{3.113}$$

The first equation gives the explicit form the canonical momentum variable P. Therefore, L_T is rewritten as follows:

$$L_T = 2\dot{Q}^2 + constant\,, \tag{3.114}$$

which is now defined in the subspace $T\mathcal{Q}|_{Q\,,\dot{Q}} \times \mathbb{R}$. It indicates that the system is always Frobenius integrable as mentioned in Section 3.6 and that two integral constants exist. In fact, L_T is nothing but describing the uniform motion in a straight line. The equation of motion is given as follows:

$$-2\ddot{Q} = 0\,. \tag{3.115}$$

This equation has a unique solution: $Q(t) = At + B$, where A and B are integral constants and the boundary conditions uniquely determine these constants. The fundamental maps are given as follows: $\kappa|_{\sigma 2(t)} : T\mathcal{Q}|_{Q\,,\dot{Q}} \to T\mathcal{Q}|_{Q\,,P}$; $\dot{Q} \mapsto P$ and $\mathfrak{D}|_{\sigma 2(t)} : X_t = Q(\partial/\partial\dot{Q}) + \dot{Q}(\partial/\partial Q) + (\partial/\partial t) \mapsto {}_*X_t = (\partial H_T/\partial P)(\partial/\partial Q) - (\partial H_T/\partial Q)(\partial/\partial P) + (\partial/\partial t)$, where $H_T =$

$P^2/4+constant$; these are introduced in a well-defined manner and invertible. The invertible map ι is $\iota|_{\sigma_3(t)}$: $\mathcal{Q}|_Q[t_1] \times \mathcal{Q}|_Q[t_2] \to \mathcal{C}|_{\sigma_3(t)}$; $(Q(t_1)\,, Q(t_2)) \mapsto (A\,, B)$ with $A = (Q(t_1 - Q(t_2))/(t_1 - t_2)$ and $B = (t_1 Q(t_2) - t_2 Q(t_1))/(t_1 - t_2)$.

The second example is the Lagrangian L_2 in Eq (3.1):

$$L_2 = \dot{q}^1 \dot{q}^3 + \frac{1}{2} q^2 (q^3)^2 \,. \tag{3.116}$$

This model has no propagating degrees of freedom but is historically crucial; it was proposed as a counter-example for the Dirac conjecture [Dirac (1950)]. The kinetic matrix K is

$$K = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \,, \tag{3.117}$$

where the following canonical momentum variables are used: $p_1 = \dot{q}^3\,, p_2 = 0\,, p_3 = \dot{q}^1$. There is a primary constraint due to rank $K = 2$:

$$\phi^{(1)} = p_2 := 0 \,. \tag{3.118}$$

The total Hamiltonian is derived as follows:

$$H_T = H_0 + \zeta \phi^{(1)} \,, \quad H_0 = p_1 p_3 - \frac{1}{2} q^2 (q^3)^2 \,. \tag{3.119}$$

The Dirac-Bergmann procedure generates a secondary and a tertiary constraint as follows:

$$\begin{aligned}
&\dot{\phi}^{(1)} = \{\phi^{(1)}\,, H_T\}_{P.b.} \approx \frac{1}{2}(q^3)^2 \\
&\therefore \phi^{(2)} = q^3 := 0\,, \\
&\phi^{(3)} = \dot{\phi}^{(2)} = \{\phi^{(2)}\,, H_T\}_{P.b.} \approx p_1 \\
&\therefore \phi^{(3)} = p_1 := 0\,.
\end{aligned} \tag{3.120}$$

$\dot{\phi}^{(3)} \approx 0$ is automatically satisfied. All $\phi^{(1)}$, $\phi^{(2)}$, and $\phi^{(3)}$ are classified into first-class constraint: all Poisson brackets among them vanish. The Shanmugadhasan-Maskawa-Nakajima theorem indicate that this system has a canonical transformation from the original coordinates to the ones such that a part of their canonical momenta themselves are the first-class constraints. In fact, the symplectic 2-form of the system is computed as follows:

$$\Omega = dq^i \wedge dp_i = d\Xi^\alpha \wedge d\Psi_\alpha\,, \tag{3.121}$$

where Ξ^α and Ψ_α are defined as follows:

$$\begin{aligned}
&\Xi^1 = q^1\,, \quad \Xi^2 = q^2\,, \quad \Xi^3 = -p_3 \\
&\Psi_1 = \phi^{(3)}\,, \quad \Psi_2 = \phi^{(1)}\,, \quad \Psi_3 = \phi^{(2)}\,.
\end{aligned} \tag{3.122}$$

Notice that the second equality in the equation of Ω is the strong equality, not weak equality. The total Hamiltonian is transformed as follows:

$$H_T = -\Psi_1 \Xi^3 - \frac{1}{2}\Xi^2(\Psi_3)^2 + \zeta\Psi_2\,. \tag{3.123}$$

This system is always Frobenius integrable as mentioned in the section 3.3. In fact, Eq (3.41) can be computed as follows:

$$
\begin{aligned}
{}_*\theta_\alpha({}_*X_T) =& \left(d\Psi_\alpha + \frac{\partial H}{\partial \Xi^\alpha}dt\right)\left(X_H + \zeta X_{\Psi_2} + \frac{\partial}{\partial t}\right) \\
=& d\Psi_\alpha(X_H) + d\Psi_\alpha(\zeta X_{\Psi_2}) + \frac{\partial H}{\partial \Xi^\alpha} \\
\approx& \{\Psi_\alpha\,, H\} + \zeta\{\Psi_\alpha\,, \Psi_2\} + \frac{\partial H}{\partial \Xi^\alpha} \\
=& 0\,, \\
&\therefore {}_*\theta_\alpha({}_*X_T) \approx 0\,.
\end{aligned}
\tag{3.124}
$$

Therefore, the system has six integral constants, of which three integral constants are occupied by the consistency conditions of the constraints. Therefore, the remaining three independent integral constants, which originated from the three equations: $\dot{\Xi}^1 = -\Xi^3$, $\dot{\Xi}^2 = \zeta$, and $\dot{\Xi}^3 = -\Xi^2\Psi_3$, have to be fixed by imposing boundary conditions in the variational principle. There are a possible quasi-canonical embedding $\tilde{\sigma}_1(t)$ and a possible canonical embedding $\sigma_1(t)$, which are defined in Sections 3.6 and 3.7, respectively.

We derive the pullback of total Lagrangian L_T by $\tilde{\sigma}_1(t)$ and compute the first-order variation of the action functional for L_T. L_T is defined as follows:

$$
\begin{aligned}
&L_T := \tilde{\sigma}_1^*(t)\left[\Psi_\alpha\dot{\Xi}^\alpha - H_T\right] \\
&\therefore L_T = \Psi_1\Xi^3 + \frac{1}{2}\Xi^2(\Psi_3)^2 + \frac{d}{dt}\left(\Psi_{\alpha'}\Xi^{\alpha'}\right)\,,
\end{aligned}
\tag{3.125}
$$

which is defined in the space $T\mathcal{Q}|_{\Xi\,,\dot{\Xi}} \times \mathbb{R}$. Here, we abbreviated the pullback operator $\tilde{\sigma}_1^*(t)$, $\alpha' \in \{1\,, 3\}$, and we used $\tilde{\sigma}_1^*(t)\Psi_2 = 0$. Then the effective first-order variation is given as follows:

$$
\delta_{\text{effective}}(\tilde{\sigma}_1^*(t)I) = \Psi_1\int_{t_1}^{t_2} dt\delta\Xi^3 + \left[\Psi_1\delta\Xi^1 + \Psi_3\delta\Xi^3\right]_{t_1}^{t_2}\,. \tag{3.126}
$$

The appropriate boundary conditions are set as follows:

$$\delta\Xi^{\alpha'}(t_1) = 0\,, \tag{3.127}$$

then $\delta\Xi^{\alpha'}(t_2) = 0$ are automatically satisfied since each solution of the equations of motion for $\Xi^{\alpha'}$ is only one integral constant, respectively. That is, each solution gives a definite value at the boundary $t = t_2$. Then the variational principle for the effective first-order variation, $\delta_{\text{effective}}(\tilde{\sigma}_1^*(t)I) := 0$, leads to $\Psi_1 = 0$. In addition, $\delta(\tilde{\sigma}_1^*(t)I) := 0$ derives $\Psi_3 = 0$. Here, we abbreviated the pullback operator $\tilde{\sigma}_1^*(t)$. Remark that the Frobenius integrability condition (3.43) in Section 3.3 restricted to $\tilde{\sigma}_1^*(t)(T\mathcal{Q}\times\mathbb{R})$ is also satisfied, and there occurs no phase space reduction. It indicates that the six integral constants hold, of which the three constants are occupied by the consistency conditions, or equivalently the embedding $\tilde{\sigma}_1^*(t)$. This fact can be also led by that Eq (3.41) given in Section 3.3 is always satisfied in this system by virtue of a zero-eigenvector $\tau^i = (0\,,\tau^2\,,0)$ and $\eta^i \approx (0\,,\eta^2\,,0)$ where τ^2 and η^2 are arbitrary function in the space $T\mathcal{Q}|_{\Xi\,,\dot{\Xi}}\times\mathbb{R}$. Then the invertible map ι is $\iota|_{\tilde{\sigma}_3}\,:\,\mathcal{Q}|_{\Xi}[t_1]\,\rightarrow\,\mathcal{C}|_{\tilde{\sigma}_3};\,(\Xi^1(t_1)\,,\Xi^3(t_1))\,\mapsto\,(c^1\,,c^2)$. In fact, we have the two equations: $\dot{\Xi}^1 = -\Xi^3$ and $\dot{\Xi}^3 = 0$. Therefore, $c_1 = \Xi^1(t_1) - \Xi^3(t_1)t_1$, $c_2 = \Xi^3(t_1)$. Remark that $\kappa|_{\tilde{\sigma}_1(t)}$ and $\mathfrak{D}|_{\tilde{\sigma}_1(t)}$ do not exist in this case since this system does not have any dynamics. The remaining one integral constant is assigned for $\dot{\Xi}^2 = \zeta$; this constant is not determined until some gauge fixing conditions are imposed.

Next, let us impose the following gauge fixing conditions to all Ξ^α: $\dot{\Xi}^1 = -\Xi^3 := 0$, $\dot{\Xi}^2 = \zeta := 0$, and $\dot{\Xi}^3 = -\Xi^2\Psi_3 := 0$. The first and the third equations are automatically satisfied by virtue of $\Xi^\alpha \approx 0$ $(\alpha\in\{1\,,2\,,3\})$. The second equation is satisfied if and only if $\zeta := 0$. Remark that all these ingredients are derived in the entire space $T^*\mathcal{Q}|_{\Psi,\Xi}\times\mathbb{R}$: the target space of the embedding $\sigma_1(t)$. Then the pullback of total Lagrangian L_T by $\sigma_1(t)$ is introduced as follows:

$$L_T = \sigma_1^*(t)\left[\Psi_\alpha \dot{\Xi}^\alpha - H_T\right] = constant\,, \tag{3.128}$$

which is defined in the null subspace $\{0\} \times \mathbb{R}$. That is, this system does not describe any dynamics. Therefore, of course, $\kappa|_{\tilde{\sigma}_1(t)}$ and $\mathfrak{D}|_{\tilde{\sigma}_1(t)}$ do not exist. Map ι is in the same situation: all the integral constants, which are implied by Eq (3.41) given in Section 3.3 by virtue of the same reason as the previous paragraph, are occupied by the consistency conditions for Ψ_α and Ξ^α, or equivalently fixing the embedding $\sigma_1(t)$.

The third example is the Lagrangian L_3 in Eq (3.1):

$$L_3 = q^1\dot{q}^2 - q^2\dot{q}^1 - (q^1)^2 - (q^2)^2\,. \tag{3.129}$$

This model is an imitation of the Dirac system for spin 1/2-particles in field theory. The kinetic matrix K is

$$K = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}\,, \tag{3.130}$$

where the following canonical momentum variables are used: $p_1 = -q^2, p_2 = q^1$. There are two primary constraints due to $\mathrm{rank}\,K = 0$:

$$\phi_1^{(1)} = p_1 + q^2 := 0\,, \quad \phi_2^{(1)} = p_2 - q^1 = 0\,. \tag{3.131}$$

The Poisson bracket is $\{\phi_1^{(1)}, \phi_2^{(1)}\}_{P.b.} = 2$ and otherwise vanish. The total Hamiltonian is derived as follows:

$$H_T = H_0 + \zeta^\alpha \phi_\alpha^{(1)}\,, \quad H_0 = (q^1)^2 + (q^2)^2\,. \tag{3.132}$$

The Dirac procedure determines all Lagrange multipliers:

$$\zeta^1 \approx -q^2\,, \quad \zeta^2 \approx q^1\,. \tag{3.133}$$

Then the consistency conditions for $\phi^{(1)}\,, \phi^{(2)}$ are satisfied: $\dot{\phi}^{(1)} \approx 0\,, \dot{\phi}^{(2)} \approx 0$. That is, all constraints are classified into second-class constraints and the propagating degrees of freedom of the system is $(2 \times 2 - 2)/2 = 1$. The Shanmugadhasan-Maskawa-Nakajima theorem indicates that the system has a canonical transformation from the original coordinates to the ones such that a part of the entire canonical coordinates are represented by the linear combination of the second-class constraints. In fact, the symplectic 2-form is computed as follows:

$$\Omega = dq^i \wedge dp_i = dQ \wedge dP + d\Theta^1 \wedge d\Theta_1\,, \tag{3.134}$$

where Θ^1, Θ_1, Q and P are defined as follows:

$$\begin{aligned} &\Theta^1 = \frac{1}{\sqrt{2}}\phi_1^{(1)}\,, \quad \Theta_1 = \frac{1}{\sqrt{2}}\phi_2^{(1)}\,, \\ &Q = \frac{1}{\sqrt{2}}(q^1 + p_2)\,, \quad P = \frac{1}{\sqrt{2}}(p_1 - q^2)\,. \end{aligned} \tag{3.135}$$

Notice that the second equality in the equation of Ω is the strong equality, not weak equality. The total Hamiltonian is transformed as follows:

$$H_T = \frac{1}{2}P^2 + \frac{1}{2}Q^2 - \frac{1}{2}(\Theta^1)^2 - \frac{1}{2}(\Theta_1)^2\,. \tag{3.136}$$

The pullback of total Lagrangian by $\sigma_2(t)$ is derived as follows:

$$\begin{aligned} L_T =&\sigma_2^*(t)\left(\Theta_1\dot{\Theta}^1 + P\dot{Q} - H_T\right) \\ =&P\dot{Q} - \frac{1}{2}Q^2 - \frac{1}{2}P^2 + \frac{1}{2}(\Theta^1)^2 + \frac{1}{2}(\Theta_1)^2\,, \\ &\therefore L_T = P\dot{Q} - \frac{1}{2}Q^2 - \frac{1}{2}P^2 + constant\,, \end{aligned} \tag{3.137}$$

which is defined in the subspace $T\mathcal{Q}|_{Q\,,\dot{Q}} \times T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}$. Here, we abbreviated the pullback operator $\sigma_2^*(t)$, which is defined in Section 3.5, in the second and the last line. Remark that the pullback of H_T by $\sigma_2(t)$ above is defined in the symplectic submanifold $(T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}\,, \Omega_{Q\,,P} = dQ \wedge dP)$. This system is Frobenius integrable as mentioned in Section 3.6. In fact, it can be shown that this system has a unique solution.

The first-order variation of the action functional of L_T is computed as follows:

$$\delta\left(\sigma_2^*(t)I\right) = \int_{t_1}^{t_2} \left[-\dot{P} - Q\right] \delta Q\, dt + \left[\dot{Q} - P\right] \delta P\, dt + \left[P\delta Q\right]_{t_1}^{t_2} . \tag{3.138}$$

The appropriate boundary conditions are set as follows:

$$\delta Q(t_2) = \delta Q(t_1) := 0\,. \tag{3.139}$$

Then the variational principle leads to the following equations:

$$-\dot{P} - Q = 0\,, \quad \dot{Q} - P = 0\,. \tag{3.140}$$

The second equation gives the explicit form for the canonical momentum variable P. Therefore, L_T is rewritten as follows:

$$L_T = \frac{1}{2}(\dot{Q})^2 - \frac{1}{2}Q^2 + constant\,, \tag{3.141}$$

which is now defined in the subspace $T\mathcal{Q}|_{Q\,,\dot{Q}} \times \mathbb{R}$. It indicates that the system is always Frobenius integrable as mentioned in Section 3.6 and that two integral constants exist. In fact, L_T is nothing but describing the one-dimensional harmonic oscillator. The equation of motion is as follows:

$$-\ddot{Q} - Q = 0\,. \tag{3.142}$$

This equation has the unique solution $Q(t) = A\,\exp(+it) + B\,\exp(-it)$ and the boundary condition uniquely determines the integral constant $A\,, B$. The fundamental maps are given as follows: $\kappa|_{\sigma_2(t)} : T\mathcal{Q}|_{Q,\dot{Q}} \to T\mathcal{Q}|_{Q,P}$; $\dot{Q} \mapsto P$ and $\mathfrak{D}|_{\sigma_2(t)} : X_t = Q(\partial/\partial\dot{Q}) + \dot{Q}(\partial/\partial Q) + (\partial/\partial t) \mapsto {}_*X_t = (\partial H_T/\partial P)(\partial/\partial Q) - (\partial H_T/\partial Q)(\partial/\partial P) + (\partial/\partial t)$, where $H_T = Q^2/2 + P^2/2 + constant$; these are introduced in a well-defined manner and invertible. The invertible map ι is $\iota|_{\sigma_3(t)} : \mathcal{Q}|_Q[t_1] \times \mathcal{Q}|_Q[t_2] \to \mathcal{C}|_{\sigma_3(t)}$; $(Q(t_1), Q(t_2)) \mapsto (A, B)$ with $A = (Q(t_1)\exp(it_2) - Q(t_2)\exp(it_1))/2i\sin(t_2 - t_1)$ and $B = (Q(t_2)\exp(-it_1) - Q(t_1)\exp(-it_2))/2i\sin(t_2 - t_1)$.

The final example is the Lagrangian L_4 in Eq (3.1):

$$L_4 = -\frac{1}{2}q\ddot{q} - \frac{1}{2}q^2 \,. \tag{3.143}$$

For this system, applying the consideration given in Section 3.2, there exists the counter-term W given as follows:

$$W = \frac{1}{2}q\dot{q} + C(q)\,, \tag{3.144}$$

where $C(q)$ is an arbitrary function of q. Then L_4 becomes as follows:

$$L_4' = L_4 + \frac{dW}{dt} = \frac{1}{2}(\dot{q})^2 - \frac{1}{2}q^2 + \frac{\partial C}{\partial q}\dot{q}\,. \tag{3.145}$$

This is none other than the Lagrangian for a one-dimensional harmonic oscillator. In fact, the first-order variation of L_4':

$$\delta I' = \int_{t_1}^{t_2} (-\ddot{q} - q)\delta q dt + \frac{d}{dt}\left[\left(\dot{q} + \frac{\partial C}{\partial q}\right)\delta q\right]_{t_1}^{t_2} \tag{3.146}$$

and the well-posed variational principle under the Dirichlet boundary condition $\delta q(t_2) = \delta q(t_1) = 0$ leads to an equation: $-\ddot{q} - q = 0$. The solution is, of course, $q(t) = A\exp(+it) + B\exp(-it)$, where A, B are integral constants that are determined by the boundary conditions. For this trivial system, we apply the two different methodologies which are introduced in Section 2.5, to formulate the well-defined variational principle without any counter-term.

That is, (i) Ostrogradsky's original formulation and (ii) Pons' modified formulation.

Let us consider applying (i) Ostrogradsky's original formulation. The configuration space, denoted by $\mathcal{Q}$, in this method is coordinated by $Q_{(1)} = q$ and $Q_{(2)} = \dot{q}$. Then the corresponding canonical momenta are given as follows: $P^{(1)} = \partial L_4/\partial Q_{(2)} - (d/dt)(\partial L_4/\dot{Q}_{(2)}) = Q_{(2)}/2$ and $P^{(2)} = \partial L_4/\dot{Q}_{(2)} = -Q_{(1)}/2$. Therefore, the rank of the kinetic matrix $K^{(2)} = \partial P^{(2)}/\partial \dot{Q}_{(2)}$ is zero, and there is a primary constraint: $\phi^{(1)} = P^{(2)} + Q_{(1)}/2 := 0$. Then the total Hamiltonian is $H_T = P^{(1)}Q_{(2)} + P^{(2)}\dot{Q}_{(2)} - L_4 + \zeta\phi^{(1)} = P^{(1)}Q_{(2)} + (Q_{(1)})^2/2 + \zeta\phi^{(1)}$, where ζ is a Lagrange multiplier. The consistency condition for $\phi^{(1)}$ generates a secondary constraint: $\phi^{(2)} = -P^{(1)} + Q_{(2)}/2 := 0$, but it expected from the definition of $P^{(1)}$. The consistency condition for $\phi^{(2)}$ determines the Lagrange multiplier ζ as $Q_{(1)}$ in the weak equality. Therefore, the procedure stops here. The Poisson brackets between $\phi^{(1)}$ and $\phi^{(2)}$ is $\{\phi^{(1)}, \phi^{(2)}\}_{P.b.} = -1$ and otherwise vanish. This system has two second-class constraints, and it indicates that the propagating degrees of freedom of the system is $(2 \times 2 - 2)/2 = 1$ and that we have to use the canonical embedding $\sigma_2(t)$ given in Section 3.5 to introduce the well-posed variational principle.

The symplectic 2-form is computed as follows: $\Omega = dQ_{(i)} \wedge dP^{(i)} = d\Theta^1 \wedge d\Theta_1 + dQ \wedge dP$, where $\Theta^1 = \phi^{(2)}$, $\Theta_1 = \phi^{(1)}$, $Q = P^{(1)} + Q_{(2)}/2$, and $P = P^{(2)} - Q_{(1)}/2$. The Poisson brackets are $\{\Theta^1, \Theta_1\}_{P.b.} = 1$, $\{Q, P\}_{P.b.} = 1$, and otherwise vanish. The original variables $Q_{(1)}$, $Q_{(2)}$, $P^{(1)}$, and $P_{(2)}$ are expressed by using the transformed variables as follows: $Q_{(1)} = \Theta^1 + Q$, $Q_{(2)} = \Theta_1 - P$, $P^{(1)} = (Q - \Theta^1)/2$, and $P^{(2)} = (P + \Theta_1)/2$. Then the total Hamiltonian is transformed as follows: $H_T = P^2/2 + Q^2/2 - 2\Theta_1 P - (\Theta^1)^2/2 + 3(\Theta_1)^2/2$ and is defined in the symplectic manifold $(T^*\mathcal{Q}|_{Q,P} \times T^*\mathcal{Q}|_\Theta \times \mathbb{R}, \Omega)$. The pullback of H_T by $\sigma_2(t)$ is $\sigma_2^*(t)H_T = P^2/2 + Q^2/2 - 2\Theta_1 P + \mathit{constant}$ in the symplectic submanifold $(T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}, \sigma_2^*(t)\Omega = dQ \wedge dP)$, and this is a Frobenius integrable system. That is, there are two integral constants. The pullback of total Lagrangian is $L_T := \sigma_2^*(t)[P\dot{Q} + \Theta_1\dot{\Theta}^1 - H_T] = P\dot{Q} - P^2/2 - Q^2/2 - 2\Theta_1 P + \mathit{constant}$ in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R}$. Therefore, the first-order variation of the action functional is given as follows:

$$\delta(\sigma_2^*(t)I) = \int_{t_1}^{t_2} \left[-\dot{P} - Q\right] \delta Q dt + \left[\dot{Q} - P - 2\Theta_1\right] \delta P dt + [P\delta Q]_{t_1}^{t_2} . \tag{3.147}$$

Under the boundary conditions:

$$\delta Q(t_2) = \delta Q(t_1) = 0 , \tag{3.148}$$

the well-posed variational principle $\delta(\sigma_2^*(t)I) := 0$ leads to the equations of motion: $-\dot{P}-Q = 0$ and $\dot{Q} - P - 2\Theta_1 = 0$. That is, using $\sigma_2^*(t)\Theta_1 = constant$, $-\ddot{Q} - Q = 0$; this is none other than the equation of a one-dimensional harmonic oscillator. Remark, here, that L_T is now defined in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \simeq T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R}$ and Frobenius integrable. In fact, the solution is $Q(t) = A\exp(+it) + B\exp(-it)$, and this includes the two integral constants: A and B. The boundary conditions fix these constants.

Finally, the maps κ, $\mathfrak{D}$, and ι are introduced as follows: $\kappa|_{\sigma_2(t)} : T\mathcal{Q}|_{Q,\dot{Q}} \to T\mathcal{Q}|_{Q,P}$; $\dot{Q} \mapsto P$ and $\mathfrak{D}|_{\sigma_2(t)} : \mathfrak{D}[T(T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R})] \to \mathfrak{D}[T(T^*\mathcal{Q}|_{Q,P} \times \mathbb{R})]$; $X_t = Q(\partial/\partial\dot{Q}) + \dot{Q}(\partial/\partial Q) + (\partial/\partial t) \mapsto {}_*X_t = (\partial H_T/\partial P)(\partial/\partial Q) - (\partial H_T/\partial Q)(\partial/\partial P) + (\partial/\partial t)$ are introduced in a well-defined manner and invertible, where $H_T = P^2/2 + Q^2/2 - 2\Theta_1 P + constant$ in $T^*\mathcal{Q}|_{Q,P} \times T\mathcal{Q}|_{\Xi,\Psi} \times \mathbb{R}$. ι is $\iota|_{\sigma_2(t)} : \mathcal{Q}|_Q[t_1] \times \mathcal{Q}|_Q[t_2] \to \mathcal{C}|_{\sigma_3(t)}$; $(Q(t_1), Q(t_2)) \mapsto (A, B)$ with $A = (Q(t_1)\exp(it_2) - Q(t_2)\exp(it_1))/2i\sin(t_2 - t_1)$ and $B = (Q(t_2)\exp(-it_1) - Q(t_1)\exp(-it_2))/2i\sin(t_2 - t_1)$.

Let us consider applying (ii) Pons' modified formulation. The original Lagrangian L_4 is represented by using a Lagrange multiplier λ as follows:

$$L_4'' = -\frac{1}{2}q\dot{x} - \frac{1}{2}q^2 + \lambda(x - \dot{q}) . \tag{3.149}$$

Regarding λ also as a position coordinate of the configuration space, the canonical momenta are derived as follows: $p = -\lambda$, $y = -q/2$, and $\pi = 0$. Therefore, the rank of the kinetic matrix $K_{ij} = \partial p_i/\partial \dot{q}^j$ (where $p_1 = p\,, p_2 = y\,, p_3 = \pi\,, q^1 = q\,, q^2 = x\,, q^3 = \lambda$) is zero, and there are three primary constraints: $\phi^{(1)}_1 = p + \lambda :\approx 0$, $\phi^{(1)}_2 = y + q/2 := 0$, and $\phi^{(1)}_3 = \pi := 0$. The total Hamiltonian is computed as follows: $H_T = q^2/2 - \lambda x + \zeta^\alpha \phi^{(1)}_\alpha$, where ζ^α are Lagrange multipliers and $\alpha \in \{1, 2, 3\}$. The consistency conditions for $\phi^{(1)}_\alpha$ become as follows: $\dot{\phi}^{(1)}_1 \approx -q - \zeta^2/2 + \zeta^3 := 0$, $\dot{\phi}^{(1)}_2 \approx \lambda + \zeta^1/2 := 0$ and $\dot{\phi}^{(1)}_3 \approx x - \zeta^1 := 0$; there is a secondary constraint: $\phi^{(2)} = \lambda + x/2$ where we used $\zeta^1 \approx x$. The consistency condition for $\phi^{(2)}$ restricts the relation between ζ^2 and ζ^3, and this determines all the multipliers as follows: $\zeta^2 \approx -q$ and $\zeta^3 \approx q/2$. The Poisson brackets among the constraints are computed as follows: $\{\phi^{(1)}_1\,, \phi^{(1)}_2\}_{P.b.} = -1/2$, $\{\phi^{(1)}_1\,, \phi^{(1)}_3\}_{P.b.} = 1$, $\{\phi^{(2)}\,, \phi^{(1)}_2\}_{P.b.} = 1/2$, $\{\phi^{(2)}\,, \phi^{(1)}_3\}_{P.b.} = 1$, and otherwise vanish. This system has four second-class constraints, and this indicates that the propagating degrees of freedom of the system is $(3\times 2-4)/2 = 1$ and that we have to use the canonical embedding $\sigma_2(t)$ given in Section 3.5 to introduce the well-posed variational principle.

The symplectic 2-form is computed as follows: $\Omega = dq \wedge dp + dx \wedge dy + d\lambda \wedge d\pi = d\Theta^1 \wedge d\Theta_1 + d\Theta^2 \wedge d\Theta_2 + dQ \wedge dP$, where $\Theta^1 = \phi^{(2)} - \phi^{(1)}_1$, $\Theta_1 = \phi^{(1)}_2$, $\Theta^2 = (\phi^{(2)} + \phi^{(1)}_1)/2$, $\Theta_2 = \phi^{(1)}_3$, $Q = q/2 - y + \pi/2$, and $P = p + x/2$. Then the total Hamiltonian is transformed as follows: $H_T = Q^2/2 + P^2/2 - (\Theta^1)^2/2$ in the symplectic manifold $(T^*\mathcal{Q}|_{Q\,,P} \times T^*\mathcal{Q}|_\Theta \times \mathbb{R}, \Omega)$. The pullback of H_T by $\sigma_2(t)$ is $\sigma^*_2(t) H_T = Q^2/2 + P^2/2 + constant$ in the symplectic submanifold $(T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}\,, \sigma^*_2(t)\Omega = dQ \wedge dP)$, and this is a Frobenius integrable system. That is, there are two integral constants. The pullback of total Lagrangian is $L_T = \sigma^*_2(t)[P\dot{Q} + \Theta_a \dot{\Theta}^a - H_T] = P\dot{Q} - Q^2/2 - P^2/2 + constant$ in the subspace $T\mathcal{Q}|_{Q\,,\dot{Q}} \times T^*\mathcal{Q}|_{Q\,,P} \times \mathbb{R}$. Therefore, the first-order variation of the action functional is given as follows:

$$\delta(\sigma^*_2(t) I) = \int_{t_1}^{t_2} \left[-\dot{P} - Q\right] \delta Q dt + \left[\dot{Q} - P\right] \delta P + \left[P \delta Q\right]^{t_2}_{t_1}\,. \tag{3.150}$$

Under the boundary conditions

$$\delta Q(t_2) = \delta Q(t_1) := 0\,, \tag{3.151}$$

the well-posed variational principle $\delta(\sigma_2^*(t)I) := 0$ leads to the equations of motion, resolving as an equation $-\ddot{Q} - Q = 0$; this is none other than the equation of a one-dimensional harmonic oscillator. Remark, here, that L_T is now defined in the subspace $T\mathcal{Q}|_{Q,\dot{Q}} \times T^*\mathcal{Q}|_{Q,P} \times \mathbb{R} \simeq T\mathcal{Q}|_{Q,\dot{Q}} \times \mathbb{R}$ and Frobenius integrable. In fact, the solution is $Q(t) = A\exp(+it) + B\exp(-it)$, and this includes the two integral constants: A and B. The boundary conditions fix these constants. The maps κ, $\mathfrak{O}$, and ι are the same as the previous case by just replacing $H_T = P^2/2 + Q^2/2 - 2\Theta_1 P + constant$ by $H_T = P^2/2 + Q^2/2 + constant$.

3.9. Summary

In this chapter, a methodology to make the variational principle well-posed in degenerate point particle systems was constructed, although that of field theories is under development. The guiding principle is stated as "*as many integral constants (/initial conditions) in the solutions of a given system as possible should be uniquely determined through the boundary conditions*". The resulting methodology can be summarized into three steps as follows:

(1). For a given system, just performing Hamilton-Dirac analysis, reveal the constraint structure.

(2). Construct constraint coordinates. (Refer to the proof of Theorem 1 (Shanmugadhasan-Maskawa-Nakajima theorem) (or Lemma 1 and/or 2) in [Tomonari (2023b)].) Then, computing the symplectic 2-form, find a new canonical coordinate system which is indicated by Theorem 1 (Shanmugadhasan-Maskawa-Nakajima theorem). Then select a suitable embedding (see Table 3.1).

(3). Consider the pullback of the Legendre transformation of the total Hamiltonian by the selected embedding: the pullback of the total Lagrangian by the selected embedding.

Table 3.1: Embeddings for each type of system. "*1st-class system*" means a system with 1st-class constraint(s). Others are defined in the same manner.

Gauge fixing	1st-class system	2nd-class system	1st- and 2nd-class system
Yes	$\sigma_1(t)$	-	$\sigma_3(t)$
No (or no gauge d.o.f)	$\tilde{\sigma}_1(t)$	$\sigma_2(t)$	$\tilde{\sigma}_3(t)$

-(i) *If one uses* $\sigma_\tau(t)$ $(\tau = 1\,,2\,,3)$, *take the first-order variation of its action functional, and just fix the emerged configurations in the boundary term at both end-points. Then the variational principle becomes well-posed.*

-(ii) *If one uses* $\tilde{\sigma}_{\tilde{\tau}}(t)$ $(\tilde{\tau} = 1\,,3)$, *take the first-order variation of its action functional, under the assumption that the pullback of primary first-class constraint coordinates by* $\tilde{\sigma}_{\tilde{\tau}}(t)$ *is set to be zero in advance. Then fix the configurations for the propagating degrees of freedom at both end-points and the configurations which correspond to higher-order (more than secondary) first-class constraint coordinates at either end-point. Then the variational principle becomes well-posed.*

The embeddings in Table 3.1 have those proper constant parameters, and these parameters correspond to the existence of the constraints of a given system. In the case of systems with only existing second-class constraints, these constant parameters form a set of conjugate pairs and drop out from the symplectic 2-form; the symplectic manifold reduces to its physical submanifold not depending on the values of these parameters. This indicates that these parameters can be set as zeros as a formality. In the case of systems with existing first-class constraints, however, the situation gets changed. The conjugate configurations with respect to (the linear combinations of) the first-class constraints are not constraints; these variables are also dynamical although not physical. Therefore, in general, the symplectic manifold does not reduce to its physical submanifold. This indicates that these conjugate configurations need those initial conditions via the boundary conditions of the variational principle. While the existence of the undetermined Lagrange multipliers forbids fixing the conjugate configurations of the primary first-class constraints on the boundaries; the primary first-class constraints have to be set as zeros in advance. In other words, these constraints cannot be taken as coordinates to be fixed for introducing the embeddings. Taking into account this regard, the configurations only of the higher-order first-class constraints should be fixed on the boundaries.

If the guiding principle is neglected, it is also possible to demand consistency only with the constraint structure of a given system. In this case, in order to make the variational principle well-posed, just evaluating the symplectic potential around the constraint surface: $\omega = P_I\delta Q^I + \Theta_a\delta\Theta^a + \Psi_\alpha\delta\Xi^\alpha \approx P_I\delta Q^I$, it reveals that fixing the configurations of the propagating degrees of freedom Q^I on the boundaries provides appropriate boundary conditions for the well-posed variational principle [Izumi et al. (2023)]. Therefore, depending on whether or not the guiding principle is assumed, there occurs a case that the well-posed variational principle needs additional surface terms. In the case of systems with only existing second-class constraints, the assumption does not change the situation: $\omega = P_I\delta Q^I + \Theta_a\delta\Theta^a \approx P_I\delta Q^I$. However, in the case of systems with existing first-class constraints, the situation gets changed; if the boundary terms appear as $\omega = P_I\delta Q^I + \Xi^\alpha\delta\Psi_\alpha$, (i) When not assuming the guiding principle, the term $\Xi^\alpha\delta\Psi_\alpha$ have to be switched in Ξ^α and Ψ_α by introducing a counter-term $W = -\Xi^\alpha\Psi_\alpha$: $\Xi^\alpha\delta\Psi_\alpha - \delta W = -\Psi_\alpha\delta\Xi^\alpha \overset{\mathfrak{C}^{(K)}}{\approx} 0$ as a necessary and sufficient condition; (ii) When assuming the guiding principle, the term $\Xi^\alpha\delta\Psi_\alpha$ vanishes since all Ψ_α are *arbitrary* constants in the restriction to an embedded phase subspace, *excepting the primary first-class constraint coordinates*: $\Psi_{\alpha_1} = 0$, *i.e.*, these are not taken as arbitrary. That is, it is possible to add some counter-terms in the completely same manner as Case (i) only for the primary first-class constraint coordinates. That is, in Case (ii), counter-terms have a different meaning: $\Xi^\alpha\delta\Psi_\alpha - \delta W = -\Psi_\alpha\delta\Xi^\alpha = -\Psi_{\alpha_1}\delta\Xi^{\alpha_1} - \Psi_{\alpha'}\delta\Xi^{\alpha'} = -\Psi_{\alpha_1}\delta\Xi^{\alpha_1} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ as a necessary and sufficient condition due to the boundary conditions either Eq (3.88) or Eq (3.89). In this case, the imposition of *full* constraints is a *sufficient* condition.

The well-posedness discussed in [Tomonari (2023b); Izumi et al. (2023)] is considered under the consistency with $\mathfrak{C}^{(K)}$. As mentioned in Section 3.1, the Dirac-Bergmann analysis itself is valid independently from the well-posedness of the variational principle. This implies the possibility of arguing the well-posedness in each constraint surface: $\mathfrak{C}^{(k)}$ ($k = 1\,, 2\,, \cdots\,, K$). Taking into account the consideration in the previous paragraph, hereinafter in the present thesis, let us treat the well-posedness under the consistency only with $\mathfrak{C}^{(1)}$ and call it the "*weak*" well-posedness of the variational principle. Otherwise, let us call the well-posedness under the consistency with full constraints that of "*strong*" one.

Chapter 4

General theory of relativity

Chapter abstract

In this chapter, the general theory of relativity, which is the most successful classical theory of gravity in modern physics, is established. First of all, the fundamental concepts of the theory such as spacetime, and weak/Einstein/strong equivalence principles are introduced. Based on these concepts, the geodesic equations and the Einstein field equations are derived from both viewpoints of physical considerations (bottom-up approach) and the variational principle (top-down approach). As mentioned in Section 3.9, we assume that the well-posedness of the variational principle demands consistency with the primary constraint(s): $\mathfrak{C}^{(1)}$. In particular, before deriving the Einstein field equations by using the variational principle, the ADM-foliation/decomposition of the spacetime is introduced. This technique is mandatory not only to apply the variational principle in a well-posed manner being consistent with $\mathfrak{C}^{(1)}$ but also to perform the Dirac-Bergmann analysis. Finally, performing the Dirac-Bergmann analysis, the propagating and gauge degrees of freedom of the theory are identified.

4.1. Spacetime and fundamental principles

In this section, the concept of spacetime and fundamental principles for establishing the general theory of relativity, that is, the principle of equivalence and of general relativity/covariance, are introduced. First of all, let us formulate Minkowski spacetime.

In the absence of gravity, the special theory of relativity describes the motions of nature, and the theory is established upon the following two fundamental principles: the principle of constant speed of light, stated as *the speed of light does not depend on inertial frames*, and the principle of special relativity/Lorentz covariance, stated as *the physical laws do not depend* *on inertial frames*. Then the first principle formulates Minkowski spacetime. Let $\mathcal{S}$ be an inertial frame equipped with coordinates (ct, x^i) $(i \in \{1\,, 2\,, \cdots\,, n\})$, where c is the speed of light, and an arbitrary particle and a photon are emitted from the origin O, coordinated by $(0, \mathbf{0})$, of the system $\mathcal{S}$. After passing time Δt, let the particle and the photon exist at a point Q coordinated by $(c\Delta t, x^i_Q)$ and a point R coordinated by $(c\Delta t, x^i_R)$, respectively. Then an observer can consider the subtraction of OR, which is the square of the *length* of the photon path, from the square of the *Euclidean distance* of QR in the n-dimensional space as follows:

$$(\Delta s)^2 = -c^2(\Delta t)^2 + \sum_{i=1}^{n}(\Delta x^i)^2\,, \tag{4.1}$$

where $\Delta x^i = x^i_R - x^i_Q$. If the time Δt is infinitesimal, *i.e.*, $\Delta t \to dt$ then the above equation inserts a distance of the $(n+1)$-dimensional space which is coordinated by (ct, x^i). Introducing the metric tensor $\eta_{\mu\nu} = \mathrm{diag}\,(-1\,, +1\,, \cdots\,, +1)$, the distance can be expressed as follows:

$$ds^2 = \eta_{\mu\nu}dx^\mu dx^\nu\,. \tag{4.2}$$

This space is nothing but Minkowski spacetime. In the special theory of relativity, all the laws of physics have to be described in Minkowski spacetime. The fundamental property of the distance ds^2 is that it does not depend on inertial frames. That is, for another inertial frame $\mathcal{S}'$, the distance is invariant: $(ds')^2 = ds^2$, and it can be shown that this crucial property is a conclusion of the first principle. This property introduces the Lorentz symmetry, in terms of group theories, $SO(1, n)$, and all physical laws have to satisfy this symmetry. Explicitly, the Lorentz symmetry is expressed as follows:

$$\eta_{\mu\nu}\Lambda^\mu{}_\rho\Lambda^\nu{}_\sigma = \eta_{\rho\sigma}\,, \tag{4.3}$$

where $\Lambda^\mu{}_\rho$ is originated from the coordinate transformation $\phi\,:\, \mathcal{S} \to \mathcal{S}';\, x^\mu \mapsto x'^\mu =$

$\Lambda^\mu{}_\rho x^\rho$. The coordinate transformation ϕ which satisfies the Lorentz symmetry is the so-called Lorentz transformation. Furthermore, more generically, the symmetry of Minkowski spacetime can be extended into the Poincaré symmetry, *i.e.*, $P^{n+1} = T^{n+1} \rtimes SO(1,n)$ with the well-defined operation $(a_1\,,\Lambda_1)\cdot(a_2\,,\Lambda_2) = (a_1 + \Lambda_1 \cdot a_2\,,\Lambda_1\cdot\Lambda_2)$, which is nothing but an affine transformation: $x^\mu \mapsto x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu$ for a constant $(n+1)$-vector a^μ in Minkowski spacetime. Therefore, the second principle is a requirement under the Lorentz transformation, and it is achieved by expressing all quantities and laws of physics in terms of tensor fields in Minkowski spacetime.

The special theory of relativity can describe physics only in inertial frames, but the real world requires the description of physics in accelerating frames. The principle of equivalence makes it possible to realize the latter requirement of nature and has three different statements: Weak Equivalence Principle (WEP), Einstein's Equivalence Principle (EEP), and Strong Equivalence Principle (SEP). The essential point of the principle is the reconsideration of the meaning of the *accelerating* frames when subjecting only to gravity.

Let us consider a freely falling test particle. The second law of Newtonian mechanics describes this motion in an equation as follows:

$$m_\mathrm{i}\mathbf{a} = -m_\mathrm{g}\nabla\Phi\,, \tag{4.4}$$

where $\mathbf{a}$, m_i, and m_g are the acceleration vector, the inertial mass, and the gravitational mass of the test particle, respectively. Φ is a Newtonian gravitational field. The WEP states that the two types of mass are equivalent: $m_\mathrm{i} = m_\mathrm{g}$, and it leads to

$$\mathbf{a} = -\nabla\Phi\,. \tag{4.5}$$

That is, the acceleration does not depend on the sort of the test particle; only depends on the gravitational field. Experimentally, the Eötvös experiment and its modern successors verify this statement in high precision. Further considerations of this result give insight into a new understanding of the acceleration; the gravitational effect cannot be distinguished from uniform acceleration in a small enough region. That is, the WEP states more generically that *in small enough regions of spacetime, the motion of freely falling particles in a gravitational field and of particles in a uniform accelerating frame are not distinguishable.* Here, spacetime is the generalized concept of Minkowski spacetime: a space, or more generically, a pseudo-Riemannian manifold, equipped with a metric tensor $g_{\mu\nu}(x)$, not restricting to $\eta_{\mu\nu}$.

The statement of the WEP restricts its application only to freely falling particles, but A. Einstein extended the statement to any other experiments that obey special relativity, which is nothing but the EEP, stated as *in small enough regions of spacetime, the laws of physics restore those of special relativity.* This means that any local experiments cannot detect a gravitational field. Remark here that the EEP is the statement only for the non-gravitational laws of physics due to its own property. Including the gravitational laws of physics, the statement is distinguished as the SEP.

In the special theory of relativity, on one hand, the laws of physics are invariant under the Poincaré transformation. On the other hand, in the presence of gravity, it demands the invariance of that under the general coordinate transformations, or more generically, diffeomorphisms, $x^\mu \mapsto x'^\mu = (\partial x'^\mu/\partial x^\nu)x^\nu$, of spacetime. Remark that in this case $\partial x'^\mu/\partial x^\nu$ is not a constant matrix like $\Lambda^\mu{}_\nu$ in the Poincaré transformation but a function matrix, or equivalently, a Jacobian matrix; a system of coordinate functions spans only a local region of the entire spacetime. This statement is nothing but the principle of general relativity/covariance and is easily realized by expressing all quantities and laws of physics in terms of tensor fields in spacetime; it is a straightforward generalization of the principle of special relativity/covariance. Explicitly, let $\phi : \mathcal{M} \to \mathcal{M}$ and T be a diffeomorphism of spacetime $\mathcal{M}$ and a tensor field of some physical quantity on $\mathcal{M}$. Then the principle claims the satisfaction of the following condition:

$$\phi^* T = T\,, \quad \text{or equivalently} \quad \mathcal{L}_{\boldsymbol{\xi}} T = 0\,, \tag{4.6}$$

where $\boldsymbol{\xi}$ is a vector field which generates the diffeomorphism ϕ and $\mathcal{L}_{\boldsymbol{\xi}}$ is the Lie derivative generated by $\boldsymbol{\xi}$. Expressing it in a component form, the first condition becomes as follows:

$$(\phi^* T)^{\mu_1 \cdots}{}_{\nu_1 \cdots}(x) = \left[\frac{\partial x^{\mu_1}}{\partial x'^{\rho_1}} \cdots \frac{\partial x'^{\sigma_1}}{\partial x^{\nu_1}} \cdots\right]_{x'=\phi(x)} T^{\rho_1 \cdots}{}_{\sigma_1 \cdots}(x')\,, \tag{4.7}$$

as desired.

So far the main concepts and principles have been introduced: (Minkowski) spacetime, the EEP, and the principle of general relativity/covariance. Based on these ingredients, the general theory of relativity is established. In particular, the EEP leads to an interpretation that a freely falling frame is equivalent to the state of a frame in *un-accelerated*, the so-called *local inertial frame*, if subjecting only to gravity, and it gives an implication of describing the trajectory of a particle in a gravitational field as geodesics.

4.2. Geodesic equations

In this section, geodesic equations are introduced in two ways: a bottom-up approach focused on the motion of particles for grasping the meaning of physics and a top-down approach based on the variational principle for formulating the geodesics in a mathematical manner. Finally, the geometrical interpretation of gravity is presented. Let us start first with the bottom-up approach for introducing geodesics. Hereinafter, the speed of light c is set as unity: $c = 1$.

In the absence of forces including gravity, although it will be revealed that gravity is not a force but the bending of spacetime, a test particle (of which mass is unity in the system of units) satisfies the following equations of motion:

$$a^{\mu} = \frac{d^2 x^{\mu}}{d\tau^2} = 0\,, \tag{4.8}$$

where $x^{\mu} = x^{\mu}(\tau)$ and τ are the position $(n{+}1)$-vector and the proper time of the test particle, respectively. Performing a general coordinate transformation $x^{\mu} \mapsto x'^{\mu} = (\partial x'^{\mu}/\partial x^{\nu})x^{\nu}$ of which Jacobian matrix being non-singular, the above equation becomes as follows:

$$a^{\rho} = 0 \mapsto a'^{\rho} = \frac{d^2 x'^{\rho}}{d\tau^2} + \Gamma'^{\rho}{}_{\mu\nu}\frac{dx'^{\mu}}{d\tau}\frac{dx'^{\nu}}{d\tau} = 0\,, \quad \Gamma'^{\rho}{}_{\mu\nu} = \frac{\partial x'^{\rho}}{\partial x^{\sigma}}\frac{\partial^2 x^{\sigma}}{\partial x'^{\mu}\partial x'^{\nu}}\,. \tag{4.9}$$

This equation is nothing but the geodesic equation in the pseudo-Riemannian geometry, if replacing $\Gamma'^{\rho}{}_{\mu\nu}$ by the so-called Christoffel symbols/Levi-Civita connection $\mathring{\Gamma}^{\rho}{}_{\mu\nu}$, given as follows:

$$\mathring{\Gamma}^{\rho}{}_{\mu\nu} = \frac{1}{2}g^{\rho\sigma}\left(\partial_{\mu}g_{\nu\sigma} + \partial_{\nu}g_{\mu\sigma} - \partial_{\sigma}g_{\mu\nu}\right)\,, \tag{4.10}$$

and the connection $\mathring{\Gamma}^{\rho}{}_{\mu\nu}$ transforms by the general coordinate transformation as follows:

$$\mathring{\Gamma}'^{\rho}{}_{\mu\nu} = \frac{\partial x^{\alpha}}{\partial x'^{\mu}}\frac{\partial x^{\beta}}{\partial x'^{\nu}}\frac{\partial x'^{\rho}}{\partial x^{\gamma}}\mathring{\Gamma}^{\gamma}{}_{\alpha\beta} + \frac{\partial x'^{\rho}}{\partial x^{\sigma}}\frac{\partial^2 x^{\sigma}}{\partial x'^{\mu}\partial x'^{\nu}}\,. \tag{4.11}$$

Then the equation describes the trajectory of the test particle as a geodesic. If $t^{\mu} = dx^{\mu}/d\tau$ is a tangent vector of the geodesic then the equation can be expressed as follows:

$$\mathring{a}^{\mu} = t^{\nu}\mathring{\nabla}_{\nu}t^{\mu} = 0\,. \tag{4.12}$$

An important insight here is that the first term in Eq (4.11) is absent in Eq (4.9); vanishing the connection $\mathring{\Gamma}^{\gamma}{}_{\alpha\beta}$ in some coordinate system is an implication of the test particle existing in a local inertial frame. Therefore, taking into account the statement of the EEP, the existence of gravity has something to do with the Levi-Civita connection. In fact, it will be revealed in the last part of this section that the connection corresponds to the gravitational force itself.

Next, let us derive the geodesic equation from the variational principle and consider its properties. The action functional is introduced as follows:

$$I[x^{\mu}(\tau)\,,e(\tau)] = \int_{\tau_1}^{\tau_2} \left[\frac{1}{2e}g_{\mu\nu}(x^{\rho})\frac{dx^{\mu}}{d\tau}\frac{dx^{\nu}}{d\tau} + \sigma\frac{e}{2}\right] d\tau\,, \tag{4.13}$$

where $\sigma = +1, 0, -1$ for space-like, null, and time-like geodesic, respectively. The auxiliary variable $e = e(\tau)$ makes it possible to treat the null geodesic, $\sigma = 0$, in a unified manner. This system has a primary constraint with respect to the auxiliary variable. Therefore, the symplectic potential becomes $\omega = \pi_e \delta e + \pi_{\mu}\delta x^{\mu} = \pi_{\mu}\delta x^{\mu}$ in the Lagrangian formulation, since $\pi_e = 0$ is automatically satisfied as an identity, where π_e and π_{μ} are the canonical momentum variables with respect to e and μ, respectively. (In the Hamiltonian formulation, it becomes ${}_{*}\omega = \pi_e \delta e + \pi_{\mu}\delta x^{\mu} \overset{\mathfrak{C}^{(1)}}{\approx} \pi_{\mu}\delta x^{\mu}$, since $\pi_e = 0$ have to be imposed: $\pi_e := 0$). It indicates that the well-posedness of the variational principle on $\mathfrak{C}^{(1)}$ demands the boundary conditions $\delta x^{\mu}(\tau_2) = \delta x^{\mu}(\tau_1) = 0$ [Tomonari (2023b); Izumi et al. (2023)]. Varying this action functional with respect to e, the following equation is derived:

$$\sigma e^2 = g_{\mu\nu}\frac{dx^{\mu}}{d\tau}\frac{dx^{\nu}}{d\tau}\,, \tag{4.14}$$

on the other hand, with respect to x^{μ}, the following equation is derived:

$$\frac{d^2x^{\rho}}{d\tau^2} + \overset{\circ}{\Gamma}{}^{\rho}{}_{\mu\nu}\frac{dx^{\mu}}{d\tau}\frac{dx^{\nu}}{d\tau} = \frac{\dot{e}}{e}\frac{dx^{\mu}}{d\tau}\,, \tag{4.15}$$

under the imposition of the boundary conditions. These two equations are nothing but the geodesic equations. The action functional (4.13) has a symmetry; it is invariant under the following one-dimensional diffeomorphism:

$$\phi\,:(\tau_1,\tau_2)\to(\tau_1',\tau_2');\;\tau\mapsto\tau'=\phi(\tau)\,. \tag{4.16}$$

Then x^μ and e are transformed as follows:

$$x^\mu(\tau)\to x'^\mu=\phi^*(x^\mu(\tau))=x^\mu(\tau'=\phi(\tau))\,,\quad e(\tau)\to e'(\tau)=\phi^*(e(\tau))=e(\tau'=\phi(\tau))\,, \tag{4.17}$$

where ϕ^* is the pull back operator of ϕ. Therefore, using this diffeomorphism, the parameter τ can be always taken under the satisfaction of the condition

$$\dot{e}(\tau)=0\,. \tag{4.18}$$

In such case, Eq (4.15) results in the geodesic equation (4.12). A parameter under the satisfaction of the condition (4.18) is called the *affine-parameter*, and it can be generically expressed as follows:

$$\tau\to\tau'=a\tau+b\,, \tag{4.19}$$

where a and b are constants. In this formulation, the proper time is redefined as a parameter τ such that $e(\tau)=1$, or equivalently, $g_{\mu\nu}(dx^\mu/d\tau)(dx^\nu/d\tau)=-1$. Notice that the proper time has a symmetry for $\tau\mapsto\tau+constant$.

Finally, let us consider the geodesic equation in spacetime which slightly deforms from Minkowski spacetime. That is, the metric tensor $g_{\mu\nu}$ is expressed as follows:

$$g_{\mu\nu}=\eta_{\mu\nu}+h_{\mu\nu}\,,\quad |h_{\mu\nu}|\ll 1\,,\quad \partial_0 h_{\mu\nu}=0\,. \tag{4.20}$$

Then the spatial part of the geodesic equation (4.15) under the imposition of the condition (4.18) is approximated as follows:

$$\frac{d^2x^i}{d\tau^2} \simeq -\overset{\circ}{\Gamma}{}^i_{\mu\nu}\frac{dx^\mu}{d\tau}\frac{dx^\nu}{d\tau}\,. \tag{4.21}$$

If $dx^i/d\tau \ll 1$ is satisfied, the above equation is further approximated as follows:

$$\frac{d^2x^i}{d\tau^2} \simeq -\overset{\circ}{\Gamma}{}^i_{00}\,, \tag{4.22}$$

where the explicit formula of the Levi-Civita connection (4.10) is used. Comparing this equation to the equation for the freely falling test particle, Eq (4.5), the following relation is derived:

$$\overset{\circ}{\Gamma}{}^i_{00} \simeq \partial_i\Phi\,, \quad \text{or} \quad h_{00} = -2\Phi\,. \tag{4.23}$$

It indicates that the Levi-Civita connection and the metric tensor are nothing but the expression of gravity and of the gravitational potential, respectively. That is, gravity is nothing but a property of spacetime how it different is from Minkowski spacetime. Therefore, the statement of the EEP is translated in terms of the Levi-Civita connection into as follows: *in small enough regions of spacetime, it exists a coordinate system such that the Levi-Civita connection vanishes*, and this statement is guaranteed by a theorem: *It exists a coordinate system such that $\tilde{\Gamma}^\rho_{\mu\nu} = 0$ if and only if the lower two indices in the connection is commutative: $\tilde{\Gamma}^\rho_{\mu\nu} = \tilde{\Gamma}^\rho_{\nu\mu}$.* Here, remark that the connection is not restricted to the Levi-Civita connection $\overset{\circ}{\Gamma}{}^\rho_{\nu\mu}$. Therefore, the EEP is now expressed only in an equation: $\tilde{\Gamma}^\rho_{\mu\nu} = \tilde{\Gamma}^\rho_{\nu\mu}$. The Levi-Civita connection $\overset{\circ}{\Gamma}{}^\rho_{\nu\mu}$ apparently satisfies this condition by virtue of its expression in Eq (4.10).

Summarizing this section, using the pseudo-Riemannian geometry, the trajectory of a particle is described by the geodesic equation (4.15) under the imposition of the condition (4.18), or equivalently, Eq (4.12), and the connection of the theory is the Levi-Civita connection (4.10). In this geometry, the EEP is automatically satisfied, and gravity and the gravitational potential are expressed by the Levi-Civita connection and the metric tensor, respectively. Since the geodesic equation is the generalization of the Newton equation for a freely falling particle, that is, Eq (4.8), therefore, a particle subjecting only to gravity does continue the uniform motion as a *straight line in spacetime*, *i.e.*, a geodesic; gravity is now engraved into a property of spacetime. Therefore, once the gravitational potential, *i.e.*, the metric tensor, is determined, the geodesic equations describe how a particle evolves in time. The Einstein field equations provide a set of field equations to govern the evolution of the metric tensor.

4.3. Einstein field equations

In this section, the Einstein field equations are derived based on two bottom-up approaches by using the Poisson equation of gravity and the equations of geodesic deviation respectively. The modern approach based on the variational principle will be presented in Section 4.5. The speed of light c is set as unity: $c = 1$. Let us start with the first approach.

The Poisson equation of gravity is given as follows:

$$\nabla^2 \Phi = 4\pi G \rho \,, \tag{4.24}$$

where G is the Newtonian constant and ρ is the matter density of sources. Using Eq (4.20), Eq (4.22), and the above equation, the following equation is derived:

$$\nabla^2 g_{00} = 8\pi G \mathring{\mathcal{T}}_{00} \,, \tag{4.25}$$

where $\mathring{\mathcal{T}}_{00} = -\rho$ is the $(0,0)$-component of the energy-momentum tensor $\mathring{\mathcal{T}}_{\mu\nu}$. Generalizing this equation in a covariant manner, the field equation should be the following form:

$$\overset{\circ}{G}_{\mu\nu} = 8\pi G \overset{\circ}{\mathcal{T}}_{\mu\nu} \,. \tag{4.26}$$

Therefore, revealing $\overset{\circ}{G}_{\mu\nu}$, the field equations for gravity are obtained, under the satisfaction of the following conditions; (i) $\overset{\circ}{G}_{\mu\nu}$ is composed of the metric tensor and its derivative up to second-order; (ii) In the Newtonian limit, Eq (4.26) restores Eq (4.25); (iii) The lower two indices of $\overset{\circ}{G}_{\mu\nu}$ are symmetric; (iv) $\overset{\circ}{G}_{\mu\nu}$ satisfies the covariant conservative property. Conditions (i) and (iii) allows that $\overset{\circ}{G}_{\mu\nu}$ is written as follows: $\overset{\circ}{G}_{\mu\nu} = A\overset{\circ}{R}_{\mu\nu} + Bg_{\mu\nu}\overset{\circ}{R}$, where $\overset{\circ}{R}_{\mu\nu}$ and $\overset{\circ}{R}$ are the Ricci tensor and the Ricci scalar, A and B are arbitrary constants. There may be some leaps to make up this form, but the validity will be able to be confirmed in the second approach. Condition (iv) leads to $A = -2B$. Therefore, $\overset{\circ}{G}_{\mu\nu}$ should be the following formula:

$$\overset{\circ}{G}_{\mu\nu} = \overset{\circ}{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \overset{\circ}{R} \,. \tag{4.27}$$

This is nothing but the so-called Einstein tensor, which is derived from the Bianchi identity: $\overset{\circ}{\nabla}_{[\rho|} \overset{\circ}{R}_{\mu\nu]\sigma\kappa} = 0$, and satisfies Condition (iv). Therefore, the Einstein field equations are derived as follows:

$$\overset{\circ}{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \overset{\circ}{R} = 8\pi G \overset{\circ}{\mathcal{T}}_{\mu\nu} \,, \quad \text{or} \quad \overset{\circ}{R}_{\mu\nu} = 8\pi G \left(\overset{\circ}{\mathcal{T}}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \overset{\circ}{\mathcal{T}} \right) \,. \tag{4.28}$$

From the second equation above, Condition (ii) leads the Poisson equation of gravity: Eq (4.25).

The second approach is based on a consideration of the tidal effect. The EEP indicates that, in small enough regions of spacetime, gravity can be removed by performing appropriate general coordinate transformation but that, in global regions of spacetime, it is not the case; the tidal effect appears. Let us consider the congruence of geodesics. The two particles in geodesics have the relative acceleration given as follows:

$$\mathring{a}^{\mu} = t^{\mu}\mathring{\nabla}_{\mu}(t^{\nu}\mathring{\nabla}_{\nu}n^{\rho})\,, \tag{4.29}$$

where n^{ρ} are the normal vector of geodesics. Using the geodesic equation (4.12) and the relation $\mathring{\mathcal{L}}_{\mathbf{n}}t^{\mu} = 0$, where $\mathring{\mathcal{L}}_{\mathbf{n}}$ is the Lie derivative with respect to the normal vector n^{μ}, the equation of geodesic congruence are derived as follows:

$$a^{\mu} = \mathring{R}^{\mu}{}_{\nu\rho\sigma}t^{\nu}t^{\rho}n^{\sigma}\,. \tag{4.30}$$

This equation describes the tidal effect between two test particles. In the Newtonian case, the following equation holds:

$$a^{i} = -n^{j}\partial_{j}\partial^{i}\Phi\,. \tag{4.31}$$

Now, let us derive the Einstein field equations. Generalizing Eq (4.31) into a covariant form, it becomes $a^{\mu} = -n^{\nu}\partial_{\nu}\partial^{\mu}\Phi$. Therefore, comparing it to Eq (4.30) and using the Poisson equation of gravity, Eq (4.24), and then tracing out the un-contracted indices, the following equation holds:

$$\mathring{R}_{\mu\nu}t^{\mu}t^{\nu} = \kappa^{2}\rho\,, \tag{4.32}$$

where κ^{2} is a constant coefficient. The right-hand side can be generalized as $\mathring{\mathcal{T}}_{\mu\nu}t^{\mu}t^{\nu}$ in a covariant form, therefore, the following relation is derived:

$$\mathring{R}_{\mu\nu} = \kappa^{2}\mathring{\mathcal{T}}_{\mu\nu} \tag{4.33}$$

This equation does not satisfy the covariant conservative property but the Bianchi identity: $\mathring{\nabla}_{[\rho|}\mathring{R}_{\mu\nu]\sigma\kappa} = 0$ leads to $\mathring{\nabla}^{\mu}\mathring{G}_{\mu\nu} = 0$, where $\mathring{G}_{\mu\nu}$ is defined in Eq (4.27). Therefore, the above equation should be modified as follows:

$$\mathring{G}_{\mu\nu} = \kappa^2 \mathring{\mathcal{T}}_{\mu\nu} \,. \tag{4.34}$$

The coefficient κ^2 can be determined by considering the Newtonian limit: $\kappa^2 = 8\pi G$. This is nothing but the Einstein field equations (4.28).

In the first approach, the form of $\mathring{G}_{\mu\nu} = A\mathring{R}_{\mu\nu} + Bg_{\mu\nu}\mathring{R}$ is assumed and it satisfies all Conditions (i) - (iv), whereas a term $Cg_{\mu\nu}$ satisfies only Conditions (i), (ii), and (iv). Therefore, if the coefficient C is small enough to be consistent with the Newtonian limit, then it would be possible to modify the Einstein equation as follows:

$$\mathring{G}_{\mu\nu} + \Lambda g_{\mu\nu} = 8\pi G \mathring{\mathcal{T}}_{\mu\nu} \,. \tag{4.35}$$

The constant coefficient, Λ, is the so-called Einstein's cosmological constant. He was motivated to introduce this term from a philosophy that the universe should be static, although modern observations indicate that the universe is expanding, and it is rather accelerating.

The Einstein field equations are composed of $(n+1)(n+2)/2$ independent equations in $(n+1)$-dimensional spacetime and non-linear partial differential equations. Therefore, it is generically difficult to solve the equations and to find the true propagating degrees of freedom. Of course, in order to reveal the latter point, the Dirac-Bergmann analysis is a powerful tool, but it demands the ADM-foliation of spacetime and the Lagrangian formulation of the theory.

4.4. ADM-foliation of spacetime and Einstein field equations

In this section, ADM-foliation of spacetime is introduced [Arnowitt et al. (1959, 1960); Deser et al. (1960); Arnowitt et al. (2008); Baez and Muniain (1995); Nakahara (2003); Carroll (2019); Padmanabhan (2014b)], and it is one of the most important fundamentals of the present thesis. The concepts introduced in this section are as follows: ADM-foliation of spacetime, the metric of the geometry, first fundamental form (projection map), covariant derivative in a foliation of spacetime, second fundamental form (extrinsic curvature), Gauss-Codazzi equations, and the ADM-foliation of Einstein field equation.

Let $\mathcal{M}$ be a $(n+1)$-dimensional manifold of spacetime that has a Cauchy surface. Then ADM-foliation of spacetime is a diffeomorphism $\phi : \mathcal{M} \to \mathbb{R} \times \mathcal{S}$ such that it decomposes the spacetime $\mathcal{M}$ as a disjoint union of hypersurfaces as follows:

$$\mathcal{M} = \bigcup_{t \in \mathcal{I}} \Sigma_t \,, \quad \Sigma_t = \{p \in \mathcal{M} | \phi^* \tau(p) = t\} \,, \tag{4.36}$$

where $\mathcal{S}$ is a n-dimensional hypersurface, t and τ are a time coordinate of $\mathcal{M}$ and of $\mathbb{R} \times \mathcal{S}$, respectively, $\mathcal{I}$ is a time interval of $\mathcal{M}$, and ϕ^* is the pullback operator of ϕ. Each hypersurface Σ_t, which is called a leaf, is diffeomorphic to $\mathcal{S}$. The ADM-foliation of spacetime is denoted as $(\mathcal{M}\,, \mathcal{S}\,, \phi)$.

Let $g = g_{\mu\nu}\, dx^\mu \otimes dx^\nu$ and n^μ be a metric tensor of $\mathcal{M}$ and a normal vector of a leaf Σ_t, respectively. Then the line element $ds^2 = g_{\mu\nu} dx^\mu dx^\nu$ is decomposed as follows:

$$\begin{aligned} ds^2 &= \epsilon N^2 d\tau^2 + h_{ij}(dx^i + N^i d\tau)(dx^j + N^j d\tau) \,, \\ h_{ij} &= [(\phi^{-1})^*]^\mu{}_i [(\phi^{-1})^*]^\nu{}_j g_{\mu\nu} \,, \end{aligned} \tag{4.37}$$

where ϵ is either -1 or $+1$ according to either time-like or space-like hypersurface Σ_t, respectively. N and N^i are the lapse function and shift vector, respectively, which is introduced as follows:

$$(\partial_t)^\mu = \epsilon N n^\mu + [(\phi^{-1})^*]^\mu{}_i N^i \,. \tag{4.38}$$

Therefore, the components of the metric tensor on $\mathcal{M}$ are expressed by the spatial metric

h_{ij}, the lapse function N, and the shift vector N^i as follows:

$$
\begin{aligned}
&g_{00} = \epsilon N^2 + h_{ij} N^i N^j \,, \\
&g_{0i} = g_{i0} = h_{ij} N^j \,, \\
&g_{ij} = h_{ij} \,.
\end{aligned}
\tag{4.39}
$$

The components of the inverse metric tensor on $\mathcal{M}$ are derived as follows:

$$
\begin{aligned}
&g^{00} = \epsilon N^{-2} \,, \\
&g^{0i} = g^{i0} = -\epsilon N^{-2} N^i \,, \\
&g^{ij} = h^{ij} + \epsilon N^{-2} N^i N^j \,.
\end{aligned}
\tag{4.40}
$$

The normal vector n^μ can be expressed in terms of the lapse function and the shift vector as follows:

$$
\begin{aligned}
&n^\mu = \epsilon N^{-1}(-1\,, N^i) = -N g^{0\mu} \,, \\
&n_\mu = (-N\,, 0) = -N \delta^0_\mu \,.
\end{aligned}
\tag{4.41}
$$

Remark that a normal vector satisfies the Frobenius theorem: $n_{[\mu} \nabla_\nu n_{\rho]} = 0$, where ∇_μ is a covariant derivative for any geometries/connections, not restricting to the Levi-Civita connection. Remark also that the expression of n_μ above can be extended into a more generic form as follows:

$$
n_\mu = (-N\,, N N_i) = -N(\delta^0_\mu - N_i \delta^i_\mu)
\tag{4.42}
$$

under the condition $N^i N_i = 0$.

In order to describe the geometry of the foliation of spacetime, let us introduce the first and second fundamental forms. The first fundamental form is defined as follows:

$$P_{\mu\nu} = g_{\mu\nu} - \epsilon n_\mu n_\nu \,, \tag{4.43}$$

or in the components form

$$\begin{aligned} P_{00} &= h_{ij} N^i N^j \,, \\ P_{0i} &= P_{i0} = h_{ij} N^j \,, \\ P_{ij} &= h_{ij} \,, \end{aligned} \tag{4.44}$$

or equivalently,

$$\begin{aligned} P^{00} &= 0 \,, \\ P^{0i} &= P^{i0} = 0 \,, \\ P^{ij} &= h^{ij} \,. \end{aligned} \tag{4.45}$$

This quantity is also called the projection map by virtue of the following properties:

$$n^\mu P_{\mu\nu} = 0 \,, \quad P^\mu{}_\nu P^\nu{}_\rho = P^\mu{}_\rho \,. \tag{4.46}$$

Hereinafter, we call it the projection map. Using this quantity, the covariant derivative on a leaf Σ_t is introduced as follows:

$$D_\rho T^{\mu_1\mu_2\cdots\mu_k}{}_{\nu_1\nu_2\cdots\nu_l} = P^\sigma{}_\rho P^{\mu_1}{}_{\tilde{\mu}_1} P^{\mu_2}{}_{\tilde{\mu}_2} \cdots P^{\mu_1}{}_{\tilde{\mu}_k} P^{\tilde{\nu}_1}{}_{\nu_1} P^{\tilde{\nu}_2}{}_{\nu_2} \cdots P^{\tilde{\nu}_l}{}_{\nu_l} \nabla_\sigma T^{\tilde{\mu}_1\tilde{\mu}_2\cdots\tilde{\mu}_k}{}_{\tilde{\nu}_1\tilde{\nu}_2\cdots\tilde{\nu}_l} \,, \tag{4.47}$$

where $T^{\tilde{\mu}_1\tilde{\mu}_2\cdots\tilde{\mu}_k}{}_{\tilde{\nu}_1\tilde{\nu}_2\cdots\tilde{\nu}_l}$ is a $(k\,,l)$-tensor in the spacetime $\mathcal{M}$ and $T^{\mu_1\mu_2\cdots\mu_k}{}_{\nu_1\nu_2\cdots\nu_l}$ is a $(k\,,l)$-tensor in a leaf Σ_t. Remark that this formula holds for any geometries/connections. In particular, in a (pseudo-)Riemannian manifold, the projection map satisfies the following properties:

$$
\begin{aligned}
&\mathring{D}_k P_{ij} = 0\,,\\
&{}^{(n)}\mathring{\Gamma}^k_{ij} = \frac{1}{2}P^{kl}(\partial_i P_{jl} + \partial_j P_{il} - \partial_l P_{ij})\,.
\end{aligned}
\tag{4.48}
$$

This is nothing but the Levi-Civita connection on a leaf Σ_t.

The second fundamental form is defined as follows:

$$
K_{\mu\nu} = \frac{1}{2}\mathcal{L}_{\mathbf{n}}P_{\mu\nu}\,,
\tag{4.49}
$$

where $\mathcal{L}_{\mathbf{n}}$ is the Lie derivative with respect to the normal vector n^μ. Remark that this quantity is viable in any geometries/connections. This quantity satisfies the following properties:

$$
\begin{aligned}
&K_{\mu\nu} = K_{\nu\mu}\,,\\
&n^\mu K_{\mu\nu} = 0\,,
\end{aligned}
\tag{4.50}
$$

and has four equivalent expressions as follows:

$$
\begin{aligned}
&\mathring{K}_{\mu\nu} = \frac{1}{2}P^\alpha{}_\mu P^\beta{}_\nu \mathring{\mathcal{L}}_{\mathbf{n}} g_{\alpha\beta}\,,\\
&\mathring{K}_{\mu\nu} = \mathring{\nabla}_\mu n_\nu - \epsilon n_\mu \mathring{a}_\nu\,,\\
&\mathring{K}_{\mu\nu} = P^\rho{}_\mu \mathring{\nabla}_\rho n_\nu\,,\\
&\mathring{K}_{\mu\nu} = \mathring{\nabla}_\mu n_\nu + n_\mu \mathring{D}_\nu \ln N\,,
\end{aligned}
\tag{4.51}
$$

where the Frobenius theorem is used. Remark that the properties in Eq (4.50) hold for any geometries/connections. That is, the quantity is symmetric with respect to the lower two indices and spatial in any geometries/connections. Using these properties, the following property is derived:

$$
\mathring{\mathcal{L}}_{\mathbf{n}}(P^\alpha{}_\mu P^\beta{}_\nu \mathring{K}_{\alpha\beta}) = P^\alpha{}_\mu P^\beta{}_\nu \mathring{\mathcal{L}}_{\mathbf{n}} \mathring{K}_{\alpha\beta}\,.
\tag{4.52}
$$

This property shows that the projection map behaves just like the metric tensor in (pseudo-)Riemannian geometry regarding the Lie derivative of the second fundamental form with respect to the normal vector. Notice that these equations excepting the fourth equation in Eq (4.51) do not depend on a concrete form of the normal vector n^μ. If n^μ is expressed in terms of the lapse function and the shift vector, *i.e.*, $n^\mu = \epsilon N^{-1}(-1, N^i)$, then the following important formula is derived:

$$ {}^{(n)}\mathring{K}_{ij} = \frac{\epsilon}{2} N^{-1}(\mathring{D}_i N_j + \mathring{D}_j N_i - \dot{h}_{ij}) \,. \tag{4.53} $$

This formula plays a crucial role in performing the Dirac-Bergmann analysis of theories of gravity. The geometrical meaning of the second fundamental form can be interpreted by considering a way of embedding a leaf Σ_t into the spacetime $\mathcal{M}$. Let C be an integral curve with respect to t^μ. Then we can verify the following relation: $t^\mu D_\mu t^\nu = P^\nu{}_\rho t^\sigma \nabla_\sigma t^\rho - \epsilon n^\nu t^\rho t^\sigma K_{\sigma\rho}$. If the curve C is a geodesic on the leaf then this relation turns into as follows: $\epsilon n^\nu t^\rho t^\sigma K_{\sigma\rho} = P^\nu{}_\rho t^\sigma \nabla_\sigma t^\rho$. This relation implies that if the curve also is a geodesic of the spacetime $\mathcal{M}$ then the second fundamental form vanishes, and vice versa. Therefore, the second fundamental form can be interpreted as a quantity that measures the difference in a way of freely falling a test particle. That is, let C' be a geodesic in the spacetime $\mathcal{M}$ and both C and C' path through a common point P. Then, to restrict a test particle on C, the parallel transformation along with the curve C' have to be modified by the amount of $\epsilon n^\nu t^\rho t^\sigma K_{\sigma\rho}$ from that of $P^\nu{}_\rho t^\sigma \nabla_\sigma t^\rho$. Therefore, the second fundamental form is interpreted as a sort of curvature. Hereinafter, we call it the extrinsic curvature.

Next, let us introduce the Gauss-Codazzi equations. The Gauss equation is given as follows:

$$ {}^{(n)}\mathring{R}^\rho{}_{\sigma\mu\nu} = P^\rho{}_\gamma P^\delta{}_\sigma P^\alpha{}_\mu P^\beta{}_\nu \mathring{R}^\gamma{}_{\delta\alpha\beta} + 2\epsilon \mathring{K}^\rho{}_{[\mu} \mathring{K}_{\nu]\sigma} \,. \tag{4.54} $$

This relation can be shown by using the relation $[\mathring{D}_\alpha\,, \mathring{D}_\beta] t^\delta = {}^{(n)}\mathring{R}^\gamma{}_{\delta\alpha\beta} t^\delta$, where t^δ is a tangent vector on a leaf Σ_t. The first and second Codazzi equations are given as follows:

$$\begin{aligned}
&P^{\alpha}{}_{\mu}P^{\beta}{}_{\nu}P^{\sigma}{}_{\gamma}n^{\delta}\mathring{R}^{\gamma}{}_{\delta\alpha\beta} = 2\mathring{D}_{[\mu}\mathring{K}_{\nu]}{}^{\sigma}\,, \\
&P^{\alpha}{}_{\mu}n^{\gamma}P^{\beta}{}_{\nu}n^{\delta}\mathring{R}_{\alpha\gamma\beta\delta} = \mathring{K}_{\mu}{}^{\rho}\mathring{K}_{\rho\nu} - \mathcal{L}_{\mathbf{n}}\mathring{K}_{\mu\nu} + \mathring{D}_{\mu}\mathring{a}_{\nu} - \epsilon\mathring{a}_{\mu}\mathring{a}_{\nu}\,,
\end{aligned} \tag{4.55}$$

respectively, where $\mathring{a}_{\mu} = n^{\nu}\mathring{\nabla}_{\nu}n_{\mu}$. These relations can be shown by using the relation $[\mathring{\nabla}_{\alpha}\,,\mathring{\nabla}_{\beta}]n^{\gamma} = \mathring{R}^{\gamma}{}_{\delta\alpha\beta}n^{\delta}$. Concerning the terms $\mathring{D}_{\mu}\mathring{a}_{\nu}$ and/or $\mathring{a}_{\mu}$, it can be replaced by using the following relations:

$$\begin{aligned}
&\mathring{a}_{\mu} = -n^{\rho}n_{\mu}\mathring{D}_{\nu}\ln N\,, \\
&\mathring{D}_{\mu}\mathring{a}_{\nu} = -\epsilon(N^{-1}\mathring{D}_{\mu}\mathring{D}_{\nu}N - \mathring{a}_{\mu}\mathring{a}_{\nu})\,.
\end{aligned} \tag{4.56}$$

From the Gauss equation (4.54), the Ricci tensor and scalar on a leaf are expressed as follows:

$$\begin{aligned}
&{}^{(n)}\mathring{R}_{\mu\nu} = P^{\alpha}{}_{\mu}P^{\beta}{}_{\nu}P^{\gamma}{}_{\delta}\mathring{R}^{\delta}{}_{\alpha\gamma\beta} + \epsilon(\mathring{K}\mathring{K}_{\mu\nu} - \mathring{K}_{\mu\rho}\mathring{K}^{\rho}{}_{\nu})\,, \\
&{}^{(n)}\mathring{R} = \mathring{R} - \epsilon(2\mathring{R}_{\mu\nu}n^{\mu}n^{\nu} + \mathring{K}^{\mu\nu}\mathring{K}_{\mu\nu} - \mathring{K}^{2})\,.
\end{aligned} \tag{4.57}$$

Contracting the first Codazzi equation, it relates the extrinsic curvature to the Ricci tensor as follows:

$$2\mathring{D}_{[\mu}\mathring{K}^{\mu}{}_{\nu]} = n^{\lambda}P^{\rho}{}_{\nu}\mathring{R}_{\lambda\rho}\,. \tag{4.58}$$

The above equations in this paragraph hold only for (pseudo-)Riemannian geometry. A generalization of these equations into metric-affine geometries is given in [Ariwahjoedi et al. (2021a,b)].

Finally, let us decompose the Einstein field equations. The Einstein tensor and the extrinsic curvature have the following relations:

$$
\begin{aligned}
&2\mathring{G}_{\mu\nu}n^{\mu}n^{\nu} = -\epsilon\,{}^{(n)}\mathring{R} + \mathring{K}^2 - \mathring{K}^{\mu\nu}\mathring{K}_{\mu\nu}\,,\\
&\mathring{D}_{\mu}\mathring{K}^{\mu}{}_{\nu} - \mathring{D}_{\nu}\mathring{K} = n^{\mu}P^{\nu}{}_{\rho}\mathring{G}_{\mu\nu}\,.
\end{aligned}
\tag{4.59}
$$

These relations are shown by using $P^{\rho\sigma}P^{\mu\nu}\mathring{R}_{\rho\mu\sigma\nu} = -2\epsilon n^{\mu}n^{\nu}\mathring{G}_{\mu\nu}$. Using these relations, the Einstein field equations (4.28) are decomposed into the following three equations:

$$
\begin{aligned}
&{}^{(n)}\mathring{R} + K^2 - \mathring{K}_{\mu\nu}\mathring{K}^{\mu\nu} = 2\kappa^2\mathcal{T}_{\mu\nu}n^{\mu}n^{\nu}\,,\\
&\mathring{D}_{\mu}\mathring{K} - \mathring{D}_{\nu}\mathring{K}^{\nu}{}_{\mu} = \kappa^2P^{\rho}{}_{\mu}n^{\sigma}\mathcal{T}_{\rho\sigma}\,,
\end{aligned}
\tag{4.60}
$$

and, using also the second equation in Eq (4.55) and the second equation in Eq (4.56),

$$
\mathring{\mathcal{L}}_{\mathbf{n}}\mathring{K}_{\alpha\beta} = -{}^{(n)}\mathring{R}_{\alpha\beta} + 2\mathring{K}^{\gamma}{}_{\alpha}\mathring{K}_{\gamma\beta} - \mathring{K}\mathring{K}_{\alpha\beta} + N^{-1}\mathring{D}_{\alpha}\mathring{D}_{\beta}N + P^{\mu}{}_{\alpha}P^{\nu}{}_{\beta}\left(\mathring{\mathcal{T}}_{\mu\nu} - \frac{1}{n-1}g_{\mu\nu}\mathring{\mathcal{T}}\right)\,, \tag{4.61}
$$

where $\epsilon = -1$; leaves are taken as space-like hypersurfaces. The third equations (4.61) describe the time evolution of the spacetime. In fact, using the following formula:

$$
\mathring{\mathcal{L}}_{\mathbf{n}}Q_{\mu\nu} = N^{-1}(\partial_0 Q_{\mu\nu} - \mathring{\mathcal{L}}_{\mathbf{n}}Q_{\mu\nu})\,, \tag{4.62}
$$

where $Q_{\mu\nu}$ is spatial tensor, *i.e.*, $n^{\mu}Q_{\mu\nu} = 0$, then Eq (4.61) is further split into as follows:

$$
\begin{aligned}
&\partial_0 h_{ij} - \mathring{\mathcal{L}}_{\mathbf{N}}h_{ij} = -2N\mathring{K}_{ij}\,,\\
&\partial_0 K_{ij} - \mathring{\mathcal{L}}_{\mathbf{N}}\mathring{K}_{ij} = N^{(3)}\mathring{R}_{ij} + N(\mathring{K}\mathring{K}_{ij} - 2\mathring{K}^{k}{}_{i}\mathring{K}_{kj}) - \mathring{D}_i\mathring{D}_jN - 2\kappa^2P^{\mu}{}_{i}P^{\nu}{}_{j}\left(\mathring{\mathcal{T}}_{\mu\nu} - \frac{1}{n-1}g_{\mu\nu}\mathring{\mathcal{T}}\right)N\,,
\end{aligned}
\tag{4.63}
$$

where $N^{\mu} = (0\,,\mathbf{N}) = (0\,,N^i)$. These equations imply the possibility of reformulating the Einstein field equations in a Hamiltonian formulation, and the first and second equations would correspond to " $\dot{q} = \partial H/\partial p$ " and " $\dot{p} = -\partial H/\partial q$ ", respectively. In this section, we have discussed based on the equations of motion. In order to verify this statement, however, it needs to establish the Lagrangian formulation of the general theory of relativity.

4.5. Reformulation based on the well-posed variational principle

In this section, Einstein-Hilbert action is introduced in the Lagrangian formulation, and, based on the well-posed variational principle on the primary constraint phase space $\mathfrak{C}^{(1)}$, the Einstein field equations are derived [Einstein (1916)]. This is the first time to consider the well-posedness of the variational principle in field theories in the current thesis, therefore, all computations are performed in detail. The Einstein-Hilbert action in the Hamiltonian formulation is also established, and the Einstein field equations as Hamilton equation are derived [Padmanabhan (2014b,a); Parattu et al. (2016a,b); Danieli (2020); Jha (2023)].

The Einstein-Hilbert action functional in vacuum is given as follows:

$$I_{GR}[g_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} d^{n+1}x\,\mathcal{L}_{GR}\,, \quad \mathcal{L}_{GR} = \mathring{R}\sqrt{-g}\,, \tag{4.64}$$

where $\mathcal{M}$ is a $(n+1)$-dimensional spacetime, g is the determinant of the metric tensor $g_{\mu\nu}$ of $\mathcal{M}$, $\mathring{R}$ is the Ricci scalar of $\mathcal{M}$, and $\kappa^2 = 8\pi G$. In order to apply the variational principle in a well-posed manner on the primary constraint phase subspace $\mathfrak{C}^{(1)}$, let us derive the canonical momentum variables of the system. Using the second relation of the contracted Gauss equation (4.57) in the case of $\epsilon = -1$ and the relation: $\mathring{R}_{\mu\nu}n^\mu n^\nu = \mathring{\nabla}_\rho(\mathring{a}^\rho - n^\rho\mathring{K}) - \mathring{K}_{\mu\nu}\mathring{K}^{\mu\nu} + \mathring{K}^2$, which can be derived from $[\mathring{\nabla}_\alpha\,, \mathring{\nabla}_\beta]n^\gamma = \mathring{R}^\gamma{}_{\delta\alpha\beta}n^\delta$, the Ricci scalar in the action functional can be decomposed as follows:

$$\mathring{R} = {}^{(n)}\mathring{R} + \mathring{K}_{\mu\nu}\mathring{K}^{\mu\nu} - \mathring{K}^2 - 2\mathring{\nabla}_\rho(n^\rho\mathring{K} - \mathring{a}^\rho)\,. \tag{4.65}$$

Therefore, the Einstein-Hilbert action functional (4.64) becomes as follows:

$$I_{GR}[N\,, N^i\,, h^{ij}] = \frac{1}{2\kappa^2}\int_{t_1}^{t_2} dt \int_{\Sigma_t} d^n x \mathcal{L}_{ADM} + \frac{1}{2\kappa^2}\int_{\partial\mathcal{M}} d^n x \left(+2\sqrt{h}\mathring{K}\right)\,, \tag{4.66}$$

where $\mathcal{L}_{ADM}$, the so-called Arnowit-Deser-Misner Lagrangian density, is defined as follows:

$$\mathcal{L}_{ADM} = N\sqrt{h}\left({}^{(n)}\mathring{R} + \mathring{K}_{\mu\nu}\mathring{K}^{\mu\nu} - \mathring{K}^2\right)\,. \tag{4.67}$$

The canonical momentum density variables of the ADM Lagrangian are derived as follows:

$$\begin{aligned} \pi_0(x) &= \frac{\delta\mathcal{L}_{ADM}(x)}{\delta\dot{N}(y)} = 0\,, \quad \pi_i(x) = \frac{\delta\mathcal{L}_{ADM}(x)}{\delta\dot{N}^i(y)} = 0\,, \\ \pi_{ij}(x) &= \frac{\delta\mathcal{L}_{ADM}(x)}{\delta\dot{h}^{ij}(y)} = \sqrt{h(x)}(\mathring{K}(x)h_{ij}(x) - \mathring{K}_{ij}(x))\delta^{(n)}(\mathbf{x}-\mathbf{y})\,. \end{aligned} \tag{4.68}$$

These results indicates that there are the total number of $(n+1)$ primary constraints as follows:

$$ {}_*\phi_0^{(1)} = \pi_0 := 0\,, \quad {}_*\phi_i^{(1)} = \pi_i := 0 \tag{4.69}$$

in the Hamiltonian formulation. In the Lagrangian formulation, these equations are satisfied as identities. The symplectic potential in the Lagrangian formulation is given as follows: $\omega = \pi_0\delta N + \pi_i\delta N^i + \pi_{ij}\delta h^{ij} = \pi_{ij}\delta h^{ij}$. (In the Hamiltonian formulation, ${}_*\omega = \pi_0\delta N + \pi_i\delta N^i + \pi_{ij}\delta h^{ij} \overset{\mathfrak{C}^{(1)}}{\approx} \pi_{ij}\delta h^{ij}$). Therefore, the well-posedness of the variational principle on the constraint phase subspace $\mathfrak{C}^{(1)}$ demands the imposition of the boundary condition as follows: $\delta h^{ij} = 0$ on the boundary $\partial\mathcal{M}$ [Tomonari (2023b); Izumi et al. (2023)].

Now, let us apply the variational principle to the Einstein-Hilbert action (4.64) under the imposition of the boundary condition $\delta h^{ij} = 0$ on $\partial\mathcal{M}$. Varying the Lagrangian density

$\mathcal{L}_{GR}$ in Eq (4.64), the following equation is derived:

$$\delta\mathcal{L}_{GR} = \mathring{G}_{\mu\nu}\delta g^{\mu\nu} + \sqrt{-g}\mathring{\nabla}_\mu\mathring{\nabla}_\nu\left(-\delta g^{\mu\nu} + g^{\mu\nu}g_{\alpha\beta}\delta g^{\alpha\beta}\right) . \tag{4.70}$$

The first term is the bulk term and it governs the dynamics of the system when coupling to matters as discussed later. The second term generates the surface term of the theory. Integrating out the second term on the spacetime $\mathcal{M}$, it becomes as follows:

$$\begin{aligned} \delta V &= \int_{\partial\mathcal{M}} dx^n \epsilon\sqrt{h}\delta\mathcal{V}\,, \\ \delta\mathcal{V} &= n_\mu\mathring{\nabla}_\nu\left(-\delta g^{\mu\nu} + g^{\mu\nu}g_{\alpha\beta}\delta g^{\alpha\beta}\right) . \end{aligned} \tag{4.71}$$

Using the relation $g_{\mu\nu}\delta g^{\mu\nu} = P_{\mu\nu}\delta P^{\mu\nu} + 2\epsilon n_\mu\delta n^\mu$ and $\delta n^\nu = n_\nu\delta g^{\mu\nu} - \epsilon n^\mu n_\alpha n_\beta\delta g^{\alpha\beta}/2$ (, or equivalently $\delta n_\rho = -\epsilon n_\rho n_\mu n_\nu\delta g^{\mu\nu}$), the density $\mathcal{V}$ is rewritten as follows:

$$\begin{aligned} \delta\mathcal{V} &= (\mathring{\nabla}_\mu n_\nu)\delta g^{\mu\nu} - \mathring{K}g_{\mu\nu}\delta g^{\mu\nu} + \mathring{\nabla}_\mu\delta\mathcal{V}^\mu\,, \\ \delta\mathcal{V}^\mu &= -n_\alpha P^\mu{}_\beta\delta g^{\alpha\beta} + n^\mu P_{\alpha\beta}\delta P^{\alpha\beta}\,. \end{aligned} \tag{4.72}$$

A direct calculation leads to the following property: $\mathring{\nabla}_\mu W^\mu = \mathring{D}_\mu W^\mu + \epsilon n^\nu\mathring{\nabla}_\nu(n_\mu W^\mu) - \epsilon W^\mu\mathring{a}_\mu$. Therefore, using this property, the density $\mathcal{V}$ becomes as follows:

$$\delta\mathcal{V} = (\mathring{K}_{\mu\nu} - \mathring{K}P_{\mu\nu})\delta P^{\mu\nu} + \frac{1}{\sqrt{h}}\delta(-2\sqrt{h}\mathring{K}) + \mathring{D}_\mu(n_\alpha P^\mu{}_\beta\delta g^{\alpha\beta})\,. \tag{4.73}$$

The third term in the above equation vanishes when integrating it out on $\partial\mathcal{M}$. Therefore, neglecting this term and using Eq (4.45), Eq (4.73) becomes as follows:

$$\delta\mathcal{V} = (\mathring{K}_{ij} - \mathring{K}h_{ij})\delta h^{ij} + \frac{1}{\sqrt{h}}\delta(-2\sqrt{h}\mathring{K})\,, \tag{4.74}$$

or Eq (4.71) becomes as follows:

$$\delta V = \int_{\partial\mathcal{M}} d^n x(-\epsilon)\pi_{ij}\delta h^{ij} + \int_{\partial\mathcal{M}} d^n x\delta(-2\epsilon\sqrt{h}\mathring{K})\,, \tag{4.75}$$

where the third equation in Eq (4.68) is used. Assembling all results, the first-order variation of the Einstein-Hilbert action (4.64) is calculated as follows:

$$\delta I_{GR} = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \mathring{G}_{\mu\nu}\delta g^{\mu\nu} + \frac{1}{2\kappa^2}\int_{\partial\mathcal{M}} d^n x(-\epsilon)\pi_{ij}\delta h^{ij} + \frac{1}{2\kappa^2}\int_{\partial\mathcal{M}} d^n x\delta(-2\epsilon\sqrt{h}\mathring{K})\,. \tag{4.76}$$

The second term vanishes under the imposition of the boundary condition $\delta h_{ij} = 0$ on $\partial\mathcal{M}$, but the third term remains. Therefore, let us modify the Einstein-Hilbert action on the ground of the following equation:

$$\delta\tilde{I}_{GR} = \frac{1}{\kappa^2}\int_{\mathcal{M}} \mathring{G}_{\mu\nu}\delta g^{\mu\nu} + \frac{1}{2\kappa^2}\int_{\partial\mathcal{M}} d^n x(-\epsilon)\pi_{ij}\delta h^{ij}\,, \tag{4.77}$$

where $\tilde{I}_{GR}$ is defined as follows:

$$\tilde{I}_{GR}[N\,, N^i\,, h^{ij}] = I_{GR}[N\,, N^i\,, h^{ij}] + \frac{1}{2\kappa^2}\int_{\partial\mathcal{M}} d^n x\left(2\epsilon\sqrt{h}\mathring{K}\right)\,. \tag{4.78}$$

The second term is nothing but the so-called Gibbons-York-Hawking counter-term [York (1972, 1986a); Gibbons and Hawking (1977); Hawking and Horowitz (1996); Padmanabhan (2014a); Parattu et al. (2016a,b); Chakraborty et al. (2017); Chakraborty and Padmanabhan (2020)]. At last, the well-posed variational principle on the constraint phase subspace $\mathfrak{C}^{(1)}$ leads to the vacuum Einstein field equations as follows:

$$\mathring{G}_{\mu\nu} = 0\,. \tag{4.79}$$

Remark that, in this case, the equations are just sufficient conditions to satisfy $\delta\tilde{I}_{GR} := 0$

due to the dependence among $\delta g^{\mu\nu}$, that is, $\delta g^{\mu\nu}$ are not independent. In fact, the number of components of $g_{\mu\nu}$ is $(n+1)(n+2)/2$ in $(n+1)$-dimensional spacetime, but at least $(n+1)$ components of them depend on other components since there exist at least that number of primary constraints; the number of $(n+1)$ components of the metric tensor can be expressed by the remaining $(n+1)(n+2)/2-(n+1)$ components. Notice, finally, that, based on Eq (4.78) in the case of $\epsilon=-1$, Eq (4.66) becomes as follows:

$$\tilde{I}_{GR}[N\,,N^i\,,h^{ij}]=\frac{1}{2\kappa^2}\int_{t_1}^{t_2}dt\int_{\Sigma_t}d^n x\mathcal{L}_{ADM}\,. \tag{4.80}$$

That is, the second term in Eq (4.66) and the second term in Eq (4.78) are canceled out one another; the canonical momentum variables in Eq (4.68), which were derived by neglecting the second term in Eq (4.66), are now justified.

Let us introduce matters. Taking into account a matter Lagrangian $\mathcal{L}_{\text{matter}}$, the net Lagrangian becomes $\mathcal{L}_{\text{net}}=\tilde{\mathcal{L}}_{EH}+\mathcal{L}_{\text{matter}}$. In the case of existing matters, the variational principle with respect to the matter fields leads to those equations of motion. Assuming these equations, the first-order variation of the net Lagrangian becomes schematically as follows:

$$\delta\mathcal{L}_{\text{matter}}=\left(\frac{\delta\mathcal{L}_{\text{matter}}}{\delta\phi}\right)\Bigg|_{g\,\text{:fixed}}\delta\phi+\left(\frac{\delta\mathcal{L}_{\text{matter}}}{\delta g^{\mu\nu}}\right)\Bigg|_{\phi\,\text{:fixed}}\delta g^{\mu\nu}=\left(\frac{\delta\mathcal{L}_{\text{matter}}}{\delta g^{\mu\nu}}\right)\Bigg|_{\phi\,\text{:fixed}}\delta g^{\mu\nu}\,, \tag{4.81}$$

or, in the form of action functional,

$$\delta I_{\text{matter}}=-\frac{1}{2}\int_{\mathcal{M}}\mathring{\mathcal{T}}_{\mu\nu}\delta g^{\mu\nu}\,d^{n+1}x\,. \tag{4.82}$$

Therefore, the variational principle leads to the Einstein field equations as follows:

$$\mathring{G}_{\mu\nu}=\kappa^2\mathring{\mathcal{T}}_{\mu\nu}\,. \tag{4.83}$$

Finally, let us derive the Hamilton equations of motion, although this formulation is not complete: it needs to take into account that the theory is a degenerate system. The ADM-Hamiltonian is derived from the Legendre transformation as follows:

$$\mathcal{H}_{ADM} = \pi_{ij}\dot{h}^{ij} - \mathcal{L}_{ADM}\,. \tag{4.84}$$

Using Eq (4.53) in the case of $\epsilon = -1$, the above equation turns into as follows:

$$\begin{aligned}\mathcal{H}_{ADM} &= N\sqrt{h}\left(\mathring{K}_{ij}\mathring{K}^{ij} - \mathring{K}^2 - {}^{(n)}\mathring{R}\right) - 2N^i\mathring{D}^j\pi_{ij} + 2\mathring{D}^i\left(\pi_{ij}N^j\right)\\ &\overset{\text{T.D.}}{=} N\sqrt{h}\left(\mathring{K}_{ij}\mathring{K}^{ij} - \mathring{K}^2 - {}^{(n)}\mathring{R}\right) - 2N^i\mathring{D}^j\pi_{ij}\,,\end{aligned} \tag{4.85}$$

where "$\overset{\text{T.D.}}{=}$" denotes the equality under the ignorance of the total divergent term. Varying $\mathcal{H}_{ADM}$, the following formula is obtained:

$$\delta\mathcal{H}_{ADM} = P_{ij}\delta h^{ij} + Q^{ij}\delta\pi_{ij} + C_0\delta N + C_i\delta N^i\,, \tag{4.86}$$

where P_{ij}, Q^{ij}, C_0, and C_i are given as follows:

$$\begin{aligned}P_{ij} =& -N\sqrt{h}\left({}^{(n)}\mathring{R}_{ij} - \frac{1}{2}h_{ij}{}^{(n)}\mathring{R}\right) - \mathring{D}^k\left(\pi_{ik}N_j + \pi_{jk}N_i - \pi_{ij}N_k\right)\\ &+ \sqrt{h}\left(\mathring{D}_i\mathring{D}_jN - h_{ij}\mathring{D}_k\mathring{D}^kN\right) + \frac{N}{2\sqrt{h}}\left(\pi_{kl}\pi^{kl} - \frac{\pi^2}{n-1}\right) - \frac{2N}{\sqrt{h}}\left(\pi_i{}^k\pi_{jk} - \frac{\pi\pi_{ij}}{n-1}\right)\,,\end{aligned} \tag{4.87}$$

$$Q^{ij} = \frac{4N}{\sqrt{h}}\left(\pi^{ij} - \frac{\pi}{n-1}h^{ij}\right) \tag{4.88}$$

$$C_0 = -\sqrt{h}{}^{(n)}\mathring{R} + \frac{1}{\sqrt{h}}\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right)\,, \tag{4.89}$$

$$C_i = -2\mathring{D}^j\pi_{ij}\,. \tag{4.90}$$

Conversely, the inverse Legendre transformation is given as follows:

$$\mathcal{L}_{ADM} = \pi_{ij}\dot{h}^{ij} - \mathcal{H}_{ADM}\,. \tag{4.91}$$

Therefore, using Eq (4.86), the first-order variation of $\mathcal{L}_{ADM}$ in the phase space is calculated as follows:

$$\delta\mathcal{L}_{ADM} \overset{T.D.}{=} \left(P_{ij} + \dot{\pi}_{ij}\right)\delta h^{ij} + \left(Q^{ij} - \dot{h}^{ij}\right)\delta\pi_{ij} - C_0\delta N - C_i\delta N^i\,. \tag{4.92}$$

The variational principle leads to the following constraint densities:

$$C_0 = 0\,, \quad C_i = 0\,, \tag{4.93}$$

and the following Hamilton equations of motion:

$$\dot{h}^{ij} = Q^{ij}\,, \quad \dot{\pi}_{ij} = -P_{ij}\,, \tag{4.94}$$

as a set of sufficient conditions. Each equation in Eq (4.94) corresponds to that of Eq (4.63), respectively. In order to apply the variational principle in a necessary and sufficient manner for deriving the Hamilton equations of motion, the methodology that is established in Sections 3.6 and 3.7 is mandatory, although it is hard to find the canonical variables that are indicated by the Shanmugadhasan-Maskawa-Nakajima theorem. In fact, no one has achieved it yet at the moment writing this thesis. If this problem is solved, the well-posedness of the variational principle on the full constraint phase subspace $\mathfrak{C}^{(K)}$ ($K = 2$ will be revealed in the next section) can be established. In this case, it may need to add another counter-term, which is different from the Gibbons-York-Hawking counter-term, to the action functional. Anyway, even if one tries to apply the method, the Dirac-Bergmann analysis is necessary to reveal the constraint structure of the theory and the propagating degrees of freedom.

4.6. Dirac-Bergmann analysis and degrees of freedom

In this section, performing the Dirac-Bergmann analysis, the degrees of freedom of gravity in the general theory of relativity is investigated [Danieli (2020); Jha (2023); Tomonari and Bahamonde (2023)]. This is the first time to apply the analysis to field theories, therefore, all computations are presented in detail. The analysis is separated into two main steps: (i) The derivation of a set of primary constraint densities and the total Hamiltonian; (ii) The verification of the consistency conditions for all constraint densities. Let us start with the main step (i): Building the total Hamiltonian.

Based on Eq (4.78), the ADM-Lagrangian (4.67) is derived without any boundary term. This is the starting point of the analysis. The canonical momentum variables and the primary constraint densities are already derived: Eq (4.68) and Eq (4.69), respectively. The fundamental Poisson brackets (PBs) are given as follows:

$$
\begin{aligned}
&\{N(x)\,,\pi_0(y)\}_{P.b.}=\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,\quad \{N^i(x)\,,\pi_j(y)\}_{P.b.}=\delta^i_j\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,\\
&\{h^{ij}(x)\,,\pi_{kl}(y)\}_{P.b.}=\delta^{(i}_k\delta^{j)}_l\delta^{(n)}(\mathbf{x}-\mathbf{y})\,.
\end{aligned}
\tag{4.95}
$$

Under these PB-algebras, the primary constraint densities Eq (4.69) are commutative with respect to the Poisson brackets (PBs). The Hessian/kinetic matrix given in Eq (2.1) (but in field theories: See Eq (7.6) in Section 7.1 for detail) is computed as follows:

$$
\mathcal{K}_{ab}\sqrt{h}=\begin{bmatrix} 0 & \mathbf{0}_{1,n} & \mathbf{0}_{1,n(n+1)/2}\\ \mathbf{0}_{n,1} & \mathbf{0}_{n,n} & \mathbf{0}_{n,n(n+1)/2}\\ \mathbf{0}_{n(n+1)/2,1} & \mathbf{0}_{n(n+1)/2,n} & K_{(i,j),(k,l)}\end{bmatrix}\cdot\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,\quad K_{(i,j),(k,l)}=\frac{\sqrt{h}}{2N}\left(h_{ij}h^{kl}-\delta^{(k}_i\delta^{l)}_j\right)\,,
\tag{4.96}
$$

where $(i,j)\,,(k,l)\in\{(1,1)\,,(1,2)\,,\cdots,(1,n)\,;(2,2)\,,(2,3)\,,\cdots,(2,n)\,;\cdots;(n,n)\}$. The rank of this matrix is six. The kernel Hamiltonian is calculated as follows:

$$\mathcal{H}_0 = NC_0 + N^iC_i\,, \tag{4.97}$$

where C and C_i are given in Eqs (4.89) and (4.90). Therefore, the total Hamiltonian is derived as follows:

$$\mathcal{H}_T = \mathcal{H}_0 + \lambda^\mu{}_*\phi^{(1)}_\mu\,, \tag{4.98}$$

where λ^μ are the Lagrange multipliers.

The next main step (ii) is the verification of the consistency conditions for all constraint densities. Those of the primary constraint densities ${}_*\phi^{(1)}_\mu \overset{\mathfrak{C}^{(1)}}{\approx} 0$ are calculated as follows:

$${}_*\phi^{(2)}_\mu = C_\mu := 0\,. \tag{4.99}$$

Notice that Eq (4.99) is nothing but Eq (4.93). The PBs between ${}_*\phi^{(1)}_\mu$ and ${}_*\phi^{(2)}_\mu$ are commutative. The PBs among the secondary constraint densities (4.99) are calculated as follows:

$$\begin{aligned}
\{{}_*\phi^{(2)}_i(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_j(t\,,\mathbf{x})\}_{P.b.} &= \left({}_*\phi^{(2)}_j(t\,,\mathbf{x})\partial^{(x)}_i - {}_*\phi^{(2)}_i(t\,,\mathbf{y})\partial^{(y)}_j\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,,\\
\{{}_*\phi^{(2)}_i(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_0(t\,,\mathbf{y})\}_{P.b.} &= {}_*\phi^{(2)}_0(t\,,\mathbf{x})\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,,\\
\{{}_*\phi^{(2)}_0(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_0(t\,,\mathbf{y})\}_{P.b.} &= \left(h^{ij}(t\,,\mathbf{x}){}_*\phi^{(2)}_j(t\,,\mathbf{x}) + h^{ij}(t\,,\mathbf{y}){}_*\phi^{(2)}_j(t\,,\mathbf{y})\right)\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,.
\end{aligned} \tag{4.100}$$

Therefore, all the secondary constraint densities are classified into first-class constraint densities. Based on these algebras, straightforward computations show that the consistency conditions for the secondary constraint densities are automatically satisfied on the constraint phase subspace $\mathfrak{C}^{(2)}$, and then The Dirac-Bergmann analysis stops here.

Another way of verifying this statement is calculations with the smeared variables. This calculation method is convenient if the system has only first-class constraints by virtue of the closed algebra (4.100). The definition of smeared variables is given as follows:

$$C_S(N) = \int_{\Sigma_t} dx^3 N C_0 \,, \quad C_V(\mathbf{N}) = \int_{\Sigma_t} dx^3 N^i C_i \,, \tag{4.101}$$

where $\mathbf{N} = N^i \partial_i$. Then, first, the following relation holds:

$$\{F(h^{ij}\,, \pi_{ij}), C_V(\mathbf{N})\}_{P.b.} = \mathcal{L}_{\mathbf{N}} F(h^{ij}\,, \pi_{ij}) \tag{4.102}$$

for arbitrary function $F(h^{ij}, \pi_{ij})$. Using this, the following algebras are derived:

$$\{C_V(\mathbf{N}_1)\,, C_V(\mathbf{N}_2)\}_{P.b.} = C_V(\mathcal{L}_{\mathbf{N}_1}\mathbf{N}_2) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \quad \{C_V(\mathbf{N})\,, C_S(N)\}_{P.b.} = C_S(\mathcal{L}_{\mathbf{N}} N) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,. \tag{4.103}$$

Neglecting spatial boundary terms, the following algebra holds:

$$\{C_S(N_1)\,, C_S(N_2)\}_{P.b.} \overset{\text{spatial T.D.}}{=} C_V\left((N_1\partial^i N_2 - N_2 \partial^i N_1)\partial_i\right) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \tag{4.104}$$

where "$\overset{\text{spatial T.D.}}{=}$" denotes the ignorance of spatial total divergence terms.[1] Using these algebras, it is obvious to verify the satisfaction of the consistency conditions for the secondary constraint densities. Therefore, the Dirac-Bergmann analysis stops here.

The Dirac-Bergmann analysis reveals that the number of $(n+1)$ primary and the same number of secondary constraint densities exist, and all the multipliers remain arbitrary.

[1]As discussed in Section 7.1 in detail, this ignorance is restricted to a system such that the diffeomorphism invariance holds, meaning that Eq (4.100) is satisfied. In this case, imposing appropriate spatial boundary conditions, *i.e.*, $N_i(t\,, \text{spatial boundary}) := 0$, the spatial total divergence terms can be neglected. However, fortunately, in the case of GR, the boundary terms are composed only of the constraint densities, therefore, even if this ignorance is not necessary.

Therefore, the propagating degrees of freedom (see Section 2.4) is given as follows:

$$\mathrm{pDoF} = \left[2 \times \frac{(n+1)(n+2)}{2} - 2 \times 0 - 2 \times \{(n+1) + (n+1)\}\right] \times \frac{1}{2} = \frac{1}{2}(n+1)(n-2)\,. \tag{4.105}$$

The gauge degrees of freedom (see Section 2.4) is the number of the primary first-class constraints as follows:

$$\mathrm{gDoF} = n + 1\,. \tag{4.106}$$

The gauge generator (see Section 2.3) is given as the linear combination of the first-class constraints: ${}_*G = \epsilon^{\mu}_{k\,*}\phi^{(k)}_{\mu}$ ($k \in \{1\,,2\}$). This gDoF inherits the principle of general relativity/covariance.

The symplectic potential becomes the following form: ${}_*\omega = P_I \delta Q^I + \Psi_\alpha \delta \Xi^\alpha \overset{\mathfrak{C}^{(2)}}{\approx} P_I \delta Q^I$, where Ψ_α are linear combinations of ${}_*\phi^{(k)}_{\mu}$ with some function coefficients, Q^I and P_I are the propagating degrees of freedom, and $I \in \{1\,,2\}$; $\alpha \in \{1\,,2\,,\cdots\,,8\}$. Since this system has only the first-class constraint densities, in order to identify appropriate boundary conditions, the symplectic potential has to be pulled back by the quasi-embedding $\tilde{\sigma}_1(t)$. (See Section 3.7.) That is, $\tilde{\sigma}^*_1(t)_*\omega \overset{\mathfrak{C}^{(2)}}{\approx} P_I(t)\delta Q^I(t) + \tilde{\Psi}_\alpha(t)\delta\Xi^\alpha(t)$, where $\tilde{\Psi}_\alpha(t) \overset{\mathfrak{C}^{(2)}}{\approx} \tilde{\sigma}^*_1(t)\Psi_\alpha$: only the primary first-class constraint densities ${}_*\phi^{(1)}_{\mu} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ in Ψ_α are set to be zero; otherwise the secondary first-class constraint densities ${}_*\phi^{(2)}_{\mu} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ in Ψ_α are set to be constant parameters. Therefore, the well-posedness of the variational principle for the *effective* action (see Section 3.7) on the full constraint phase subspace $\mathfrak{C}^{(2)}$ demands the boundary conditions $\delta Q^I = 0$ and, in generically, $\delta\Xi^\alpha = 0$, on the boundary $\partial\mathcal{M}$. However, the explicit expressions of these variables are difficult to lead, as mentioned in the final paragraph in Section 4.5. No one has achieved it yet at the moment writing this thesis.

4.7. Summary

In this chapter, the general theory of relativity was constructed; the geodesic equations and the Einstein field equations are derived based on the well-posed variational principle being consistent with the primary constraint densities. In particular, the latter case showed that the Gibbons-York-Hawking term is automatically derived and the well-posedness being consistent with all constraint densities expect to generate new sorts of counter-terms. Every modified/extended theory of gravity has to be able to restore the Einstein field equations as a special case under the satisfaction of some specific conditions. Then the dynamics is described by the geodesic equations of the spacetime of a given theory of gravity. The ADM-foliation/decomposition introduced in Section 4.4 plays a crucial role in performing the Dirac-Bergmann analysis of theories of gravity. An example of the analysis for the general theory of relativity was given in Section 4.6. This technique can also apply to modified/extended theories of gravity and provides one of the fundamental ingredients to the present thesis.

Chapter 5

Gauge approach to gravity

Chapter abstract

In this chapter, a mathematical framework for the gauge approach to gravity is constructed. First of all, three fundamental bundles, *i.e.*, fiber bundle, G-bundle, and principal G-bundle are defined. For the principal G-bundle, the Ehresmann connection and its curvature are introduced. After that, vector bundles together with gauge fields and those curvature (field strengths) are derived. Internal space bundles, which play a crucial role in constructing the metric-affine gauge theories of gravity, are also derived, in particular, focusing on frame fields and Weitzenböch connection. Finally, a gauge approach derivation of the Einstein field equations is described. This chapter gives mathematical basics for the succeeding chapters.

5.1. Fiber bundles and G-bundles

In this section, the basics of fiber bundles for physics are briefly introduced [Kobayashi (1989); Baez and Muniain (1995); Kobayashi and Nomizu (1996); Sharpe (1997); Nakahara (2003)]. First, fiber bundles are defined, and restrictions of the application to physics are described. Second, G-bundles are introduced. Finally, the construction of G-bundles is explained aiming to clarify geometrical meanings.

A fiber bundle is a structure between two topological spaces, denoted by a total space $\mathcal{E}$ and a base space $\mathcal{M}$, related by a continuous surjective map (, or equivalently, projection map,) $\pi : \mathcal{E} \to \mathcal{M}$ such that, for an open set U, $\pi^{-1}(U)$ is homeomorphic to the direct product of U and a *given* topological space $\mathcal{F}$, *i.e.*, $\varphi : \mathcal{E}|_U = \pi^{-1}(U) \to U \times \mathcal{F}$; $(p\,,\xi) \mapsto \{p\} \times \mathcal{F} = \mathcal{F}_p = \phi(p\,,\xi)$. This homeomorphism is called *local* trivialization. Then the fiber bundle is denoted as $\mathfrak{B} = (\mathcal{E}\,,\mathcal{M}\,,\pi\,,\mathcal{F})$, and $\mathcal{F}$ is called the standard fiber of the fiber bundle. On the fiber bundle, a quantity s which is defined on $\mathcal{M}$ and valued in $\mathcal{E}$, that is $s:\mathcal{M}\to\mathcal{E}$, can be introduced as satisfying $\pi\circ s=id$. This map is called a section of $\mathcal{E}$ on $\mathcal{M}$, and the set of all sections is denoted as " $\Gamma(\mathcal{E})$ ".

For applications to physics, the two topological spaces $\mathcal{E}$ and $\mathcal{M}$ are often assumed as some differential manifolds, so is for the fiber F. Then the projection map π is also assumed to be differentiable. In particular, $\mathcal{M}$ is taken to be a spacetime manifold, and then, of course, coordinate transformations on local regions in $\mathcal{M}$ are considered. That is, for an atlas of charts $\{\phi_i:\,U_i\to\mathbb{R}^d|\,i\in I\}$, where $\mathfrak{U}=\{U_i\}_{i\in I}$ is an open covering of $\mathcal{M}$ and d is the dimension of $\mathcal{M}$, and $p\in U_i\cap U_j$, a coordinate transformation is given as follows: $\phi_i\circ{\phi_j}^{-1}:\mathbb{R}^d\to\mathbb{R}^d;\,(x^1\,,\cdots,x^d)=\phi_i(p)\mapsto(y^1\,,\cdots,y^d)=\phi_j(p)$. Then, making a set by gathering all transition functions " $t_{ij}=\phi_i\circ{\phi_j}^{-1}$ " and inducing the composition of functions " $\circ$ " as a binary operation into the set, denoted by $G=(t_{ij}\,,\circ)$, G forms (a subgroup of) a general linear group $GL(d\,;\mathbb{R})$.

For the total space $\mathcal{E}$, the resemble concepts of a chart and an atlas of charts in a manifold can be introduced: G-chart(, or equivalently, local trivialization,) and G-atlas, where G is a *given* Lie group. That is, for $U_i\in\mathfrak{U}$, a G-chart is a homeomorphism given as follows: $\varphi_i:\,\mathcal{E}|_{U_i}=\pi^{-1}(U_i)\to U_i\times\mathcal{F};\,(p\,,\xi)\mapsto\{p\}\times\mathcal{F}=\mathcal{F}_p=\phi_i(p\,,\xi)$. Then the set of all G-charts is defined as G-atlas: $\{\varphi_i|\,i\in I\}$. If a G-atlas is given, for each point $p\in U_i\cap U_j$, there exists an element $\tau_{ij}(p)\in G$ such that $\varphi_i\circ{\varphi_j}^{-1}:\,(U_i\cap U_j)\times\mathcal{F}\to(U_i\cap U_j)\times\mathcal{F};\,(p\,,\xi)\mapsto(p\,,\tau_{ij}(p)\eta)$. This map is denoted also as " $\tau_{ij}=\varphi_i\circ{\varphi_j}^{-1}$ " and called a transition function, and it plays the role of a coordinate transformation for each fiber. In this way, the group structure of G is implemented into the fiber bundle $\mathfrak{B}$ as the way of the transformation of the fiber $\mathcal{F}$. This sort of fiber bundle is called as a G-bundle with a structure group G and denotesd by $\mathfrak{G}=(\mathcal{E}\,,\mathcal{M}\,,\pi\,,\mathcal{F}\,,G)$.

Conversely, if a set of transition functions $\tau_{ij}\in G$, where G is a Lie group, is provided, then a G-bundle can be constructed as follows: Let $\mathcal{M}$ and $\{U_i\}_{i\in I}$ be a differential manifold and an open covering of $\mathcal{M}$. Giving a differential manifold F, a set of the direct product manifolds and its disjoint union are constructed: $\{U_i \times \mathcal{F}\}_{i\in I}$ and $\mathcal{E}' = \coprod_{i\in I} U_i \times \mathcal{F}$, respectively. Now, using the transition functions τ_{ij}, an equivalence relation, denoted by " $\sim$ ", in $\mathcal{E}'$ can be induced in a well-defined manner. That is, for $(p\,,\xi) \in U_i \times \mathcal{F}$ and $(q\,,\eta) \in U_j \times \mathcal{F}$, the equivalence relation " $\sim$ " is defined as satisfying the following two conditions: (i) $p = q$; (ii) $\xi = \tau_{ij}\eta$. Let $[(p\,,\xi)]$ be an equivalent class of the representative element $(p\,,\xi)$. Then the quotient space of $\mathcal{E}'$ by " $\sim$ ", $i.e.$, $\mathcal{E} = \mathcal{E}'/\sim$, becomes G-bundle. In fact, the projection map and the local trivialization are given as $\pi\,:\,\mathcal{E}|_U = U \times \mathcal{F} \to \mathcal{M}$; $[(p\,,\xi)] \mapsto p$ and $\varphi\,:\,\pi^{-1}(U) \to U \times \mathcal{F}$; $[(p\,,\xi)] \mapsto (p\,,\xi)$, respectively: $\mathfrak{G} = (\mathcal{E}\,,\mathcal{M}\,,\pi\,,\mathcal{F}\,,G)$.

Famous examples of G-bundles are a cylinder and a Möbius strip. Let $\mathfrak{B} = (\mathcal{S}^1 \times \mathcal{F}\,,\mathcal{S}^1\,,\pi\,,\mathcal{F})$ be a fiber bundle, where $\mathcal{S}^1$ and $\mathcal{F}$ are a circle and an interval $[-1\,,1]$. Then, if a group $G_{\text{cylinder}} = \{e\}$ is given then the G-bundle, $\mathfrak{G} = (\mathcal{S}^1 \times \mathcal{F}\,,\mathcal{S}^1\,,\pi\,,\mathcal{F}\,,G_{\text{cylinder}})$, becomes a cylinder. If a group $G_{\text{Moebius}} = \{e\,,-e\}$ is given then the G-bundle, $\mathfrak{G} = (\mathcal{S}^1 \times \mathcal{F}\,,\mathcal{S}^1\,,\pi\,,\mathcal{F}\,,G_{\text{Moebius}})$, becomes a Möbius strip.

For applications to physics, G-bundles need more additional structure. In particular, connection/covariant derivative and curvature/field strength are mandatory. In order to formulate these concepts, a right action of the group G to a G-bundle is introduced, (the left action of the group G to G-bundle is nothing but a generalization of coordinate transformations) and it invokes a new geometric structure: the principal bundles.

5.2. Principal G-bundles, Ehresmann connections, and curvatures

In this section, making a relation between the fiber, $\mathcal{F}$, and the structure group, G, to a G-bundle, $\mathfrak{G} = (\mathcal{E}\,,\mathcal{M}\,,\pi\,,\mathcal{F}\,,G)$, as a group action, a principal G-bundle is introduced [Kobayashi (1989); Kobayashi and Nomizu (1996); Sharpe (1997)]. For the principal G-bundle, a connection so-called Ehresmann connection is formulated, and its fundamental properties are derived [Kobayashi (1989); Kobayashi and Nomizu (1996)]. Let us start by introducing a principal G-bundle.

A principal G-bundle is a G-bundle with a right action of the group G, *i.e.*, $R:\ \mathcal{P}\times G \to \mathcal{P}$; $(u\,,g)\mapsto u\cdot g$, acting on the total space $\mathcal{P}$ in the following manner: $(u\cdot g)g' = u\cdot(gg')$ and $u\cdot g = u$, and it satisfies the following conditions; (i) $\pi(u\cdot g)=\pi(u)$; (ii) $\pi(u)=\pi(u')$ implies the existence of an element $g\in G$ as follows $u' = u\cdot g$ (simply transitivity). In addition, assume that (iii) all sections $\sigma_i:\ U_i \to \pi^{-1}(U_i) = U_i\times G$ are differentiable, where $U_i\in\mathfrak{U}$ and $\mathfrak{U}$ is an open covering of the base space $\mathcal{M}$. " $\cdot$ " denotes the right action of the group G. Conditions (i) and (ii) identify the fiber $\mathcal{F}$ with the structure group G. Therefore, the principal G-bundle is denoted as $\mathfrak{P}=(\mathcal{P}\,,\mathcal{M}\,,\pi\,,G\,;\,R)$. Condition (iii) leads to a local trivialization $\varphi_i:\ \mathcal{P}|_{U_i}\to U_i\times G$; $\sigma_i(p)\mapsto(p\,,g)$ for $U_i\in\mathfrak{U}$, where the relation, *i.e.*, $\sigma_i(p)=\sigma_i(p)\cdot e=\sigma_i(p)\cdot(g^{-1}g)=(\sigma_i(p)\cdot g^{-1})\cdot g=\sigma'_i(p)\cdot g$ for $g\in G$, is used. The transition functions are defined by using the local trivializations, $\{\varphi_i\}_{i\in I}$, with respect to the *right* action of the structure group G as usual: $\{\tau_{ij}=\varphi_i^{-1}\circ\varphi_j\}$.

A famous example of a principal G-bundle is the Hopf fibration. Let $\mathfrak{G}=(\mathcal{S}^3\,,\mathcal{S}^2\,,\pi\,,F\,,U(1))$ be a $U(1)$-bundle with a fiber F, where $U(1)$ is the 1-rank unitary group. Introducing a right action of $U(1)$ into $\mathfrak{G}$, for the projection map $\pi:\ (x^1\,,x^2\,,x^3\,,x^4)\mapsto(\xi^1\,,\xi^2\,,\xi^3)$ such that $\xi^1=2(x^1x^3+x^2x^4)\,,\xi^2=2(x^2x^3-x^1x^4)\,,\xi^3=(x^1)^2+(x^2)^2-(x^3)^2-(x^4)^2$, becomes a principal $U(1)$-bundle: $\mathfrak{P}=(\mathcal{S}^3\,,\mathcal{S}^2\,,\pi\,,U(1)\,;\,R)$. Notice that, since the elements in $U(1)$ can be expressed as $\exp(i\theta)$ for $\theta\in(-\pi\,,\pi)$, the right action is not distinguished from the left action of the group.

Next, let us introduce the Ehresmann connection. The definition is given as follows:

$$\begin{aligned}&\text{(i)}\quad \omega(A^*)=A\quad (A\in\mathfrak{g})\,,\\&\text{(ii)}\quad {R_g}^*\omega(X)=Ad_g(\omega)=g^{-1}\omega g\,,\end{aligned}\tag{5.1}$$

where $\mathfrak{g}$ is the Lie algebra of the structure group G, ω is a $\mathfrak{g}$-valued 1-form, $\omega\in\mathfrak{g}\otimes T^*\mathcal{P}$, ${R_g}^*$ is the pull back operator of the right action with respect to an element $g\in G$, and Ad_g

is the adjoint representation with respect to $g \in G$. A^* is the so-called fundamental vector field defined as follows:

$$A^*{}_u f(u) = \frac{d}{dt}\left[f\left(ug(t)\right)\right]\Big|_{t=0}\,, \tag{5.2}$$

where $u \in P$, $g(t) = \exp(tA) \in G$, and f is an arbitrary function on $\mathcal{P}$. The right action, $R : \mathcal{P} \times G \to \mathcal{P}$, induces the differential map $dR : T\mathcal{P} \times TG \to T\mathcal{P}$; it means that the right action of $\mathfrak{g} = T_eG$ to $\mathcal{P}$ is well-defined. Therefore, the specific form of the fundamental vector field can be written as follows:

$$A^*{}_u = uA\,, \tag{5.3}$$

and it of course belongs to $T_u\mathcal{P}$.

The Ehresmann connection has two different expressions: the geometric and algebraic formulations. The geometric formulation is given as follows: a $\mathfrak{g}$-valued 1-form ω on $\mathcal{P}$ is the Ehresmann connection if and only if the following conditions are satisfied:

$$\begin{aligned} &\text{(i)} \quad T_u\mathcal{P} = V_u\mathcal{P} \oplus H_u\mathcal{P}\,, \\ &\text{(ii)} \quad {R_g}^*(H_u\mathcal{P}) = H_{ug}\mathcal{P}\,, \end{aligned} \tag{5.4}$$

where $V_u\mathcal{P}$ and $H_u\mathcal{P}$ are the vertical and horizontal subspaces, respectively, defined as follows:

$$V_u\mathcal{P} = \{X \in T_u\mathcal{P} \,|\, \pi_*(X) = 0\}\,, \quad H_u\mathcal{P} = \{X \in T_u\mathcal{P} \,|\, \omega(X) = 0\}\,, \tag{5.5}$$

where π_* is the push forward operator of the projection map π. In particular, the vertical subspace is expressed equivalently as follows:

$$V_u\mathcal{P} = \{A^*_u = uA \in T_u\mathcal{P} \,|\, A \in \mathfrak{g}\}\,. \tag{5.6}$$

The equivalence of the two definitions (5.1) and (5.4) is obvious from the definitions of the horizontal and vertical subspaces. Since the Principal G-bundle $\mathcal{P}$ is expressed as a direct product $\pi^{-1}(U) = U \times G$ in a local region, the above properties give a geometrical interpretation that U and G represent the horizontal and vertical direction on $\pi^{-1}(U) \subset \mathcal{P}$, respectively.

The curvature/field strength of the Ehresmann connection in the geometrical representation (5.4) is introduced as follows:

$$\Omega(X\,,Y) = d\omega(X^H\,,Y^H)\,, \tag{5.7}$$

where Ω is a $\mathfrak{g}$-valued 2-form on $\mathcal{P}$, X and Y belong to $T\mathcal{P}$, and X^H and Y^H belong to $H\mathcal{P}$. Expanding this, the following equation is derived:

$$\Omega(X\,,Y) = -\frac{1}{2}\omega\left([X^H\,,Y^H]\right)\,. \tag{5.8}$$

Therefore, the flatness, which is of course expressed as $\Omega = 0$, of the principal G-bundle $\mathcal{P}$ is equivalent to satisfying the following condition:

$$[X^H\,,Y^H] = 0\,. \tag{5.9}$$

This condition means that the horizontal subspace $H\mathcal{P} = \bigsqcup_{u\in\mathcal{P}} H_u\mathcal{P}$ is Frobenius integrable, and it restores the entire of the total space $\mathcal{P}$; in other words, if $\Omega \neq 0$, the Frobenius theorem restores only a part of the total space $\mathcal{P}$ as a submanifold. Notice that the vertical subspace $V\mathcal{P} = \bigsqcup_{u\in\mathcal{P}} V_u\mathcal{P}$ is always Frobenius integrable, and it restores the total space $\mathcal{P}$.

Finally, let us introduce the algebraic formulation of the Ehresmann connection. This formulation plays the main role in establishing gauge theories. The algebraic formulation is given as follows: for the Ehresmann connection ω in Eq (5.1),

$$\omega_i = \sigma_i^* \omega\,, \tag{5.10}$$

where $U_i \in \mathfrak{U}$, σ_i^* is the pull back operator of $\sigma_i : U_i \to \pi^{-1}(U_i)$. Then the following relation is satisfied:

$$\omega_j = {\tau_{ij}}^{-1} \omega_i \tau_{ij} + {\tau_{ij}}^{-1} d\tau_{ij}\,, \tag{5.11}$$

where $\tau_{ij} \in G$ is the transition function on $U_i \cup U_j$ for $U_i\,, U_j \in \mathfrak{U}$. Conversely, if the relations (5.11) are given then the Ehressmann connection in Eq (5.1) is derived. The proof of this statement is not trivial but easy to give as follows: Eq (5.10) is transformed from U_i to U_j by using the transition function τ_{ij} as $\omega_j = \omega((\sigma_i \tau_{ij})_* X)$, where $X \in T\mathcal{P}$. Here, $(\sigma_i \tau_{ij})_* X$ is calculated as follows: $(\sigma_i \tau_{ij})_* X = \sigma_{i*}(u)(X)\tau_{ij}(u) + A^*_{\sigma_j(u)}(X)$, where x_t is a curve in $\mathcal{P}$ such that $x_0 = u$ and $(dx_t/dt)|_{t=0} = X$. Eq (5.3) is also used. Therefore, $\omega_j = [{\tau_{ij}}^{-1}(\sigma_i^*\omega)\tau_{ij} + {\tau_{ij}}^{-1} d\tau_{ij}](X)$, $i.e.$, $\omega_j = {\tau_{ij}}^{-1}\omega_i \tau_{ij} + {\tau_{ij}}^{-1} d\tau_{ij}$, where Eq (5.1) are used. Conversely, if Eq (5.11) holds then, using the fact that ${\tau_{ij}}^{-1} d\tau_{ij}$ is Maurer-Cartan form (left-invariant $\mathfrak{g}$-valued 1-form with respect to the group action of $L : G \times \mathcal{P} \to \mathcal{P}$) [Kobayashi (1989); Kobayashi and Nomizu (1996)], it is shown that $\tilde{\omega}_i = {\tau_{ij}}^{-1}(\pi^*\omega_i)\tau_{ij} + {\tau_{ij}}^{-1} d\tau_{ij}$ is also valid on $\pi^{-1}(U_i \cap U_j)$; $\tilde{\omega}_i$ is defined on the entire region of $\mathcal{P}$: $\omega = {\tau_{ij}}^{-1}(\pi^*\omega_i)\tau_{ij} + {\tau_{ij}}^{-1} d\tau_{ij}$. Taking into account $\omega_i(A^*) = 0$, ω derives the first condition in Eq (5.1). (The satisfaction of the second condition in Eq (5.1) is obvious.) The pull back of ω by a section σ_i leads to $\omega_i = {\sigma_i}^*(\omega)$.

The curvature/field strength of the Ehresmann connection in the algebraic representation (5.11) is introduced as follows:

$$\Omega_i = d\omega_i + \frac{1}{2}[\omega_i\,, \omega_i]\,. \tag{5.12}$$

This expression can be derived by calculating the pull back of the definition (5.7) by a section σ_i and is now defined on $\mathfrak{g}$-valued 2-form on $\mathcal{M}$. For the curvature Ω_j on U_j, the following relation is easily verified:

$$\Omega_j = Ad_{\tau_{ij}}(\Omega_i) = {\tau_{ij}}^{-1}\Omega_i\tau_{ij}\,, \tag{5.13}$$

where τ_{ij} is the transition function from U_i to U_j. These quantities also live as $\mathfrak{g}$-valued 2-forms on $\mathcal{M}$.

For applications to physics, sections in a principal G-bundle, $\mathfrak{P}$, have to express the fields that describe physical phenomena. In order to achieve this, representations of the structure group G and those actions to the total space $\mathcal{P}$ are introduced, and then a new sort of fiber bundle is invoked: the vector bundles.

5.3. Vector bundles, gauge fields, and curvatures

In this section, introducing a representation of the structure group G of a principal G-bundle $\mathfrak{P} = (\mathcal{P}\,, \mathcal{M}\,, \pi\,, G\,;\, R)$, denoted by $\rho:\ G \to \mathrm{End}(V)$ for a r-dimensional representation space V, an associated vector bundle is introduced [Kobayashi (1989); Kobayashi and Nomizu (1996); Sharpe (1997); Nakahara (2003)]. Inheriting its properties, the generic definition of vector bundles is also given. Then gauge fields/connection 1-form in covariant exterior derivative and its curvature are introduced, respectively [Kobayashi (1989); Kobayashi and Nomizu (1996)]. Sections of a vector bundle are nothing but fields that describe physical phenomena. Therefore, these concepts play a central role in constructing a theory of physics. First of all, let us introduce an associated vector bundle.

An associated vector bundle is derived from a quotient space of $\mathcal{P} \times V$ with an equivalent relation, denoted by " $\sim$ ", of the structure group G such that, for $(\xi\,, u)$ and $(\eta\,, v)$ in $\mathcal{P} \times V$, these two elements are equivalent if and only if the following two relations hold: (i) $\xi = R_g\eta$; (ii) $u = \rho^{-1}(g)v$. The quotient space is $\mathcal{V}_\rho = \mathcal{P} \times_\rho V = (\mathcal{P} \times V)/\sim$ and an equivalent class is denoted as $[(\xi\,, v)]$. Then the structure $\mathfrak{V} = (\mathcal{V}_\rho\,, \mathcal{M}\,, \pi\,, V\,;\, R\,, \rho)$ has a one-to-one correspondence on a local region $U \subset \mathcal{M}$ as follows: $\mathcal{P}|_U \times V \to U \times G \times V\,;\, (\sigma(p)\,, v) \mapsto (p\,, e\,, v)$, where $p \in U$, σ is a section of $\mathcal{P}$ on U, and e is the unit element of G, since the group action R is simply transitive. Therefore, the quotient space $\mathcal{V}$ can be identified in a local region U with $\mathcal{V}_\rho|_U = U \times V$. That is, the representation space V is nothing but the standard fiber of the associated vector bundle $\mathcal{V}_\rho$. This property also indicates the existence of local trivializations as follows: $\varphi_i \,:\, \pi^{-1}(U_i) \to U_i \times V$, where $U_i \in \mathfrak{U}$ and the projection map is given as follows: $\pi \,:\, \mathcal{V}_\rho \to \mathcal{M}\,;\, [(\sigma_i(p)\,, v)] \mapsto p$, where σ_i is a section of $\mathcal{P}$ on $U_i \in \mathfrak{U}$. Based on these properties, it would be interpreted that an associated vector bundle is nothing but a result of replacing the structure group G by a representation space V using a group representation ρ in a principal G-bundle.

Based on the properties of an associated vector bundle described above, the generic definition of vector bundles is defined as follows: a fiber bundle $\mathfrak{V} = (\mathcal{V}\,, \mathcal{M}\,, \pi\,, V)$ such that (i) the fiber V is a vector space; (ii) for each $U_i \in \mathfrak{U}$, a local trivialization $\varphi_i : \mathcal{V}|_{U_i} = \pi^{-1}(U_i) \to U \times V$ exists. Conversely, if a vector bundle is given then a principal G-bundle exits such that its associated vector bundle by the representation $\rho = id$ coincides with the original vector bundle: " $\mathcal{V} = {}^\exists\mathcal{V}'_{\rho=id}$ " [Kobayashi and Nomizu (1996)]. Therefore, in order to reveal the properties of vector bundles, it is enough to consider that of associated vector bundles.

Next, let us introduce gauge fields/connection 1-form of an associated vector bundle. In order to define the operation of covariant exterior derivative, it needs to prepare V-valued p-form, denoted by $\tilde{\xi}$, on $\mathcal{P}$ as a section on $V \otimes \bigwedge^p T^*\mathcal{P}$ as follows: for $X_1\,, \cdots, X_p \in \Gamma(T\mathcal{P})$, it satisfies

$$\tilde{\xi}(X_1\,, \cdots, X_p) = u^{-1}(\xi(\pi_* X_1\,, \cdots, \pi_* X_p))\,, \tag{5.14}$$

where $\xi \in \Gamma(\mathcal{V}_\rho \otimes \bigwedge^p T^*\mathcal{M})$. If $p = 0$ then $\tilde{\xi}$ is a V-valued function given as follows:

$$\tilde{\xi} \,:\, \mathcal{P} \to V\,;\, u \mapsto u^{-1}(\xi(\pi(u)))\,. \tag{5.15}$$

This V-valued p-from $\tilde{\xi}$ on $\mathcal{P}$ obviously satisfies the following two properties:

$$
\begin{aligned}
&\text{(i)} \quad R_g^* \tilde{\xi} = \rho^{-1}(g) \tilde{\xi}\,, \\
&\text{(ii)} \quad X_1 \in H\mathcal{P} \quad \text{then} \quad \tilde{\xi}(X_1\,, \cdots, X_p) = 0\,.
\end{aligned}
\tag{5.16}
$$

These two properties lead to a one-to-one correspondence between $\tilde{\xi} \in \Gamma(V \otimes \bigwedge^p T^*\mathcal{P})$ and $\xi \in \Gamma(\mathcal{V}_\rho \otimes \bigwedge^p T^*\mathcal{M})$ in Eq (5.14). Then the covariant exterior derivative, denoted by d_D, of $\tilde{\xi} \in \Gamma(V \otimes \bigwedge^p T^*\mathcal{P})$ is introduced in a well-defined manner as follows:

$$
d_D \tilde{\xi}(X_1\,, \cdots, X_p) = d\tilde{\xi}(X_1^H\,, \cdots, X_p^H)\,, \tag{5.17}
$$

where $X_1\,, \cdots, X_p \in \Gamma(T\mathcal{P})$ and $X_1^H\,, \cdots, X_p^H \in \Gamma(H\mathcal{P})$. In terms of the Ehresmann connection, the above equation can be expressed as follows:

$$
d_D \tilde{\xi} = d\tilde{\xi} + d\rho(\omega) \wedge \tilde{\xi}\,, \tag{5.18}
$$

where $d\rho$ is the representation of the Lie algebra $\mathfrak{g}$ induced by ρ. Then the properties in Eq (5.16) lead also to $d_D\tilde{\xi} \in \Gamma(V \otimes \bigwedge^{p+1} T^*\mathcal{P})$. For $\alpha \in \Gamma(\bigwedge^p T\mathcal{M})$ and $\tilde{\xi} \in \Gamma(V \otimes \bigwedge^q T^*\mathcal{P})$, the following formula holds:

$$
d_D(\tilde{\xi} \wedge \alpha) = d_D\tilde{\xi} \wedge \alpha + (-1)^q \tilde{\xi} \wedge d(\pi^*\alpha)\,. \tag{5.19}
$$

The one-to-one correspondence between $\tilde{\xi} \in \Gamma(V \otimes \bigwedge^p T^*\mathcal{P})$ and $\xi \in \Gamma(\mathcal{V}_\rho \otimes \bigwedge^p T^*\mathcal{M})$ leads to the covariant exterior derivative in $\Gamma(V \otimes \bigwedge^p T^*\mathcal{P})$; just removing " $\tilde{}$ ", " ^{H} ", " $d\rho$ ", and " π^* ", from Eqs (5.17), (5.18) and (5.19), and just replacing $T\mathcal{P}$ by $T\mathcal{M}$, $H\mathcal{P}$ by $T\mathcal{M}$, and V by $\mathcal{V}_\rho$, the covariant exterior derivative d_D in $\Gamma(\mathcal{V}_\rho \otimes \bigwedge^p T^*\mathcal{M})$ is introduced in a well-defined manner. Notice that in this case the Ehresmann connection becomes a section of $\mathrm{End}(\mathcal{V}) \times \mathrm{T}^*\mathcal{M}$: $\omega = \omega^i{}_{j\mu} e_i \otimes e^j \otimes dx^\mu$. This Ehresmann connection is, in particular, called gauge fields. Since the theorem " $\mathcal{V} = {}^\exists\mathcal{V}'_{\rho=id}$ " [Kobayashi and Nomizu (1996)] as mentioned in the previous paragraph guarantees that a vector bundle has its associated principal G-bundle, all formulae above, *i.e.*, Eqs (5.18) and (5.19), can apply also to any given vector bundle.

For a vector bundle $\mathfrak{V} = (\mathcal{V}, \mathcal{M}, \pi, V)$, the covariant derivative of a section of $\mathcal{V}$ can be derived by considering a special case of the covariant exterior derivative; let p in Eq (5.18) set zero. Then d_D becomes a linear operator as follows: $d_D : \Gamma(\mathcal{V}) \to \Gamma(\mathcal{V} \otimes T^*M)\,;\, \xi \mapsto d_D\xi$. In particular, for a function f on $\mathcal{M}$, it satisfies $d_D(f\xi) = df \otimes \xi + f d_D\xi$. The image of ξ by d_D is defined as the covariant derivative of ξ and denoted by $d_D\xi = \nabla\xi$. Explicitly, it is expressed as follows:

$$d_D\xi = \nabla\xi = (d + \omega)\xi\,. \tag{5.20}$$

From the definition of d_D, the covariant derivative ∇ can be interpreted as a linear operator as follows: for a vector field $X \in \Gamma(T\mathcal{M})$, $\nabla_X : \Gamma(\mathcal{V}) \to \Gamma(\mathcal{V})\,;\, \xi \mapsto \nabla_X\xi$ such that (i) $\nabla_{fX}\xi = f\nabla_X\xi$; (ii) $\nabla_{X+Y}\xi = \nabla_X\xi + \nabla_Y\xi$, where f is a function on $\mathcal{M}$, $X\,, Y \in \Gamma(T\mathcal{M})$, and $\xi \in \Gamma(\mathcal{V})$. In other words, $\nabla_X \in \mathrm{End}(\Gamma(\mathcal{V}))$. Then Eq (5.20) becomes as follows:

$$\nabla_X\xi = X(\xi) + \omega(X)\xi\,. \tag{5.21}$$

Since the fiber V of the vector bundle $\mathcal{V}$ is vector space, $\mathcal{V}|_U = \pi^{-1}(U) = U \times V$ has a basis of $\Gamma(\mathcal{V})$: $e_I = e_I(p)$ for $p \in U$, where $I \in \{1\,, \cdots, r\}$ and r is the dimension of V. Therefore, Eqs (5.20) and (5.21) can be rewritten as follows:

$$\begin{aligned} \nabla\xi &= (d\xi^I + \omega^I{}_J\xi^J)e_I\,, \\ \nabla_\mu\xi &= (\partial_\mu\xi^I + \omega^I{}_{J\mu}\xi^J)e_I\,, \end{aligned} \tag{5.22}$$

respectively, where $X = \partial_\mu$. Defining the components of $\nabla_\mu \xi$ as $(\nabla_\mu \xi)^I$, *i.e.*, $\nabla_\mu \xi = (\nabla_\mu \xi)^I e_I$, the second equation becomes as follows:

$$(\nabla_\mu \xi)^I = \partial_\mu \xi^I + \omega^I{}_{J\mu} \xi^J \,. \tag{5.23}$$

This is a familiar form of covariant derivative in physics. For a component ξ^I the second formula in Eq (5.22) becomes more familiar form: $\nabla_\mu \xi^I = \partial_\mu \xi^I + \omega^I{}_{J\mu} \xi^J$.

Finally, let us introduce the curvature (2-form on $\mathcal{M}$) of the covariant derivative ∇ given in (5.20). Based on Eq (5.7), the following equation is derived:

$$R(X\,, Y)\xi = \frac{1}{2}\left(\nabla_X \nabla_Y - \nabla_Y \nabla_X - \nabla_{[X\,,Y]}\right)\xi \,, \tag{5.24}$$

where R is End($\mathcal{V}$)-valued 2-form on $\mathcal{M}$, X and Y are vector fields on $\mathcal{M}$, and ξ is a section of the vector bundle $\mathcal{V}$. This formula is called the Ricci identity. Calculating it for $\xi = e_I$, the following equations are derived:

$$\begin{aligned} R e_I &= \Omega_I{}^J \otimes e_J \,, \\ \Omega_I{}^J &= d\omega_I{}^J + \omega_K{}^J \wedge \omega_I{}^K = d_D \omega_I{}^J \,, \end{aligned} \tag{5.25}$$

where Eq (5.18) is used. The first equation and second relation are the so-called structure equation and curvature form of the covariant derivative ∇, respectively. Notice that the curvature form coincides with Eq (5.12). That is, it is nothing but a relation replaced ω_i, which lives as a $\mathfrak{g}$-valued 1-form on $\mathcal{M}$, by $\omega_I{}^J$, which lives as a End($\mathcal{V}$)-valued 1-form on $\mathcal{M}$. Therefore, for the gauge transformation of Eq (5.11), the curvature 2-form changes as Eq (5.13).

So far, it is revealed that the connection 1-form ω and curvature 2-form Ω are the first- and second-order covariant exterior derivative of a basis e_I of the fiber V, respectively.

Considering the third-order covariant exterior derivative of e_I, or more generically, $\xi \in \Gamma(\mathcal{V})$, the following identity is derived

$$d_D R = 0\,. \tag{5.26}$$

This is nothing but the so-called Bianchi identity.

Depending on the structure group G and its representation, the mathematical theory presented above can describe a specific physics. For instance, for $G = U(1)$, Maxwell's electromagnetic interaction is obtained [Weyl (1929); O'Raifeartaigh and Straumann (1998)]. The structure group $G = U(1) \times SU(2)$ and $G = SU(3)$ describe the electroweak interaction [Weinberg (1967); Salam (1968)] and the quantum chromodynamics/strong interaction [Greenberg (1964); Han and Nambu (1965)], as non-abelian gauge Yang-Mills gauge theory [Yang and Mills (1954)], respectively. In addition, identifying irreducible representations for each theory, gauge fields/particles are taken into account. In the same manner, it may be expected that a theory of gravity is also obtained from the proper structure group and its representation [Utiyama (1956)]. This is the motivation for gauge theories of gravity. Before introducing these theories, let us relate the Ehresmann connection to the affine connection.

5.4. Internal space bundles, frame fields, and Weitzenböch connections

In this section, the main concepts for gauge theories of gravity, and internal space bundles, in particular, focusing on frame fields/vielbein, are introduced. Relating it, an important formula, *i.e.*, the Weitzenböch connection, between the so-called spin connection and the affine connection is derived. This relation plays a crucial role in formulating the metric-affine gauge theories of gravity as presented in the next Chapter 6.

Frame fields/vielbein are the components of a bundle morphism, denoted by $\mathbf{e}$, from a vector bundle $\mathfrak{V} = (\mathcal{V}\,, \mathcal{M}\,, \pi)$ to the tangent bundle of a spacetime manifold $\mathfrak{T} = (T\mathcal{M}\,, \mathcal{M}\,, \iota)$.

That is, for any open set U of an open covering of $\mathcal{M}$ and a smooth function $f : M \to M$, the bundle map $\mathbf{e} = \pi^{-1} \circ f \circ \iota : \mathcal{V} \to T\mathcal{M}\,;\, \mathcal{V}|_U \mapsto \mathbf{e}(\mathcal{V}|_U) = T\mathcal{M}|_U$ defines a set of sections as follows:

$$e_I = \mathbf{e}(\xi_I) = e_I{}^\mu \partial_\mu \,, \tag{5.27}$$

where ξ_I and ∂_μ are a basis of sections of $\mathcal{V}|_U$ and the local coordinate/holonomic basis of $T\mathcal{M}|_U$, respectively. Then the set of components $e_I{}^\mu$, or equivalently, e_I, and the vector bundle $\mathfrak{V}$ are called frame fields/vielbein with respect to the vector bundle $\mathfrak{V}$ and the internal space bundle, respectively. Remark that both e_I and $e_I{}^\mu$ are sections of the tangent bundle $T\mathcal{M}$, although the indices represent that of the internal space bundle $\mathcal{V}$. Therefore, the bundle morphism can be written also as follows:

$$\mathbf{e} = e_I{}^\mu \partial_\mu \otimes \xi^I \,, \tag{5.28}$$

where ξ^I are the dual basis of ξ_I. This is a section of the vector bundle of the tensor product, *i.e.*, $T\mathcal{M} \otimes \mathcal{V}^*$. The projection map of the constructed bundle is obtained just by taking the tensor product of each projection map in the order; so are the local trivializations.

The inverse map of $\mathbf{e}$ can be introduced in a well-defined manner by virtue of its definition $\mathbf{e} = \pi^{-1} \circ f \circ \iota$. That is, $\mathbf{e}^{-1} = \iota^{-1} \circ f^{-1} \circ \pi : T\mathcal{M} \to \mathcal{V}\,;\, T\mathcal{M}|_U \mapsto \mathbf{e}^{-1}(T\mathcal{M}|_U) = \mathcal{V}|_U$. Using this map, the dual basis of ξ_I, *i.e.*, ξ^I, are pulled back to $T^*\mathcal{M}$ as follows:

$$e^I = (\mathbf{e}^{-1})^*(\xi^I) = e^I{}_\mu dx^\mu \,, \tag{5.29}$$

where dx^μ are the dual basis of ∂_μ. Then the components $e^I{}_\mu$, or equivalently, e^I, are called co-frame fields/co-vielbein with respect to the internal space bundle $\mathfrak{V}$. Remark that both e^I and $e^I{}_\mu$ are sections of the co-tangent vector bundle $T^*\mathcal{M}$. Therefore, the inverse map can be expressed as follows:

$$(\mathbf{e}^{-1})^* = e^I{}_\mu dx^\mu \otimes \xi_I \, . \tag{5.30}$$

This is a section of the dual vector bundle $T^*\mathcal{M} \otimes \mathcal{V}$ of $T\mathcal{M} \otimes \mathcal{V}^*$. The projection map and local trivializations are also introduced in a dual manner.

The frame fields/co-frame fields satisfy the following relations:

$$e_I{}^\mu e^J{}_\mu = \delta_I^J \, , \quad e_I{}^\mu e^I{}_\nu = \delta_\nu^\mu \, . \tag{5.31}$$

For a metric tensor of the tangent space $g = g_{\mu\nu} dx^\mu \otimes dx^\nu$ and a metric of the internal space bundle $g = g_{IJ} \xi^I \otimes \xi^J$, pulling back it by $\mathbf{e}$ and $(\mathbf{e}^{-1})^*$, the following relation are obtained:

$$g_{IJ} = e_I{}^\mu e_J{}^\nu g_{\mu\nu} \, , \quad g_{\mu\nu} = e^I{}_\mu e^J{}_\nu g_{IJ} \, , \tag{5.32}$$

respectively. The total number of independent variables in the tangent bundle is, on one hand, $(n+1)(n+2)/2$ for the metric tensor $g_{\mu\nu}$. On the other hand, that in the internal space bundle is the total number of $(n+1)(n+1)$ for the frame fields $e_I{}^\mu$ and of $(n+1)(n+2)/2$ for the metric tensor g_{IJ}, respectively. Therefore, in order to make the correspondence between $g_{\mu\nu}$, and, $e_I{}^\mu$ and g_{IJ} in a one-to-one manner, the internal space variables have to be imposed some conditions. In many applications in theories of gravity, the internal space bundle is taken to be a trivial vector bundle $\mathcal{M} \times \mathbb{R}^{n+1}$. This indicates that all components of the metric g_{IJ} are constant; it reduces the number of the independent variables in the internal space bundle into the number of the frame fields. The remaining extra degrees of freedom, *i.e.*, $(n+1)(n+2)/2 - (n+1)(n+1) = n(n+1)/2$, can be erased by imposing a gauge symmetry of the (co-)frame fields. In the case of the trivial bundle $\mathcal{M} \times \mathbb{R}^{n+1}$, the structure group G is sometimes set to be the Lorentz group: $G = SO(n\,,1)$. Then, since an element of $G = SO(n\,,1)$ has the number of $n(n+1)/2$ independent components, the (co-)frame fields are restricted by the group via the transition functions. Therefore, in this case, the number of independent variables on each bundle coincides with one another.

The covariant derivative of sections of the internal space bundle is also given by Eq (5.20) or Eq (5.22) in the previous section 5.3. Since the frame field $\mathbf{e}$ can be expressed as Eq (5.28), *i.e.*, a section of the tensor product bundle $T^*\mathcal{M}\otimes\mathcal{V}$, the covariant derivative of $\mathbf{e}$, denoted by $\mathcal{D}\mathbf{e}$, becomes as follows:

$$\mathcal{D}\mathbf{e} = (de^I{}_\mu - \tilde{\Gamma}^\rho_{\nu\mu} e^I{}_\rho dx^\nu + \omega^I{}_{J\mu} e^J{}_\nu dx^\nu) dx^\mu \otimes \xi_I \,, \tag{5.33}$$

where $\Gamma^\rho_{\mu\nu}$ and $\omega^I{}_{J\mu}$ are the affine connection of the tangent bundle and the spin connection of the internal space bundle. In component form, the above formula is expressed as follows:

$$\mathcal{D}_\mu e^I{}_\nu = \partial_\mu e^I{}_\nu - \tilde{\Gamma}^\rho_{\mu\nu} e^I{}_\rho + \omega^I{}_{J\mu} e^J{}_\nu \,. \tag{5.34}$$

In the same way, $\mathcal{D}_\mu e_I{}^\nu$ is calculated as follows:

$$\mathcal{D}_\mu e_I{}^\nu = \partial_\mu e_I{}^\nu + \tilde{\Gamma}^\nu_{\mu\rho} e_I{}^\rho - \omega^J{}_{I\mu} e_J{}^\nu \,. \tag{5.35}$$

These formulae are the result from $\mathcal{V}|_U \simeq T\mathcal{M}|_U$ on a local region U in $\mathcal{M}$; this local relation implies that the affine connection and the spin connection can be identified in the local region U. The transition functions $\tau_{ij} = \varphi_i^{-1} \circ \varphi_j$ of the internal space bundle $\mathcal{V}$ form its structure group G. Therefore, for $\Lambda \in G$, Eq (5.11) leads to the transformation of the spin connection as follows:

$$\omega^I{}_{J\mu} \to \omega'^I{}_{J\mu} = (\Lambda^{-1})^I{}_K \partial_\mu \Lambda^K{}_J + (\Lambda^{-1})^I{}_K \omega^K{}_{L\mu} \Lambda^L{}_J \,. \tag{5.36}$$

Then the co-frame fields $e^I{}_\mu$ and those covariant derivatives $\mathcal{D}_\mu e^I{}_\nu$ are transformed as $e^I{}_\mu \to e'^I{}_\mu = \Lambda^I{}_J e^J{}_\mu$ and $\mathcal{D}_\mu e'^I{}_\nu = \Lambda^I{}_J \mathcal{D}_\mu e^J{}_\nu$, respectively. $\mathcal{D}_\mu e_I{}^\nu$ transforms in the same manner under the gauge transformation (5.36): $\mathcal{D}_\mu e'^{\ \nu}_I = (\Lambda^{-1})^J{}_I \mathcal{D}_\mu e_J{}^\nu$.

Finally, let us derive the Weitzenböch connection. A section, denoted by X, of the tangent bundle $T\mathcal{M}$ is of course expressed as $X = X^\mu \partial_\mu$. Pulling back X^μ to the internal space bundle by using co-frame fields $e^I{}_\mu$, the components of a section on the internal space are obtained: $\tilde{X}^I = e^I{}_\mu X^\mu$, or equivalently, $X^\mu = e^\mu{}_I \tilde{X}^I$. Therefore, X is equivalent to $\tilde{X} = \tilde{X}^I \xi_I$. The covariant derivative of X and $\tilde{X}$ become as follows:

$$\nabla X = (\partial_\nu X^\mu + \tilde{\Gamma}^\mu_{\nu\rho} X^\rho) \partial_\mu \otimes dx^\nu \tag{5.37}$$

and

$$\mathcal{D}\tilde{X} = (e^I{}_\nu \partial_\mu X^\nu + X^\nu \partial_\mu e^I{}_\nu + \omega^I{}_{J\mu} e^J{}_\nu X^\nu) \xi_I \otimes dx^\mu\,, \tag{5.38}$$

respectively. Using the pull back of ∂_μ by the frame fields $e_I{}^\mu$, $\xi_I = e_I{}^\mu \partial_\mu$, the left-hand side of the second formula becomes as follows:

$$\mathcal{D}\tilde{X} = (\partial_\nu X^\mu + X^\rho e_I{}^\mu \partial_\nu e^I{}_\rho + \omega^I{}_{J\nu} e_I{}^\mu e^J{}_\rho X^\rho) \partial_\mu \otimes dx^\nu\,. \tag{5.39}$$

This formula is of course the same as the first one; the covariant derivatives ∇X and $\mathcal{D}\tilde{X}$ are also equivalent. Therefore, the following relation is derived:

$$\tilde{\Gamma}^\rho_{\mu\nu} = e_I{}^\rho \partial_\mu e^I{}_\nu + \omega^I{}_{J\mu} e_I{}^\rho e^J{}_\nu\,. \tag{5.40}$$

This is the so-called Weitzenböch connection, which relates the spin connection to the affine connection via the (co-)frame fields. Notice that Eq (5.40) implies $\mathcal{D}_\mu e^I{}_\nu = 0$, or equivalently, $\mathcal{D}_\mu e_I{}^\nu = 0$. These properties are sometimes called vielbein *postulate* but, as shown in the above, always satisfied. That is, it is not a *postulate*. In addition, taking into account the gauge invariant property of them, it guarantees that these properties hold in the global region of $\mathcal{M}$.

The metric-vielbein relation (5.32) and the Weitzenböch connection (5.40) play a fundamental role of gauge theories of gravity. That is, assume that an action of gravy is given as follows:

$$I[g_{\mu\nu}\,,\tilde{\Gamma}^{\rho}_{\mu\nu}] = \int_{\mathcal{M}} \mathcal{L}(g_{\mu\nu}\,,\partial_\rho g_{\mu\nu}\,,\cdots;\,\tilde{\Gamma}^{\rho}_{\mu\nu}\,,\partial_\lambda\tilde{\Gamma}^{\rho}_{\mu\nu}\,,\cdots)\,\sqrt{-g}\,d^{n+1}x\,. \tag{5.41}$$

Then, using the metric-vielbein relation and the Weitzenböch connection, the above action is rewritten in terms of the metric of the internal space, the (co-)frame fields, and the spin connection as follows:

$$I[g_{IJ}\,,e^I{}_\mu\,,\omega^I{}_{J\mu}] = \int_{\mathcal{M}} \mathcal{L}(g_{IJ}\,,\partial_\rho g_{IJ}\,,\cdots;\,e^I{}_\mu\,,\partial_\rho e^I{}_\mu\,,\cdots;\,\omega^I{}_{J\mu}\,,\partial_\lambda\omega^I{}_{J\mu}\,,\cdots)\,\det(\mathbf{e}^{-1})\,d^{n+1}x\,, \tag{5.42}$$

where $\det(\mathbf{e}^{-1})$ denotes the determinant of the co-frame fields. This quantity is well-defined by virtue of $\mathcal{V}|_U \simeq T\mathcal{M}|_U$. Remark that the theory given in Eq (5.42) does not always restore that in Eq (5.41). Conversely, starting with constructing an internal space bundle $\mathfrak{V} = (\mathcal{V}\,,\mathcal{M}\,,\pi)$, a generic theory which is described by the action functional (5.42) is obtained. This theory is much richer than the original theory given by Eq (5.41) since impositions of proper gauge conditions would give rise to a lot of theories of gravity. As a special case, for the trivial internal space bundle $\mathcal{V} = \mathcal{M} \times \mathbb{R}^{n+1}|_U$, Eq (5.42) becomes as follows:

$$I[e^I{}_\mu\,,\omega^I{}_{J\mu}] = \int_{\mathcal{M}} \mathcal{L}(e^I{}_\mu\,,\partial_\rho e^I{}_\mu\,,\cdots;\,\omega^I{}_{J\mu}\,,\partial_\lambda\omega^I{}_{J\mu}\,,\cdots)\,\det(\mathbf{e}^{-1})\,d^{n+1}x\,. \tag{5.43}$$

The metric tensor g_{IJ} has those components as constant and defined on the global region of $\mathcal{M} \times \mathbb{R}^{n+1}$. This theory is always equivalent to that given by Eq (5.41).

5.5. A derivation of Einstein field equations based on gauge approach to gravity

In this section, the Einstein field equations (4.28) are derived in the way of the gauge theories of gravity that is provided in the previous section 5.4 [Palatini (1919); Utiyama (1956); Baez and Muniain (1995)].

The action functional given as Eq (5.43) of the internal space bundle $\mathfrak{V} = (\mathcal{V} = \mathcal{M} \times \mathbb{R}^{n+1}\,, \mathcal{M}\,, \pi)$ realize this purpose. First, in order to specify the metric g_{IJ}, the following metric-preserving condition is imposed:

$$vg(\xi\,, \xi') = g(\mathcal{D}_v \xi\,, \xi') + g(\xi\,, \mathcal{D}_v \xi')\,, \tag{5.44}$$

where v is a vector field on $\mathcal{M}$, and, ξ and ξ' are sections of the internal space $\mathcal{M} \times \mathbb{R}^{n+1}$. Considering it with respect to the basis of sections of the internal space $\mathcal{M} \times \mathbb{R}^{n+1}$, $i.e.$, ξ_I, the connection $\omega^I{}_{J\mu}$ satisfies the following property:

$$\omega_{IJ\mu} = -\omega_{JI\mu}\,. \tag{5.45}$$

Therefore, under the metric-preserving condition, this connection is nothing but the Lorentz connection: $\omega^{(L)}{}_{IJ\mu} \in \mathfrak{so}(n\,, 1)$. This satisfies the demand from the EEP. Second, a specific Lagrangian in Eq (5.43) is given as follows:

$$I[e^I{}_\mu\,, \tilde{\omega}^I{}_{J\mu}] = \int_{\mathcal{M}} \mathcal{L} \det(\mathbf{e}^{-1})\, dx^{n+1} = \int_{\mathcal{M}} e^\mu{}_I e^\nu{}_J \tilde{\Omega}^{IJ}{}_{\mu\nu} \det(\mathbf{e}^{-1})\, dx^{n+1}\,, \tag{5.46}$$

where $\tilde{\Omega}^{IJ}{}_{\mu\nu}$ is the curvature form given in Eq (5.25). Explicitly, $\tilde{\Omega}^{IJ}{}_{\mu\nu}$ is written as follows:

$$\tilde{\Omega}^{IJ}{}_{\mu\nu} = \tilde{\nabla}_{[\mu} \tilde{\omega}^{IJ}{}_{\nu]} + \tilde{\omega}^I{}_{K[\mu} \tilde{\omega}^{KJ}{}_{\nu]}\,, \tag{5.47}$$

where $\tilde{\nabla}_\mu$ is the covariant derivative of the Weitzenböch connection $\tilde{\Gamma}^\rho_{\mu\nu}$ given in Eq (5.40).

To apply the variational principle in a well-posed manner with respect to the constraint phase space $\mathfrak{C}^{(1)}$, let us clarify appropriate boundary conditions. The action functional (5.46) can be rewritten as follows [Lagraa et al. (2017); Lagraa and Lagraa (2018)]:

$$I[e^I{}_\mu\,, \tilde{\omega}^I{}_{J\mu}] = \int_\mathcal{M} \left[A^{iI0J}(\tilde{\nabla}_0 \tilde{\omega}_{IJi} - \tilde{\nabla}_i \tilde{\omega}_{IJ0}) - A^{iIjJ} \tilde{\Omega}_{IJij}\right] \,\det(\mathbf{e}^{-1})\, dx^{n+1}\,, \tag{5.48}$$

where $A^{\mu I\nu J}$ is defined as follows:

$$A^{\mu I\nu J} = e^{I\mu} e^{J\nu} - e^{I\nu} e^{J\mu}\,. \tag{5.49}$$

Canonical momentum variables are calculated as follows:

$$\pi^{\mu I} = \frac{\delta \mathcal{L}}{\delta(\tilde{\nabla}_0 e_{I\mu})} = 0\,, \quad \mathcal{P}^{iIJ} = \frac{\delta \mathcal{L}}{\delta(\tilde{\nabla}_0 \tilde{\omega}_{IJi})} = A^{iI0J}\,, \quad \mathcal{P}^{0IJ} = \frac{\delta \mathcal{L}}{\delta(\tilde{\nabla}_0 \tilde{\omega}_{IJ0})} = A^{0I0J} = 0\,. \tag{5.50}$$

All of these variables become primary constraint densities, and these constraint densities specify the phase subspace $\mathfrak{C}^{(1)}$. Then the symplectic potential is given as follows: $\theta = \pi^{\mu I} \delta e_{I\mu} + \mathcal{P}^{iIJ} \delta \tilde{\omega}_{IJi} + \mathcal{P}^{0IJ} \delta \tilde{\omega}_{IJ0} = \mathcal{P}^{iIJ} \delta \tilde{\omega}_{IJi}$. Therefore, the variational principle becomes well-posed on the constraint phase subspace $\mathfrak{C}^{(1)}$ under the imposition of boundary conditions $\delta \tilde{\omega}_{IJi} = 0$ on $\partial \mathcal{M}$.

Varying Eq (5.46) with respect to the frame fields $e_I{}^\alpha$, the following equation is derived:

$$\delta_e I = 2 \int_\mathcal{M} \left(\tilde{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \tilde{R}\right) \eta^{IJ} e_I{}^\mu \delta(e_J{}^\beta) \det(\mathbf{e}^{-1}) dx^{n+1}\,. \tag{5.51}$$

Note that there are no boundary terms: this is consistent with the appropriate boundary conditions that are derived in the previous paragraph. Therefore, the variational principle leads to the following equations in a well-posed manner:

$$\tilde{G}_{\mu\nu} = \tilde{R}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} \tilde{R} = 0 \, . \tag{5.52}$$

Varying Eq (5.46) with respect to the connection $\omega^I{}_{J\mu}$ around the Lorentz connection ${\omega^{(L)}}^I{}_{J\mu}$: $\tilde{\omega}^I{}_{J\mu} = {\omega^{(L)}}^I{}_{J\mu} + {\tilde{\omega}'}^I{}_{J\mu}$, the following equation is derived:

$$\begin{aligned} \delta I_\omega = & \int_{\mathcal{M}} g^{\mu\nu} (-C^\alpha_{\alpha\beta} \delta C^\beta_{\mu\nu} + C^\beta_{\gamma\mu} \delta C^\gamma_{\beta\nu} - C^\alpha_{\mu\nu} \delta C^\beta_{\beta\alpha} + C^\alpha_{\beta\nu} \delta C^\beta_{\mu\alpha}) \det(\mathbf{e^{-1}}) dx^{n+1} \\ & + \int_{\partial\mathcal{M}} (n_\nu g^{\mu\nu} \delta C^\rho_{\rho\mu} - g^{\mu\nu} n_\rho \delta C^\rho_{\mu\nu}) \det(\mathbf{e^{-1}}) dx^n \, , \end{aligned} \tag{5.53}$$

where $C^\rho_{\mu\nu} = e_I{}^\rho e^J{}_\mu {\tilde{\omega}'}^I{}_{J\nu}$. Applying the appropriate boundary conditions $\delta C^\nu_{\mu I} = 0$ that are derived in the previous paragraph, the above equation becomes as follows:

$$\delta I_\omega = \cdots + \int_{\partial\mathcal{M}} (n_\nu g^{0\nu} \delta C^\rho_{\rho 0} - g^{\mu 0} n_\rho \delta C^\rho_{\mu 0}) \det(\mathbf{e^{-1}}) dx^n \, . \tag{5.54}$$

Remark that the frame fields are fixed in this variation. To erase this boundary term, let us impose a gauge condition as follows:

$${\tilde{\omega}'}^I{}_{J0} = 0 \, , \quad \text{or equivalently,} \quad C^\mu_{\nu 0} = 0 \, . \tag{5.55}$$

This is the so-called temporal gauge condition. Then the boundary term is removed from the first-order variation of the action as follows:

$$\delta I_\omega = \int_{\mathcal{M}} g^{\mu\nu} (-C^\alpha_{\alpha\beta} \delta C^\beta_{\mu\nu} + C^\beta_{\gamma\mu} \delta C^\gamma_{\beta\nu} - C^\alpha_{\mu\nu} \delta C^\beta_{\beta\alpha} + C^\alpha_{\beta\nu} \delta C^\beta_{\mu\alpha}) \det(\mathbf{e^{-1}}) dx^{n+1} \, . \tag{5.56}$$

Therefore, the variational principle leads to the following conditions are derived:

$$C^\mu_{\nu i} = 0 \, , \quad \text{or equivalently,} \quad {\tilde{\omega}'}^I{}_{Ji} = 0 \, . \tag{5.57}$$

Taking into account Eqs (5.55) and (5.57), the Weitzenböch connection (5.40) becomes as follows:

$$\tilde{\Gamma}^{\rho}_{\mu\nu} = e_I{}^{\rho}\partial_\mu e^I{}_\nu + \omega^{(L)I}{}_{J\mu} e_I{}^{\rho} e^J{}_\nu \,. \tag{5.58}$$

This is equivalent to the Christoffel/Levi-Civita connection given in Eq (4.10). That is, Eq (5.52) becomes the Einstein field equations in vacuum. In the case of coupling matter with this theory, using the covariant derivative of spinor fields ψ

$$\mathcal{D}_\mu = \partial_\mu - \frac{i}{4}\omega^{(L)IJ}{}_\mu \sigma_{IJ} \,, \quad \sigma_{IJ} = \frac{i}{2}[\gamma_I \,, \gamma_J] \,, \tag{5.59}$$

where γ_I are Dirac matrices, and pull-backed Dirac matrices $\gamma^\mu(x) = e_I{}^\mu(x)\gamma^I$, the Lagrangian of matters are constructed as " $i\bar{\psi}\gamma^\mu \mathcal{D}_\mu \psi - m\bar{\psi}\psi$ " on a generic spacetime $\mathcal{M}$. Other fields are also coupled with gravity in the same manner provided in Section 4.5.

5.6. Summary

In this chapter, the mathematical basics for the gauge approach to gravity were introduced. The gauge approach to gravity provides a method to construct gravity theories based on a local symmetry just like the Yang-Mills gauge field theories in the elementary particle physics. In particular, the ingredients introduced in Sections 5.2 and 5.4 are repetitively utilized for constructing the metric-affine gauge theories of gravity in the next chapter. A local symmetry is introduced into the internal space and leads to possible geometric quantities. The Weitzenböch connection bridges these geometric quantities on a spacetime manifold to ones on an internal space via (co-)frame fields, and vice versa. This dual structure plays a crucial role in constructing the metric-affine gauge theories of gravity.

Chapter 6

Metric-affine gauge theories of gravity

Chapter abstract

In this chapter, the metric-affine gauge theories of gravity are constructed. First, based on Sections 5.2 and 5.4, three fundamental geometric quantities, *i.e.*, curvature, torsion, and non-metricity are introduced. Second, using the so-called Möbius representation of a gauge group, the metric-affine geometries are classified into eight subclasses: Riemann-Cartan, teleparallel, Riemann, Minkowski, Weyl-Cartan, Weyl, metric-affine, and symmetric teleparallel geometries. In this formulation, each geometric quantity is given by the covariant exterior derivative of each corresponding potential. Third, The geometrical trinity of gravity, which is composed of the three subclasses: Riemann (general relativity), symmetric teleparallel, and torsion teleparallel, is established. These three subclasses are equivalent up to boundary terms in the meaning of action functional. Finally, two extensions of the geometrical trinity of gravity, that is, quadratic extension and non-linear extension, are introduced. The latter extension plays a main role in the next Chapter 7.

6.1. Curvatures, torsions, and non-metricities

In this section, based on the tangent bundle $T\mathcal{M}$ of a spacetime manifold $\mathcal{M}$, three fundamental geometric quantities, *i.e.*, curvature, torsion, and non-metricitie are introduced [Kobayashi (1989); Kobayashi and Nomizu (1996); Nakahara (2003)]. Throughout those introductions, the positioning of the affine connection in these quantities is also clarified. Let us first reformulate curvature and define torsion. To do this, it needs to introduce an associated principal bundle from the tangent bundle.

Each fiber $T_p\mathcal{M}$ of the tangent bundle $T\mathcal{M}$ has a basis $\{e_i\}$, where $p \in \mathcal{M}$ and $i \in$

$\{1\,,2\,,\cdots\,,n+1\}$. $n+1$ is the dimension of each fiber, or equivalently, that of the spacetime manifold. Then an isomorphism from $\mathbb{R}^{n+1}$ to $T_p\mathcal{M}$, $i.e.$, $u\,:\,\mathbb{R}^{n+1}\to\langle e_1\,,e_2\,,\cdots\,,e_{n+1}\rangle = T_p\mathcal{M}$ always exists, where $\langle\cdots\rangle$ denotes a vector space spanned by the basis " $\cdots$ ". Gathering all such u, denotes the set as $L(\mathcal{M})_p$ and then construct a disjoint union as follows: $L(\mathcal{M}) = \bigsqcup_{p\in\mathcal{M}} L(\mathcal{M})_p$. For each $L(\mathcal{M})_p$, a right action R of $GL(n+1\,;\mathbb{R})$ is defined in a well-defined manner as follows: $R_g\,:\,L(\mathcal{M})_p\times GL(n+1\,;\mathbb{R})\to L(\mathcal{M})_p\,;\,(u\,,g)\mapsto u\circ g$ since $R_g(u)=u\circ g$ is nothing but a basis transformation of $T_p\mathcal{M}$. Then a manifold structure is inserted into the disjoint union $L(\mathcal{M})$ by using the inverse map of a local trivialization $\varphi_U\,:\,L(\mathcal{M})|_U\to U\times GL(n+1\,;\mathbb{R})\,;\,\sigma_U(p)\circ g\to(p\,,g)$, where σ_U is a set of a basis of $T_p\mathcal{M}$ at point $p\in U$. Based on these structures, the disjoint union $L(\mathcal{M})$ becomes a principal $GL(n+1;\mathbb{R})$-bundle associated to the tangent bundle $T\mathcal{M}$: $\mathfrak{L}=(L(\mathcal{M})\,,\mathcal{M}\,,\iota\,,GL(n+1\,;\mathbb{R})\,;\,R)$, where the projection map is given as follows: $\iota\,:\,L(\mathcal{M})\to\mathcal{M}\,;\,L(\mathcal{M})|_p\mapsto p$.

From Chapter 5, in particular, Sections 5.2 and 5.3, the associated principal bundle $L(\mathcal{M})$ has, on one hand, the Ehresmann connection, $\omega\in\Gamma\left(\mathfrak{gl}(n+1\,;\,\mathbb{R})\otimes T^*L(\mathcal{M})\right)$, defined as Eq (5.1). These 1-forms ω lives in the dual space of the vertical space $VL(\mathcal{M})$. On the other hand, the associated principal bundle $L(\mathcal{M})$ has its proper $\mathbb{R}^{n+1}$-valued 1-forms on $L(\mathcal{M})$, denoted by θ^i, defined as follows:

$$\theta^i(X)=\sigma_U^{-1}(p)(\iota_*X)\,, \tag{6.1}$$

where X is a vector field on $L(\mathcal{M})$ and σ_U is a section of $L(\mathcal{M})$. Then the pull back of θ^i becomes the dual basis of a basis of a tangent space $T_p\mathcal{M}$: $\sigma_U^*\theta^i(e_j)=\delta^i_j$, where $\{e_i\}$ denotes a basis of $T_p\mathcal{M}$. Therefore, these 1-forms θ^i lives in the dual space of the horizontal space $HL(\mathcal{M})$. Remark that the existence of such 1-forms is a proper characteristic of associated principle bundles since generic principle bundles do not have any basis of those fibers.

For the Ehresmann connection ω, the curvature 2-form is defined by Eq (5.7). Similarly, for the 1-forms θ^i, $\mathbb{R}^r$-valued 2-form θ^i is defined as follows:

$$T(X\,,Y) = d\theta(X^H\,,Y^H)\,, \tag{6.2}$$

where $X\,,Y \in \Gamma(TL(\mathcal{M}))$, $\theta \in \langle\theta^i\rangle$, and $X^H\,,Y^H \in HL(\mathcal{M})$. This quantity is called the torsion tensor of the spacetime manifold $\mathcal{M}$. In the same manner as the curvature 2-form given in Eq (5.12), the torsion 2-form has the algebraic expression given as follows:

$$\sigma_U^* T = d\sigma_U^*\theta + \frac{1}{2}[\sigma_U^*\omega\,,\sigma_U^*\theta]\,. \tag{6.3}$$

This relation holds on the spacetime manifold $\mathcal{M}$. Here, U is an open set of $\mathcal{M}$. Since the curvature 2-form Ω given in Eq (5.7) and the torsion 2-form given in the above vanish for $X\,,Y \in VL(\mathcal{M})$, these quantities can be expressed in algebraic forms as follows:

$$\Omega = \Omega^i{}_j e_i \otimes \theta^j \tag{6.4}$$

and

$$T = \Theta^i \otimes e_i\,, \tag{6.5}$$

respectively, where $\Omega^i{}_j$ and Θ^i are defined as follows:

$$\Omega^i{}_j = \frac{1}{2}R^i{}_{jkl}\theta^k \wedge \theta^l \tag{6.6}$$

and

$$\Theta^i = \frac{1}{2}T^i{}_{jk}\theta^j \wedge \theta^k\,, \tag{6.7}$$

respectively. Eqs (6.4) and (6.5) are a $\mathfrak{gl}(n+1\,;\mathbb{R})$-valued 2-form on $L(\mathcal{M})$ and a $T\mathcal{M}$-valued 2-form on $L(\mathcal{M})$, respectively.

Now, let us apply the framework given in Section 5.3 to the associated principle bundle $L(\mathcal{M})$ and its geometrical quantities Ω and T. For the representation $\rho = id$, the principal bundle $L(\mathcal{M})$ turns back into the original vector bundle $T\mathcal{M}$. Then the Ehresmann connection ω becomes a section of End($T\mathcal{M}$)-valued 1-form on $\mathcal{M}$; this connection ω is nothing but the affine connection. That is, a connection of the tangent bundle is defined as an affine connection. Then, for the curvature 2-form, on one hand, it becomes a section of End($T\mathcal{M}$)-valued 2-form on $\mathcal{M}$, and the Ricci identity (5.24) and the structure equation (5.25) hold. On the other hand, for the torsion 2-form, it becomes $T\mathcal{M}$-valued 2-form on $\mathcal{M}$, and the resemble formula to the curvature 2-form is derived as follows:

$$\tilde{T}(X\,, Y) = \frac{1}{2}\left(\tilde{\nabla}_X Y - \tilde{\nabla}_Y X - [X\,, Y]\right)\,, \tag{6.8}$$

where X and Y are vector fields on $\mathcal{M}$, *i.e.*, sections of $T\mathcal{M}$. Hereinafter, we denote the quantities in the affine connection by putting " $\tilde{}$ " over those notations. Calculating it for a basis $\{e_i\}$ of $T\mathcal{M}|_U$, where U is an open set of $\mathcal{M}$, the following equations are derived:

$$\tilde{T}(e_i\,, e_j) = \left(d\theta^k + \omega^k{}_l \wedge \theta^l\right)(e_i\,, e_j) \otimes e_k\,, \tag{6.9}$$

where θ^i are the dual basis of e_i; these θ^i correspond to Eq (6.1). Comparing the above equation with Eq (6.5), the components Θ^i are determined as follows:

$$\tilde{\Theta}^i = d\theta^i + \omega_j{}^i \wedge \theta^j = d_{\tilde{D}}\theta^i\,, \tag{6.10}$$

where $\omega_i{}^j$ are the components of the Ehresmann connection ω and d_D is the covariant exterior derivative of the connection ω. This equation is called Cartan's first structure equation. The equation of the curvature 2-form, *i.e.*,

$$\tilde{\Omega}_i{}^j = d\omega_i{}^j + \omega_k{}^j \wedge \omega_i{}^k = d_{\tilde{D}}\omega_i{}^j \,, \tag{6.11}$$

is called Cartan's second structure equation.

In the existence of the torsion, in addition to the Bianchi identity given in Eq (5.26), another identity that relates the curvature to the torsion exists:

$$d_{\tilde{D}}\tilde{T} = \tilde{R}e_i \wedge \theta^i \,. \tag{6.12}$$

This identity is defined on $T\mathcal{M} \otimes \bigwedge^3 T^*\mathcal{M}$. Acting it to three vector fields X, Y, and Z, the above identity is expressed as follows:

$$\tilde{R}(X\,,Y)Z + \tilde{R}(Y\,,Z)X + \tilde{R}(Z\,,X)Y = 2(d_{\tilde{D}}\tilde{T})(X\,,Y\,,Z)\,. \tag{6.13}$$

These identities (6.12) and (6.13) are called Bianchi's first identity. The Bianchi identity is given in Eq (5.26) with replacing d_D by $d_{\tilde{D}}$ is then called the Bianchi's second identity, distinguishing from the first one.

Next, let us introduce the non-metricity tensor. Assume that a metric tensor $g = g_{ij}\theta^i \otimes \theta^j$ of the tangent bundle is given. Then the metric tensor generically satisfies the following relation:

$$dg(X\,,Y) = (\tilde{\nabla}g)(X\,,Y) + g(\tilde{\nabla}X\,,Y) + g(X\,,\tilde{\nabla}Y)\,, \tag{6.14}$$

or equivalently,

$$Zdg(X\,,Y) = (\tilde{\nabla}_Z g)(X\,,Y) + g(\tilde{\nabla}_Z X\,,Y) + g(X\,,\tilde{\nabla}_Z Y)\,, \tag{6.15}$$

where X, Y, and Z are vector fields on $\mathcal{M}$. Then the quantity $\tilde{\nabla}g$, or equivalently, $\tilde{\nabla}_X g$ is defined as the non-metricity tensor and denoted by $\tilde{Q}$, or equivalently, $\tilde{Q}_X$. For the basis $\{e_i\}$, the non-metricity tensor is expressed as follows:

$$\tilde{Q} = d_{\tilde{D}} g \,, \tag{6.16}$$

or equivalently,

$$\begin{aligned} \tilde{Q}_{ij} &= \tilde{\nabla} g_{ij} = dg_{ij} - \omega_i{}^k g_{kj} - \omega_j{}^k g_{ik} \,, \\ \tilde{Q}_{kij} &= \tilde{\nabla}_k g_{ij} = dg_{ij}(e_k) - \omega_{ik}{}^l g_{lj} - \omega_{jk}{}^l g_{il} \,. \end{aligned} \tag{6.17}$$

Both the curvature tensor and the torsion tensor have those Bianchi identities. The non-metricity tensor is the same as these quantities. Considering the exterior covariant derivative of it, the following identity is derived:

$$d_{\tilde{D}} \tilde{Q} = \tilde{R} \theta^i \wedge g e_i \,. \tag{6.18}$$

This identity is called the zero-th Bianchi identity.

Finally, let us express these geometrical quantities, $i.e.$, curvature $\tilde{R}$, torsion $\tilde{T}$, and non-metricity $\tilde{Q}$, in terms of the standard coordinate basis, $i.e.$, $\{x^\mu\}$ and those partial derivatives $\{\partial_\mu\}$. In this basis, the affine connection ω is denoted as $\tilde{\Gamma}$, and the italic indices $i\,, j\,, k\,, \cdots$ are replaced by the greek indices $\mu\,, \nu\,, \rho\,, \cdots$. Then the Ricci identity (5.24) of the curvature tensor is expressed as follows:

$$\tilde{R}^\sigma{}_{\mu\nu\rho} = 2\partial_{[\nu} \tilde{\Gamma}^\sigma_{\rho]\mu} + 2\tilde{\Gamma}^\sigma_{\lambda[\nu} \tilde{\Gamma}^\lambda_{\rho]\mu} = \partial_\nu \tilde{\Gamma}^\sigma_{\rho\mu} - \partial_\rho \tilde{\Gamma}^\sigma_{\nu\mu} + \tilde{\Gamma}^\sigma_{\lambda\nu} \tilde{\Gamma}^\lambda_{\rho\mu} - \tilde{\Gamma}^\sigma_{\lambda\rho} \tilde{\Gamma}^\lambda_{\nu\mu} \,. \tag{6.19}$$

For the torsion tensor, using Eq (6.8), the following expression is derived:

$$\tilde{T}^\rho{}_{\mu\nu} = 2\tilde{\Gamma}^\rho_{[\mu\nu]} = \tilde{\Gamma}^\rho_{\mu\nu} - \tilde{\Gamma}^\rho_{\nu\mu} \,. \tag{6.20}$$

These expressions can be also derived from Eqs (6.6) and (6.7), respectively. The non-metricity tensor is expressed as follows:

$$\tilde{Q}_{\rho\mu\nu} = \partial_\rho g_{\mu\nu} - 2\tilde{\Gamma}^\lambda_{\rho(\mu} g_{|\lambda|\nu)} = \partial_\rho g_{\mu\nu} - \tilde{\Gamma}^\lambda_{\rho\mu} g_{\lambda\nu} - \tilde{\Gamma}^\lambda_{\rho\nu} g_{\lambda\mu} \,. \tag{6.21}$$

Remark that the order of the lower two indices in $\tilde{\Gamma}$ has to be as this order.

Conversely, using the torsion and non-metricity tensors, the affine connection is decomposed as follows [Schouten (1954); Hehl et al. (1989, 1995); Heisenberg (2019); Beltrán Jiménez et al. (2019)]:

$$\tilde{\Gamma}^\rho{}_{\mu\nu} = \mathring{\Gamma}^\rho{}_{\mu\nu} + K^\rho{}_{\mu\nu} + L^\rho{}_{\mu\nu} \,, \tag{6.22}$$

where the contorsion tensor $K^\rho{}_{\mu\nu}$ and the disformation tensor $L^\rho{}_{\mu\nu}$ are defined as follows:

$$K^\rho{}_{\mu\nu} = \frac{1}{2} T^\rho{}_{\mu\nu} + T_{(\mu}{}^\rho{}_{\nu)} \tag{6.23}$$

and

$$L^\rho{}_{\mu\nu} = \frac{1}{2} Q^\rho{}_{\mu\nu} - Q_{(\mu}{}^\rho{}_{\nu)} \tag{6.24}$$

respectively. This decomposition can be shown by a straightforward calculation. According to this decomposition, the curvature tensor (6.19) is also decomposed into as follows:

$$\tilde{R}^\sigma{}_{\mu\nu\rho} = \mathring{R}^\sigma{}_{\mu\nu\rho} + 2\mathring{\nabla}_{[\nu} N^\sigma{}_{\rho]\mu} + 2N^\sigma{}_{[\nu|\lambda|} N^\lambda{}_{\rho]\mu} \,, \tag{6.25}$$

where $\mathring{R}^\sigma{}_{\mu\nu\rho}$ is the curvature tensor of the Levi-Civita connection $\mathring{\Gamma}^\rho_{\mu\nu}$, $N^\rho{}_{\mu\nu}$ is the distorsion tensor defined as follows:

$$N^\rho{}_{\mu\nu} = \tilde{\Gamma}^\rho{}_{\mu\nu} - \mathring{\Gamma}^\rho{}_{\mu\nu} \,. \tag{6.26}$$

That is, the distorsion tensor is nothing but the difference between the affine connection and the Levi-Civita connection and can be taken as the contorsion tensor and/or the disformation tensor.

In Section 5.4, a frame field $\mathbf{e}$ is nothing but a bundle map from an internal space bundle $\mathfrak{V} = (\mathcal{V}, \mathcal{M}, \pi)$ to the tangent bundle $\mathfrak{T} = (T\mathcal{M}, \mathcal{M}, \iota)$. Notice that the isomorphism "$u : \mathbb{R}^{n+1} \to \langle e_1, e_2, \cdots, e_{n+1} \rangle = T_p\mathcal{M}$" is possible to play the role of a frame field by replacing the basis $\{e_i\}$ by $\{\partial_\mu\}$. Therefore, all statements for the frame fields in Section 5.4 hold also for the sections of the associated principle bundle $L(\mathcal{M})$. This means also that the italic indices $i, j, k, \cdots$ are identified as the capital indices $I, J, K, \cdots$. In particular, the affine connection (6.22) is equivalent to the Weitzenböch connection (5.40). That is, the following important equation holds:

$$e_I{}^\rho \partial_\mu e^I{}_\nu + \omega^I{}_{J\mu} e_I{}^\rho e^J{}_\nu = \mathring{\Gamma}^\rho{}_{\mu\nu} + K^\rho{}_{\mu\nu} + L^\rho{}_{\mu\nu} \, . \tag{6.27}$$

This equation relates the gauge structure of the internal space to the metric-affine geometry.

6.2. Metric-affine gauge approach to gravity and its subclass

In this section, based on the following gauge groups, *i.e.*, affine group $A(n+1;\mathbb{R}) = T(n+1;\mathbb{R}) \rtimes GL(n+1;\mathbb{R})$ [Hayashi and Shirafuji (1980); Baekler et al. (2011)], Weyl group $W(n+1;\mathbb{R}) = D(n+1;\mathbb{R}) \rtimes A(n+1;\mathbb{R})$ [Charap and Tait (1974); Kopczyński et al. (1988); Hehl et al. (1989); Blagojevic (2001)], and metric-affine group $MA(n+1;\mathbb{R}) = S(n+1;\mathbb{R}) \rtimes W(n+1;\mathbb{R})$ [Hehl et al. (1995, 1989); Tomonari (2023a)], the full theory is classified into eight subclasses: (i) Riemann-Cartan geometry: U_{n+1}, (ii) Teleparallel geometry: T_{n+1}, (iii) Riemann geometry: V_{n+1}, (iv) Minkowski geometry: M_{n+1}, (v) Weyl-Cartan geometry: Y_{n+1}, (vi) Weyl geometry: W_{n+1}, (vii) metric-affine geometry: L_{n+1}, and (viii) symmetric teleparallel geometry: S_{n+1}. Throughout these considerations, the relations between each gauge group structure and the relevant geometries are clarified. Further, the so-called spin, dilation, and shear currents are introduced, and the relations between each gauge group structure and these currents are briefly discussed. First of all, let us reconstruct the metric-affine geometry from the viewpoint of the gauge group structure in a bottom-up approach.

Let us first consider the case of the affine group: $A(n+1\,;\mathbb{R}) = T(n+1\,;\mathbb{R}) \rtimes GL(n+1\,;\mathbb{R})$. This group forms an internal space bundle introduced in Section 5.4. The group multiplication of $A(n+1\,;\mathbb{R})$, denoted by " $\circ$ ", is defined as follows:

$$(s_1\,, t_1) \circ (s_2\,, t_2) = (s_1 \cdot s_2\,, s_1 t_2 + t_1)\,, \tag{6.28}$$

where $s_1 = s_1(p)\,, s_2 = s_2(p) \in GL(d\,;\mathbb{R})$, $t_1 = t_1(p)\,, t_2 = t_2(p) \in T(d\,;\mathbb{R})$ for $p \in \mathcal{M}$, and " $\cdot$ " is the group multiplication of $GL(n+1\,;\mathbb{R})$. This law of multiplication is the common one for the semi-direct products. The Lie algebra of this group, denoted by $\mathfrak{a}(n+1\,;\mathbb{R}) = \mathfrak{t}(n+1\,;\mathbb{R}) \rtimes \mathfrak{gl}(n+1\,;\mathbb{R})$, is given as follows:

$$[P_i\,, P_j] = 0 \quad [L^i{}_j\,, P_k] = {C^{(A)}}^{il}{}_{jk} P_l\,, \quad [L^i{}_j\,, L^k{}_l] = {C^{(A)}}^{ikn}{}_{jlm} L^m{}_n\,, \tag{6.29}$$

where P_i and L^i_j are the generator of the Lie groups $T(n{+}1\,;\mathbb{R})$ and $GL(n{+}1\,;\mathbb{R})$, respectively. ${C^{(A)}}^{il}{}_{jk}$ and ${C^{(A)}}^{ikn}{}_{jlm}$ are structure constants. In this case, ${C^{(A)}}^{il}{}_{jk} = \delta^i{}_k \delta^l{}_j$ and ${C^{(A)}}^{ikn}{}_{jlm} = \delta^i{}_l \delta^k{}_m \delta^n{}_j - \delta^i{}_m \delta^k{}_j \delta^n{}_l$. The affine group $A(d\,;\mathbb{R})$ can be regarded as a subgroup of $GL(n{+}2\,;\mathbb{R})$ as follows:

$$A_{\text{Mobius}}(n+1\,;\mathbb{R}) = \left\{ \begin{bmatrix} g(p) & \tau(p) \\ 0 & 1 \end{bmatrix} \middle|\, g(p) \in GL(n+1\,;\mathbb{R})\,, \tau(p) \in T(n+1\,;\mathbb{R}) \right\}. \tag{6.30}$$

This representation is called the Möbius representation [Kobayashi (1972); Mielke (1987); Hehl et al. (1995)]. Then the ordinary matrix product of the elements of $A_{\text{Mobius}}(n+1\,;\mathbb{R})$ restores the semi-direct product defined in Eq (6.28) in as the first row of the result of the matrix computations. In addition, acting an element $\Lambda(p) \in A_{\text{Mobius}}$ on ${}^T(x\,,1)$, where $x = x(p)$ is the coordinates of the point $p \in \mathcal{M}$, it is revealed that the first component of the result is nothing but the affine transformation of the point p as follows: $\Lambda(p)\,{}^T(x\,,1) = {}^T(s(p)x(p)+\tau(p)\,,1)$. Therefore, the action of the affine group $A(n+1\,;\mathbb{R})$ leaves the $(n+1)$-dimensional hyperplane $\mathbb{R}^{n+1}$ invariant.

In this representation, the affine connection is given as follows [Kobayashi and Nomizu (1996)]:

$$\omega^{(A)} = \begin{bmatrix} \omega^{(E)} & \omega^{(T)} \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \omega^{(E)\,i}{}_j \otimes L^j{}_i & \omega^{(T)\,i} \otimes P_i \\ 0 & 0 \end{bmatrix}, \tag{6.31}$$

where $\omega^{(E)}$ and $\omega^{(T)}$ are a $\mathfrak{gl}(n+1\,;\mathbb{R})$-valued 1-form on $\mathcal{M}$ and a $\mathfrak{t}(n+1\,;\mathbb{R})$-valued 1-form on $\mathcal{M}$, respectively. Then, for a frame transformation $e^i \to e'^i = \Lambda^i{}_j e^j$, $\mathfrak{a}(n+1\,;\mathbb{R})$-valued 1-form $\omega^{(A)}$ on $\mathcal{M}$ is transformed as follows:

$$\omega^{(A)} \to \omega'^{(A)} = \Lambda^{-1} d\Lambda + \Lambda^{-1}\omega^{(A)}\Lambda\,, \tag{6.32}$$

where $\Lambda \in A_{\text{Mebius}}(n+1\,;\mathbb{R})$, or equivalently,

$$\begin{aligned} &\omega^{(E)} \to \omega'^{(E)} = s^{-1} ds + s^{-1}\omega^{(E)} s\,, \\ &\omega^{(T)} \to \omega'^{(T)} = s^{-1} d_D t + s^{-1}\omega^{(T)}\,, \quad d_D t = dt + d\rho(\omega^{(E)})t \end{aligned} \tag{6.33}$$

where $s \in GL(n+1\,;\mathbb{R})$ and $t \in T(n+1\,;\mathbb{R})$. The first transformation law in Eq (6.33) indicates that $\omega^{(E)}$ is nothing but the Ehresmann connection of the principal $GL(n+1\,,;\mathbb{R})$-bundle. Therefore, $d_D t = dt + d\rho(\omega^{(E)})t$ is actually the covariant exterior derivative of t with respect to the connection $\omega^{(E)}$, where $d\rho$ is a representation of the Lie algebra $\mathfrak{gl}(n+1\,;\mathbb{R})$. Similarly, the curvature 2-form is given as follows:

$$\Omega^{(A)} = d\omega^{(A)} + \omega^{(A)} \wedge \omega^{(A)} = \begin{bmatrix} \Omega^{(E)} & \Omega^{(T)} \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} d\omega^{(E)} + \omega^{(E)} \wedge \omega^{(E)} & d\omega^{(T)} + \omega^{(E)} \wedge \omega^{(T)} \\ 0 & 0 \end{bmatrix}. \tag{6.34}$$

Then $\Omega^{(A)}$ is a $\mathfrak{gl}(n{+}1\,;\mathbb{R})$-valued 2-form on $\mathcal{M}$. For a frame transformation $e^i \to e'^i = \Lambda^i{}_j e^j$, $\Omega^{(A)}$ is transformed as follows:

$$\Omega^{(A)} \to \Omega'^{(A)} = \Lambda^{-1}\Omega^{(A)}\Lambda\,. \tag{6.35}$$

This is the same only in the form as Eq (5.13). That is, $\omega^{(T)}$ is not an Ehresmann connection of the principal $T(d\,;\mathbb{R})$-bundle; the above law is not a gauge transformation law.

Eq (6.3), or equivalently, Eq (6.10) implies the meaning of $\Omega^{(T)} = d\omega^{(T)} + \omega^{(E)} \wedge \omega^{(T)}$. That is, if the $\omega^{(T)}$ is equivalent to the coframe field $\mathbf{e}^{-1}$, $\Omega^{(T)}$ is nothing but the torsion of the spacetime manifold $\mathcal{M}$. To confirm this speculation, let us introduce an auxiliary vector field $\xi = \xi^i P_i$. Then the coframe field $\mathbf{e}^{-1}$ can be expressed as follows:

$$\mathbf{e}^{-1} = \omega^{(T)} + d_D\xi\,, \tag{6.36}$$

where $\mathbf{e}^{-1} = e^i \otimes P_i = e^i{}_\mu dx^\mu \otimes P_i$ and $\omega^{(T)} = \omega^{(T)\,i} \otimes P_i = \omega^{(T)\,i}{}_\mu dx^\mu \otimes P_i$. Therefore, if the following condition holds then the statement is shown:

$$d_D\xi := 0\,. \tag{6.37}$$

Under the imposition of the above condition, the affine connection (6.31) and curvature 2-form become as follows [Kobayashi (1972)]:

$$\omega^{(C)} = \begin{bmatrix} \omega^{(E)} & \mathbf{e}^{-1} \\ 0 & 0 \end{bmatrix}, \quad \Omega^{(C)} = d\omega^{(C)} + \omega^{(C)} \wedge \omega^{(C)} = \begin{bmatrix} \Omega^{(E)} & T, \\ 0 & 0 \end{bmatrix}, \tag{6.38}$$

where $\Omega^{(E)}$ and T are givens as follows:

$$T = d\mathbf{e}^{-1} + \omega^{(E)} \wedge \mathbf{e}^{-1} = d_D\mathbf{e}^{-1}\,, \quad \Omega^{(E)} = d\omega^{(E)} + \omega^{(E)} \wedge \omega^{(E)} = d_D\omega^{(E)}\,. \tag{6.39}$$

These two equations are nothing but Cartan's first and second structure equations. This connection $\omega^{(C)}$ is the so-called Cartan connection, although only the part " $\omega^{(E)}$ " in $\omega^{(C)}$ is an Ehresmann connection; the remaining part " $\mathbf{e}^{-1}$ " has nothing to do with Ehresmann connections, therefore, strictly speaking, this use " connection " is just an abuse of jargon. Note that, for a frame transformation $e^i \to e'^i = \Lambda^i{}_j e^j$, $\Omega^{(E)}$ and T transform as follows:

$$\Omega^{(E)} \to \Omega'^{(E)} = \Lambda^{-1}\Omega^{(E)}\Lambda\,, \quad T \to T' = \Lambda^{-1}T\,, \tag{6.40}$$

respectively. Remark also that this decomposition is valid only in the satisfaction of Eq (6.37).

The geometry based on the affine group $A(n+1\,;\mathbb{R}) = T(n+1\,;\mathbb{R}) \rtimes GL(n+1\,;\mathbb{R})$ is, therefore, the so-called (i) Riemann-Cartan geometry, which includes not only curvature but also torsion. The Riemann-Cartan geometry is denoted by " U_{n+1} ", where $n+1$ is the dimension of the geometry. U_{n+1} has four subclasses depending on whether or not the curvature and/or torsion vanishes; (ii-a) " T_{n+1} ": The curvature vanishes: $\Omega^{(E)} = 0$ then the geometry turns into teleparallel geometry; (iii) " V_{n+1} ": The torsion vanishes: $T = 0$ then the geometry turns into Riemann geometry; (iv) " M_{n+1} ": The curvature and torsion vanish: $\Omega^{(E)} = 0$ and $T = 0$ then the geometry turns into Minkowski geometry. Therefore, the Riemann-Cartan geometry provides geometrical extensions of the general theory of relativity. In particular, the existence of torsion gives rise to a new subclass, *i.e.*, T_{n+1}, for theories of gravity.

Next, let us extend the affine group to the so-called Weyl group: $W(n+1\,;\mathbb{R}) = D(n+1\,;\mathbb{R}) \rtimes A(n+1\,;\mathbb{R})$. The Lie algebra of $W(n+1\,;\mathbb{R})$, *i.e.*, $\mathfrak{w}(n+1\,;\mathbb{R}) = \mathfrak{d}(n+1\,;\mathbb{R}) \rtimes \mathfrak{a}(n+1\,;\mathbb{R})$, is identified by the affine algebra (6.29) and the following algebra:

$$[D\,, P_i] = C^{(W)j}{}_i P_j\,, \quad [D\,, L^i{}_j] = 0\,, \tag{6.41}$$

where $C^{(W)j}{}_i$ is structure constant. In this case, $C^{(W)j}{}_i = \delta^j{}_i$ [Charap and Tait (1974)]. The

Möbius representation of the Weyl group is given as follows [Tomonari (2023a)]:

$$W_{\text{Mobius}}(n{+}1\,;\mathbb{R}) = \left\{ \begin{bmatrix} g(p) & \tau(p) & \text{đ}(p) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \middle|\, g(p) \in GL(n{+}1\,;\mathbb{R})\,, \tau(p) \in T(n{+}1\,;\mathbb{R})\,, \text{đ} \in D(n{+}1\,;\mathbb{R}) \right\}. \tag{6.42}$$

This is of course a subgroup of $GL(n+3\,;\mathbb{R})$. Then the Weyl connection is defined as follows [Tomonari (2023a)]:

$$\omega^{(A)} = \begin{bmatrix} \omega^{(E)} & \omega^{(T)} & \omega^{(D)} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} \omega^{(E)\,i}{}_j \otimes L^j{}_i & \omega^{(T)\,i} \otimes P_i & \tilde{\omega}^{(D)} \otimes D \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{6.43}$$

where

$$\tilde{\omega}^{(D)} = \frac{1}{n+1}\ln(-\det(g))\mathbf{e}^{-1}\,. \tag{6.44}$$

The same consideration as the case of the affine group leads the following transformation law [Tomonari (2023a)]:

$$\begin{aligned} &\omega^{(E)} \to \omega'^{(E)} = s^{-1}ds + s^{-1}\omega^{(E)}s\,, \\ &\omega^{(T)} \to \omega'^{(T)} = s^{-1}d_D t + s^{-1}\omega^{(T)}\,, \quad d_D t = dt + d\rho(\omega^{(E)})t\,, \\ &\omega^{(D)} \to \omega'^{(D)} = s^{-1}d_D \text{đ} + s^{-1}\omega^{(D)}\,, \quad d_D \text{đ} = d\text{đ} + d\rho(\omega^{(E)})\text{đ} \end{aligned} \tag{6.45}$$

for the frame transformation $e^i \to e'^i = \Lambda^i{}_j e^j$. Therefore, the $\mathfrak{d}(n+1\,;\mathbb{R})$-valued 1-form $\omega^{(D)}$ is not an Ehresmann connection. Alternatively, this valued 1-form becomes a potential to generate the following geometric quantity [Tomonari (2023a)]:

$$\Delta = d_\nabla \omega^{(D)} - \frac{1}{n+1}\ln(|\det(g)|)\,T = \frac{1}{n+1}\,\mathrm{Tr}\,(\,d_\nabla\, g\,)\,\mathbf{e}^{-1} = \frac{1}{n+1}\,\mathrm{Tr}\,(\,Q\,)\,\mathbf{e}^{-1}\,. \tag{6.46}$$

where " Tr " is the trace operator and $Q = d_\nabla g$ is the non-metricity 2-form defined in Eq (6.16). Remark that the commutativity of the generators D and $E^I{}_J$ ensures $\omega^{(E)} \wedge \omega^{(D)} = 0$. This quantity Δ is the so-called dilation 2-form. Notice that if the torsion 2-form vanishes: $T = 0$, Eq (6.46) turn to simply to be [Tomonari (2023a)]

$$\Delta = d_\nabla \omega^{(D)} = \frac{1}{n+1} \mathrm{Tr}\,(\,d_\nabla\, g\,)\,\mathbf{e}^{-1} = \frac{1}{n+1} \mathrm{Tr}\,(\,Q\,)\,\mathbf{e}^{-1}\,, \tag{6.47}$$

The torsion-free condition can be realized by taking the auxiliary field ζ in Eq (6.36) as follows [Tomonari (2023a)]:

$$d_\nabla \omega^{(T)} + {d_\nabla}^2 \zeta := 0\,. \tag{6.48}$$

Remark that ${d_\nabla}^2 = d_\nabla d_\nabla$ does not vanish unlike the ordinary exterior derivative: $d^2 = dd = 0$. Based on the classification of the Riemann-Cartan geometry, such geometry can contain the subclasses V_{n+1} and E_{n+1} (or M_{n+1}).

The geometry based on the Weyl group $W(n+1\,;\mathbb{R}) = D(n+1\,;\mathbb{R}) \rtimes A(n+1\,;\mathbb{R})$ is richer than the Riemann-Cartan geomrtry by virtue of the exixtence of the dilation. This geometry is called (v) the Weyl-Cartan geometry and denoted as " Y_{n+1} ". On one hand, Y_{n+1} contains U_{n+1} as a special case of vanishing the dilation: $\Delta = 0$. On the other hand, Y_{n+1} gives new subclasses; (vi-a) " W_{n+1} ": The torsion vanishes: $T = 0$ then the geometry turns into the Weyl geometry; (ii-b) T_{n+1}: The curvature vanishes: $\Omega^{(E)} = 0$ then the geometry turns into one of the teleparallel geometry with the dilation.

Further generalization of the Weyl geometry is possible; the dilation given in Eq (6.46) implies the existence of a geometry such that the non-metricity tensor is generated from a covariant exterior derivative of some potential quantity. Consider the metric-affine group: $MA(n+1\,;\mathbb{R}) = S(n+1\,;\mathbb{R}) \rtimes W(n+1\,;\mathbb{R})$. The Lie algebra of $MA(n+1\,;\mathbb{R})$, $\mathfrak{ma}(n+1\,;\mathbb{R}) = \mathfrak{s}(n+1\,;\mathbb{R}) \rtimes \mathfrak{w}(n+1\,;\mathbb{R})$, is identified by the affine algebra (6.29) and the following algebra [Tomonari (2023a)]:

$$[D^i{}_j\,,P_k]=C^{(MA)}{}^{il}{}_{jk}P_l\,,\quad [D^i{}_j\,,L^k{}_l]=0\,,\quad [D^i{}_j\,,D^k{}_l]=C^{(MA)}{}^{ikm}{}_{jln}D^m{}_n\,, \tag{6.49}$$

where $C^{(MA)}{}^{il}{}_{jk}$ and $C^{(MA)}{}^{ikm}{}_{jln}$ are structure constants. In this case, $C^{(MA)}{}^{il}{}_{jk}=\delta^i{}_k\delta^l{}_j$ and $C^{(MA)}{}^{ikn}{}_{jlm}=0$. Notice that this algebra is nothing but a generalization of the Weyl algebra (6.41); in the case of its dimension being one, Eq (6.49) results in Eq (6.41). The Möbius representation of the metric-affine group is given as follows [Tomonari (2023a)]:

$$MA_{\text{ Mobius}}(n+1\,;\mathbb{R})=\left\{\begin{bmatrix} g(p) & \tau(p) & \text{đ}(p) & \mathfrak{s}(p)\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}\middle|\, g(p)\in GL(n+1\,;\mathbb{R})\,,\tau(p)\in T(n+1\,;\mathbb{R})\,,\right.$$
$$\left.\text{đ}\in D(n+1\,;\mathbb{R})\,,\ \mathfrak{s}\in S(n+1\,;\mathbb{R})\right\}. \tag{6.50}$$

This is a subgroup of $GL((n+2)(n+3)/2+1\,;\mathbb{R})$. Then the metric-affine connection is introduced as follows [Tomonari (2023a)]:

$$\omega^{(A)}=\begin{bmatrix}\omega^{(E)} & \omega^{(T)} & \omega^{(D)} & \omega^{(S)}\\ 0&0&0&0\\ 0&0&0&0\\ 0&0&0&0\end{bmatrix}=\begin{bmatrix}\omega^{(E)}{}^i{}_j\otimes L^j{}_i & \omega^{(T)}{}^i\otimes P_i & \omega^{(D)}\otimes D & \omega^{(S)i}{}_j\otimes D^j{}_i\\ 0&0&0&0\\ 0&0&0&0\\ 0&0&0&0\end{bmatrix}, \tag{6.51}$$

where

$$
\begin{aligned}
\omega^{(S)i}{}_j &= \tilde{\omega}^{(S)}\delta^i{}_j\,, \\
\tilde{\omega}^{(S)} &= \left(g - \frac{1}{n+1}\ln(-\det(g))\right)\mathbf{e}^{-1}\,.
\end{aligned}
\tag{6.52}
$$

For a frame transformation, $\omega^{(S)}$ obeys the same rule as $\omega^{(T)}$, $\omega^{(D)}$ in Eq (6.45). Then the $\mathfrak{s}(n+1\,;\mathbb{R})$-valued 1-form $\omega^{(S)}$ becomes a potential to generate the following geometric quantity [Tomonari (2023a)]:

$$
\not{\Delta} = d_{\nabla}\omega^{(S)} - \left(g - \frac{1}{n+1}\ln(|\det(g)|)\right)T = Q\,\mathbf{e}^{-1} - \Delta = \left(Q - \frac{1}{n+1}\,\mathrm{Tr}\,(\,Q\,)\right)\,\mathbf{e}^{-1}\,. \tag{6.53}
$$

This quantity $\not{\Delta}$ is the so-called shear 2-form. Remark that the commutativity of the generators D and $E^I{}_J$ ensures $\omega^{(E)} \wedge \omega^{(S)} = 0$. Notice that the case of vanishing torsion turns Eq (6.53) to be [Tomonari (2023a)]

$$
\not{\Delta} = d_{\nabla}\omega^{(S)} = Q\,\mathbf{e}^{-1} - \Delta = \left(Q - \frac{1}{n+1}\,\mathrm{Tr}\,(\,Q\,)\right)\,\mathbf{e}^{-1}\,. \tag{6.54}
$$

Taking into account the dilation 2-form, the non-metricity 2-form is restored as follows;

$$
Q = \not{Q} + \frac{1}{n+1}\mathrm{Tr}\,(Q) \tag{6.55}
$$

as a 1-form on $\mathcal{M}$, where $\not{Q}$ is defined as $\not{\Delta} = \not{Q}\mathbf{e}^{-1}$ under Eq (6.53). Therefore, the existence of both the dilation and shear 2-forms is equivalent to that of the non-metricity 2-form, and vice versa. Notice, finally, that Eq (6.55) holds not depending on whether or not Condition (6.48) is satisfied.

The geometry based on the metric-affine group $MA(n{+}1\,;\mathbb{R}) = S(n{+}1\,;\mathbb{R}) \rtimes W(n{+}1\,;\mathbb{R})$ is the most generic geometry by virtue of the existence not only the dilation but also the shear. This geometry is nothing but (vii) the metric-affine geometry and denoted as " L_{n+1} ". On one hand, L_{n+1} contains Y_{n+1} as a special case of vanishing the shear: $\not{\Delta} = 0$. On the other hand, L_{n+1} gives new subclasses: (vi-b) W_{n+1}: The torsion vanishes: $T = 0$ then the geometry turns into the most generic subclass of the Weyl geometry with the shear; (viii) " S_{n+1} ": The torsion and the curvature vanish: $T = 0$ and $\Omega^{(E)} = 0$ then the geometry turns into the symmetric telepalallel; (ii-c) T_{n+1}: The curvature vanishes: $\Omega^{(E)} = 0$ then the geometry turns into the most generic subclass of the teleparallel geometry with the dilation and the shear: the non-metricity.

Finally, let us consider the relation between the above classification and the field equations. The action functional is given as follows [Hehl et al. (1989)]:

$$I_{\rm MAG} = \int_{\mathcal{M}} \mathcal{L}\,{\rm vol} = \int_{\mathcal{M}} \mathcal{L}_{\rm MAG}(g_{ij}\,, e^i\,, \omega^{(E)}{}_i{}^j\,, Q_{ij}\,, T^i\,, R_i{}^j)\,{\rm vol} + \mathcal{L}_{\rm matter}(g_{ij}\,, e^i\,, \Phi\,, \mathcal{D}\Phi)\,{\rm vol}\,, \tag{6.56}$$

where e^i is the coframe fields, Φ denotes a set of matter fields, and $\mathcal{D}$ is the covariant derivative given in Eq (5.59). " vol " is the volume form on $\mathcal{M}$. Varying this action functional, the following field equations are derived:

$$\begin{aligned}
&\mathcal{D}\left(2\frac{\partial \mathcal{L}_{\rm MAG}}{\partial Q_{ij}}\right) + 2\frac{\partial \mathcal{L}_{\rm MAG}}{\partial g_{ij}} = -\sigma^{ij}\,,\\
&\mathcal{D}\left(\frac{\partial \mathcal{L}_{\rm MAG}}{\partial T^i}\right) + \frac{\partial \mathcal{L}_{\rm MAG}}{\partial e^i} = -\Sigma_i\,,\\
&\mathcal{D}\left(2\frac{\partial \mathcal{L}_{\rm MAG}}{\partial R_i{}^j}\right) + e^i \wedge \frac{\partial \mathcal{L}_{\rm MAG}}{\partial T^j} + 2g_{jk}\frac{\partial \mathcal{L}_{\rm MAG}}{\partial Q_{ki}} = -\Pi^i{}_j\,,
\end{aligned} \tag{6.57}$$

where σ^{ij}, Σ^i, and $\Pi^i{}_j$ are the metric stress-energy tensor, the canonical energy-momentum tensor, and the hypermomentum, respectively, given as follows:

$$\sigma^{ij} = 2\frac{\delta \mathcal{L}_{\rm matter}}{\delta g_{ij}}\,, \quad \Sigma_i = \frac{\delta \mathcal{L}_{\rm matter}}{\delta e^i}\,, \quad \Pi^i{}_j = \frac{\delta \mathcal{L}_{\rm matter}}{\delta \omega^{(E)}{}_i{}^j}\,. \tag{6.58}$$

The equations of motion of the matter fields Φ are given by the Euler-Lagrange equations as usual. The connection decomposition (, strictly speaking, the pull back of it by the coframe field,) in Eq (6.22) implies that the hypermomentum is decomposed as follows:

$$\Pi^{ij} = \tau^{ij} + \frac{1}{n+1} g^{ij}\Pi + \slashed{\Pi}^{ij}\,, \tag{6.59}$$

where the spin current τ^{ij} and shear current $\slashed{\Pi}^{ij}$ are given as follows:

$$\tau^{ij} = \frac{\delta\mathcal{L}}{\delta K_{ij}}\,, \quad \slashed{\Pi}^{ij} = \frac{\delta\mathcal{L}}{\delta \slashed{Q}_{ij}} = \Pi^{(ij)} - \frac{1}{n+1} g^{ij}\Pi\,, \tag{6.60}$$

The dilation current Π is the trace of the hypermomentum, which is also given as follows:

$$\Pi = \frac{1}{2}\frac{\delta\mathcal{L}}{\delta Q}\,. \tag{6.61}$$

Therefore, the gauge structures are engraved also into the hypermomentum structure. That is, the metric-affine geometry L_{n+1} includes all components: the spin, the dilation, and the shear current. the Weyl-Cartan geometry Y_{n+1} contains the spin and the dilation current. The affine geometry U_{n+1} has only the spin current. In the Riemann geometry V_{n+1}, the teleparallel geometry T_{n+1}, and the Minkowski geometry M_{n+1}, the hypermomentum vanishes.

Summarizing, the most generic class is the metric affine geometry denoted as L_{n+1} of which the gauge group is the metric-affine group $MA(n+1\,;\mathbb{R}) = S(n+1\,;\mathbb{R}) \rtimes W(n+1\,;\mathbb{R})$. L_{n+1} is described by the three geometric quantities: the curvature R, the torsion T, and the non-metricity Q and has two subclasses: the Weyl-Cartan geometry Y_{n+1}, which is described by the curvature R, the torsion T, and the dilation Δ, and the symmetric teleparallel geometry S_{n+1}, which is described by the non-metricity Q. In the viewpoint of the equations of motion, the entire class L_{n+1} has all the three currents: the spin, the dilation, and the shear current. The subclass Y_{n+1} has its gauge group as the Weyl group $W(n{+}1\,;\mathbb{R}) = D(n{+}1\,;\mathbb{R}) \rtimes A(n{+}1\,;\mathbb{R})$. The possible subclasses of Y_{n+1} are Weyl geometry W_{n+1}, which is described by the curvature R and the dilation Δ, and the Riemann-Cartan geometry U_{n+1}, which is described by the curvature R and the torsion T. In the viewpoint of the equations of motion, this subclass Y_{n+1} has the spin and dilation currents. The latter geometry U_{n+1} has its gauge group as the affine group $A(n+1\,;\mathbb{R}) = T(n+1\,;\mathbb{R}) \rtimes GL(n+1\,;\mathbb{R})$ and the three subclasses: the Riemann geometry V_{n+1}, which is described by the curvature R, the teleparallel geometry T_{n+1}, which is described by the torsion T, and the Minkowski geometry M_{n+1}, which is described by vanishing all the three geometric quantities. From the viewpoint of the equations of motion, this subclass U_{n+1} has only the spin current. The subclasses V_{n+1}, T_{n+1}, and M_{n+1} do not have any hypermomentum.

Remark that the geometric classification based on whether or not each of the three geometric quantities vanish(es) does not take into account the gauge group structure of the theory. However, notice that the four geometries V_{n+1}, T_{n+1}, S_{n+1}, and M_{n+1} are the common subclasses in the algebraic classification and the geometrical classification. In addition, V_{n+1} and M_{n+1} are nothing but the geometry of the general and the special theory of relativity, respectively. Therefore, let us focus on these two subclasses in the next chapter: gravity theories based on the teleparallel geometry T_{n+1} and the symmetric teleparallel geometry S_{n+1}: the so-called geometrical trinity of gravity/general relativity.

Notice, finally, that, if it is possible to further extend the metric-affine gauge group using a semi-direct product then a new geometric quantity would be discovered, and then it would also be possible to construct a new subclass of gravity. The investigation of this perspective is for an intriguing future work including its realizability.[2]

[2]See Appendix C.

6.3. Geometrical trinity of gravity

In this section, the so-called geometrical trinity of gravity, of which geometries are taken in a set of subclasses, *i.e.*, V_{n+1}, T_{n+1}, S_{n+1}, in the metric-affine gauge theories of gravity, is established [Beltrán Jiménez et al. (2019)]. Since these subclasses satisfy the common condition of vanishing curvature, let us start by introducing the most generic class of the teleparallel gravity: (ii-c) [Beltrán Jiménez et al. (2020a); Gomes et al. (2023b); Bahamonde et al. (2023a); Heisenberg (2023)]. In order to construct the Lagrangian of the theory, it needs to unveil the relation between the Ricci scalar of the Levi-Civita connection in the (pseudo-)Riemann geometry and the geometric quantities in the metric-affine geometry.

The decomposition of the curvature tensor given in Eq (6.25) provides the fundamental relation to establishing the metric-affine gauge theories of gravity. Contracting Eq (6.25), the following relation is derived:

$$\tilde{R} = \mathring{R} + \mathbb{T} + \mathbb{Q} + T^{\rho\mu\nu}Q_{\mu\nu\rho} - T^{\mu}Q_{\mu} + T^{\mu}\bar{Q}_{\mu} + \tilde{\nabla}_{\mu}(Q^{\mu} - \bar{Q}^{\mu} + 2T^{\mu})\,, \tag{6.62}$$

where $Q_{\mu} = g^{\nu\rho}Q_{\mu\nu\rho}$, $\bar{Q}_{\rho} = g^{\mu\nu}Q_{\mu\nu\rho}$, $T^{\mu} = g^{\mu\nu}T^{\rho}{}_{\nu\rho}$, and $\mathbb{T}$ and $\mathbb{Q}$ are defined as follows:

$$\mathbb{T} = \frac{1}{2}\left(\frac{1}{4}T_{\mu\nu\rho} + \frac{1}{2}T_{\nu\mu\rho} - g_{\mu\nu}T_{\rho}\right)T^{\mu\nu\rho} \tag{6.63}$$

and

$$\mathbb{Q} = \frac{1}{4}Q_{\mu\nu\rho}Q^{\mu\nu\rho} - \frac{1}{2}Q_{\mu\nu\rho}Q^{\nu\mu\rho} - \frac{1}{4}Q_{\mu}Q^{\mu} + \frac{1}{2}Q_{\mu}\bar{Q}^{\mu}\,, \tag{6.64}$$

respectively. Here, we abbreviated " $\tilde{}$ " for each geometric quantity excepting the Ricci scalar and the covariant derivative " $\tilde{\nabla}$ ". The latter scalar quantity is also expressed in terms of the disformation tensor given in Eq (6.24) as follows:

$$\mathbb{Q} = g^{\mu\nu}\left(L^{\rho}{}_{\rho\lambda}L^{\lambda}{}_{\mu\nu} - L^{\rho}{}_{\lambda\mu}L^{\lambda}{}_{\nu\rho}\right)\,. \tag{6.65}$$

Notice that the decomposition (6.62) can represent the Ricci scalar in terms of the geometric quantities in the metric-affine gauge theories of gravity. Therefore, generalizing the pseudo-Riemannian geometry of the Einstein-Hilbert action functional given in Eq (4.64) into the metric-affine geometry and replacing the Ricci scalar in the action functional by the quantities in the metric-affine geometry, the following action functional is derived:

$$I_{\mathrm{MAG}}[g_{\mu\nu}\,,\tilde{\Gamma}^{\rho}_{\mu\nu}\,,\Phi] = \frac{1}{2\kappa^2}\int_{\mathcal{M}}[\tilde{R} - \mathbb{T} - \mathbb{Q} - T^{\rho\mu\nu}Q_{\mu\nu\rho} + T^{\mu}Q_{\mu} - T^{\mu}\bar{Q}_{\mu} \\ - \tilde{\nabla}_{\mu}(Q^{\mu} - \bar{Q}^{\mu} + 2T^{\mu})]\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,. \tag{6.66}$$

This action functional is defined in the tangent bundle of the spacetime manifold. In order to move to the internal space bundle, it is just to replace the variables $g_{\mu\nu}$ and $\tilde{\Gamma}^{\rho}_{\mu\nu}$ by $e^{I}{}_{\mu}$ and $\omega^{I}{}_{J\mu}$ making use of Eq (5.32) and Eq (5.40). In the case of the teleparallel gravity (ii-c), the vanishing curvature is assumed: $R^{\sigma}{}_{\mu\nu\rho} = 0$. Therefore, the action functional becomes as follows:

$$I_{GTEGR}[g_{\mu\nu}\,,\Gamma^{\rho}_{\mu\nu}\,,\Phi] = \frac{1}{2\kappa^2}\int_{\mathcal{M}}[\,-\mathbb{T} - \mathbb{Q} - T^{\rho\mu\nu}Q_{\mu\nu\rho} - T^{\mu}Q_{\mu} - T^{\mu}\bar{Q}_{\mu} \\ - \tilde{\nabla}_{\mu}(Q^{\mu} - \bar{Q}^{\mu} + 2T^{\mu})]\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,. \tag{6.67}$$

This theory is called the General Teleparallel Equivalnt to General Relativity (GTEGR) and provides the basics of the geometrical trinity of gravity. Here, notice that the assumption of vanishing curvature tensor, this condition is called teleparallel condition/teleparallelism in the metric-affine gauge theories of gravity, leads to the following connection:

$$\Gamma'^{\rho}_{\mu\nu} = 0\,, \tag{6.68}$$

in some coordinate system. Conversely, this connection trivially satisfies the teleparallel condition. In addition, for a general coordinate transformation: $x^\mu \to x'^\mu = x'^\mu(x^\nu)$, recall that the affine connection obeys the following transformation law:

$$\Gamma^\rho_{\mu\nu} = \frac{\partial x'^\rho}{\partial x^\lambda}\frac{\partial x^\kappa}{\partial x'^\mu}\frac{\partial x^\sigma}{\partial x'^\nu}\Gamma'^\lambda_{\kappa\sigma} + \frac{\partial x^\rho}{\partial x'^\lambda}\frac{\partial^2 x'^\lambda}{\partial x^\mu \partial x^\nu}\,. \tag{6.69}$$

This law holds by virtue of the transformation law for the Levi-Civita connection $\overset{\circ}{\Gamma}{}^\rho_{\mu\nu}$ and that both the contorsion and the disformation in Eq (6.22) are tensorial quantities. Under the imposition of Eq (6.68), the affine connection with the teleparallel condition in a generic coordinate system is, on one hand, expressed as follows:

$$\Gamma^\rho_{\mu\nu} = (\Lambda^{-1})^\rho{}_\lambda \partial_\mu \Lambda^\lambda{}_\nu\,, \tag{6.70}$$

where $\Lambda^\mu{}_\nu = \partial x^\mu / \partial x'^\nu$. This connection also satisfies the teleparallel condition. On the other hand, the relation given in Eq (5.40) always has the following form in some local region:

$$\Gamma^\rho_{\mu\nu} = e_I{}^\rho \partial_\mu e^I{}_\nu \tag{6.71}$$

by virtue that any vector bundle has the so-called standard flat connection in some local region: $\omega^I{}_{J\mu} = 0$. In the case of restricting such local region, the matrix components $\Lambda^\mu{}_\nu$ can be replaced by the coframe field components $e^I{}_\mu$. In particular, the case that the internal space bundle is $\mathcal{M} \times \mathbb{R}^{n+1}$ makes it possible to identify the index " λ " in Eq (6.70) with the index " I " in Eq (6.71) and the matrix components $\Lambda^\mu{}_\nu$ with the coframe field components $e^I{}_\mu$. In this special case, $e^I{}_\mu$, or equivalently, $\Lambda^\mu{}_\nu$, belongs to the general linear group $GL(n+1\,;\mathbb{R})$, which is nothing but the structure group of the internal space bundle. Hereinafter, we assume this special case.

Next, let us consider the case of vanishing non-metricity tensor: $Q^\rho{}_{\mu\nu} = 0$. The GTEGR action functional turns into as follows:

$$I_{\rm TEGR}[g_{\mu\nu}\,,\Gamma^{\rho}_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}}\left[-\mathbb{T} - 2\nabla_\mu T^\mu\right]\sqrt{-g}\,d^{n+1}x + I_{\rm matter}[\Phi\,,\mathcal{D}\Phi]\,. \tag{6.72}$$

This theory is called Teleparallel Equivalent to General Relativity (TEGR) and implies the equivalence to the general theory of relativity up to boundary terms [Einstein (1928); Unzicker and Case (2005)]. Varying this, the following equations of motion are derived:

$$\begin{aligned}
&\mathbb{T}_{\mu\nu} - \frac{1}{2}\mathbb{T}g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,, \quad \mathbb{T}_{\mu\nu} = \left(\nabla_\rho + T_\rho\right)S_{(\mu\nu)}{}^{\rho} + t_{\mu\nu}\,,\\
&\left(\nabla_\rho + T_\rho\right)\left[\sqrt{-g}S_{[\mu}{}^{\rho}{}_{\nu]}\right] = 0\,,
\end{aligned} \tag{6.73}$$

where the symmetric tensors $S_\rho{}^{\mu\nu}$, which is called the torsion conjugate tensor, and $t_{\mu\nu}$ are defined as follows:

$$\begin{aligned}
S_\rho{}^{\mu\nu} &= \frac{\partial\mathbb{T}}{\partial T^\rho{}_{\mu\nu}} = \frac{1}{4}T_\rho{}^{\mu\nu} + \frac{1}{2}T^{[\mu}{}_\rho{}^{\nu]} - \delta_\rho{}^{[\mu}T^{\nu]}\,,\\
t_{\mu\nu} &= \frac{\partial\mathbb{T}}{\partial g^{\mu\nu}} = \frac{1}{2}S_{(\mu|}{}^{\lambda\kappa}T_{\nu)\lambda\kappa} - T^{\lambda\kappa}{}_{(\mu}S_{\lambda\kappa|\nu)}\,.
\end{aligned} \tag{6.74}$$

The first equations in Eq (6.73) has the same form as the Einstein field equations.

The TEGR action functional is also written in terms of (co)frame fields. The assumption of vanishing non-metricity tensor leads to the following equation:

$$2e_i{}^\rho\partial_\beta e^i{}_{(\mu}g_{\nu)\rho} = \partial_\beta g_{\mu\nu}\,. \tag{6.75}$$

This equation is easily solved in terms of coframe field components as follows:

$$g_{\mu\nu} = e^I{}_\mu e^J{}_\nu c_{IJ}\,, \tag{6.76}$$

where c_{IJ} is arbitrary constant symmetric tensor. This solution includes the case of Eq (5.32);

c_{IJ} is nothing but the internal space metric η_{IJ}. The torsion tensor is also expressed as follows:

$$T^{\rho}{}_{\mu\nu} = 2e^{\rho}{}_{I}\partial_{[\mu}e^{I}{}_{\nu]}\,. \tag{6.77}$$

Of course, this relation corresponds to Eq (5.40). Using Eq (5.32), or more generically Eq (6.76), and Eq (5.40), or equivalently, Eq (6.77), Eq (6.72) becomes as follows:

$$I_{\text{TEGR}}[e^{I}{}_{\mu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \left[-\mathbb{T} - 2\mathcal{D}_I T^I\right] \det(\mathbf{e}^{-1})\, d^{n+1}x + I_{\text{matter}}[\Phi\,, \mathcal{D}\Phi]\,. \tag{6.78}$$

The action functionals Eq (6.72) and Eq (6.78) correspond to each other in a one-to-one manner. (See Section 5.4 in detail.)

Finally, let us consider the case of vanishing torsion tensor: $T^{\rho}{}_{\mu\nu} = 0$. The GTEGR action functional turns into as follows:

$$I_{\text{STEGR}}[g_{\mu\nu}\,, \Gamma^{\rho}_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \left[-\mathbb{Q} - \nabla_{\mu}(Q^{\mu} - \bar{Q}^{\mu})\right] \sqrt{-g}\, d^{n+1}x + I_{\text{matter}}[\Phi\,, \mathcal{D}\Phi]\,. \tag{6.79}$$

This is called Symmetric Teleparallel Equivalent to General Relativity (STEGR) [Nester and Yo (1999)] and implies the equivalence to the general relativity up to boundary terms. Varying this, the following equations of motion are derived:

$$\begin{aligned} &\mathbb{Q}_{\mu\nu} - \frac{1}{2}\mathbb{Q}g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,, \quad \mathbb{Q}_{\mu\nu} = \frac{1}{\sqrt{-g}}\nabla_{\rho}\left[\sqrt{-g}P^{\rho}{}_{\mu\nu}\right] + q_{\mu\nu}\,, \\ &\nabla_{\mu}\nabla_{\nu}\left(\sqrt{-g}P^{\mu\nu}{}_{\rho}\right) = 0\,. \end{aligned} \tag{6.80}$$

where the symmetric tensors $P^{\rho}{}_{\mu\nu}$, which is called the non-metricity conjugate tensor, and

$q_{\mu\nu}$ are defined as follows:

$$
\begin{aligned}
P^{\rho}{}_{\mu\nu} &= \frac{1}{2}\frac{\partial \mathbb{Q}}{\partial Q_{\rho}{}^{\mu\nu}} = -\frac{1}{4}Q^{\rho}{}_{\mu\nu} + \frac{1}{2}Q_{(\mu}{}^{\rho}{}_{\nu)} + \frac{1}{4}g_{\mu\nu}Q^{\rho} - \frac{1}{4}\left(g_{\mu\nu}\bar{Q}^{\rho} + \delta^{\rho}{}_{(\mu}Q_{\nu)}\right) \\
q_{\mu\nu} &= \frac{\partial \mathbb{Q}}{\partial g^{\mu\nu}} = P_{(\mu|\lambda\kappa}Q_{\nu)}{}^{\lambda\kappa} - 2P^{\lambda\kappa}{}_{(\nu}Q_{\lambda\kappa|\mu)} \,.
\end{aligned} \tag{6.81}
$$

Note that the non-metricity scalar $\mathbb{Q}$ can be expressed by using the non-metricity conjugate tensor $P^{\rho}{}_{\mu\nu}$ as follows:

$$
\mathbb{Q} = P_{\rho\mu\nu}Q^{\rho\mu\nu} \,. \tag{6.82}
$$

The first equations in Eq (6.80) has the same form as the Einstein field equations.

The STEGR action functional is of course written in terms of (co)frame fields by using Eqs (5.32) and (5.40). This is the same formulation as the TEGR case. Whereas, in the STEGR case, a specific formulation exists; the theory can be expressed in terms of the so-called Stükelberg fields. To see this, let us focus on a proper solution of the following equation:

$$
\partial_{\mu}e^{I}{}_{\nu} = 0 \,. \tag{6.83}
$$

This equation is derived from the assumption of vanishing torsion tensor and easily solved in terms of the so-called Stükelberg fields, denoted by $\xi^{I} = \xi^{I}(x)$, as follows:

$$
e^{I}{}_{\mu} = \frac{\partial \xi^{I}}{\partial x^{\mu}} \,. \tag{6.84}
$$

Then the affine connection becomes as follows:

$$
\Gamma^{\rho}_{\mu\nu} = \frac{\partial x^{\rho}}{\partial \xi^{I}}\partial_{\mu}\partial_{\nu}\xi^{I} \,. \tag{6.85}
$$

Therefore, the STEGR action functional given in Eq (6.79) becomes as follows:

$$I_{\text{STEGR}}[\xi^I\,, e^I{}_\mu] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \left[-\mathbb{Q} - \mathcal{D}_I(Q^I - \bar{Q}^I)\right]\,\det(\mathbf{e}^{-1})\,d^{n+1}x + I_{\text{matter}}[\Phi\,, \mathcal{D}\Phi]\,. \quad (6.86)$$

Notice that the above action functional contains the second-order derivative terms of the Stükelberg fields ξ^μ. This is the reason why the action functional includes the variables $e^I{}_\mu = \partial_\mu \xi^I$; higher-order terms have to be treated as independent variables in its own right. Such higher-order terms could cause the Ostrogradski ghost modes as explained in Sections 2.5 and 2.6. However, the work given in [Hu et al. (2023)] showed that the theory does not suffer from such ghost modes. Notice also that, under the condition of fixing the internal space metric, the use of the variables $e^I{}_\mu$ is equivalent to that of the variables $g_{\mu\nu}$: $I_{\text{STEGR}}[\xi^I\,, e^I{}_\mu] = I_{\text{STEGR}}[\xi^I\,, g_{\mu\nu}]$. Since the original action functional (6.79) includes the derivatives of the metric tensor only up to first-order, this alternative expression is an implication of the absence of the Ostrogradski ghost modes.

The STEGR subclass has a special case known as the so-called Coincident General Relativity (CGR) [Beltrán Jiménez et al. (2018)]. This special theory can be derived by imposing the so-called coincident gauge condition to the STEGR subclass [Beltrán Jiménez and Koivisto (2022)]. In order to clarify this gauge condition, let us go back to Eq (6.85). This equation is apparently invariant under the following global transformation:

$$\xi^I(x) \to \xi'^I(x) = M^I{}_J \xi^J(x) + \zeta^I\,, \quad (6.87)$$

where $M^I{}_J \in GL(n+1\,;\mathbb{R})$ and ζ^I are arbitrary constant $(n+1)$-vector components. Since the internal space bundle is locally isomorphic to $U \times \mathbb{R}$, a section on the bundle can be identified with that on the tangent bundle $T\mathcal{M}$ by virtue of the local relation $U \times \mathbb{R} \simeq T\mathcal{M}|_U$, where U is an open set of $\mathcal{M}$. This indicates that the internal space indices $I\,, J\,, K\,, \cdots$ can be replaced by the spacetime indices $\mu\,, \nu\,, \rho\,, \cdots$. Therefore, Eq (6.87) gives the following equation in a local region:

$$\xi^I(x) = M^I{}_\mu x^\mu + \zeta^I\,. \tag{6.88}$$

This relation is equivalent to the case just replacing $\xi^I(x)$ by x^μ in Eq (6.87) as follows:

$$\xi^I(x) = \delta^I{}_\mu x^\mu + A^I\,, \tag{6.89}$$

where A^I are arbitrary constant $(n+1)$-vector components. That is, the coincident gauge is nothing but a condition on the Stükelberg fields such that it restricts to those that are obtained only from an affine transformation of a spacetime point. This indicates also that, based on Eq (6.84), the co-frame fields are obtained from a given spacetime coordinates. Notice that in this gauge Eq (6.84) turns into $e^I{}_\mu = \delta^I{}_\mu$, and it is nothing but the coefficients of " x^μ " in Eq (6.89). This is the another signal of the local relation: " $U \times \mathbb{R} \simeq T\mathcal{M}|_U$ " [Tomonari and Bahamonde (2023)]. Under the imposition of the coincident gauge, *i.e.*, Eq (6.88), Eq (6.85) becomes as follows:

$$\Gamma^\rho_{\mu\nu} = 0\,. \tag{6.90}$$

This indicates that the coincident gauge condition changes the covariant derivative " ∇ " to the partial derivative " ∂ ".

The CGR action functional is of course directly obtained from Eq (6.79) just replacing " ∇ " in the action functional by " ∂ ". However, this naive replacement unfortunately blinds the essence of the theory. Therefore, using Eq (6.65), let us express the STEGR action functional and impose the coincident gauge condition.

$$I_{\mathrm{STEGR}}[g_{\mu\nu}\,, \Gamma^\rho_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \left[-g^{\mu\nu}\left(L^\rho{}_{\rho\lambda}L^\lambda{}_{\mu\nu} - L^\rho{}_{\lambda\mu}L^\lambda{}_{\nu\rho}\right)\right]\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,, \mathcal{D}\Phi]\,, \tag{6.91}$$

where the boundary terms are neglected. Imposing the coincident gauge condition (6.88) and using the decomposition (6.22), the disformation tensor can be expressed by the Levi-Civita connection as follows:

$$L^{\rho}{}_{\mu\nu} = -\mathring{\Gamma}^{\rho}_{\mu\nu}\,. \tag{6.92}$$

Therefore, the CGR action functional is given as follows:

$$I_{\mathrm{CGR}}[g_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} \left[g^{\mu\nu}\left(\mathring{\Gamma}^{\rho}{}_{\rho\lambda}\mathring{\Gamma}^{\lambda}{}_{\mu\nu} - \mathring{\Gamma}^{\rho}{}_{\lambda\mu}\mathring{\Gamma}^{\lambda}{}_{\nu\rho}\right)\right]\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,. \tag{6.93}$$

Notice that this is nothing but the Einstein-Hilbert action functional *without boundary terms*. That is, the dynamics of CGR is equivalent to that of the general relativity.

The theories discussed in this section, *i.e.*, the geometrical trinity of gravity, so far are just equivalent subclasses to the general theory of relativity from the viewpoint of the action functional up to boundary terms. That is, there is no departure from the general theory of relativity. However, by extending these theories in a proper manner, the situations get changed; the theories may acquire the possibility to provide explanations for dark energy and dark matter and also to generate new propagating degrees of freedom and symmetry breaking.

6.4. Modified theories of geometrical trinity of gravity

In this section, two ways of extension/modification of the geometrical trinity of gravity, *i.e.*, quadratic extensions and non-linear extensions, are presented. Let us start by investigating the quadratic extension of TEGR and STEGR.

The TEGR action functional (6.72) (, or equivalently, Eq (6.78),) contains terms up to quadratic with respect to the torsion tensor $T^{\rho}{}_{\mu\nu}$ and its contraction T^{ρ} under neglecting boundary terms. Therefore, the possible quadratic Lagrangian with respect to these quantities are given as follows:

$$
\begin{aligned}
I_{\mathrm{qTEGR}} &= -\frac{1}{2\kappa^2}\int_{\mathcal{M}} \hat{\mathbb{T}}\,\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,,\\
\hat{\mathbb{T}} &= c_1 T_{\rho\mu\nu}T^{\rho\mu\nu} + c_2 T_{\mu\rho\nu}T^{\rho\mu\nu} + c_3 T_\rho T^\rho\,,
\end{aligned}
\tag{6.94}
$$

where c_1, c_2, and c_3 are arbitrary constant parameters. Therefore, the extension of TEGR in this manner forms the theory of a three-parameters family. These three parameters have to do with the emergence of new degrees of freedom of the theory [Blixt et al. (2019b,a, 2021); D'ambrosio and Heisenberg (2021); Heisenberg (2023)]. However, a complete Hamiltonian analysis has not been performed yet at the moment of writing this thesis. Remark that in the case of $c_1 = 1/4\,, c_2 = 1/2\,, c_3 = -1$ the theory results in the TEGR action functional (6.72) (, or equivalently, Eq (6.78)). Varying Eq (6.94), the following field equations are derived:

$$
\begin{aligned}
&\hat{\mathbb{T}}_{\mu\nu} - \frac{1}{2}\hat{\mathbb{T}}g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,, \quad \hat{\mathbb{T}}_{\mu\nu} = (\nabla_\rho + T_\rho)\,\hat{S}_{(\mu\nu)}{}^{\rho} + \hat{t}_{\mu\nu}\,,\\
&(\nabla_\rho + T_\rho)\left(\sqrt{-g}\hat{S}_{[\mu}{}^{\rho}{}_{\nu]}\right) = 0\,,
\end{aligned}
\tag{6.95}
$$

where $\hat{S}_\rho{}^{\mu\nu}$ and $\hat{t}_{\mu\nu}$ are defined as follows:

$$
\begin{aligned}
\hat{S}_\rho{}^{\mu\nu} &= \frac{\partial\hat{\mathbb{T}}}{\partial T^\rho{}_{\mu\nu}} = c_1 T_\rho{}^{\mu\nu} + c_2 T^{[\mu}{}_{\rho}{}^{\nu]} + c_3\delta_\rho{}^{[\mu}T^{\nu]}\,,\\
\hat{t}_{\mu\nu} &= \frac{\partial\hat{\mathbb{T}}}{\partial g^{\mu\nu}} = \frac{1}{2}\hat{S}_{(\mu|}{}^{\rho\kappa}T_{\nu)\rho\kappa} - T^{\rho\kappa}{}_{(\mu}\hat{S}_{\rho\kappa|\nu)}\,.
\end{aligned}
\tag{6.96}
$$

Eq (6.95) is the field equations with respect to the metric tensor and to the connection, respectively. Notice that in the case of $c_1 = 1/4\,, c_2 = 1/2\,, c_3 = -1$ the theory results in the equations of motion of TEGR: Eq (6.73) with Eq (6.74).

In the same way as the TEGR case, the STEGR action functional (6.79) (, or equivalently, Eq (6.86),) can be extended into the theory of a five-parameters family as follows:

$$
\begin{aligned}
& I_{\mathrm{qSTEGR}} = -\frac{1}{2\kappa^2}\int_{\mathcal{M}} \hat{\mathbb{Q}}\,\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,, \\
& \hat{\mathbb{Q}} = c_1 Q_{\rho\mu\nu}Q^{\rho\mu\nu} + c_2 Q_{\mu\rho\nu}Q^{\rho\mu\nu} + c_3 Q_\rho Q^\rho + c_4 \bar{Q}_\rho \bar{Q}^\rho + c_5 Q_\rho \bar{Q}^\rho\,,
\end{aligned}
\tag{6.97}
$$

where c_1, c_2, c_3, c_4, and c_5 are arbitrary constant parameters. Notice that the fourth term " $\bar{Q}_\rho\bar{Q}^\rho$ " is a proper term in this extended theory; the original action functional (6.79) (, or equivalently, Eq (6.86)) does not contain this sort of term. These parameters relate to new degrees of freedom of the theory [D'ambrosio and Heisenberg (2021); Heisenberg (2023)]. However, a complete Hamiltonian analysis has not been performed yet at the moment of writing this thesis. Remark that the case of $c_1 = 1/4\,, c_2 = -1/2\,, c_3 = -1/4\,, c_4 = 0\,, c_5 = 1/2$ results in the STEGR action functional (6.79) (, or equivalently (6.86)). Varying Eq (6.97), the following field equations with respect to the metric tensor and the connection are derived:

$$
\begin{aligned}
& \frac{2}{\sqrt{-g}}\nabla_\rho\left(\sqrt{-g}\hat{P}^\rho{}_{\mu\nu}\right) + \hat{q}_{\mu\nu} - \frac{1}{2}\hat{\mathbb{Q}}g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,, \\
& \nabla_\mu\nabla_\nu\left(\sqrt{-g}\hat{P}^{\mu\nu}{}_\rho\right) = 0\,,
\end{aligned}
\tag{6.98}
$$

respectively, where $P^\rho{}_{\mu\nu}$ and $\hat{q}_{\mu\nu}$ are defined as follows:

$$
\begin{aligned}
& \hat{P}^\rho{}_{\mu\nu} = \frac{1}{2}\frac{\partial\hat{\mathbb{Q}}}{\partial Q_\rho{}^{\mu\nu}} = c_1 Q^\rho{}_{\mu\nu} + c_2 Q_{(\mu}{}^\rho{}_{\nu)} + c_3 g_{\mu\nu}Q^\rho + c_4\delta^\rho{}_{(\mu}Q_{\nu)} + \frac{1}{2}c_5\left(g_{\mu\nu}\bar{Q}^\rho + \delta^\rho{}_{(\mu}Q_{\nu)}\right)\,, \\
& \hat{q}_{\mu\nu} = \frac{\partial\hat{\mathbb{Q}}}{\partial g^{\mu\nu}} = \hat{P}_{(\mu|\lambda\kappa}Q_{\nu)}{}^{\lambda\kappa} - 2\hat{P}^{\lambda\kappa}{}_{(\mu}Q_{\lambda\kappa|\nu)}\,.
\end{aligned}
\tag{6.99}
$$

The relation " $\hat{\mathbb{Q}} = \hat{P}_{\rho\mu\nu}Q^{\rho\mu\nu}$ " also holds. Notice that the case of $c_1 = 1/4\,, c_2 = -1/2\,, c_3 = -1/4\,, c_4 = 0\,, c_5 = 1/2$ results in the STEGR field equations: Eq (6.80) with Eq (6.81).

Finally, let us consider the non-linear extension of TEGR and STEGR. The main idea of this extension is the same known as the so-called $f(R)$-gravity [Buchdahl (1970)]:

$$I_{\mathrm{fGR}}[g_{\mu\nu}] = \frac{1}{2\kappa^2}\int_{\mathcal{M}} f(\mathring{R})\,\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi]\,. \tag{6.100}$$

Varying this, the following field equations are derived:

$$f'(\mathring{R})R_{\mu\nu} - \frac{1}{2}f(\mathring{R})g_{\mu\nu} + (g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)f'(\mathring{R}) = \kappa^2\mathcal{T}_{\mu\nu}\,, \tag{6.101}$$

where $f'(\mathring{R}) = df(\mathring{R})/d\mathring{R}$. This extension contains the Einstein-Hilbert action functional (4.64) as a special case of $f(\mathring{R}) = \mathring{R}$; this is nothing but a linear case. Further, the case of $f(\mathring{R}) = \mathring{R} - 2\Lambda$ leads to the following equations:

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,. \tag{6.102}$$

This is nothing but the Einstein field equations with the cosmological constant: Eq (4.35). Therefore, non-linear extensions need to be $f''(\mathring{R}) \neq 0$, where $f''(\mathring{R}) = d^2f(\mathring{R})/d\mathring{R}^2$.

In the TEGR case, the extended action functional is given as follows:

$$I_{\mathrm{fTEGR}} = -\frac{1}{2\kappa^2}\int_{\mathcal{M}} f(\mathbb{T})\,\sqrt{-g}\,d^{n+1}x + I_{\mathrm{matter}}[\Phi\,,\mathcal{D}\Phi] \tag{6.103}$$

Varying this, the field equations with respect to the metric tensor and the connection are given as follows:

$$\begin{aligned}&(\nabla_\rho + T_\rho)\left(f'(\mathbb{T})S_{(\mu\nu)}{}^{\rho}\right) + f'(\mathbb{T})t_{\mu\nu} - \frac{1}{2}f(\mathbb{T})g_{\mu\nu} = \kappa^2\mathcal{T}_{\mu\nu}\,,\\ &(\nabla_\rho + T_\rho)\left(f'(\mathbb{T})S_{[\mu}{}^{\rho}{}_{\nu]}\right)\,,\end{aligned} \tag{6.104}$$

respectively. In the case of $f(\mathbb{T}) = \mathbb{T}$, the theory results in the TEGR case: Eq (6.73). The first equations are rewritten by using the Einstein tensor $G_{\mu\nu}$ as follows:

$$f'(\mathbb{T})G_{\mu\nu} - \frac{1}{2}\left(f(\mathbb{T}) - f'(\mathbb{T})\mathbb{T}\right) g_{\mu\nu} + f''(\mathbb{T})S_{(\mu\nu)}{}^{\rho}\partial_\rho \mathbb{T} = \kappa^2 \mathcal{T}_{\mu\nu} \,. \tag{6.105}$$

The cases of $f(\mathbb{T}) = \mathbb{T}$ and $f(\mathbb{T}) = \mathbb{T} - 2\Lambda$ results in the Einstein field equations (4.28) and (4.35), respectively. In particular, even if a non-linear case, it is possible to obtain the Einstein field equations with the cosmological constant (4.35) as an effective theory: let us consider the case of $\mathbb{T} = \mathbb{T}_0 = \textit{constant}$. Then the third term in Eq (6.105) vanishes, and then the following equations are derived:

$$G_{\mu\nu} + \Lambda_{\text{eff}}\, g_{\mu\nu} = \kappa^2 \mathcal{T}_{\text{eff}\,\mu\nu} \,, \tag{6.106}$$

where Λ_{eff} and $\mathcal{T}_{\text{eff}\,\mu\nu}$ are defined as follows:

$$\Lambda_{\text{eff}} = -\frac{1}{2f'(\mathbb{T}_0)}\left(f(\mathbb{T}_0) - f'(\mathbb{T}_0)\mathbb{T}_0\right) \,, \quad \mathcal{T}_{\text{eff}\,\mu\nu} = \frac{1}{f(\mathbb{T}_0)}\mathcal{T}_{\mu\nu} \,. \tag{6.107}$$

Notice that this sort of effectiveness is absent in the $f(\mathring{R})$-gravity. In order to understand this difference, the Dirac-Bergmann analysis is available. In fact, the authors in [Blagojević and Nester (2020)] unveiled that the theory has a specific sector (s4) in their notation and the corresponding term emerges caused by the difference of the constraint structure by virtue of the violation of the local Lorentz symmetry.

In the STEGR case, the extended action functional is given as follows:

$$I_{\text{fSTEGR}} = -\frac{1}{2\kappa^2}\int_{\mathcal{M}} f(\mathbb{Q})\,\sqrt{-g}\,d^{n+1}x + I_{\text{matter}}[\Phi\,, \mathcal{D}\Phi] \tag{6.108}$$

Varying this, the following field equations are derived:

$$\begin{aligned}
&\frac{2}{\sqrt{-g}}\nabla_\rho\left(\sqrt{-g}f'(\mathbb{Q})P^\rho{}_{\mu\nu}\right)+f'(\mathbb{Q})q_{\mu\nu}-\frac{1}{2}f(\mathbb{Q})g_{\mu\nu}=\kappa\mathcal{T}_{\mu\nu}\,,\\
&\nabla_\mu\nabla_\nu\left(\sqrt{-g}f'(\mathbb{Q})P^{\mu\nu}{}_\rho\right)=0\,,
\end{aligned} \tag{6.109}$$

with respect to the metric tensor and the connection, respectively. The former equations can be rewritten as follows:

$$f'(\mathbb{Q})G_{\mu\nu}-\frac{1}{2}\left(f(\mathbb{Q})-f'(\mathbb{Q})\mathbb{Q}\right)g_{\mu\nu}+2f''(\mathbb{Q})P^\rho{}_{\mu\nu}\partial_\rho\mathbb{Q}=\kappa^2\mathcal{T}_{\mu\nu}\,. \tag{6.110}$$

These equations are also resemble structure to the non-linear extension of the TEGR case; (i) The case of $f(\mathbb{Q})=\mathbb{Q}$ and $f(\mathbb{Q})=\mathbb{Q}-2\Lambda$ results in the Einstein field equations (4.28) and (4.35), respectively; (ii) The case of $\mathbb{Q}=\mathbb{Q}_0=\mathit{constant}$ leads to an effective field equations: Eq (6.106) with the following Λ_{eff} and $\mathcal{T}_{\text{eff}\,\mu\nu}$:

$$\Lambda_{\text{eff}}=-\frac{1}{2f'(\mathbb{Q}_0)}\left(f(\mathbb{Q}_0)-f'(\mathbb{Q}_0)\mathbb{Q}_0\right)\,,\quad \mathcal{T}_{\text{eff}\,\mu\nu}=\frac{1}{f(\mathbb{Q}_0)}\mathcal{T}_{\mu\nu}\,. \tag{6.111}$$

Notice also that this sort of effectiveness is absent in the $f(\mathring{R})$-gravity. Similar to the non-linear extension of TEGR, the Dirac-Bergmann analysis would unveil the reason for the difference from the viewpoint of constraint structures.

6.5. Summary

In this chapter, the metric-affine gauge theories of gravity were constructed. There were eight possible geometries depending on the corresponding Möbius representation of each gauge group. In particular, the subclasses that are called the geometrical trinity of gravity, *i.e.*, GR (Riemann), TEGR (Teleparallel Equivalent to GR), and STEGR (Symmetric Teleparalle Equivalent to GR) are important since these subclasses are equivalent to one another up to boundary terms in the meaning of action functional and include general relativity. These subclasses satisfy the teleparallel condition, or equivalently, the Weitzenböch gauge condition. STEGR includes a special subclass so-called Coincident GR (CGR) which satisfies the coincident gauge. In addition, if it is possible further to extend the metric-affine gauge group using a semi-direct product then a new geometric quantity would be discovered, and then it would also be possible to construct a new subclass of gravity. The investigation of this perspective is for an intriguing future work. In the next chapter, the Dirac-Bergmann analysis will be performed for each subclass and its non-linear extension to unveil those propagating degrees of freedom.

Chapter 7

Dirac-Bergmann analysis of geometrical trinity of gravity and its extension

Chapter abstract

In this chapter, the Dirac-Bergmann analysis is performed for each subclass of the geometrical trinity of gravity and its non-linear extension. In order to apply the analysis, which was introduced in Section 2.2 but restricted to point particle systems, to field theories, three fundamental issues are clarified. These issues are commonly caused by the spatial derivatives of the Dirac delta function. And then a prescription that circumvents the issues is proposed. Based on the prescription, the analysis is performed for TEGR, CGR, non-linear extensions of GR, TEGR, and CGR, and the propagating degrees of freedom of each theory is unveiled. Throughout these analyses, the three issues in field theories of the Dirac-Bergmann analysis are concretely clarified for each subclass, and the reason why the prescription is valid for removing the issues is investigated. I emphasize that these analyses are not a complete manipulation of the issues; it is just a *prescription* to circumvent the issues and make it possible to perform the Dirac-Bergmann analysis. Therefore, the results could be valid only for some classes of solutions. Finally, this chapter is summarized with the outlook for these works.

7.1. Issues of Dirac-Bergmann analysis in field theories and a prescription

In this section, three issues concerning spatial derivative terms in Poisson brackets are clarified. A correct understanding of these issues is important when applying the Dirac-Bergmann analysis to field theories. A prescription that settles these issues is also given. Let us first scrutinize each step of the extension of the analysis into field theories.

The Dirac-Bergmann analysis of the general theory of relativity, which is one of the analyses in field theories, was already performed in Section 4.6. The analysis revealed that the theory has the number of $(n+1)$ gauge degrees of freedom (gDoF) and that of $(n+1)(n-2)/2$ propagating degrees of freedom (pDoF). The former result is reasonable since this number is the same as that of the maximal and independent generators of a diffeomorphism. The validity of the latter result can also be confirmed by using the Einstein field equations of motion (4.28) and the Bianchi identity: $\mathring{\nabla}_{[\rho|}\mathring{R}_{\mu\nu]\sigma\kappa} = 0$. That is, contracting the Bianchi identity, $\mathring{\nabla}_{\mu}G^{\mu\nu} = 0$ is derived, and it can be expanded as follows: $\partial_0 G^{0\nu} + \partial_i G^{i\nu} + \mathring{\Gamma}^{i}_{\ i\rho}G^{\rho\nu} + \mathring{\Gamma}^{\nu}_{\ \mu\rho}G^{\mu\rho} = 0$. The second, third, and fourth terms include the time derivative terms up to second-order, therefore, the first term should be the same order with respect to the time derivative. This indicates that $G^{0\nu}$ contains the time derivative terms up to first-order; the Einstein field equations with respect to time-space components become constraint densities, and that number is $n+1$. Therefore, the number of pDoF is $(n+1)(n+2)/2 - (n+1) - (n+1) = (n+1)(n-2)/2$. However, it is difficult to perform this sort of degrees of freedom counting when the theory gets complicated including the geometrical trinity of gravity and its extensions. In such cases, a systematic method would be a powerful tool to achieve this purpose. The Dirac-Bergmann analysis provides this convenience although we have to manage to do with the following issues.

The extension of the Dirac-Bergmann analysis into field theories is achieved in a straightforward manner as usual; it just introduces density variables and those fundamental Poisson brackets (PBs). That is, integrating field variables $\varphi^a(t\,,\mathbf{x})$, denote it as $\Phi^a(t)$, on a hypersurface Σ_t in the spacetime manifold, it just regards as variables in point particle systems as follows:

$$\Phi^a(t) = \int_{\Sigma_t} \varphi^a(t\,,\mathbf{x})\,\sqrt{|h|}\,d^n x\,, \tag{7.1}$$

where a stands for schematic index of the fields and h is the determinant of the metric h_{ij} of Σ_t. Then, in this formulation, the fields $\varphi^a(t\,,\mathbf{x})\sqrt{|h|}$ are, in particular, called density variables. The Lagrangian density of a given system is composed in terms of these fields like $\mathcal{L}(\varphi^a\,,\nabla_\mu\varphi^a\,,\cdots)\sqrt{|g|}$, and the action functional is defined as follows:

$$I[\phi^a(t)] = \int_{t_1}^{t_2}\int_{\Sigma_t}\mathcal{L}(\varphi^a\,,\nabla_\mu\varphi^a\,,\cdots)\,\sqrt{|g|}\,d^nx\,dt = \int_{t_1}^{t_2} L(\Phi^a(t)\,,(\nabla_\mu\Phi^a)(t)\,,\cdots)\,dt\,, \quad (7.2)$$

where $|g| = N\sqrt{|h|}$ is the determinant of the metric tensor $g_{\mu\nu}$ of the spacetime manifold. Then the canonical momentum density variables are introduced as follows:

$$\pi_a(t\,,\mathbf{x}) = \frac{\delta I}{\delta\dot{\varphi}^a}\,. \quad (7.3)$$

In this formulation, therefore, φ^a play the role of configuration variables. Then the fundamental PBs are introduced as follows:

$$\{\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{y})\}_{P.b.} = \delta^a{}_b\delta^{(n)}(\mathbf{x}-\mathbf{y})\,. \quad (7.4)$$

In the right-hand side, there is no time dependence of φ^a and π_a on the same leaf Σ_t. Here, the PB itself is defined as follows:

$$\{F(\varphi^a\,,\pi_b)\,,G(\varphi^a\,,\pi_b)\}_{P.b.} = \int_{\Sigma_t}\sum_c\left(\frac{\delta F}{\delta\varphi^c}\frac{\delta G}{\delta\pi_c} - \frac{\delta G}{\delta\varphi^c}\frac{\delta F}{\delta\pi_c}\right)d^nz\,, \quad (7.5)$$

where F and G are functional with respect to the canonical variables φ^a and π_a. Based on the above formulation, the Dirac-Bergmann analysis is applied to field theories. An important example is of course the analysis of the general theory of relativity. The variables φ^a correspond to the lapse function, $N = N(t\,,\mathbf{x})$, the shift vector, $N^i = N^i(t\,,\mathbf{x})$, and the induced metric, $h_{ij} = h_{ij}(t\,,\mathbf{x})$. The corresponding canonical momentum variables, $\pi_0(t\,,\mathbf{x})$,

$\pi_i(t\,,\mathbf{x})$, and $\pi_{ij}(t\,,\mathbf{x})$ are given as Eq (4.68) in Section 4.5. The fundamental PBs are defined as Eq (4.95).

In order to investigate the existence of primary constraint densities, it is necessary to introduce the Hessian/Kinetic matrix

$$\begin{aligned}\mathcal{K}_{ab}(x\,,y)\,\sqrt{|h|} &= \frac{\delta}{\delta\dot{\varphi}^a(x)}\frac{\delta}{\delta\dot{\varphi}^b(y)}\int_{\Sigma_t}\mathcal{L}(\varphi^a(z)\,,\nabla_\mu\varphi^a(z)\,,\cdots)\,\sqrt{|h|}\,d^nz \\ &= K_{ab}(\varphi^a(x)\,,\nabla_\mu\varphi^a(x)\,,\cdots)\,\delta^{(n)}(x-y)\,,\end{aligned} \tag{7.6}$$

and to scrutinize the rank of the matrix density: $K_{ab}(\varphi^a(x)\,,\nabla_\mu\varphi^a(x)\,,\cdots)$. If the matrix density is degenerate and has its rank of $n+1-r$ then there exist the number of r primary constraint densities. Let us denote these primary constraint densities as follows:

$${}_*\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\ \overset{\mathfrak{C}^{(1)}}{\approx}\ 0\,, \tag{7.7}$$

where α_1 ranges $1\,,2\,,\cdots\,,r$. Then the total Hamiltonian density is introduced as follows:

$$\mathcal{H}_T(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x})) = \mathcal{H}_0(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))+\lambda^{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\,{}_*\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\,, \tag{7.8}$$

or abbreviating the arguments with respect to the support manifold (the spacetime manifold $\mathcal{M}$),

$$\mathcal{H}_T(\varphi^a\,,\pi_b) = \mathcal{H}_0(\varphi^a\,,\pi_b) + \lambda^{\alpha_1}(\varphi^a\,,\pi_b)\,{}_*\phi^{(1)}_{\alpha_1}(\varphi^a\,,\pi_b)\,, \tag{7.9}$$

where $\lambda^{\alpha_1} = \lambda^{\alpha_1}(\phi^a\,,\pi_b)$ are Lagrange multipliers. Remark that the variable dependence. That is, if it was $\lambda^{\alpha_1} = \lambda^{\alpha_1}(x) = \lambda^{\alpha_1}(t\,,\mathbf{x})$ then these variables are not the Lagrange multipliers; these variables are instead auxiliary field variables, although it also is mathematically inappropriate. A great amount of authors mistakes in this regard. Remember over and over again that we are considering the extremum problem in the phase space but not in the spacetime manifold. That is, for each spacetime point x, we consider the first-order variation of the total Hamiltonian density with respect to $\varphi^a(x) \to \varphi^a(x) + \delta\varphi^a(x)$ and $\pi_a(x) \to \pi_a(x) + \delta\pi_a(x)$: not to the spacetime points. As an example of these quantities, in the case of the general theory of relativity, the Hessian matrix K_{ab} is given by Eq (4.96), and its rank is six. Therefore, there are four primary constraint densities: Eq (4.69), and the total Hamiltonian is derived as Eqs (4.98) and (4.97).

So far, every extension of ingredients in the Dirac-Bergmann analysis to field theories has been straightforwardly achieved, and no problematic situation has occurred. The next step is, of course, the computations of consistency conditions for the derived constraint densities. In this step, we will encounter three issues with the analysis of field theories [Sundermeyer (1982); Blagojević and Nester (2020); D'Ambrosio et al. (2023); Tomonari and Bahamonde (2023); Heisenberg (2023)]. Let us consider the consistency conditions of the primary constraint densities as follows:

$$
\begin{aligned}
&{}_{*}\dot{\phi}^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\\
&\quad=\left\{{}_{*}\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\,,\mathcal{H}_T(\varphi^a(t\,,\mathbf{y})\,,\pi_b(t\,,\mathbf{y}))\right\}_{P.b.}\\
&\quad\overset{\mathfrak{C}^{(1)}}{\approx}\left\{{}_{*}\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\,,\mathcal{H}_0(\varphi^a(t\,,\mathbf{y})\,,\pi_b(t\,,\mathbf{y}))\right\}_{P.b.}+\lambda^{\beta_1}(\varphi^a(t\,,\mathbf{y})\,,\pi_b(t\,,\mathbf{y}))\,\mathcal{D}_{\alpha_1\beta_1}(x\,,y)\sqrt{|h|}:=0\,,
\end{aligned}
\tag{7.10}
$$

where " $:=$ " denotes the equation as an imposition and $D_{\alpha_1\beta_1}(\varphi^a\,,\pi_b)$ is defined as follows:

$$
\mathcal{D}_{\alpha_1\beta_1}(x\,,y)\,\sqrt{|h|}\,=\left\{{}_{*}\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))\,,{}_{*}\phi^{(1)}_{\beta_1}(\varphi^a(t\,,\mathbf{y})\,,\pi_b(t\,,\mathbf{y}))\right\}_{P.b.}\,. \tag{7.11}
$$

This matrix density is called the Dirac matrix density. The Dirac matrix in point particle systems is already defined in Eq (2.27). Remark that if $\lambda^{\beta_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))$ are not Lagrange multipliers but auxiliary fields $\lambda^{\beta_1}(t\,,\mathbf{x})$ then the weak equal " $\overset{\mathfrak{C}^{(1)}}{\approx}$ " is just an equal " $=$ ". This is easily verified from the definition of Poisson bracket (7.5). Therefore, needless to say, Eqs (7.10) and (7.11) are defined on the phase space: not on the support manifold (spacetime manifold) itself. In field theories, Eq (7.11) can be *schematically* calculated as follows:

$$
\begin{aligned}
&\mathcal{D}_{\alpha_1\beta_1}(x\,,y)\,\sqrt{|h|}\; = \\
&\quad f_1({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\cdots)_{\alpha_1\beta_1}\delta^{(n)}(\mathbf{x}-\mathbf{y}) \\
&\quad + f_2({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\cdots\,;\,\varphi^c(\varphi^a(x)\,,\pi_b(x))\,,\partial_i\varphi^c(\varphi^a(x)\,,\pi_b(x))\,,\cdots\,; \\
&\qquad\qquad \pi_c(\varphi^a(x)\,,\pi_b(x))\,,\partial_i\pi_c(\varphi^a(x)\,,\pi_b(x))\,,\cdots)_{\alpha_1\beta_1}\delta^{(n)}(\mathbf{x}-\mathbf{y}) \\
&\quad + g^{(i)}_1({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\cdots)_{\alpha_1\beta_1}\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \\
&\quad + g^{(i)}_2({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(x)\,,\pi_b(x))\,,\cdots\,;\,\varphi^c(\varphi^a(x)\,,\pi_b(x))\,,\partial_i\varphi^c(\varphi^a(x)\,,\pi_b(x))\,,\cdots\,; \\
&\qquad\qquad \pi_c(\varphi^a(x)\,,\pi_b(x))\,,\partial_i\pi_c(\varphi^a(x)\,,\pi_b(x))\,,\cdots)_{\alpha_1\beta_1}\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \\
&\quad + \cdots \\
&\quad + h^{(i)}_1({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(y)\,,\pi_b(y))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(y)\,,\pi_b(y))\,,\cdots)_{\alpha_1\beta_1}\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \\
&\quad + h^{(i)}_2({}_*\phi^{(1)}_{\alpha_1}(\varphi^a(y)\,,\pi_b(y))\,,\partial_{i*}\phi^{(1)}_{\alpha_1}(\varphi^a(y)\,,\pi_b(y))\,\cdots\,;\,\varphi^c(\varphi^a(y)\,,\pi_b(y)))\,,\partial_i\varphi^c(\varphi^a(y)\,,\pi_b(y))\,,\cdots\,; \\
&\qquad\qquad \pi_c(\varphi^a(y)\,,\pi_b(y))\,,\partial_i\pi_c(\varphi^a(y)\,,\pi_b(y))\,,\cdots)_{\alpha_1\beta_1}\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y})
\end{aligned}
\tag{7.12}
$$

where we abbreviated " $(t\,,\mathbf{x})$ " as " x ". f_1, $g^{(i)}_1$, and $h^{(i)}_1$ are functionals that are composed only of the primary constraint densities and those spatial derivatives. f_2, $g^{(i)}_2$, and $h^{(i)}_2$ are functionals that are constituted not only of the primary constraint densities and those spatial derivatives but also of the canonical variables φ^a, π_b, and those spatial derivatives, such that not vanishing under the imposition of the primary constraint densities. In particular, if f_1, $g^{(i)}_1$, and $h^{(i)}_1$ do not contain any spatial derivatives then these terms vanish under the imposition of the primary constraint densities. The terms including $h^{(i)}_1$ and $h^{(i)}_2$ give rise to total derivative terms. The terms including $g^{(i)}_1$ and $g^{(i)}_2$ give rise to the same sort of terms as " $h_1^{(i)}\partial_i\delta(\cdot)$ " and " $h_2^{(i)}\partial_i\delta(\cdot)$ ", respectively, and as " $f_1\delta(\cdot)$ " and " $f_2\delta(\cdot)$ ", respectively. Therefore, Eq (7.12) can be written *schematically* as follows:

$$\mathcal{D}_{\alpha_1\beta_1}(x\,,y)\,\sqrt{|h|}\;=F_{\alpha_1\beta_1}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})+\partial_i\left[H^{(i)}_{\alpha_1\beta_1}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]\,, \tag{7.13}$$

where $F_{\alpha_1\beta_1}$ and $H^{(i)}_{\alpha_1\beta_1}$ are specific functionals of ${}_*\phi^{(1)}_{\alpha_1}$, φ^a, π_a, and those spatial derivatives. So far, only primary constraint densities have been considered but this manipulation works as well in the same manner for higher-order constraint densities. Remark that if $g_1^{(i)}$ and $g_2^{(i)}$ are composed only of the constraint densities up to those linear combinations then the manipulation of integral by parts does not need since, just imposing the constraints, these functionals vanish. The PB-algebras (4.99) in Section 4.6 of the general theory of relativity has this property.

Now, let us clarify the issues of the Dirac-Bergmann analysis in field theories. The first issue relates to the existence of the inverse matrix of the Dirac matrix density $\mathcal{D}_{\alpha_1\beta_1}(x\,,y)\,\sqrt{|h|}$; the second term $\partial_i\left[H^{(i)}_{\alpha_1\beta_1}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]$ in Eq (7.13) generically leads to the following equations:

$$\begin{aligned}\int_{\Sigma_t}\left(\mathcal{D}_{\alpha_1\gamma_1}(x\,,z)\,\sqrt{|h|}\right)\left((\mathcal{D}^{-1})^{\gamma_1\beta_1}(z\,,y)\,\sqrt{|h|}^{\,-1}\right)\,d^n z\\ =\delta^{(n)}(\mathbf{x}-\mathbf{y})\delta_{\alpha_1}{}^{\beta_1}+\text{total divergent terms on }\partial\Sigma_{\rm t}\,,\end{aligned} \tag{7.14}$$

where $\partial\Sigma_t$ denotes the boundary of the leaf Σ_t. That is, the total divergent terms on $\partial\Sigma_t$ may disturb the well-defined calculation of the inverse matrix. That is, the question here is the method to define the inverse matrix. More fundamentally, "*the first issue concerns the method to define the degeneracy/rank of the matrix under the existence of the boundary terms.*" Since the rank determines the total number of primary constraint densities, therefore, this issue cannot be ignored. It is also crucial in particular for a system that has second-class constraint densities since the definition has something to do with determining the multipliers.

The second issue relates to the mathematical meaning of the density equations. In order to obtain the mathematical meaning of Eq (7.13) in a well-defined manner, the density equations should be integrated over on a leaf Σ_t with respect to $\mathbf{x}$ and $\mathbf{y}$ as follows:

$$\begin{aligned}\int_{\Sigma_t}\int_{\Sigma_t} \mathcal{D}_{\alpha_1\beta_1}(x\,,y)\,\sqrt{|h|}\,d^n x d^n y &= \left\{\int_{\Sigma_t} {}_*\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))d^n x\,, \int_{\Sigma_t} {}_*\phi^{(1)}_{\beta_1}(\varphi^a(t\,,\mathbf{y})\,,\pi_b(t\,,\mathbf{y}))d^n y\right\}_{P.b.} \\ &= \int_{\Sigma_t} \tilde{F}_{\alpha_1\beta_1}\,d^n x + \left[n_i \tilde{H}^{(i)}_{\alpha_1\beta_1}\right]_{\partial\Sigma_t}\,,\end{aligned} \tag{7.15}$$

where $\partial\Sigma_t$ denotes the boundary of the leaf Σ_t. Here, remark that, when integrating over Eq (7.13), there may occur the cancellation between the terms from $F_{\alpha_1\beta_1}$ and $H^{(i)}_{\alpha_1\beta_1}$. Taking into account this cancellation, $F_{\alpha_1\beta_1}$ and $H^{(i)}_{\alpha_1\beta_1}$ are redefined as $\tilde{F}_{\alpha_1\beta_1}$ and $\tilde{H}^{(i)}_{\alpha_1\beta_1}$, respectively. Excepting the last term $\left[n_i \tilde{H}^{(i)}_{\alpha_1\beta_1}\right]_{\partial\Sigma_t}$, all other terms are the so-called smeared variables. That is, the boundary terms may disturb to make the smeared algebras closed. To make matters worse, if $F_{\alpha_1\beta_1} \overset{\mathfrak{C}^{(1)}}{\approx} 0$, the existence of the boundary terms relates directly to whether or not a primary constraint density, ${}_*\phi^{(1)}_{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x})) \overset{\mathfrak{C}^{(1)}}{\approx} 0$, is classified into first-class constraint: if the boundary terms are absent then there is a possibility to be the primary constraint density as a first-class one. Furthermore, even if non-vanishing boundary terms do not appear in the consistency conditions for the primary constraint densities, that for higher-order constraint densities would face the same problem. That is, "*the second issue is whether should the boundary terms be also taken into account when classifying a constraint into either first- or second-class constraint density.*" This issue is the most crucial for counting degrees of freedom. As a special case, we can use the normal vector given in Eq (4.41), and then the boundary terms in Eq (7.15) always vanish. In this case, another issue occurs; which equation, either Eq (7.13) or Eq (7.15), should be applied for the classification? Furthermore, this issue implies that the constraint structure of a given theory depends on the way of taking a foliation. For a diffeomorphism invariant theory, this property is at a glance pathological.

How to resolve this situation? These are also the second issue.

The final issue relates to determining the Lagrange multipliers. Applying the schematic relation (7.13) to the consistency conditions (7.10), the following *schematic* equations are derived:

$$\left(A^{(i)}\partial_i\vec{\lambda}+B\vec{\lambda}+\vec{C}\right)\delta^{(n)}(\mathbf{x}-\mathbf{y})=\vec{0}\,, \tag{7.16}$$

or equivalently, integrating over with respect to either $\mathbf{x}$ or $\mathbf{y}$ on a leaf Σ_t,

$$A^{(i)}\partial_i\vec{\lambda}+B\vec{\lambda}+\vec{C}=\vec{0}\,, \tag{7.17}$$

where A^i, B, and $\vec{C}$ are the matrices and the vector that are determined by the given action functional (7.2) and composed of the phase space variables φ^a, π_b and those spatial derivatives, respectively. $\vec{\lambda}$ is the column matrix of which components are the Lagrange multipliers $\lambda^{\alpha_1}(\varphi^a(t\,,\mathbf{x})\,,\pi_b(t\,,\mathbf{x}))$ given in Eq (7.10). Notice here that the terms " $\partial_i\left[H^{(i)}_{\alpha_1\beta_1}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]$ " in Eq (7.13) give rise to the first term " $A^i\partial_i\vec{\lambda}$ " from the second terms in Eq (7.10) due to the Leibniz law. Explicitly, Eq (7.17) can be expanded into as follows:

$$A^{(i)}\left[\frac{\partial\vec{\lambda}}{\partial\varphi^a}\partial_i\varphi^a+\frac{\partial\vec{\lambda}}{\partial\pi_b}\partial_i\pi_b\right]+B\vec{\lambda}+\vec{C}=\vec{0}\,. \tag{7.18}$$

On one hand, if $A^{(i)}=0$ then the above equation becomes an ordinary linear algebraic equation, and the situation is the same as the point particle systems as explained in Section 2.2; the multipliers λ^{α_1} as the same number of the rank of the matrix B are determined, and otherwise secondary constraint densities occur. On the other hand, if the rank of $A^{(i)}$ is not zero then the situation gets changed; the above equation turns into partial differential equations of *functionals* (PDEs of functionals) with respect to the phase space variables φ^a and π_b. When the PDEs are solved, of course, the function forms of the Lagrange multipliers are determined, and then the equation generically turns into the differential equations with respect to the phase space variables themselves. That is, the above equation determines φ^a and π_b in terms of the coordinate variables $\mathbf{x}$ on the leaf Σ_t. However, the equations of motion also determine the variables φ^a and π_b in terms of the coordinate variables $\mathbf{x}$ (and t). Therefore, "*the third issue is whether or not the solved phase space variables φ^a and π_b in these two different ways are always consistent.*" Remark that, hereinafter, we use the term "*solvable*" for such PDEs in the means that all the Lagrange multipliers are expressed in terms of the phase space variables under the satisfaction of this consistency.

These three issues of the Dirac-Bergmann analysis in field theories are commonly caused by the problematic terms " $\partial_i \left[H^{(i)}_{\alpha_1\beta_1}\, \delta^{(n)}(\mathbf{x}-\mathbf{y}) \right]$ " in Eq (7.13). Therefore, it is mandatory to unveil a valid treatment of the problematic terms. Furthermore, this problem relates directly to the well-posedness of PBs. Based on the considerations in the previous three paragraphs, the most naive treatment to settle these issues is to discard the problematic terms. That is, if it is possible, Eq (7.14) turns out to give a definition of the inverse matrix of the Dirac matrix density in the usual manner just like Eq (7.6) and then the total number of first-class constraint densities becomes maximum number (See Section 2.2); Eq (7.15) plays a role in classifying a constraint into first- or second-class constraint in a usual manner just like the point particle cases; Eq (7.17) becomes an ordinary linear algebraic equations. Since the consistency conditions have to be calculated by using the well-defined PB-algebras in advance, it makes sense to consider the discard of the problematic terms in the step of calculating the PB-algebras. Remark, here, that, in the general theory of relativity, all primary constraint densities are commutative with respect to the PB-algebras; the terms $F_{\alpha_1\beta_1}$ in Eq (7.13) vanish and the terms " $\partial_i \left[H^{(i)}_{\alpha_1\beta_1}\, \delta^{(n)}(\mathbf{x}-\mathbf{y}) \right]$ " in Eq (7.13) do not appear. Therefore, the issues above do not occur.

In order to determine PB-algebras in a well-defined manner, the relations (7.13) should be considered by integrating over. That is, Eq (7.15) has a key for the well-definedness. In particular, the possibility of vanishing the boundary terms " $\left[n_i H^{(i)}_{\alpha_1\beta_1} \right]_{\partial\Sigma_t}$ " in the equations would relate to whether or not the problematic terms could be discarded. Then the possible reasons to make the naive treatment of the spatial boundary terms mentioned in the previous paragraph would be that Possibility (i): If the spatial normal vector n_i is orthogonal to $H^{(i)}_{\alpha_1\beta_1}$ on the leaf Σ_t then the boundary terms vanishes (This include the specific use of Eq (4.41)); Possibility (ii): The boundary terms could be vanished under the imposition of appropriate spatial boundary conditions to φ^a and/or π_a. In the latter case, the variables that are fixed on the spatial boundary $\partial\Sigma_t$ should be unphysical variables. Possibility (iii): The spacetime manifold is foliated into leaves with no boundaries. In particular, it seems that Possibility (ii) is the most realizable and applicable to the wide range of theories. Extending this statement into all other PBs that appear in the Dirac-Bergmann analysis, it is reasonable since the well-definedness is a mathematical property although this statement needs to be proven, in this thesis, let us assume that the following prescription [Tomonari and Bahamonde (2023)]:[3]

Prescription 1.

For functionals $\mathcal{F}^{(i)}$ on a phase space which are coordinated by $\varphi^a(t\,,\mathbf{x})$ and $\pi_a(t\,,\mathbf{x})$, the term " $\partial_i\left[\mathcal{F}^{(i)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]$ " in PB-algebras can be discarded by setting properly spatial boundary conditions of the "unphysical variables" in $\varphi^a(t\,,\mathbf{x})$ and $\pi_a(t\,,\mathbf{x})$ on the boundary of a leaf Σ_t. Here, the index i runs from 1 to the dimension of a leaf Σ_t, i.e., n, and h are the determinant of the metric on a leaf Σ_t.

■

Here, "*unphysical*" means that a variable corresponds to a constraint in the conjugate manner

[3] In the original paper [Tomonari and Bahamonde (2023)], the statement was deserted for the terms like " $\sqrt{h(x)}A(x)\partial^{(x)}_i\delta^{(n)}(\vec{x}-\vec{y})$ ". In the current thesis, we already integrated by parts this sort of term in Eq (7.13). That is, if we expand as $\sqrt{h(x)}A(x)\partial^{(x)}_i\delta^{(n)}(\vec{x}-\vec{y}) = \partial^{(x)}_i(\sqrt{h(x)}A(x)\delta^{(n)}(\vec{x}-\vec{y})) - \delta^{(n)}(\vec{x}-\vec{y})\partial^{(x)}_i(\sqrt{h(x)}A(x))$ then the first term is nothing but ones that have been considered in the current thesis. (The second term is encapsulated into the first term of Eq (7.13).) The important point here is that these two statements are equivalent since, in order to evaluate the PBs, we integrate them over twice; every term above turns into a spatial boundary term and appropriate spatial boundary conditions erase them.

and we assume that the classification of constraint densities into either first- or second-class is determined by the use of Eq (7.15). This makes sense since the Dirac delta function has its mathematical meaning in a well-defined manner when integrated over and since before performing the calculation for determining multipliers the PB-algebras should be given in a well-defined manner in advance.

The possibilities (i) (excepting the specific use of Eq (4.41)) and (iii) could also be viable but it would strongly depend on each theory. Therefore, in this thesis, we do not assume these specific possibilities. Remark, here, that, in the case of the general theory of relativity, the secondary constraint densities given in Eq (4.100) contains the spatial derivative of the Dirac delta function. However, these terms are not problematic in this meaning; the coefficients of these terms are composed of the secondary constraint densities, as already mentioned. Therefore, the imposition of the secondary constraint densities removes them without applying Prescription 1. Notice, finally, that the imposition of spatial boundary conditions restricts the solution space of a given theory [Heisenberg (2023)]. That is, the Dirac-Bergmann analysis based on Prescription 1 gives the propagating degrees of freedom for the restricted solutions by the spatial boundary condition. For example, let us consider the Schwarzschild and FLRW spacetime as two solutions of the Einstein field equations. If we impose the asymptotically flatness as a spatial boundary condition then FLRW spacetime no longer belongs to the solution space of the Einstein field equations. Therefore, in compensation for the use of Prescription 1, the Dirac-Bergmann analysis does not always unveil all propagating degrees of freedom of a given theory. This is the meaning of the word, "*prescription*", and it guarantees the reliable results of the Dirac-Bergmann analysis that do not suffer from the three issues instead of its generality.

There is an important remark: the specific choice of the normal vector given in Eq (4.41) always satisfies Prescription 1. For a diffeomorphism theory, on one hand, since taking an ADM-foliation itself decomposes a spacetime manifold into another one which has a topology

$\mathbb{R}\times S$ in a diffeomorphic manner (See Section 4.4 in detail) and this manipulation is equivalent to a choice of a coordinate system, without any loss of generality, it means that Prescription 1 can be applied and always provide the full pDoF of a given theory. On the other hand, for a theory with violating its diffeomorphism invariant characteristics, the theory generically depends on coordinate systems, or equivalently, the choices of ADM-foliations. It indicates that the theory generically has several sectors and each sector generically derives a different pDoF from that of the other sectors. In this regard, a detailed survey in $f(T)$-gravity is given in [Tomonari and Bahamonde (2023)].

In the succeeding sections, the Dirac-Bergmann analysis of the geometrical trinity of gravity and its non-linear extension is performed under the imposition of Prescription 1 when facing the three issues. These cases are also good examples for the application of Prescription 1, or more fundamentally, for making the understanding of the three issues deeper.

7.2. Degrees of freedom of TEGR

In this section, the Dirac-Bergmann analysis of TEGR is performed [Blagojevic and Nikolic (2000); Blagojevic and Vasilic (2000); Maluf and da Rocha-Neto (2000); Ferraro and Guzmán (2016)], and the propagating and gauge degrees of freedom are clarified. In the case of TEGR, it is unveiled that the spatial boundary terms appear in PB-algebras but the analysis does not need Prescription 1; this is just the same situation as the general theory of relativity. The following derivation particularly obeys the authors of Ref [Ferraro and Guzmán (2016)].

Let us start with the action functional of TEGR given in Eq (6.78) in Section 6.3. The Lagrangian density is introduced as follows:

$$S_{\mathrm{TEGR}} = \int_{\mathcal{M}} d^{n+1}x\,\mathcal{L}_{\mathrm{TEGR}}\,,\quad \mathcal{L}_{\mathrm{TEGR}} = -\frac{1}{2\kappa^2}\det(\mathbf{e}^{-1})\mathbb{T}\,, \tag{7.19}$$

where we discarded the boundary term in Eq (6.78). Hereinafter, we use the unit $2\kappa^2 = 1$

and $e = \det(\mathbf{e}^{-1})$. Expressing in terms of (co)frame fields, Eq (7.19) becomes as follows:

$$\mathcal{L}_{\mathrm{TEGR}} = -\frac{1}{2}\, e\, \partial_\mu e^I{}_\nu \partial_\rho e^J{}_\sigma e^\mu{}_K e^\nu{}_L e^\rho{}_M e^\sigma{}_N \mathfrak{M}_{IJ}{}^{KLMN}\,, \tag{7.20}$$

where $\mathfrak{M}_{IJ}{}^{KLMN}$ is called the supermetric and defined as follows:

$$\mathfrak{M}_{IJ}{}^{KLMN} = 2 g_{IJ} g^{K[M} g^{N]L} - 4\delta_I^{[M} g^{N][K} \delta_J^{L]} + 8\delta_I^{[K} g^{L][M} \delta_J^{N]}\,, \tag{7.21}$$

where g_{IJ} is the metric of the internal space. Notice that the supermetic is antisymmetric with respect to the indices $(K\,, L)$ and $(M\,, N)$. The canonical momentum density variables are computed as follows:

$$\pi_I{}^\mu = -e\, \partial_\nu e^J{}_\rho e^0{}_K e^\mu{}_L e^\nu{}_M e^\rho{}_N \mathfrak{M}_{IJ}{}^{KLMN}\,. \tag{7.22}$$

The fundamental PBs are introduced as follows:

$$\{e^I{}_\mu(t\,, \mathbf{x})\,, \pi_J{}^\nu(t\,, \mathbf{y})\}_{P.b.} = \delta^I_J \delta^\nu_\mu \delta^{(n)}(\mathbf{x} - \mathbf{y})\,. \tag{7.23}$$

The antisymmetric property of the supermetric with respect to K and L leads apparently to the number of $(n+1)$ primary constraint densities as follows:

$$_*\phi^{(1)}_I = \pi_I{}^0 := 0\,. \tag{7.24}$$

These trivial constraint densities give an insight into finding other remaining primary constraint densities. Eq (7.24) can be deformed as follows:

$$_*\phi^{(1)}_I = e^0{}_J \delta^K_I \pi_K{}^\mu e^J{}_\mu := 0\,. \tag{7.25}$$

This implies the following quantity:

$$\mathfrak{G}^J{}_I = \pi_I{}^\mu e^J{}_\mu = -e\, C_{IK}{}^{JL} e^\mu{}_L \partial_0 e^K{}_\mu - e\, \partial_i e^L{}_\mu\, e^0{}_K e^i{}_M e^\mu{}_N \mathfrak{M}_{IL}{}^{KJMN}\,. \tag{7.26}$$

In order to turn these quantities into constraint densities, multiplying $V^I{}_{(X)J}$ to the above equations

$$\mathfrak{G}_{(X)} = V^I{}_{(X)J} \mathfrak{G}^J{}_I\,, \tag{7.27}$$

and then impose the following conditions:

$$V^I{}_{(X)J} C_{IK}{}^{JL} := 0\,. \tag{7.28}$$

Here, the index " (X) " is a dummy one. For instance, $V^I{}_{KJ} = e^0{}_J \delta^I_K$ satisfies Eq (7.28), and then Eq (7.27) restores the primary constraint densities (7.25), or equivalently, Eq (7.24). In this case, the dummy index " (X) " is taken as K. In the same way, let us take $V^I{}_{(X)J}$ as $2\delta^I_{[J} g_{K]L}$: $V^I{}_{KLJ} = 2\delta^I_{[J} g_{K]L}$. Then $V^I{}_{KLJ}$ satisfies Eq (7.28), and then the number of $n(n+1)/2$ primary constraint densities are derived as follows:

$$_*\phi^{(1)}_{IJ} = 2 g_{K[J} \pi_{I]}{}^i e^K{}_i + 4\, e\, \partial_i e^K{}_j\, e^0{}_{[J} e^i{}_I e^j{}_{K]} := 0\,. \tag{7.29}$$

Then the PB-algebras among $_*\phi^{(1)}_I$ and $_*\phi^{(1)}_{IJ}$ are computed as follows:

$$\begin{aligned}
&\{{}_*\phi^{(1)}_I(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_J(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi^{(1)}_{IJ}(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_K(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi^{(1)}_{IJ}(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_{KL}(t\,,\mathbf{y})\}_{P.b.} = \left(g_{JL}\,{}_*\phi^{(1)}_{IK} + g_{IK}\,{}_*\phi^{(1)}_{JL} - g_{JK}\,{}_*\phi^{(1)}_{IL} - g_{IL}\,{}_*\phi^{(1)}_{JK}\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(1)}}{\approx} 0\,,
\end{aligned} \tag{7.30}$$

where we abbreviated the argument " $(t\,,\mathbf{x})$ " on the right hand side in the third PB-algebras. These PB-algebras do not include the spatial derivative of δ-function. Notice that the third PB-algebras are exactly the same as the Lorentz algebra. Therefore, it is expected that the primary constraint densities ${}_*\phi^{(1)}_{IJ}(t\,,\mathbf{x})$ becomes the generator of the local Lorentz transformation and are classified into first-class constraint densities.

Next, let us calculate the consistency conditions for the primary constraint densities. The total Hamiltonian is composed as follows:

$$\mathcal{H}_T = \mathcal{H}_0 + \lambda^I\,{}_*\phi^{(1)}_I + \lambda^{IJ}\,{}_*\phi^{(1)}_{IJ}\,, \tag{7.31}$$

where $\mathcal{H}_0$ is the kernel Hamiltonian and λ^I and λ^{IJ} are Lagrange multipliers. Remark that the multipliers are the functionals of the canonical variables $e^I{}_\mu$ and $\pi_I{}^\mu$. The kernel Hamiltonian is derived from the temporal component of the Euler-Lagrange equations under the primary constraint densities. That is,

$$\begin{aligned}
&\partial_\mu \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial(\partial_\mu e^I{}_0)} - \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial e^I{}_0} \overset{\mathfrak{C}^{(1)}}{\approx} \partial_i \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial(\partial_i e^I{}_0)} - \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial e^I{}_0} = -\partial_i \pi_I{}^i - \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial e^I{}_0} = 0\,,\\
&\therefore \quad \partial_i \pi_I{}^i + \frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial e^I{}_0} = 0\,.
\end{aligned} \tag{7.32}$$

The second term on the left-hand side is calculated as follows:

$$\frac{\partial \mathcal{L}_{\mathrm{TEGR}}}{\partial e^I{}_0} = e_I{}^0 \left[\partial_i (e^J{}_0 \pi_J{}^i) - \mathcal{H}_0\right] - e^J{}_0 e_I{}^0 \partial_i \pi_J{}^i + 2 e_I{}^j \partial_{[i} e^J{}_{j]} \pi_J{}^i\,. \tag{7.33}$$

Substituting the second formulae into the first equations, the following equations are derived:

$$e^J{}_j e_I{}^j \partial_i \pi_J{}^i + e_I{}^0 \left[\partial_i (e^J{}_0 \pi_J{}^i) - \mathcal{H}_0\right] + 2 e_I{}^j \partial_{[i} e^J{}_{j]} \pi_J{}^i = 0\,. \tag{7.34}$$

The temporal component gives the kernel Hamiltonian as follows:

$$\mathcal{H}_0 = e^I{}_0 e_I{}^j e^J{}_j \partial_i \pi^i{}_J + \partial_i(e^I{}_0 \pi_I{}^i)\,. \tag{7.35}$$

The consistency conditions for the primary constraint densities ${}_*\phi^{(1)}_I \overset{\mathfrak{C}^{(1)}}{\approx} 0$ generate the secondary constraint densities as follows:

$$\begin{aligned} {}_*\phi^{(2)}_0 &= {}_*\dot{\phi}^{(1)}_0 \overset{\mathfrak{C}^{(1)}}{\approx} \mathcal{H}_0 - \partial_i(e^I{}_0 \pi^i{}_I) := 0\,, \\ {}_*\phi^{(2)}_i &= {}_*\dot{\phi}^{(1)}_0 \overset{\mathfrak{C}^{(1)}}{\approx} \partial_j(e^I{}_i \pi_I{}^j) := 0\,. \end{aligned} \tag{7.36}$$

Notice that the first constraint densities of the above equations imply that the total Hamiltonian is composed only of the constraint densities with a total divergent term as follows:

$$\mathcal{H}_T = {}_*\phi^{(2)}_0 + \lambda^I\, {}_*\phi^{(1)}_I + \lambda^{IJ}\, {}_*\phi^{(1)}_{IJ} + \partial_i(e^I{}_0 \pi^i{}_I) \overset{\mathfrak{C}^{(2)}}{\approx} \partial_i(e^I{}_0 \pi^i{}_I)\,. \tag{7.37}$$

Therefore, taking into account the PB-algebras (7.30), the consistency conditions for the Lorentz generators ${}_*\phi^{(1)}_{IJ} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ are automatically satisfied up to boundary terms. The PB-algebras among ${}_*\phi^{(2)}_I \overset{\mathfrak{C}^{(2)}}{\approx} 0$ are calculated as follows:

$$\begin{aligned} \{{}_*\phi^{(2)}_i(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_j(t\,,\mathbf{x})\}_{P.b.} &= \left({}_*\phi^{(2)}_j(t\,,\mathbf{x})\partial^{(x)}_i - {}_*\phi^{(2)}_i(t\,,\mathbf{y})\partial^{(y)}_j\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \\ \{{}_*\phi^{(2)}_i(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_0(t\,,\mathbf{y})\}_{P.b.} &= {}_*\phi^{(2)}_0(t\,,\mathbf{x})\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \\ \{{}_*\phi^{(2)}_0(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_0(t\,,\mathbf{y})\}_{P.b.} &= \left(h^{ij}(t\,,\mathbf{x}){}_*\phi^{(2)}_j(t\,,\mathbf{x}) + h^{ij}(t\,,\mathbf{y}){}_*\phi^{(2)}_j(t\,,\mathbf{y})\right)\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,. \end{aligned} \tag{7.38}$$

Notice that these PB-algebras are exactly the same as the ones of general relativity given in Eq (4.100). This fact means that TEGR has the same gauge symmetry as the one of general relativity. The PB-algebras among ${}_*\phi_I^{(1)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ and ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ are calculated as follows:

$$\begin{aligned}
&\{{}_*\phi_I^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_I^{(2)}(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi_I^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_0^{(2)}(t\,,\mathbf{y})\}_{P.b.} = (e_I{}^0{}_*\phi_0^{(2)} + e_I{}^i{}_*\phi_i^{(2)})\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,,\\
&\{{}_*\phi_{IJ}^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_i^{(2)}(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi_{IJ}^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_0^{(2)}(t\,,\mathbf{y})\}_{P.b.} = -e^K{}_0 g_{K[I}e_{J]}{}^0{}_*\phi_0^{(2)}\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,.
\end{aligned} \tag{7.39}$$

Using these PB-algebras and the total Hamiltonian (7.37), the consistency condition for the secondary constraint densities ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ are automatically satisfied up to boundary terms. Therefore, the Dirac-Bergman analysis stops here. The propagating degrees of freedom of TEGR in a $(n+1)$-dimensional spacetime is given as follows:

$$\text{pDoF} = (n+1)^2 - \frac{(n+1)(n+4)}{2} = \frac{1}{2}(n+1)(n-2)\,. \tag{7.40}$$

The gauge degrees of freedom is given as follows:

$$\text{gDoF of Diffeomorphism} = n+1 \tag{7.41}$$

for the diffeomorphism (covariance) symmetry and

$$\text{gDoF of Lorentz} = \frac{1}{2}n(n+1) \tag{7.42}$$

for the local Lorentz symmetry.

Finally, notice that the PB-algebras (7.30), (7.38), and (7.39) do not need the Prescription 1 since the coefficients of these PB-algebras are composed by the linear combination of the primary and/or secondary constraint densities. This structure prevents moving from the spatial differential operator to the Lagrange multipliers. That is, TEGR does not suffer from the third issue explained in Section 7.1. In addition, if the constraint densities are satisfied on the spatial boundary then TEGR is also free from the second issue explained in Section 7.1. The first issue does not arise since TEGR has only first-class constraint densities: the Dirac matrix cannot be defined. Therefore, the pDoF given in Eq (7.40) holds for any solutions of TEGR.

7.3. Degrees of freedom of Coincident GR

In this section, the Dirac-Bergmann analysis of Coincident GR (CGR) is performed [D'Ambrosio et al. (2020)], and the propagating and gauge degrees of freedom are clarified. In the case of TEGR, it is unveiled that the spatial boundary terms appear in PB-algebras, but the analysis does not need Prescription 1; this is just the same situation as general relativity.

Let us start by decomposing the CGR action functional in the ADM-foliation manner. The action functional of CGR is already derived as Eq (6.93) in Section 6.3. The action functional can be rewritten as follows:

$$S_{\mathrm{CGR}} = \int_{\mathcal{M}} d^{n+1}x\sqrt{-g}\,\frac{1}{4}\,M^{\alpha\beta\sigma\rho\mu\nu}Q_{\alpha\beta\sigma}Q_{\rho\mu\nu}\,, \tag{7.43}$$

where $2\kappa^2 = 1$ and $M^{\alpha\beta\sigma\rho\mu\nu}$ is set as follows:

$$M^{\alpha\beta\sigma\rho\mu\nu} = g^{\alpha\rho}g^{\beta\sigma}g^{\mu\nu} - g^{\alpha\rho}g^{\beta\mu}g^{\sigma\nu} + 2g^{\alpha\nu}g^{\beta\mu}g^{\sigma\rho} - 2g^{\alpha\beta}g^{\mu\nu}g^{\sigma\rho}\,. \tag{7.44}$$

Remark that $Q_{\alpha\beta\gamma} = \nabla_\alpha g_{\beta\gamma}$ is now in the coincident gauge: $Q_{\alpha\beta\gamma} = \partial_\alpha g_{\beta\gamma}$. Applying the ADM-foliated metric Eq (4.37) and, after performing very long but straightforward algebraic calculations, the above action can be rewritten as follows [D'Ambrosio et al. (2020)]:

$$S_{\mathrm{CGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x\sqrt{h}\left[N\left({}^{(n)}Q + K^{ij}K_{ij} - K^2\right) + \mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_3\right]\,, \tag{7.45}$$

where ${}^{(n)}Q$, $\mathcal{B}_1$, $\mathcal{B}_2$, and $\mathcal{B}_3$ are set as follows:

$$
{}^{(n)}Q = \frac{1}{4}\left[-h^{il}h^{jm}h^{kn} + 2h^{in}h^{jm}h^{kl} + h^{il}h^{jk}h^{mn} - 2h^{ij}h^{mn}h^{kl}\right]Q_{ijk}Q_{lmn}\,, \tag{7.46}
$$

$$
\begin{aligned}
\mathcal{B}_1 =& h^{ij}h^{kl}(Q_{jkl} - Q_{kjl})\partial_i N\,,\\
\mathcal{B}_2 =& K\partial_i N^i + \dot{N}\frac{\partial_i N^i}{N^2} - \frac{(\partial_i N^i)(N^j\partial_j N)}{N^2}\,,\\
\mathcal{B}_3 =& \frac{(N^i\partial_j N)(\partial_i N^j)}{N^2} - \frac{\partial_i N^j}{2N}\left(2\partial_j N^i + N^i h^{mn}Q_{jmn}\right) + \dot{N}^k\frac{1}{2N^2}(Nh^{ij}Q_{kij} - 2\partial_k N)\,.
\end{aligned} \tag{7.47}
$$

The sum of these boundary terms multiplying $\sqrt{h}$, *i.e.*, $\sqrt{h}\mathcal{B}_1$, $\sqrt{h}\mathcal{B}_2$, and $\sqrt{h}\mathcal{B}_3$, are calculated, neglecting spatial boundary terms, as follows:

$$
\sqrt{h}(\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_3) = -N\sqrt{h}\mathring{D}_i({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i) + \partial_\mu N^j\partial_j(\sqrt{h}n^\mu) - \partial_i N^i\partial_\mu(\sqrt{h}n^\mu)\,. \tag{7.48}
$$

Remark that this ignorance is irrelevant to the Priscription 1. Therefore, the action becomes as follows:

$$
\begin{aligned}
S_{\mathrm{CGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x \Big[& N\sqrt{h}\left\{{}^{(n)}Q + K^{ij}K_{ij} - K^2 - \mathring{D}_i({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i)\right\}\\
& -\partial_i N^i\partial_\mu(\sqrt{h}n^\mu) + \partial_\mu N^j\partial_j(\sqrt{h}n^\mu)\Big]\,.
\end{aligned} \tag{7.49}
$$

This is none other than the ADM-foliation of CGR [D'Ambrosio et al. (2020)]. Notice that the derivation of Eq (7.49) neglected only spatial boundary terms. Integrating the second term in Eq (7.49) by parts: $-\partial_i N^i\partial_\mu(\sqrt{h}n^\mu) = -\partial_i[N^i\partial_\mu(\sqrt{h}n^\mu)] + \partial_\mu[N^i\partial_i(\sqrt{h}n^\mu)] - (\partial_\mu N^i)(\partial_i\sqrt{h}n^\mu)$, the third term is canceled out with the third term in Eq (7.49). The remnant terms are only boundary terms; these terms can be neglected by introducing appropriate counter-terms just like the case of general relativity. (See Section 4.5 in detail.)

Therefore, we get the final result:

$$S_{\mathrm{CGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x N\sqrt{h}\left[{}^{(n)}Q + K^{ij}K_{ij} - K^2 - \mathring{D}_i({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i)\right] . \tag{7.50}$$

Note that the above derivation does not need the Gauss equation, unlike the case of the general theory of relativity. (See Sections 4.4 and 4.5.) We just manipulated complicated algebraic calculations.

The Dirac-Bergmann analysis is performed for the action functional Eq (7.50). The canonical momentum variables are calculated as follows:

$$\pi_0 = 0\,, \quad \pi_i = 0\,, \quad \pi_{ij} = \sqrt{h}(Kh_{ij} - K_{ij})\,, \tag{7.51}$$

and therefore, the primary constraint densities are given as follows:

$${}_*\phi_0^{(1)} = \pi_0 := 0\,, \quad {}_*\phi_i^{(1)} = \pi_i := 0\,. \tag{7.52}$$

These constraint densities restrict the entire phase space to a subspace $\mathfrak{C}^{(1)}$. The total Hamiltonian density is derived as follows:

$$\mathcal{H}_T = N\mathcal{C}_0^{(\mathrm{CGR})} + N^i\mathcal{C}_i^{(\mathrm{CGR})} + \lambda^\mu{}_*\phi_\mu^{(1)}\,, \tag{7.53}$$

where $\mathcal{C}_0^{(\mathrm{CGR})}$ and $\mathcal{C}_i^{(\mathrm{CGR})}$ are set as follows:

$$\mathcal{C}_0^{(\mathrm{CGR})} = -\sqrt{h}\left[{}^{(n)}Q - \mathring{D}_i({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i)\right] + \frac{1}{\sqrt{h}}\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right)\,, \quad \mathcal{C}_i^{(\mathrm{CGR})} = -2\mathring{D}^j\pi_{ij}\,. \tag{7.54}$$

The fundamental PB-algebras are the same as those of the general theory of relativity: Eq (4.95). Therefore, the consistency conditions for the primary constraint densities Eqs (7.52) lead to four secondary constraint densities:

$$
{}_*\phi_0^{(2)} = \mathcal{C}_0^{(\mathrm{CGR})} := 0\,, \quad {}_*\phi_i^{(2)} = \mathcal{C}_i^{(\mathrm{CGR})} := 0\,, \tag{7.55}
$$

and these constraint densities restrict $\mathfrak{C}^{(1)}$ to a new subspace $\mathfrak{C}^{(2)}$. We can show that the smeared PB-algebras of Eq (7.55) satisfy the same PB-algebras as those of the general theory of relativity given in Eq (4.103) and (4.104) [D'Ambrosio et al. (2020)], and it indicates that CGR has the same gauge symmetry as the general theory of relativity. That is, the analysis stops here. Therefore, CGR has

$$
\mathrm{pDoF} = \frac{1}{2}(n+1)(n-2) \tag{7.56}
$$

and

$$
\mathrm{gDoF} = n+1\,. \tag{7.57}
$$

That is, CGR is completely equivalent to GR from both viewpoints of dynamics and gauge symmetry. [4]

7.4. Degrees of freedom of non-linear extension of GR

In this section, the Dirac-Bergmann analysis of the non-linear extension of the general theory of relativity, denoted by "fGR", is performed [Sotiriou and Faraoni (2010); Deruelle et al. (2009); Capozziello and De Laurentis (2011); Liang et al. (2017)], and the propagating and gauge degrees of freedom are clarified. In the case of fGR, it is unveiled that the spatial boundary terms generically appear in PB-algebras due to the existence of the non-linearity,

[4] However, the original Lagrangian density given in Eq (6.93) discards the boundary term of the Ricci scalar in the Einstein-Hilbert action functional. It means that the diffeomorphism invariance is at least partly violated, (it is also guessed from the imposition of the coincident gauge since this gauge destroys the covariance of the theory,) and it might imply that the analysis gives rise to some second-class constraint densities. I would like to leave to scrutinize the validity of the work [D'Ambrosio et al. (2020)] from this perspective for future work.

and the analysis generically needs Prescription 1; this is the departure from the case of the general theory of relativity from the viewpoint of constraint mechanics. That is, the theory suffers from the second issue, and, caused by it, the first issue may also occur. Further, it might happen the third issue. It means that the result is viable only for the solutions that satisfy the spatial boundary condition that is demanded by Prescription 1.

The action functional of the non-linear extension of the general theory of relativity is already given as Eq (6.100) in Section 6.4:

$$S_{\mathrm{fGR}} = \int_{\mathcal{M}} d^{n+1}x\sqrt{-g}f(\mathring{R})\,, \tag{7.58}$$

where $2\kappa^2 = 1$, $f'(\mathring{R}) = df(\mathring{R})/d\mathring{R}$, and $f'' \neq 0$. Introducing an auxiliary field φ, Eq (7.58) is decomposed as follows:

$$S_{\mathrm{fGR}} = \int_{\mathcal{M}} d^{n+1}x\sqrt{-g}\left[f'(\varphi)\mathring{R} + f(\varphi) - \varphi f'(\varphi)\right]\,. \tag{7.59}$$

Using the Gauss equation Eq (4.57) to decompose $\mathring{R}$, this action becomes as follows:

$$\begin{aligned} S_{\mathrm{fGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x N\sqrt{h}\left[f'\left({}^{(n)}\mathring{R} - K^2 + K^{ij}K_{ij} - \varphi\right) + f\right] \\ - 2\int_{\mathcal{M}} d^{n+1}x\sqrt{-g}\left[f'\mathring{\nabla}_\mu\left(n^\nu\mathring{\nabla}_\nu n^\mu - n^\mu\mathring{\nabla}_\nu n^\nu\right)\right]\,. \end{aligned} \tag{7.60}$$

Compared to Eq (4.66), the boundary terms cannot be neglected due to the existence of the non-linearity of f'. Integrating by parts and then neglecting the boundary terms, Eq (7.60) becomes as follows [Liang et al. (2017)]:

$$
\begin{aligned}
S_{\rm fGR} = &\int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x N\sqrt{h}\left[f'\left({}^{(n)}\mathring{R} - K^2 + K^{ij}K_{ij} - \varphi\right) + f\right] \\
&+ \int_{\mathcal{I}} dt \int_{\Sigma_t} d^n x N\sqrt{h}\left[\frac{2K}{N}\left(N^i\mathring{D}_i f' - f''\dot{\varphi}\right) + 2\mathring{D}_i f'\mathring{D}^i \ln N\right] .
\end{aligned}
\tag{7.61}
$$

The canonical momentum variables are calculated as follows:

$$
\pi_0 = 0\,, \quad \pi_i = 0\,, \quad \pi_{ij} = \sqrt{h}\left[f'\left(Kh_{ij} - K_{ij}\right) - \frac{h_{ij}}{N}\left(N^k\mathring{D}_k f' - f''\dot{\varphi}\right)\right]\,, \quad \pi_\varphi = -2K\sqrt{h}f'' .
\tag{7.62}
$$

In the case of $f' = constant$, as expected, Eq (7.62) becomes Eq (4.68). The primary constraint densities are given as follows:

$$
{}_*\phi_0^{(1)} = \pi_0 := 0\ , \quad {}_*\phi_i^{(1)} = \pi_i := 0\,,
\tag{7.63}
$$

and these constraint densities identify the subspace $\mathfrak{C}^{(1)}$. The total Hamiltonian density is calculated as follows:

$$
\mathcal{H}_T = N\mathcal{C}_0^{\rm (fGR)} + N^i\mathcal{C}_i^{\rm (fGR)} + \lambda^\mu{}_*\phi_\mu^{(1)} = \mathcal{H}_0 + \lambda^\mu{}_*\phi_\mu^{(1)}
\tag{7.64}
$$

where λ^μ are Lagrange multipliers, and $\mathcal{C}_\mu^{\rm (fGR)}$ are defined as follows:

$$
\begin{aligned}
\mathcal{C}_0^{\rm (fGR)} =& -\sqrt{h}\left[f + f'\left({}^{(n)}\mathring{R} - \varphi\right)\right] + \frac{1}{\sqrt{h}f'}\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right) + 2\sqrt{h}\mathring{D}_i\mathring{D}^i f' \\
&- \frac{1}{n\sqrt{h}f''}\pi\pi_\varphi + \frac{n-1}{n\sqrt{h}f'}\left(\frac{f'}{f''}\right)^2\pi_\varphi^2, \\
\mathcal{C}_i^{\rm (fGR)} =& \pi_\varphi\mathring{D}_i\varphi - 2\mathring{D}^j\pi_{ij} .
\end{aligned}
\tag{7.65}
$$

In the case of $f' = constant$, Eq (7.65) coincides with Eqs (4.89) and (4.90). The consistency conditions for the primary constraint densities, ${}_*\phi^{(1)}_\mu \overset{\mathfrak{C}^{(1)}}{\approx} 0$, are gives four secondary constraint densities as follows:

$$ {}_*\phi^{(2)}_0 = \mathcal{C}^{(\mathrm{fGR})}_0 := 0\,, \quad {}_*\phi^{(2)}_i = \mathcal{C}^{(\mathrm{fGR})}_i := 0\,, \tag{7.66} $$

under the same fundamental PB-algebras Eq (4.95) and

$$ \{\varphi(x), \pi_\varphi(y)\}_{P.b.} = \delta^{(n)}(\mathbf{x}-\mathbf{y})\,. \tag{7.67} $$

These constraint densities restrict $\mathfrak{C}^{(1)}$ to a new subspace $\mathfrak{C}^{(2)}$. The consistency conditions for these secondary constraint densities are computed as follows:

$$ \begin{aligned} &\{{}_*\phi^{(2)}_i(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_j(t\,,\mathbf{y})\}_{P.b.} = \\ &\qquad \left({}_*\phi^{(2)}_j(t\,,\mathbf{x})\partial^{(x)}_i - {}_*\phi^{(2)}_i(t\,,\mathbf{y})\partial^{(y)}_j\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \\ &\{{}_*\phi^{(2)}_0(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_i(t\,,\mathbf{y})\}_{P.b.} = \\ &\qquad {}_*\phi^{(2)}_0(t\,,\mathbf{x})\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) + \partial_j\left[H^{(j)}_i\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right] \overset{\mathfrak{C}^{(2)}}{\approx} \partial_j\left[H^{(j)}_i\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]\,, \\ &\{{}_*\phi^{(2)}_0(t\,,\mathbf{x})\,,{}_*\phi^{(2)}_0(t\,,\mathbf{y})\}_{P.b.} = \\ &\qquad \left(h^{ij}(t\,,\mathbf{x}){}_*\phi^{(2)}_j(t\,,\mathbf{x}) + h^{ij}(t\,,\mathbf{y}){}_*\phi^{(2)}_j(t\,,\mathbf{y})\right)\partial^{(x)}_i\delta^{(n)}(\mathbf{x}-\mathbf{y}) + \partial_i\left[H^{(i)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right] \overset{\mathfrak{C}^{(2)}}{\approx} \\ &\qquad \partial_i\left[H^{(i)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]\,, \end{aligned} \tag{7.68} $$

where $H^{(j)}_i$ and $H^{(i)}$ are composed of the phase space variables, the secondary constraint densities, and those spatial derivatives up to second-order. Notice that these functionals appear due to the non-linearlity of f; if f is a linear functional then $H^{(j)}_i$ and $H^{(i)}$ vanish. The concrete forms of these functionals are very complicated and may include terms that do not vanish under the imposition of the constraint densities. That is, here, the second issue arises.

However, it does not matter. Since the $f(\mathring{R})$-gravity is a diffeomorphism invariant theory, without any loss of generality, we can choose an ADM-foliation such that the Prescription 1 demands. Therefore, if we use Prescription 1, then the PB-algebras turn into that of the general theory of relativity, and $f(\mathring{R})$-gravity has

$$\text{pDoF} = \frac{1}{2}(n+1)(n-2) + 1 \tag{7.69}$$

and

$$\text{gDoF} = n + 1\,. \tag{7.70}$$

Comparing to the case of the general theory of relativity, one additional pDoF appears and the gauge symmetry does not change.

The calculations of the PB-algebras among the secondary constraint densities are performed under the imposition of Prescription 1 (or other possibilities (i), (iii) explained in Section 7.1), and then it is shown that the PB-algebras are the same as the ones of the general theory of relativity. In other words, in general, the analysis performed in this section is reliable only for the solutions that satisfy the boundary conditions: the shift vector on the spatial boundary vanishes. This is a good example to scrutinize the influence of the spatial boundary terms on the classification of constraint densities, $i.e.$, the second issue. If the spatial boundary terms can be neglected then the pDoF is given by Eq (7.69) and the shift vector has to vanish at least on the spatial boundary. Otherwise, the pDoF may generically be changed additionally from $(n+1)(n-2)/2+1$ since the secondary constraint densities are no longer classified into first-class constraint densities. [5] However, since the

[5] It is known that another sort of extra degrees of freedom is obtained by separating the conformal mode in the general theory of relativity [Chamseddine and Mukhanov (2013)] and by considering the invertible/disformal transformation of gravity [Jiroušek et al. (2023, 2022)]. If the boundary terms cannot be ignored, does the additional DoF become some sort of DoF similar to the above? This interpretation might be a possible story since the Dirac-Bergmann analysis generically counts out the degrees of freedom of a given theory including propagate but unphysical (ghost) modes. However, these statements have to be proven more rigorously, and this problem is unsolved at the moment of writing this thesis.

action functional given in Eq (7.61) indicates that the theory is diffeomorphism invariant, the change of the constraint structure depending on the way of taking an ADM-foliation would be a contradiction. As already mentioned in the final remark in Section 7.1, the result of the analysis on a diffeomorphism invariant theory should be independent of the choice of ADM-foliation. Therefore, it makes sense to neglect the boundary terms, and it should hold even for the well-definedness of all PBs in the analysis of $f(\mathring{R})$-gravity.

7.5. Degrees of freedom of non-linear extension of TEGR

In this section, the Dirac-Bergmann analysis of the non-linear extension of TEGR, denoted by "fTEGR", is performed [Li et al. (2011); Ferraro and Guzmán (2018); Blagojević and Nester (2020)], and the propagating and gauge degrees of freedom are clarified. In the case of fTEGR, it is unveiled that the spatial boundary terms appear in PB-algebras and the analysis generically needs Prescription 1; this is the departure from the case of the general theory of relativity from the viewpoint of constraint mechanics. In addition, differing from the fGR case, it is also unveiled that fTEGR suffers from the second issue and third issue. The second issue may also cause the first issue. This means that the result is viable only for the solutions that satisfy the spatial boundary condition that is demanded by Prescription 1.

We performed the Dirac-Bergmann analysis of GR, TEGR, CGR, $f(\mathring{R})$-gravity in a $(n+1)$-dimensional spacetime. However, since the non-linear extension of TEGR is described by (co-)frame fields, it makes the theory far more complicated than the metric formalism. Therefore, first of all, the analysis is performed in a 4-dimensional spacetime, and then, the case of a generic dimension is estimated.

The Lagrangian density of TEGR is already given as Eq (7.19) in Section 7.2. The Lagrangian density of the theory is given as follows:

$$S_{\text{fTEGR}} = \int_{\mathcal{M}} d^4x \, \mathcal{L}_{\text{fTEGR}} \,, \quad \mathcal{L}_{\text{fTEGR}} = -\frac{1}{2\kappa^2} \det(\mathbf{e}^{-1}) \, f(\mathbb{T}) \tag{7.71}$$

Hereinafter, we use the unit $2\kappa^2 = 1$ and $e = \det(\mathbf{e}^{-1})$. Using an auxiliary field φ, the above Lagrangian density is decomposed as follows [Blagojević and Nester (2020)]:

$$\mathcal{L}_{\text{fTEGR}} = e\left[\varphi \mathbb{T} - V(\varphi)\right] \tag{7.72}$$

under the imposition of the following condition:

$$\frac{\delta \mathcal{L}_{\text{fTEGR}}}{\delta \varphi} := 0\,, \tag{7.73}$$

where $V = V(\varphi)$ is a function such that $V'(\varphi)$ is invertible and $V''(\varphi) \neq 0$. This method of decomposing the Lagrangian density is different from that of $f(\mathring{R})$-gravity, but it has the advantage of simplifying the analysis of a non-linear theory in terms of the vielbein formalism. That is, the explicit form of the torsion tensor

$$T^I{}_{\mu\nu} = e^I{}_\rho T^\rho{}_{\mu\nu} = \partial_\mu e^I{}_\nu + \omega^I{}_{J\mu} e^J{}_\nu - \partial_\nu e^I{}_\mu + \omega^I{}_{J\nu} e^J{}_\mu = \partial_\mu e^I{}_\nu - \partial_\nu e^I{}_\mu\,, \tag{7.74}$$

indicates that $T^I{}_{0\mu}$ can be used equivalently as velocity variables of the co-frame fields, where the Weitzenböch gauge (, or equivalently, the teleparallel condition,) is applied. In this formalism, canonical momentum variables of the decomposed Lagrangian density (7.72) with respect to the velocity $T^I{}_{0\mu}$ are computed as follows: First, we compute

$$\mathcal{H}_{IJK} = \frac{\delta \mathcal{L}_{\text{fTEGR}}}{\delta T^{IJK}} = e\,\varphi\left(\frac{1}{4} T_{IJK} + \frac{1}{2} T_{[KJ]I} - g_{I[J} T_{K]}\right)\,. \tag{7.75}$$

Then the canonical momentum variables are given as follows:

$$\pi_I{}^\mu = \frac{\delta \mathcal{L}_{\text{fTEGR}}}{\delta T^I{}_{0\mu}} = \mathcal{H}_I{}^{0\mu} = e^0{}_J e^\mu{}_K \mathcal{H}_I{}^{JK}\,. \tag{7.76}$$

The canonical momentum variable with respect to the auxiliary field φ is given as follows:

$$\pi_\varphi = \frac{\delta \mathcal{L}_{\mathrm{fTEGR}}}{\delta(\partial_0 \varphi)} = 0\,. \tag{7.77}$$

Therefore, primary constraint densities are derived as follows:

$${}_*\phi_I^{(1)} = \pi_I{}^0 := 0 \quad {}_*\phi_\varphi^{(1)} = \pi_\varphi := 0\,. \tag{7.78}$$

Taking into account the considerations in Section 7.2, it expects that there exist further primary constraint densities corresponding to the generators of local Lorentz transformation.

In order to find the remaining other primary constraint densities, the (1+3)-decomposition of a vector is introduced as follows:

$$V_\perp = n^I V_I \quad V_{\bar{I}} = V_I - n_I V_\perp\,, \tag{7.79}$$

where $\mathbf{V} = V^I \xi_I$ is a vector of the internal space and $\mathbf{n} = n^I \xi_I$ is a normal vector to a leaf Σ_t. ξ_I are a basis of sections of the internal space. Using this decomposition and recalling the process of deriving the canonical momentum variables (7.29) from Eq (7.26), the following quantities

$$\begin{aligned}
&\hat{\pi}_{I\bar{J}} = \pi_I{}^\mu e_{J\mu} = \frac{\varphi}{N} \mathcal{H}_{I\perp\bar{J}}\,, \\
&\mathcal{H}_{I\perp\bar{J}} = T_{I\perp\bar{J}} + (T_{\bar{J}\perp I} - T_{\perp\bar{J}I}) - 2(n_I V_{\bar{J}} - g_{I\bar{J}} V_\perp)
\end{aligned} \tag{7.80}$$

lead to the remaining primary constraint densities as follows:

$${}_*\phi_{IJ}^{(1)} = \mathcal{H}_{IJ} + \varphi B_{IJ} := 0\,, \tag{7.81}$$

where $\mathcal{H}_{IJ}$ and B_{IJ} are defined as follows:

$$\begin{aligned}
&\mathcal{H}_{IJ} = \hat{\pi}_{I\bar{J}} - \hat{\pi}_{\bar{J}I}\,,\\
&B_{IJ} = -\frac{2}{N}(T^{\perp}{}_{\bar{I}\bar{J}} - n_I T^{\bar{K}}{}_{\bar{K}\bar{J}} + n_J T^{\bar{K}}{}_{\bar{K}\bar{I}})\,.
\end{aligned} \tag{7.82}$$

Therefore, fTEGR has the number of $(4+1)+6 = 11$ primary constraint densities. Then the total Hamiltonian is derived as follows:

$$\mathcal{H}_T = N\mathcal{H}_{\perp} + N^i\mathcal{H}_i + \lambda^I{}_*\phi^{(1)}_I + \lambda^{\varphi}{}_*\phi^{(1)}_{\varphi} + \frac{1}{2}\lambda^{IJ}{}_*\phi^{(1)}_{IJ} + \partial_i(\pi_I{}^i e^I{}_0)\,, \tag{7.83}$$

where $\mathcal{H}_{\perp}$ and $\mathcal{H}_i$ are defined as follows:

$$\begin{aligned}
&\mathcal{H}_{\perp} = \hat{\pi}_I{}^{\bar{J}} T^I{}_{\perp\bar{J}} - \frac{1}{N}\mathcal{L}_{fTEGR} - n^I\partial_j\pi_I{}^j\,,\\
&\mathcal{H}_i = \pi_I{}^j T^I{}_{ij} - e^I{}_i\partial_j\pi_I{}^j\,,
\end{aligned} \tag{7.84}$$

and λ^I, λ^{φ}, and λ^{IJ} are Lagrange multipliers. The PB-algebras are computed as follows:

$$\begin{aligned}
&\{{}_*\phi^{(1)}_I(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_J(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi^{(1)}_I(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_{JK}(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi^{(1)}_{IJ}(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_{KL}(t\,,\mathbf{y})\}_{P.b.}\\
&\quad = \left(g_{JL}\,{}_*\phi^{(1)}_{IK} + g_{IK}\,{}_*\phi^{(1)}_{JL} - g_{JK}\,{}_*\phi^{(1)}_{IL} - g_{IL}\,{}_*\phi^{(1)}_{JK}\right)\delta^{(3)}(\mathbf{x}-\mathbf{y}) + \frac{4}{N}\varphi_{\bar{M}}g_{NL}\delta^{\perp\bar{M}N}_{IJK}\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,
\end{aligned} \tag{7.85}$$

where $\varphi_{\bar{I}} = \partial_{\bar{I}}\varphi$. We abbreviated the argument " $(t\,,\mathbf{x})$ " on the right-hand side in the third PB-algebras. Notice that the third PB-algebras implies that some of ${}_*\phi^{(1)}_{IJ} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ are classified into second-class constraint densities; there occurs a departure from the TEGR case. (Compare to the PB-algebras (7.30) in Section 7.2.) The PB-algebras between ${}_*\phi^{(1)}_{\varphi} \overset{\mathfrak{C}^{(1)}}{\approx} 0$

and others are computed as follows:

$$
\begin{aligned}
&\{{}_*\phi^{(1)}_{\varphi}(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_{I}(t\,,\mathbf{y})\}_{P.b.} = 0\,,\\
&\{{}_*\phi^{(1)}_{\varphi}(t\,,\mathbf{x})\,,{}_*\phi^{(1)}_{IJ}(t\,,\mathbf{y})\}_{P.b.} = -B_{IJ}(t\,,\mathbf{x})\delta^{(3)}(\mathbf{x}-\mathbf{y})\,.
\end{aligned}
\tag{7.86}
$$

The second PB-algebras imply that all the constraint densities ${}_*\phi^{(1)}_{IJ} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and ${}_*\phi^{(1)}_{\varphi} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ are classified into second-class constraint densities. Therefore, fTEGR does not have the full local Lorentz symmetry.

Next, let us investigate the consistency conditions for these primary constraints: ${}_*\phi^{(1)}_{I} \overset{\mathfrak{C}^{(1)}}{\approx} 0$, ${}_*\phi^{(1)}_{IJ} \overset{\mathfrak{C}^{(1)}}{\approx} 0$, and ${}_*\phi^{(1)}_{\varphi} \overset{\mathfrak{C}^{(1)}}{\approx} 0$. From the PB-algebras (7.85) and (7.86), it is easy to confirm the first case relative to the second and third ones. The conditions

$$
{}_*\dot{\phi}^{(1)}_{I} = \{{}_*\phi^{(1)}_{I}\,,\mathcal{H}_T\}_{P.b.} \overset{\mathfrak{C}^{(1)}}{\approx} N_I\mathcal{H}_\perp + e_I{}^i\mathcal{H}_i := 0 \tag{7.87}
$$

lead to the following secondary constraints:

$$
{}_*\bar{\phi}^{(2)}_{0} = \mathcal{H}_\perp := 0\,,\quad {}_*\bar{\phi}^{(2)}_{i} = \mathcal{H}_i := 0\,. \tag{7.88}
$$

In order to construct a closed PB-algebra, the above constraints can be modified as follows [Mitrić (2019)]:

$$
{}_*\phi^{(2)}_{0} = {}_*\bar{\phi}^{(2)}_{0} + {}_*\phi^{(1)}_{\varphi}\partial_\perp\varphi \overset{\mathfrak{C}^{(2)}}{\approx} 0\,,\quad {}_*\phi^{(2)}_{i} = {}_*\bar{\phi}^{(2)}_{i} + {}_*\phi^{(1)}_{\varphi}\partial_i\varphi \overset{\mathfrak{C}^{(2)}}{\approx} 0\,. \tag{7.89}
$$

Then these modified PB-algebras form the following PB-algebras:

$$
\begin{aligned}
&\{{}_*\phi_i^{(2)}(t\,,\mathbf{x})\,,{}_*\phi_j^{(2)}(t\,,\mathbf{y})\}_{P.b.} \overset{\mathfrak{C}^{(2)}}{\approx} \\
&\qquad \left({}_*\phi_j^{(2)}(t\,,\mathbf{x})\partial_i^{(x)} - {}_*\phi_i^{(2)}(t\,,\mathbf{y})\partial_j^{(y)}\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}) \overset{\mathfrak{C}^{(2)}}{\approx} 0\,, \\
&\{{}_*\phi_0^{(2)}(t\,,\mathbf{x})\,,{}_*\phi_i^{(2)}(t\,,\mathbf{y})\}_{P.b.} \overset{\mathfrak{C}^{(2)}}{\approx} \\
&\qquad {}_*\phi_0^{(2)}(t\,,\mathbf{x})\partial_i^{(x)}\delta^{(n)}(\mathbf{x}-\mathbf{y}) + \partial_j\left[H_i^{(j)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right] \overset{\mathfrak{C}^{(2)}}{\approx} \partial_j\left[H_i^{(j)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]\,, \\
&\{{}_*\phi_0^{(2)}(t\,,\mathbf{x})\,,{}_*\phi_0^{(2)}(t\,,\mathbf{y})\}_{P.b.} = \\
&\qquad \left(h^{ij}(t\,,\mathbf{x}){}_*\phi_j^{(2)}(t\,,\mathbf{x}) + h^{ij}(t\,,\mathbf{y}){}_*\phi_j^{(2)}(t\,,\mathbf{y})\right)\partial_i^{(x)}\delta^{(n)}(\mathbf{x}-\mathbf{y}) + \partial_i\left[H^{(i)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right] \overset{\mathfrak{C}^{(2)}}{\approx} \\
&\qquad \partial_i\left[H^{(i)}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]\,,
\end{aligned}
\tag{7.90}
$$

where $H_J^{(I)}$ and $H^{(I)}$ are composed of the phase space variables, the secondary constraint densities, and those spatial derivatives up to second-order, which arise due to the non-linearity f, or equivalently, V. Remark that the above algebras hold only in the weak equality on the constraint phase subspace restricted at least by ${}_*\phi_\varphi^{(1)} \overset{\mathfrak{C}^{(1)}}{\approx} 0$, ${}_*\phi_I^{(1)} \overset{\mathfrak{C}^{(1)}}{\approx} 0$, and ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$. Here, notice that we face the second issue. If the total divergent terms in the second and third PB-algebras remain then the secondary constraint densities ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ are classified into second-class constraint densities, and then the third issue occurs. Therefore, in order to restrict our consideration to algebraically solvable cases, let us apply Prescription 1. Then the PB-algebras of the secondary constraint densities ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ becomes commutative ones. In addition, applying the Castellani algorithm [Castellani (1982)] to the primary constraint densities ${}_*\phi_I^{(1)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ and ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$, taking into account the second PB-algebras in Eq (7.85) and the first PB-algebras in Eq (7.85), *at least* these constraint densities form a closed PB-algebra up to linear combinations of these constraint densities. Therefore, under Prescription 1, ${}_*\phi_I^{(1)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ and ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ are classified into first-class constraint densities. The satisfaction of the consistency conditions for these first-class constraint densities are now trivial; the

Dirac-Bergmann procedure on the sector ${}_*\phi_I^{(1)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ and ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ stops here. Remark that the action functional given in Eq (7.72) implies that the theory is diffeomorphism invariant. Therefore, the application of Prescription 1 does not change the generality of the result of the analysis, as already mentioned in Section 7.1.

The consistency condition for the primary constraint densities ${}_*\phi_{IJ}^{(1)} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ and ${}_*\phi_\varphi^{(1)} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ determine some of the Lagrange multipliers λ^I, λ^φ, and λ^{IJ} by virtue of the PB-algebras (7.85) and (7.86). The secondary constraint densities with respect to these constrain densities are computed as follows:

$$\begin{aligned} {}_*\phi_\varphi^{(2)} &= -N\partial_\varphi\tilde{\mathcal{H}}_\perp - \frac{1}{2}\lambda^{MN}B_{MN} := 0\,, \\ {}_*\phi_{IJ}^{(2)} &= G_{IJ}{}^K\partial_K\varphi := 0\,, \end{aligned} \tag{7.91}$$

where $\tilde{\mathcal{H}}_\perp$ denotes $\mathcal{H}_\perp$ evaluated on shell and $G_{IJ}{}^K$ are determined from the following relations:

$$\begin{aligned} &G_{IJ}{}^\perp = NB_{IJ}\,, \\ &G_{IJ}{}^{\bar{K}} = \frac{2}{N}\delta^{\perp\bar{K}\bar{N}}_{IJM}\lambda^M{}_{\bar{N}} - N\varphi^{-1}g^{\bar{K}\bar{M}}\left(n_I\hat{\pi}_{(\bar{M}\bar{J})} - n_J\hat{\pi}_{(\bar{M}\bar{I})}\right) - \delta^{\bar{K}\bar{M}\bar{N}}_{\bar{I}\bar{J}\bar{R}}T^{\bar{R}}{}_{\bar{M}\bar{N}}\,. \end{aligned} \tag{7.92}$$

These secondary constraint densities lead to the following equations:

$$\begin{aligned} \lambda_{\perp\bar{J}}B^{\perp\bar{J}} + \frac{1}{2}\lambda_{\bar{I}\bar{J}}B^{\bar{I}\bar{J}} &\overset{\mathfrak{C}^{(2)}}{\approx} -N\partial_\varphi\hat{\mathcal{H}}_\perp\,, \\ B_{IJ}\bar{\lambda}_\varphi + \frac{2}{N}\varphi_{\bar{K}}\delta^{\perp\bar{K}\bar{N}}_{IJM}\lambda^M{}_N &\overset{\mathfrak{C}^{(2)}}{\approx} X_{IJ}\,, \end{aligned} \tag{7.93}$$

respectively, where $\bar{\lambda}_\varphi$, $\varphi_{\bar{I}}$, and X_{IJ} are defined as follows:

$$\begin{aligned}
&\bar{\lambda}_\varphi = \lambda_\varphi - N^I \partial_I \varphi \,, \\
&\varphi_{\bar{I}} = \partial_{\bar{I}} \varphi \\
&X_{IJ} = \varphi_{\bar{K}} \left[N\varphi^{-1} g^{\bar{K}\bar{M}} \left(n_I \hat{\pi}_{(\bar{M}\bar{J})} - n_J \hat{\pi}_{(\bar{M}\bar{I})} \right) + \delta^{\bar{K}\bar{M}\bar{N}}_{\bar{I}\bar{J}\bar{R}} T^{\bar{R}}{}_{\bar{M}\bar{N}} \right] .
\end{aligned} \tag{7.94}$$

Performing $(1+3)$-decomposition, the following three equation are derived:

$$\begin{aligned}
B^{\perp\bar{N}} \lambda_{\perp\bar{N}} + B^{\bar{N}} \lambda_{\bar{N}} &\overset{\mathfrak{C}^{(2)}}{\approx} -N \partial_\varphi \tilde{\mathcal{H}}_\perp \,, \\
B^{\perp\bar{M}} \bar{\lambda}_\varphi - Z_K \epsilon^{\bar{K}\bar{M}\bar{N}} \lambda_{\bar{N}} &\overset{\mathfrak{C}^{(2)}}{\approx} X^{\perp\bar{M}} \,, \\
B^{\bar{M}} \bar{\lambda}_\varphi - Z_K \epsilon^{\bar{K}\bar{M}\bar{N}} \lambda_{\perp\bar{N}} &\overset{\mathfrak{C}^{(2)}}{\approx} X^{\bar{M}} \,,
\end{aligned} \tag{7.95}$$

where $Z_{\bar{I}}$, $F_{\bar{I}}$, and $\lambda_{\bar{I}}$ are defined as follows:

$$Z_{\bar{I}} = \frac{2}{N} \varphi_{\bar{I}} \quad B_{\bar{I}} = \frac{1}{2} \epsilon_{\bar{I}\bar{M}\bar{N}} B^{\bar{M}\bar{N}} \quad \lambda_{\bar{I}} = \frac{1}{2} \epsilon_{\bar{I}\bar{M}\bar{N}} \lambda^{\bar{M}\bar{N}} \quad X^{\bar{I}} = \varphi_{\bar{K}} \epsilon^{\bar{K}\bar{M}\bar{N}} T^{\bar{I}}{}_{\bar{M}\bar{N}} \,. \tag{7.96}$$

Let us consider the case of $\varphi_{\bar{I}} \neq 0$. Combining the contraction of the second and third equations in Eq (7.95) with $\varphi_{\bar{M}}$, the following equation is derived:

$$\left[\left(\varphi_{\bar{M}} B^{\perp\bar{M}} \right)^2 + \left(\varphi_{\bar{M}} B^{\bar{M}} \right)^2 \right] \bar{\lambda}_\varphi \overset{\mathfrak{C}^{(2)}}{\approx} \left(\varphi_{\bar{M}} B^{\perp\bar{M}} \right) \varphi_{\bar{N}} X^{\perp\bar{N}} + \left(\varphi_{\bar{M}} B^{\bar{M}} \right) \varphi_{\bar{N}} X^{\bar{N}} \,. \tag{7.97}$$

This equation with the first relation in Eq (7.94) determines the multiplier λ_φ when $\left(\varphi_{\bar{M}} F^{\perp\bar{M}} \right)^2 + \left(\varphi_{\bar{M}} B^{\bar{M}} \right)^2 \neq 0$. Then a new secondary constraint density arises as follows:

$${}_*\phi^{(2)} = \left(\varphi_{\bar{M}} B^{\perp\bar{M}} \right) \left(\varphi_{\bar{N}} X^{\bar{N}} \right) - \left(\varphi_{\bar{M}} B^{\bar{M}} \right) \left(\varphi_{\bar{N}} X^{\perp\bar{N}} \right) := 0 \,. \tag{7.98}$$

The emergence of the additional constraint density implies that some of the remaining multipliers λ^I and λ^{IJ} are determined since the PB-algebras between ${}_*\phi^{(2)}$ and ${}_*\phi^{(2)}_{IJ}$ are not commutative under the imposition of all constraint densities [Blagojević and Nester (2020)].

The transformed multipliers $\lambda_{\perp\bar{I}}$ and $\lambda_{\bar{I}}$ can be decomposed into parallel and orthogonal components as follows:

$$\begin{aligned}
&\lambda_{\perp\bar{I}} = \lambda_{\perp}\varphi_{\bar{I}} + \hat{\lambda}_{\perp\bar{I}}\,, \quad \hat{\lambda}_{\perp\bar{I}}\varphi^{\bar{I}} = 0\,, \\
&\lambda_{\bar{I}} = \lambda\varphi_{\bar{I}} + \hat{\lambda}_{\bar{I}}\,, \quad \hat{\lambda}_{\bar{I}}\varphi^{\bar{I}} = 0\,.
\end{aligned} \tag{7.99}$$

Combining these decomposition with Eq (7.94), the following equation are derived:

$$\lambda_{\perp}\left(B^{\perp\bar{I}}\varphi_{\bar{I}}\right) + \lambda\left(B^{\bar{I}}\varphi_{\bar{I}}\right) = -N\partial_{\varphi}\hat{\mathcal{H}}_{\perp} - B^{\perp\bar{I}}\hat{\lambda}_{\perp\bar{I}} - B^{\bar{I}}\hat{\lambda}_{\bar{I}}\,. \tag{7.100}$$

In addition, the consistency condition for the secondary constraint density ${}_*\phi^{(2)} \overset{\mathfrak{C}^{(1)}}{\approx} 0$ leads to the following equation:

$$\begin{aligned}
&\lambda_{\perp}\left(\varphi^{\bar{I}}\{{}_*\phi^{(1)}_{\perp\bar{I}}\,, {}_*\phi^{(2)}\}_{P.b.}\right) + \lambda\left(\frac{1}{2}\epsilon^{\bar{M}\bar{N}\bar{K}}\varphi_{\bar{K}}\{{}_*\phi^{(1)}_{MN}\,, {}_*\phi^{(2)}\}_{P.b.}\right) \\
&\qquad \overset{\mathfrak{C}^{(2)}}{\approx} \text{multiplier independent and known terms}\,.
\end{aligned} \tag{7.101}$$

Therefore, the following equation is derived:

$$\lambda(x)D(x\,, x') = G(x')\,, \tag{7.102}$$

where $D(x\,, x')$ and $G(x')$ are defined as follows:

$$\begin{aligned}
&D(x\,, x') = \left(B^{\perp\bar{I}}\varphi_{\bar{I}}\right)\left(\frac{1}{2}\epsilon^{\bar{J}\bar{K}\bar{L}}\varphi_{\bar{L}}\{{}_*\phi^{(1)}_{\bar{J}\bar{K}}\,, {}_*\phi^{(2)}\}_{P.b.}\right) - \left(B^{\bar{I}}\varphi_{\bar{I}}\right)\left(\varphi^{\bar{J}}\{{}_*\phi^{(1)}_{\perp\bar{J}}\,, {}_*\phi^{(2)}\}_{P.b.}\right)\,, \\
&G(x') = \text{all known terms}\,.
\end{aligned} \tag{7.103}$$

Here, the term $D(x\,, x')$ contains the spatial derivatives of the Dirac delta function: schematically, " $A(x)\partial_i^{(x)}\delta^{(3)}(\mathbf{x}-\mathbf{y})$ ". Integrating Eq (7.102) by parts, the following PDE is derived:

$$A^i\partial_i u + \alpha u = G\,, \tag{7.104}$$

schematically. This is nothing but Eq (7.17); there gives rise to the third issue. However, applying Prescription 1 (we already imposed it to make the constraint densities ${}_*\phi_I^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ first-class constraint densities), the first term in the left-hand side does not appear since all terms such like " $A(x)\partial_i^{(x)}\delta^{(3)}(\mathbf{x}-\mathbf{y})$ " in the PB-brackets are erased by the imposition of the spatial boundary condition $N_i(t\,,\partial\Sigma_t) = 0$. As mentioned in the final remark in Section 7.1, since $f(T)$-gravity is a diffeomorphism invariant theory, the imposition of Prescription 1 holds the generality of the analysis. Therefore, Eq (7.102) becomes just a linear algebraic equation, and it is always solvable as long as $D \neq 0$; the Dirac-Bergmann procedure stops here. The pDoF of $f(T)$-gravity is

$$\text{pDoF} = \frac{1}{2}\left[(16+1) - 8\times 2 - 8\right] = 5\,, \tag{7.105}$$

the gDoF is

$$\text{gDoF} = 4\,. \tag{7.106}$$

The local Lorentz gauge symmetry is broken due to the third PB-algebras in Eq (7.85) and the second PB-algebras in Eq (7.86). In general, for a $(n+1)$-dimensional spacetime, the pDoF and gDoF are given as follows [Blagojević and Nester (2020)]:

$$\text{pDoF} = \frac{1}{2}(n+1)(n-2) + n \tag{7.107}$$

and

$$\text{gDoF} = n+1\,. \tag{7.108}$$

The local Lorentz gauge symmetry is of course broken. Remark that the authors [Li et al. (2011)] also derived the same result but overlooked the third issue. In the work [Blagojević and Nester (2020)], other three possible cases are mentioned; (i) If $\varphi_{\bar{I}} \neq 0$ and $D = 0$ then pDoF is N/A; (ii) If $\varphi_{\bar{I}} \neq 0$ and ${}_*\dot{\phi}^{(2)} \overset{\mathfrak{C}^{(2)}}{\approx} 0$ then pDoF $= 4$; (iii) If $\varphi_{\bar{I}} = 0$ then pDoF $= 2$. Here, we used Prescription 1. (The original work in [Blagojević and Nester (2020)] takes into account the spatial derivatives of the Dirac delta function.) There is a remark: the work in [Blagojević and Nester (2020)] overlooked a generic sector of (iii), which is indicated by the work [Ferraro and Guzmán (2018)]. In this work, the authors find out (iii)' If $\varphi_{\bar{I}} = 0$ then pDoF $= 3$. The difference between (iii) and (iii)' is that Sector (iii) implicitly demands also $\varphi = constant$. That is, $\varphi = \varphi(t)$ in Sector (iii)' implies that one propagates but unphysical DoF exists. In this regard, a detailed consideration is given in [Tomonari and Bahamonde (2023)].

An important lesson from the analysis of $f(T)$-gravity is that the violation of the local Lorentz symmetry provided several sectors and each sector has a different pDoF from the other sectors. As mentioned in the final remark in Section 7.1, for a diffeomorphism invariant theory, without any loss of generality, Prescription 1 can be applicable. Therefore, the above analysis unveiled the full pDoF of each sector. However, for a theory with violating its diffeomorphism invariance, the result of the analysis depends on the choice of an ADM-foliation. That is, the analysis under the use of Prescription 1 does generically not provide the full pDoF of the theory. Nevertheless, this sort of analysis has an advantage for circumventing the three issues. In other words, as long as an analysis suffers from the three issues, any result cannot be beyond a speculation. The use of Prescription 1 would unveil the pDoF only of a special sector, which is not the full pDoF of the most generic sector, but the results are exact, meaning that it is not a speculation since no pathological PDE(s) of Lagrange multiplier(s) emerges, and, therefore, reliable. This situation happens rather in the analysis of the coincident $f(Q)$-gravity.

7.6. Degrees of freedom of non-linear extension of CGR

In this section, the Dirac-Bergmann analysis of the non-linear extension of CGR, denoted by " fCGR ", is performed [Hu et al. (2022); Tomonari and Bahamonde (2023)], and the propagating and gauge degrees of freedom are clarified. In the case of fCGR, it is unveiled that the spatial boundary terms appear in PB-algebras and the analysis generically needs Prescription 1; this is the departure from the case of the general theory of relativity from the viewpoint of constraint mechanics. In addition, differing from the fGR and fTEGR cases, it is also unveiled that fCGR suffers from the first issue and third issue. This means that the result is viable only for the solutions that satisfy the spatial boundary condition that is demanded by Prescription 1.

We performed the Dirac-Bergmann analysis of GR, TEGR, CGR, $f(\mathring{R})$-gravity in a $(n+1)$-dimensional spacetime. As we will see, however, the existence of the second-class constraint densities makes it difficult to understand whether the consistency conditions determine the multipliers or derive new constraint densities since the size of the Dirac matrix becomes bigger. Therefore, in this section, for simplicity, we perform the analysis for $f(Q)$ in a $(3+1)$-dimensional spacetime and then estimate the general case of the dimension of $(n+1)$. A general proof would be completed by applying the mathematical induction.

In the same manner as the case of $f(\mathring{R})$-gravity, the CGR can be extended non-linearly into as follows:

$$S_{\rm fCGR} = \int_{\mathcal{M}} d^4x\sqrt{-g}f(Q)\,, \tag{7.109}$$

where f is an arbitrary function of the nonmetricity scalar. By introducing an auxiliary variable we obtain:

$$S_{\rm fCGR} = \int_{\mathcal{M}} d^4x\sqrt{-g}\left[f'Q + f - \varphi f'\right]\,, \tag{7.110}$$

where f is an arbitrary function of the auxiliary variable φ and $f'' = d^2f/d\varphi^2 \neq 0$. From

Section 7.3, using the ADM-foliation of Q given in Eq (7.49), Eq (7.110) can be decomposed as follows:

$$S_{\mathrm{fCGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^3x \left[N\sqrt{h} f' \left\{ {}^{(3)}Q + K^{ij}K_{ij} - K^2 - \mathring{D}_i \left({}^{(3)}Q^i - {}^{(3)}\bar{Q}^i \right) \right\} + N\sqrt{h}\left(f - \varphi f'\right) \right.$$
$$\left. + f' \left\{ \partial_\mu N^i \partial_i \left(\sqrt{h} n^\mu \right) - \partial_i N^i \partial_\mu \left(\sqrt{h} n^\mu \right) \right\} + \sqrt{h} f' \mathring{D}_i \left\{ N \left({}^{(3)}Q^i - {}^{(3)}\bar{Q}^i \right) \right\} \right] . \tag{7.111}$$

Remark that this foliation takes all boundary terms into account. Integrating by parts and neglecting the spatial boundary terms by imposing appropriate spatial boundary conditions on $\partial\Sigma_t$, we get

$$S_{\mathrm{fCGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^3x \left[N\sqrt{h} \left\{ f' \left({}^{(3)}Q + K^{ij}K_{ij} - K^2 \right) - \mathring{D}_i \left\{ f' \left({}^{(3)}Q^i - {}^{(3)}\bar{Q}^i \right) \right\} \right\} + f - \varphi f' \right\}$$
$$\left. + f' \left\{ \partial_\mu N^i \partial_i \left(\sqrt{h} n^\mu \right) - \partial_i N^i \partial_\mu \left(\sqrt{h} n^\mu \right) \right\} \right] . \tag{7.112}$$

Further, integrating by parts the first term of and the second term of the boundary term with respect to the spatial derivative and the spacetime derivative, respectively, and neglecting each the boundary term on $\partial\Sigma_t$ and $\partial\mathcal{M}$, respectively, we obtain the following formula:

$$S_{\mathrm{fCGR}} = \int_{\mathcal{I}} dt \int_{\Sigma_t} d^3x \left[N\sqrt{h} \left\{ f' \left({}^{(3)}Q + K^{ij}K_{ij} - K^2 \right) - \mathring{D}_i \left\{ f' \left({}^{(3)}Q^i - {}^{(3)}\bar{Q}^i \right) \right\} \right\} + f - \varphi f' \right\}$$
$$\left. + \frac{\sqrt{h}}{N} \left(N^i \partial_j N^j - N^j \partial_j N^i \right) \partial_i f' - \frac{\sqrt{h}}{N} \left(\partial_i f' \right) \dot{N}^i + \frac{\sqrt{h}}{N} f'' \left(\partial_i N^i \right) \dot{\varphi} \right] . \tag{7.113}$$

That is, the non-linearity of f changes the constraint structure of CGR. This action was first derived in [Hu et al. (2022)] by a different method that resembles the GR case. At first glance, the Lagrangian density is not a scalar, and it would indicate that this theory generically has only second-class constraint densities. That is, this theory has no diffeomorphism invariance.

It would be expected from the ignorance of the surface terms like " $\partial\Gamma$ " in Eq (6.93) for the comparison to the Ricci scalar and indicates that the diffeomorphism symmetry is at least partly broken. A related consideration is shown in Ref [Mukhopadhyay and Padmanabhan (2006)].

The canonical momentum variables are computed as follows:

$$\begin{aligned}
\pi_0 =&\frac{\delta S_{\text{fCGR}}(t\,,\mathbf{x})}{\delta \dot{N}(t\,,\mathbf{y})} = 0,\\
\pi_i =&\frac{\delta S_{\text{fCGR}}(t\,,\mathbf{x})}{\delta \dot{N}^i(t\,,\mathbf{y})} = -\frac{\sqrt{h}}{N} f''\partial_i\varphi\delta^{(3)}(\mathbf{x}-\mathbf{y}),\\
\pi_{ij} =&\frac{\delta S_{\text{fCGR}}(t\,,\mathbf{x})}{\delta \dot{h}^{ij}(t\,,\mathbf{y})} = \sqrt{h}f'\left(K_{ij}-Kh_{ij}\right)\delta^{(3)}(\mathbf{x}-\mathbf{y}),\\
\pi_\varphi =&\frac{\delta S_{\text{fCGR}}(t\,,\mathbf{x})}{\delta \dot{\varphi}(t\,,\mathbf{y})} = \frac{\sqrt{h}}{N} f''\partial_i N^i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,
\end{aligned} \tag{7.114}$$

The canonical momentum variables with respect to the shift vectors depart from the ordinary CGR case; it depends on the lapse function, the 3-metric h_{IJ}, and the non-linearity part by f''. The canonical momentum with respect to the auxiliary variable φ generates a constraint density, which is different from the case of $f(\mathring{R})$-gravity. That is, in coincident $f(Q)$-gravity, the auxiliary variable φ does not have any physical feature unlike $f(\mathring{R})$-gravity.

The Hessian matrix of the system has the size of 11×11 - components only being non-vanishing components with respect to the canonical momenta π_{ij}. All other components of the matrix vanish. Therefore, the rank of the Hessian matrix is six, and it implies that the system has five primary constraint densities given as follows:

$$\begin{aligned}
{}_*\phi^{(1)}_0 =&\pi_0 := 0\,,\\
{}_*\phi^{(1)}_i =&\pi_i + \frac{\sqrt{h}}{N} f''\partial_i\varphi := 0\,,\\
{}_*\phi^{(1)}_\varphi =&\pi_\varphi - \frac{\sqrt{h}}{N} f''\partial_i N^i := 0\,.
\end{aligned} \tag{7.115}$$

This feature also implies that the *physical* DoF of the system is up to six. These constraint densities restrict the entire phase space to the subspace $\mathfrak{C}^{(1)}$. The PB-algebras among these primary constraint densities are computed as follows:

$$
\begin{aligned}
\{{}_*\phi_0^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_i^{(1)}(t\,,\mathbf{y})\}_{P.b.} =& \frac{1}{N^2}\sqrt{h}f''\partial_i\varphi\delta^{(3)}(\mathbf{x}-\mathbf{y}) = A_i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,, \\
\{{}_*\phi_0^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_\varphi^{(1)}(t\,,\mathbf{y})\}_{P.b.} =& -\frac{1}{N^2}\sqrt{h}f''\partial_i N^i\delta^{(3)}(\mathbf{x}-\mathbf{y}) = B\delta^{(3)}(\mathbf{x}-\mathbf{y})\,, \\
\{{}_*\phi_i^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_\varphi^{(1)}(t\,,\mathbf{y})\}_{P.b.} =& \frac{1}{N}\sqrt{h}f'''\partial_i\varphi\delta^{(3)}(\mathbf{x}-\mathbf{y}) = C_i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,
\end{aligned}
\tag{7.116}
$$

where we used Prescription 1 proposed in Section 7.1. Explicitly, the problematic term occurs in the third PB given in Eq (7.116) as follows:

$$
\begin{aligned}
&\{{}_*\phi_i^{(1)}(t\,,\mathbf{x})\,,{}_*\phi_\varphi^{(1)}(t\,,\mathbf{y})\}_{P.b.} \\
&= C_i\delta^{(3)}(\mathbf{x}-\mathbf{y}) + \left[\left(\frac{\sqrt{h}}{N}f''\right)\Bigg|_x \partial_i^{(x)} + \left(\frac{\sqrt{h}}{N}f''\right)\Bigg|_y \partial_i^{(y)}\right]\delta^{(n)}(\mathbf{x}-\mathbf{y})\,.
\end{aligned}
\tag{7.117}
$$

Taking into account that $\phi_I^{(1)}(x)$ and $\phi_\varphi^{(1)}(y)$ are density variables, in order to reveal the meaning of the above equations in mathematically correct manner, we have to integrate it out with respect to d^nx and d^ny on a leaf Σ_t. Then the first term in Eq (7.117) turns into the smeared one, and then the second terms become generically as follows:

$$
\begin{aligned}
&\int_{\Sigma_t}\int_{\Sigma_t}\left[\left(\frac{\sqrt{h}}{N}f''\right)\Bigg|_x \partial_i^{(x)}\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]dx^ndy^n \\
&= \int_{\Sigma_t}\int_{\Sigma_t}\left[\partial_i^{(x)}\left(\frac{\sqrt{h}}{N}f''\delta^{(n)}(\mathbf{x}-\mathbf{y})\right) - \partial_i^{(x)}\left(\frac{\sqrt{h}}{N}f''\right)\delta^{(3)}(\mathbf{x}-\mathbf{y})\right]dx^ndy^n \\
&= -\,N_i\sqrt{h}f''\left(1-\mathfrak{D}(\mathbf{x}\rightleftarrows\mathbf{y})\right)\Big|_{\partial\Sigma_t}\,,
\end{aligned}
\tag{7.118}
$$

where we assumed $n_\mu = (-N\,,NN_i)$ with $N^iN_i = 0$ and $\mathfrak{D}(\mathbf{x}\rightleftarrows\mathbf{y})$ denotes the Lebesgue integration of the second term. If the naive replacement of " y " in the spatial derivative by " x " is possible then $\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$, and Eq (7.118) vanishes. Therefore, in this case, if we fix the shift vectors $N_i = 0$ as the spatial boundary condition, that is, applying Prescription 1, the problematic term is removed from the analysis, and it is always consistent with the coincident gauge since the gauge restricts only to the Stükelberg fields via the affine transformation of a given coordinate system. This is reasonable since the shift vectors are just unphysical variables. In fact, the action functional (7.113) contains only the first-order time derivative of N_i, and it indicates that N_i cannot be any physical variable; it affects only the constraint structure of the system. It would also be possible to impose $f'' = 0$ on $\partial\Sigma_t$. (If $\varphi^2 \in f''$ then we modify the term φ^2 as $\alpha\varphi^2$ with $\alpha \to 0$ on $\partial\Sigma_t$). Hereinafter, we use this prescription also for PBs, which is formulated in detail in Section 7.1. Therefore, these five primary constraint densities are classified into second-class constraint densities, and, as we will see, the Dirac matrix has its rank two. Note, here, that the theory is free from the second issue at least for the primary constraint densities. Otherwise, only one additional secondary second-class constraint density appears and the Dirac procedure stops, and then the pDoF of the theory turns out to be eight [Hu et al. (2022)], although the normal vector should be taken as Eq (4.41) with Eq (4.42) and $N_i \neq 0$ at least on the spatial boundary. Since the coincident $f(Q)$-gravity does not have diffeomorphism invariance, this difference of the shift vectors indicates that we perform the analysis for another sector from the sector analyzed by the authors in [Hu et al. (2022)]. This discrepancy of pDoF is caused by the difference in the rank of the Dirac matrix density, and this problematic situation has something to do with the first issue. In addition, strictly speaking, in the work [Hu et al. (2022)], the third issue explained in Section 7.1 is overlooked in the calculation of the consistency conditions for the primary constraint densities, therefore, a more exact analysis is mandatory.

The Legendre transformation of the coincident $f(Q)$-gravity is calculated as follows:

$$\mathcal{H}_0 = N\mathcal{C}_0^{(\mathrm{fCGR})} + N^i\mathcal{C}_i^{(\mathrm{fCGR})}\,, \tag{7.119}$$

where $\mathcal{C}_0^{(\mathrm{fCGR})}$ and $\mathcal{C}_i^{(\mathrm{fCGR})}$ are defined as follows:

$$
\begin{aligned}
\mathcal{C}_0^{(\mathrm{fCGR})} =& -\sqrt{h}\left[f'^{(3)}Q - \mathring{D}_i\left\{f'\left({}^{(3)}Q^i - {}^{(3)}\bar{Q}^i\right)\right\} + f - \varphi f' - \frac{1}{hf'}\left(\pi^{ij}\pi_{ij} - \frac{1}{2}\pi^2\right)\right], \\
\mathcal{C}_i^{(\mathrm{fCGR})} =& -2\mathring{D}^j\pi_{ij} - \frac{\sqrt{h}}{N}f''\left(\partial_j N^j\partial_i\varphi - \partial_i N^j\partial_j\varphi\right).
\end{aligned}
\tag{7.120}
$$

Therefore, the total Hamiltonian density of the system is introduced as follows:

$$
\mathcal{H}_T = \mathcal{H}_0 + \lambda_{0*}\phi_0^{(1)} + \lambda^i{}_*\phi_i^{(1)} + \lambda_{\varphi*}\phi_\varphi^{(1)}. \tag{7.121}
$$

The PB-algebras among the primary constraint densities and the density $\mathcal{H}_0$ are given in Appendix A.

The consistency conditions for the primary constraint densities ${}_*\phi_\alpha^{(1)}$ are given as follows:

$$
{}_*\dot{\phi}_\alpha^{(1)} = \{{}_*\phi_\alpha^{(1)}, \mathcal{H}_T\}_{P.b.} \approx \{{}_*\phi_\alpha^{(1)}, \mathcal{H}_0\}_{P.b.} + \lambda^\beta\{{}_*\phi_\alpha^{(1)}, {}_*\phi_\beta^{(1)}\}_{P.b.} := 0, \tag{7.122}
$$

where α, β run in the range of $\alpha, \beta \in \{0, 1, 2, 3, \varphi\}$. Since all these primary constraint densities are classified into second-class constraint densities, it is necessary to investigate the rank of the Dirac matrix $D_{\alpha\beta}^{(1)}\delta^{(3)}(\mathbf{x} - \mathbf{y}) := \{{}_*\phi_\alpha^{(1)}, {}_*\phi_\beta^{(1)}\}_{P.b.}$:

$$
D^{(1)} = \begin{bmatrix}
0 & A_1 & A_2 & A_3 & B \\
-A_1 & 0 & 0 & 0 & C_1 \\
-A_2 & 0 & 0 & 0 & C_2 \\
-A_3 & 0 & 0 & 0 & C_3 \\
-B & -C_1 & -C_2 & -C_3 & 0
\end{bmatrix}, \tag{7.123}
$$

where A_i, C_i, and B are defined by Eq (7.116). Applying the fundamental matrix transformations to Eq (7.123), we get the following matrix:

$$D'^{(1)} = P^{(1)} D^{(1)} Q^{(1)} = \begin{bmatrix} 0 & 0 & 0 & 0 & B \\ 0 & 0 & A_{12} & A_{13} & 0 \\ 0 & -A_{12} & 0 & A_{23} & 0 \\ 0 & -A_{13} & -A_{23} & 0 & 0 \\ -B & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{7.124}$$

where we set $A_{ij} := 2A_{[i}C_{j]}$. $P^{(1)}$ and $Q^{(1)}$ are set as follows:

$$P^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{C_1}{B} & 1 & 0 & 0 & -\frac{A_1}{B} \\ -\frac{C_2}{B} & 0 & 1 & 0 & -\frac{A_2}{B} \\ -\frac{C_3}{B} & 0 & 0 & 1 & -\frac{A_3}{B} \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad Q^{(1)} = \begin{bmatrix} 1 & -\frac{C_1}{B} & -\frac{C_2}{B} & -\frac{C_3}{B} & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -\frac{A_1}{B} & -\frac{A_2}{B} & -\frac{A_3}{B} & 1 \end{bmatrix}. \tag{7.125}$$

The straightforward computations lead to $A_{ij} = 0$. Therefore, The Dirac matrix $D^{(1)}$ has a rank of two. It indicates that two multipliers are determined, and then three secondary constrain densities appear. Using these fundamental matrices $P^{(1)}$ and $Q^{(1)}$, and the Dirac matrix $D^{(1)}$, the consistency conditions Eq (7.122) becomes as follows:

$$P^{(1)}{}_{\alpha}{}^{\beta}\{{}_{*}\phi^{(1)}_{\beta}, \mathcal{H}_0\}_{P.b.} + D'^{(1)}_{\alpha\beta}\lambda^{(1)^{\beta}}\delta^{(3)}(\mathbf{x}-\mathbf{y}) := 0\,, \tag{7.126}$$

where we set

$$\lambda^{(1)^{\alpha}} = Q^{(1)^{-1}}{}^{\alpha}{}_{\beta}\lambda^{\beta}\,. \tag{7.127}$$

For $\alpha = \varphi$ and $\alpha = 0$, the corresponding multipliers $\lambda_\varphi^{(1)}$ and $\lambda_0^{(1)}$ are determined as follows:

$$\lambda_\varphi^{(1)} = -\frac{1}{B}\{{}_*\phi_0^{(1)}\,, \mathcal{H}_0\}_{P.b.}\,, \quad \lambda_0^{(1)} = \frac{1}{B}\{{}_*\phi_\varphi^{(1)}\,, \mathcal{H}_0\}_{P.b.}\,. \tag{7.128}$$

The explicit formulae of these multipliers are derived by using the formulae given in Appendix A. The multipliers $\lambda^{(1)^i}$ remain arbitrary. Converting $\lambda^{(1)^\alpha}$ into the original multipliers λ^α, we get

$$\begin{aligned}\lambda_0 =& \frac{1}{B}\{\phi_\varphi^{(1)}, \mathcal{H}_0\}_{P.b.} - \frac{C_i}{B}\lambda^{(1)^i}\,,\\ \lambda_\varphi =& -\frac{1}{B}\{\phi_0^{(1)}, \mathcal{H}_0\}_{P.b.} - \frac{A_i}{B}\lambda^{(1)^i}\,,\\ \lambda^i =& \lambda^{(1)^i}\,.\end{aligned} \tag{7.129}$$

The secondary constraint densities are derived in the correspondence to the undetermined multipliers $\lambda^i = \lambda^{(1)^i}$ ($i \in \{1, 2, 3\}$):

$${}_*\phi_i^{(2)} = P^{(1)}{}_i{}^\alpha\{{}_*\phi_\alpha^{(1)}\,, \mathcal{H}_0\}_{P.b.} = -\frac{C_i}{B}\{{}_*\phi_0^{(1)}\,, \mathcal{H}_0\}_{P.b.} + \{{}_*\phi_i^{(1)}\,, \mathcal{H}_0\}_{P.b.} - \frac{A_i}{B}\{{}_*\phi_\varphi^{(1)}\,, \mathcal{H}_0\}_{P.b.} := 0\,. \tag{7.130}$$

The explicit formulae of these secondary constraint densities can be derived by using the formulae given in Appendix A and it reveals that all the secondary constraint densities are classified into second-class constraint densities. These constraint densities restrict $\mathfrak{C}^{(1)}$ to the new subspace $\mathfrak{C}^{(2)}$.

Using Eq (7.129), the multipliers λ_0 and λ_φ in the total Hamiltonian density Eq (7.121) are replaced by λ^i:

$$\mathcal{H}_T = \mathcal{H}_0^{(2)} + \lambda^i{}_*\Phi_i^{(2)}\,, \tag{7.131}$$

where $\mathcal{H}_0^{(2)}$ and ${}_*\Phi_i^{(2)}$ are set as follows:

$$\begin{aligned}\mathcal{H}_0^{(2)} =&\mathcal{H}_0 - \frac{1}{B}\{{}_*\phi_0^{(1)}\,, \mathcal{H}_0\}_{P.b.}{}_*\phi_\varphi^{(1)} + \frac{1}{B}\{{}_*\phi_\varphi^{(1)}\,, \mathcal{H}_0\}_{P.b.}{}_*\phi_0^{(1)}\,,\\ {}_*\Phi_i^{(2)} =&{}_*\phi_i^{(1)} - \frac{A_i}{B}{}_*\phi_\varphi^{(1)} - \frac{C_i}{B}{}_*\phi_0^{(1)} \approx 0\,.\end{aligned} \tag{7.132}$$

In the next section, we calculate the tertiary constraint densities.

The consistency conditions for the secondary constraint densities ${}_*\phi_i^{(2)}$ are given as follows:

$${}_*\dot{\phi}_i^{(2)} = \{{}_*\phi_i^{(2)}\,, \mathcal{H}_0^{(2)}\}_{P.b.} + \lambda^j\{{}_*\phi_i^{(2)}\,, {}_*\Phi_j^{(2)}\}_{P.b.} := 0\,. \tag{7.133}$$

The existence of tertiary constraint densities depends on the rank of the matrix $D_{ij}^{(2)}\delta^{(3)}(\mathbf{x}-\mathbf{y}) = \{{}_*\phi_i^{(2)}\,, {}_*\Phi_j^{(2)}\}_{P.b.}$. Using the formulae in Appendix A, we get the following result:

$$D_{ij}^{(2)} = \partial_i\varphi(\alpha\partial_j\varphi + \Delta_j)\,, \tag{7.134}$$

where $\Delta_i := \beta_i{}^j\partial_j\varphi$ and the explicit formulae of α and $\beta_i{}^j$ are given in Appendix B. In matrix form, $D^{(2)}$ is expressed as follows:

$$D^{(2)} = \begin{bmatrix}\varphi_1(\alpha\varphi_1+\Delta_1) & \varphi_1(\alpha\varphi_2+\Delta_2) & \varphi_1(\alpha\varphi_3+\Delta_3)\\ \varphi_2(\alpha\varphi_1+\Delta_1) & \varphi_2(\alpha\varphi_2+\Delta_2) & \varphi_2(\alpha\varphi_3+\Delta_3)\\ \varphi_3(\alpha\varphi_1+\Delta_1) & \varphi_3(\alpha\varphi_2+\Delta_2) & \varphi_3(\alpha\varphi_3+\Delta_3)\end{bmatrix}\,, \tag{7.135}$$

where $\varphi_i := \partial_i\varphi$. Applying the fundamental matrix transformations to Eq (7.135), we get

$$D'^{(2)} = P^{(2)}D^{(2)}Q^{(2)} = \begin{bmatrix}\varphi_1(\alpha\varphi_1+\Delta_1) & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\,, \tag{7.136}$$

where $P^{(2)}$ and $Q^{(2)}$ are set as follows:

$$P^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ -\varphi_2 & \varphi_1 & 0 \\ -\varphi_3 & 0 & \varphi_1 \end{bmatrix} , \quad Q^{(2)} = \begin{bmatrix} 1 & -\frac{\alpha\varphi_2+\Delta_2}{\alpha\varphi_1+\Delta_1} & -\frac{\alpha\varphi_3+\Delta_3}{\alpha\varphi_1+\Delta_1} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} . \tag{7.137}$$

Therefore, the matrix $D^{(2)}$ has its rank of one. This indicates that one multiplier is determined and then two tertiary constraint densities appear. The consistency conditions in Eq (7.133) can be rewritten as follows:

$$P^{(2)}{}_i{}^j \{{}_*\phi_j^{(2)}, \mathcal{H}_0^{(2)}\}_{P.b.} + D'^{(2)}_{ij} \lambda^{(2)^j} \delta^{(3)}(\mathbf{x}-\mathbf{y}) := 0 \, , \tag{7.138}$$

where $\lambda^{(2)^i}$ is set as follows:

$$\lambda^{(2)^i} = Q^{(2)^{-1}}{}^i{}_j \lambda^j \, . \tag{7.139}$$

Therefore, the multiplier to the x-component, $\lambda^{(2)^1}$, is determined as follows:

$$\lambda^{(2)^1} = -\frac{1}{\varphi_1(\alpha\varphi_1+\Delta_1)} P^{(2)^{1i}} \{{}_*\phi_i^{(2)}, \mathcal{H}_0^{(2)}\}_{P.b.} = -\frac{1}{\varphi_1(\alpha\varphi_1+\Delta_1)} \{{}_*\phi_1^{(2)}, \mathcal{H}_0^{(2)}\}_{P.b.} \, , \tag{7.140}$$

where we used $P^{(2)}$ in Eq (7.137). The explicit formula of Eq (7.140) can be derived by using Eq (7.130), the first formula in Eq (7.132), and the formulae given in Appendix A. The multipliers $\lambda^{(2)^{i'}}$ ($i' \in \{2,3\}$) remain arbitrary. Converting $\lambda^{(2)^i}$ into the original multipliers λ^i, we get

$$\begin{aligned} \lambda^1 =& -\frac{1}{\varphi_1(\alpha\varphi_1+\Delta_1)} \{{}_*\phi_1^{(2)}, \mathcal{H}_0^{(2)}\}_{P.b.} - \frac{\alpha\varphi_2+\Delta_2}{\alpha\varphi_1+\Delta_1} \lambda^{(2)^2} - \frac{\alpha\varphi_3+\Delta_3}{\alpha\varphi_1+\Delta_1} \lambda^{(2)^3} \, , \\ \lambda^{i'} =& \lambda^{(2)^{i'}} \, . \end{aligned} \tag{7.141}$$

The tertiary constraint densities are derived in the correspondence to the undetermined multipliers $\lambda^{i'} = \lambda^{(2)i'}$:

$$
{}_*\phi^{(3)}_{i'} := P^{(2)}{}_{i'}{}^{j}\{{}_*\phi^{(2)}_{j}\,, \mathcal{H}^{(2)}_0\}_{P.b.} := 0\,, \tag{7.142}
$$

that is,

$$
\begin{aligned}
{}_*\phi^{(3)}_2 &:= -\,\varphi_2\{{}_*\phi^{(2)}_1\,, \mathcal{H}^{(2)}_0\}_{P.b.} + \varphi_1\{{}_*\phi^{(2)}_2\,, \mathcal{H}^{(2)}_0\}_{P.b.} := 0\,,\\
{}_*\phi^{(3)}_3 &:= -\,\varphi_3\{{}_*\phi^{(2)}_1\,, \mathcal{H}^{(2)}\}_{P.b.} + \varphi_1\{{}_*\phi^{(2)}_3\,, \mathcal{H}^{(2)}_0\}_{P.b.} := 0\,.
\end{aligned} \tag{7.143}
$$

The explicit formulae can be derived by using Eq (7.130), the first formula in Eq (7.132), and the formulae given in Appendix A and it reveals that all the tertiary constraint densities are classified into second-class constraint densities. These constraint densities restrict $\mathfrak{C}^{(2)}$ to the new subspace $\mathfrak{C}^{(3)}$.

Using Eq (7.142), the total Hamiltonian density Eq (7.131) is rewritten as follows:

$$
\mathcal{H}_T = \mathcal{H}^{(3)}_0 + \lambda^{i'}{}_*\Phi^{(3)}_{i'}\,, \tag{7.144}
$$

where $\mathcal{H}^{(3)}_0$ and ${}_*\Phi^{(3)}_{i'}$ are set as follows:

$$
\begin{aligned}
\mathcal{H}^{(3)}_0 =&\mathcal{H}^{(2)}_0 - \frac{1}{\varphi_1(\alpha\varphi_1+\Delta_1)}\{{}_*\phi^{(2)}_1\,, \mathcal{H}^{(2)}_0\}_{P.b.*}\Phi^{(2)}_1,\\
{}_*\Phi^{(3)}_{i'} =&{}_*\Phi^{(2)}_{i'} - \frac{\alpha\varphi_{i'}+\Delta_{i'}}{\alpha\varphi_1+\Delta_1}{}_*\Phi^{(2)}_1\,.
\end{aligned} \tag{7.145}
$$

The consistency conditions for the tertiary constraint densities ${}_*\phi^{(3)}_{i'}$ are given as follows:

$$
{}_*\dot{\phi}^{(3)}_{i'} = \{{}_*\phi^{(3)}_{i'}\,, \mathcal{H}^{(3)}_0\}_{P.b.} + \lambda^{j'}\{{}_*\phi^{(3)}_{i'}\,, {}_*\Phi^{(3)}_{j'}\}_{P.b.} := 0\,. \tag{7.146}
$$

The existence of quaternary constraints depends on the rank of the matrix $D^{(3)}_{i'j'}\delta^{(3)}(\mathbf{x}-\mathbf{y}) := \{{}_*\phi^{(3)}_{i'}\,, {}_*\Phi^{(3)}_{j'}\}_{P.b.}$. It is easy to confirm that the rank of $D^{(3)}$ is two (full-rank; its determinant does not vanish) since the spatial boundary terms no longer vanish without accidental cases due to that the primed indices run the range only of $2, 3$, although it is very tedious to lead to the explicit formula of $D^{(3)}$ and its determinant. Therefore, the remaining multipliers are determined and then the procedure stops here excepting accidental cases. Since there are five primary, three secondary, and two tertiary constraint densities and all the constraint densities are classified into second-class constraint densities, therefore, the pDoF and the gDoF of coincident $f(Q)$-gravity are

$$\text{pDoF} = \frac{1}{2} \times (22 - 5 - 3 - 2) = 6\,, \quad \text{and} \quad \text{gDoF} = 0\,. \tag{7.147}$$

For simplicity, so far, we considered that the spacetime manifold has $(3+1)$ dimensions, however, it would be possible to extend this result for any spacetime dimension. This analysis would also give an implication of pDoF and gDoF. Let $\mathcal{M}$ be a $(n+1)$-dimensional spacetime manifold. To do this, we have to consider the two cases depending on whether n is odd or even. If n is an odd number then we might get $n+2$ primary, n secondary, and $n-1$ tertiary constraint densities and all these constraint densities would be classified into second-class constraint densities. Therefore, when n is an odd number, we have

$$\text{pDoF} = \frac{1}{2}(n^2 + 3)\,, \quad \text{and} \quad \text{gDoF} = 0\,, \tag{7.148}$$

respectively. If n is an even number then we might get $n + 2$ primary, n secondary, $n - 1$ tertiary, and 1 quaternary constraint densities, and all these constraint densities would be classified into second-class constraint densities. Therefore, when n is an even number, we have

$$\text{pDoF} = \frac{1}{2}n^2 + 1\,, \quad \text{and} \quad \text{gDoF} = 0\,. \tag{7.149}$$

These pDoFs are just an estimation based on the result of the analysis in the case of a $(3 + 1)$-dimensional spacetime. However, it would be possible to strictly prove these results by applying mathematical induction.

There is a remark: If the Lebesgue measure in Eq (7.118) is unity, *i.e.*, $\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$, then the terms like " $A(x)\partial_i^{(x)}\delta^{(3)}(\mathbf{x}-\mathbf{y})$ " in Eq (7.117) automatically vanish. In this case, another scenario is possible: the case of the absence of Prescription 1. Then the PB-algebras in the second term in Eq (7.133) contain the spatial boundary terms, and then the matrix given in Eq (7.134) could be non-singular (full-rank). This means that the tertiary constraints do not appear and the procedure stops here with the pathological PDEs of the Lagrange multipliers (third issue): this is a resemble situation to the fTEGR case. The same issue would arise also in Eqs (7.122) and (7.123). Therefore, *if all of these PDEs are solvable,* the pDoF becomes seven [Tomonari and Bahamonde (2023)]. Notice that this is another sector from the sector we have considered in the previous paragraphs so far and this perspective would be consistent with the recent works of the cosmological perturbation [Gomes et al. (2023a); Heisenberg et al. (2023)] in the non-trivial branch I [Gomes et al. (2023b)]. Where the non-trivial branch I is one of five branches, which are the classification of the Stükelberg fields according to the possible Möbius representation in the teleparallel theories of gravity. A detailed description is given in [Gomes et al. (2023b)].

7.7. Summary

In this chapter, the Dirac-Bergmann analysis performed for each subclass of the geometrical trinity of gravity, *i.e.*, GR, TEGR, and CGR, and for each non-linear extension. Before performing the analysis, the three issues in consistency conditions were revealed. These issues were commonly caused by the existence of the total divergent terms like " $\partial_i\left[H^{(i)}_{\alpha_1\beta_1}\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\right]$ ". Then Prescription 1 was introduced, and it demanded appropriate spatial boundary conditions if it is necessary. Since all computations of consistency conditions have to be based on the well-defined PB-algebras, Prescription 1 should be imposed at every step of evaluating PB-algebras when emerging new constraints. As the points to be careful, for a theory with the characteristics of diffeomorphism invariance, without any loss of generality, Prescription 1 can be applicable. If this is not the case, however, the application of Prescription 1 provides the result of a special sector of the full theory. Nevertheless, this prescription circumvents the three issues, therefore, the result is exact and reliable; it is not a speculation.

For the analyses of GR and TEGR, on one hand, the analysis leads to two pDoF for each theory without Prescription 1. For that of CGR, there is a question as mentioned in footnote 4. The investigation of this question is a future work. On the other hand, for the analyses of non-linear extensions of these theories, we assumed the imposition of Prescription 1. This prescription generically demanded the spatial boundary condition of vanishing the shift vector on the spatial boundary: $N_i(t\,,\partial\Sigma_t) := 0$. Otherwise, for fGR and fTEGR, some additional degrees of freedom appeared due to the breaking of the closed PB-algebras of first-class constraints (second issue), and then, caused by it, the Dirac matrix arises. It might cause a reduction of its rank (first issue). fCGR had the same issue as the latter case. fTEGR and fCGR suffered from the pathological PDEs of the multipliers (third issue; See Eq (7.17) in Section 7.1). fGR might also had such concern. The status of each subclass to these issues is summarized as 7.1 as follows:

Table 7.1: Presence of issues in each non-linear extension of the geometrical trinity of gravity. " ◯ " denotes the theory is free from the issue, " $\times$ " denotes the theory suffers from the issue, and Prescription 1 would be necessary. " △ " denotes the necessity of further investigating.

Subclass	GR	TEGR	CGR	fGR	fTEGR	fCGR
1st issue	◯	◯	△	△	△	$\times$
2nd issue	◯	◯	△	$\times$	$\times$	◯
3rd issue	◯	◯	△	△	$\times$	$\times$

Prescription 1 removed these issues from the non-linear extended theories. For diffeomorphism theories, *i.e.*, $f(\mathring{R})$- and $f(T)$-gravity, the generality of the results were remained.

However, the coincident $f(Q)$-gravity, the result was restricted to a special sector. An analysis of the most generic sector is already performed in [Hu et al. (2022)], but the analysis suffered from the first and third issues. In this regard, the most detailed investigation is mandatory.

In particular, in the case of the non-linear extension of CGR, there are three possible cases. The first criterion is the satisfaction of $\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$. Since this is a mathematical fact, it should be proved whether or not this statement holds, and the fact is common for all subclasses once the truth is unveiled. The second criterion is the ignorance of the total divergent term $\partial_i \left[H^{(i)}_{\alpha_1\beta_1}\, \delta^{(n)}(\mathbf{x}-\mathbf{y}) \right]$ under the imposition of some spatial boundary condition. In this thesis, we have imposed $N_i(t\,,\mathbf{x}) = 0$ on the spatial boundaries commonly to all subclasses or taken a specific foliation characterized by the normal vector given in Eq (4.41). The current status is given in the following table 7.2:

Table 7.2: Three possibilities of pDoF in coincident $f(Q)$-gravity. " $\bigcirc$ " and " $\times$ " denote the satisfaction and non-satisfaction of the condition, respectively. "BS" and "SB" denote the bulk space and spatial boundaries, respectively.

Condition	$\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$	$N_i(t\,,\mathbf{x}) = 0$ (Ignorance of $\partial_i \left[H^{(i)}_{\alpha_1\beta_1}\, \delta^{(n)}(\mathbf{x}-\mathbf{y}) \right]$)	pDoF
Case 1	$\times$	$\times$ (Both on BS and SB)	8
Case 2	$\bigcirc$	$\times$ (Only on SB)	7
Case 3	Either $\bigcirc$ or $\times$	$\bigcirc$ (Only on SB)	6

The most reasonable approach to settle this controversy is to clarify whether or not $\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$ holds. If $\mathfrak{D}(\mathbf{x} \rightleftarrows \mathbf{y}) = 1$ then Case 2 or 3 are possible cases since the problematic term in the PB-algebras among the primary constraints vanish without applying Prescription 1 [Tomonari and Bahamonde (2023)]. In this case, there appear at least the number of three secondary constraint densities. In these cases, the most generic case is Case 2 with no restriction to the shift vector although this case suffers form the first issue and third issue; the latter is the same situation as that $f(T)$-gravity faced in Eq (7.104). Applying

Prescription 1 to Case 2, two tertiary constraints arise, and Case 3 is resulted; this situation is different from the $f(T)$-gravity case. Otherwise, only Case 1 is possible case [Hu et al. (2022)] although it suffers from the first issue and third issue. Case 1 and/or Case 2 is compatible with the recent works of the cosmological perturbation [Gomes et al. (2023b); Heisenberg et al. (2023)] in the non-trivial branch I [Gomes et al. (2023a)]. Case 3 is still alive for the trivial branch and non-trivial branch II, in which two tensor modes and up to two scalar modes exist as propagating modes. A detailed description of these branches is given in [Gomes et al. (2023b)].

It would be also viable either to alternate the method to count out the pDoF or to generalize CGR itself into a theory without the coincident gauge: restoring STEGR. Concerning the former case, the authors in [Errasti Díez et al. (2020, 2024)] proposed a new method of degrees of freedom counting for first-order field theories. In this methodology, all procedures proceed in Lagrange formulation; we do not make use of the problematic PB-algebras. Fortunately, the method is applicable to CGR and fCGR since these subclasses are composed of up to first-order derivatives. Concerning the latter case, when the diffeomorphism invariance is restored, the analysis would be performed being analogous to the case of $f(T)$-gravity in terms of vielbein formalism. Otherwise, an alternative formulation proposed in [Hu et al. (2023)] is also viable. These considerations are important for future work.

Finally, we summarize the current status of the Dirac-Bergmann analysis of the geometrical trinity of gravity and its non-linear extension. The analysis can be performed in the following two formalisms: (i) Metric formalism and (ii) Vielbein formalism. In (i), the analysis can unveil the pDoF and the presence of diffeomorphism symmetry from the viewpoint of gauge theory. In (ii), the analysis can unveil the pDoF and the presence not only of diffeomorphism symmetry but also of internal space symmetry from the viewpoint of gauge theory. Therefore, theoretically speaking, it is enough to analyze the latter case, although computations are far more complicated relative to the former case. In this perspective, we could summarize the current status of our theories as follows:

Table 7.3: "MF" and "VF" denote the Dirac-Bergmann analysis in the metric formalism and the vielbein formalism, respectively. " $\bigcirc$ " denotes the analysis is performed and has a common understanding. " $\times$ " denotes the analysis is not performed. " $\triangle$ " denotes the analysis is performed, but there is no common understanding.

Subclass	GR	TEGR	CGR	fGR	fTEGR	fCGR
MF	$\bigcirc$	$\times$	$\triangle$	$\bigcirc$	$\times$	$\triangle$
VF	$\bigcirc$	$\bigcirc$	$\times$	$\times$	$\bigcirc$	$\times$

The analysis of GR in the vielbein formalism is performed in the works [Deser and Isham (1976); Henneaux (1983); Charap and Nelson (1983a,b); D'Adda et al. (1985); Charap (1987); Charap et al. (1988)]. Fulfilling this table by $\bigcirc$ is a great future work.

Chapter 8

Conclusions

This thesis has quested the following three pillars: the well-posedness of variational principle, the classification of the metric-affine gauge theories of gravity based on the unified understanding of the geometric quantities in the metric-affine geometry, *i.e.,* curvature, torsion, and non-metricity in the Möbius representations, and the Hamiltonian/Dirac-Bergmann analysis of the geometrical trinity of gravity and its non-linear extension.

The summary and future directions of the first pillar are given as follows: In Chapter 2, a theory of analytical mechanics for theories of gravity, focusing on degenerate and higher-order derivative point particle systems, was established. The Hamiltonian/Dirac-Bergmann analysis unveiled the constraint structures such as the gauge symmetries and the possible propagating degrees of freedom of a given degenerate system. In Chapter 3, a methodology to make the variational principle well-posed in degenerate point particle systems was constructed. Throughout the consideration in Summary 3.9, in this thesis, the well-posedness only with the primary constraints is assumed. This methodology is still developing in the following two points; (i) The elucidation of the difference of treatment between the secondary or more higher-order first-class constraints and that in the primary first-class constraints; (ii) The extension to field theories in a generic manner. In Chapter 4, the general theory of relativity was reconstructed. In particular, the geodesic equations and the Einstein field equations are derived based on the well-posed variational principle being consistent with the primary constraints. In particular, the latter derivation showed that the Gibbons-York-Hawking term is automatically derived and the well-posedness being consistent with all constraints would generate other sort of counter-terms but specific formulae were not unveiled; this is a future work.

The summary and future directions of the second pillar are given as follows: In Chapter 5, a mathematical framework for gauge approach to gravity, *i.e.,* a bundle theory, is reviewed. The Ehresmann connection and its curvature on a principle G-bundle was introduced, and using these ingredients, the internal space bundle and frame fields were introduced together with the Weitzenböch connection. The gauge structures of the metric-affine gauge theories of gravity were engraved into the internal space. In Chapter 6, deriving the tangent bundle of a spacetime manifold from a principal G-bundle, curvature tensor, and torsion tensor were introduced. The curvature was automatically derived from the Ehresmann connection of the given principle G-bundle, but the torsion was deduced as an analogy of the derivation of the curvature. The non-metricity tensor was introduced separately from the above approach and in an ad hoc manner by considering the covariant derivative. In order to construct these three quantities in a unified manner and classify the metric-affine gauge theories of gravity into eight subclasses, the Möbius representations were applied. Then teleparallel equivalent to general relativity (TEGR) and symmetric teleparallel equivalent to general relativity (STEGR) were formulated. In particular, for the STEGR subclass, imposing the coincident gauge condition, coincident general relativity (CGR) is derived. Further, those quadratic and non-linear extensions were also introduced. Notice, finally, that if it is possible to further extend the metric-affine gauge group using a semi-direct product then a new geometric quantity would be discovered, and then it would also be possible to construct a new subclass of gravity. The investigation of this perspective is for an intriguing future work.

The summary and future directions of the third pillar are given as follows: In Chapter 7, the Dirac-Bergmann analysis was performed for each subclass of the geometrical trinity of gravity and its non-linear extension. First of all, the three issues on the Dirac-Bergmann analysis were clarified. The first issue was that "*the method to define the degeneracy/rank of the matrix under the existence of the boundary terms*". This issue concerns the rank of the

Dirac matrix, and, therefore, it determines the total number of second-class constraints; this issue relates not only to the propagating degrees of freedom counting but also to the determination of Lagrange multipliers. The second issue was that "*whether should the boundary terms be also taken into account when classifying a constraint into either a first- or second-class constraint*". This issue concerns the gauge symmetry of a given theory, and, therefore, the constraint structure of the given theory, since first-class constraints form the generator of the symmetry. This issue becomes crucial in particular for diffeomorphism invariant theories in those consistencies. The third issue was that "*whether or not the solved phase space variables ϕ^a and π_b in the consistency conditions Eq (7.16), or equivalently, Eq (7.17), and that of the field equations of motion are always consistent*". Where the meaning of this *consistency* is that whether or not the functional forms of the Lagrange multipliers exist such that the solutions of Eq (7.16) provide that of the field equations motion. Only when this consistency is satisfied, the Dirac-Bergmann analysis can count out the propagating degrees of freedom of a given theory. All of these issues are caused by the spatial boundary term like " $\partial_i \left[H^{(i)}_{\alpha_1\beta_1} \delta^{(n)}(\mathbf{x}-\mathbf{y}) \right]$ " in Eq (7.13), or more fundamentally, " $A(x)\partial^{(x)}_i \delta^{(3)}(\mathbf{x}-\mathbf{y})$ " in Eq (7.12). To manipulate the issues and make it possible to perform the Dirac-Bergmann analysis reliably, Prescription 1 was proposed, stating that appropriate spatial boundary conditions remove the spatial boundary terms from all PBs. In compensation for the use of Prescription 1, the solution space of the given theory was restricted; the Dirac-Bergmann analysis does not always unveil all propagating degrees of freedom of a given theory. In more detail, for a theory with the characteristics of diffeomorphism invariance, on one hand, the usage did not spoil any generality. On the other hand, for a theory with violating its diffeomorphism invariance, the result of the analysis lost its generality and generically provided that of a special sector. Finally, based on Prescription 1, the Dirac-Bergmann analysis for each subclass was performed, and the following results were obtained. (See Table 8.1.)

As for future directions of the third pillar, there are three problems; (i) To reveal the

Table 8.1: Degrees of freedoms (DoF) of each subclass in 4-dimentional spacetime. "pDoF", "gDoF(Diffeo.)", and "gDoF(Lorentz)" denote propagating DoF, diffeomorphism symmetry, and local Lorentz symmetry, respectively. All analyses are based on Prescription 1. " ($\triangle$) " denotes that further investigation *based on the Dirac-Bergmann analysis* is necessary (See also Table 7.3 in Section 7.7.)

Subclass	GR	TEGR	CGR	fGR	fTEGR	fCGR
pDoF	2	2	2 ($\triangle$)	$2+1$	$2+3$	$2+4$
gDoF(Diffeo.)	4	4	4 ($\triangle$)	4	4	0
gDoF(Lorentz)	6	6	6 ($\triangle$)	6 ($\triangle$)	0	6 ($\triangle$)

existence of each issue in each subclass (See Table 7.1 in Section 7.7); (ii) To perform the Dirac-Bergmann analysis based on Prescription 1 for uncompleted subclasses (See Table 7.3 in Section 7.7); (iii) To settle down the controversies in coincident $f(Q)$-gravity (See Table 7.2 in Section 7.7.) More essentially, it should be investigated a mathematically correct way to manipulate the spatial boundary terms. In particular, it is important to unveil whether or not the consistency in the third issue is always satisfied since this problem relates directly to the validity of the Dirac-Bergmann analysis.

Finally, as the future direction of this thesis, when completing the above problems (for each subclass), the cosmological perturbation should be performed. (See Figure 1.1.) In this stage, we should scrutinize the existence of (infinitely) strong couplings against a background spacetime, which is a discrepancy between the true DoF derived from the Dirac-Bergmann analysis and/or other alternative methodologies [Kaparulin et al. (2013); Errasti Díez et al. (2020, 2024)] and the estimated DoF in the cosmological perturbation around a background spacetime. In particular, aiming to the application to cosmology, the investigations of those existences against Minkowski spacetime, the flat and non-flat FLRW spacetime are important. If there exists a (infinitely) strong coupling then the theory cannot be applied to cosmology since the perturbation theory breaks down. For instance, the Dirac-Bergmann analysis unveiled that $f(T)$-gravity has five pDoF in a generic sector (See Section 7.5), whereas the linear perturbations around Minkowski spacetime [Golovnev and Guzman (2021); Beltrán Jiménez et al.

(2021)], the flat and non-flat FLRW spacetime [Bahamonde et al. (2023b)] lead to only two pDoF. This situation suggests that $f(T)$-gravity should not be applied in its current form to cosmology in a theoretically consistent manner. The recent work also indicates that the same pathology may appear in the coincident $f(Q)$-gravity [Beltrán Jiménez et al. (2020b); Beltrán Jiménez and Koivisto (2021); Gomes et al. (2023a)]. That is, on one hand, the linear perturbation theories around Minkowski spacetime and (the flat and non-flat) FLRW spacetime lead to two, and, four, five, six or seven with respect to its connection dependence, respectively. On the other hand, as shown in Section 7.6, the possible pDoF of the theory is six in a special sector [Tomonari and Bahamonde (2023)] or, either seven [Tomonari and Bahamonde (2023)] or eight [Hu et al. (2022)] in a generic sector. The modified/extended theories of gravity are valid for constructing cosmology only when the issues are cured in some way, and the theory becomes a healthy one. Then, for each healthy theory, the power spectrum of each ingredient should be derived for comparison to the recent observations. (See Figure 1.1.) The perturbations and the power spectra of several subclasses are already calculated. For GR and fGR, see Refs [De Felice and Tsujikawa (2010); Koivisto (2006); Li et al. (2012)], for example. For TEGR and fTEGR, see Refs [Chen et al. (2011); Izumi and Ong (2013); Bahamonde et al. (2023a,b)], for example. For CGR and fCGR, see Refs [Beltrán Jiménez et al. (2020b); Gomes et al. (2023b,a); Heisenberg et al. (2023)], for example. For perturbations of the metric-affine gauge theories of gravity, see Ref [Aoki et al. (2023)] for example. It would be intriguing to scrutinize the late-time accelerated expansion of the universe (, or equivalently, dark energy problem, cosmological constant problem,) and the tension problems based on healthy models.

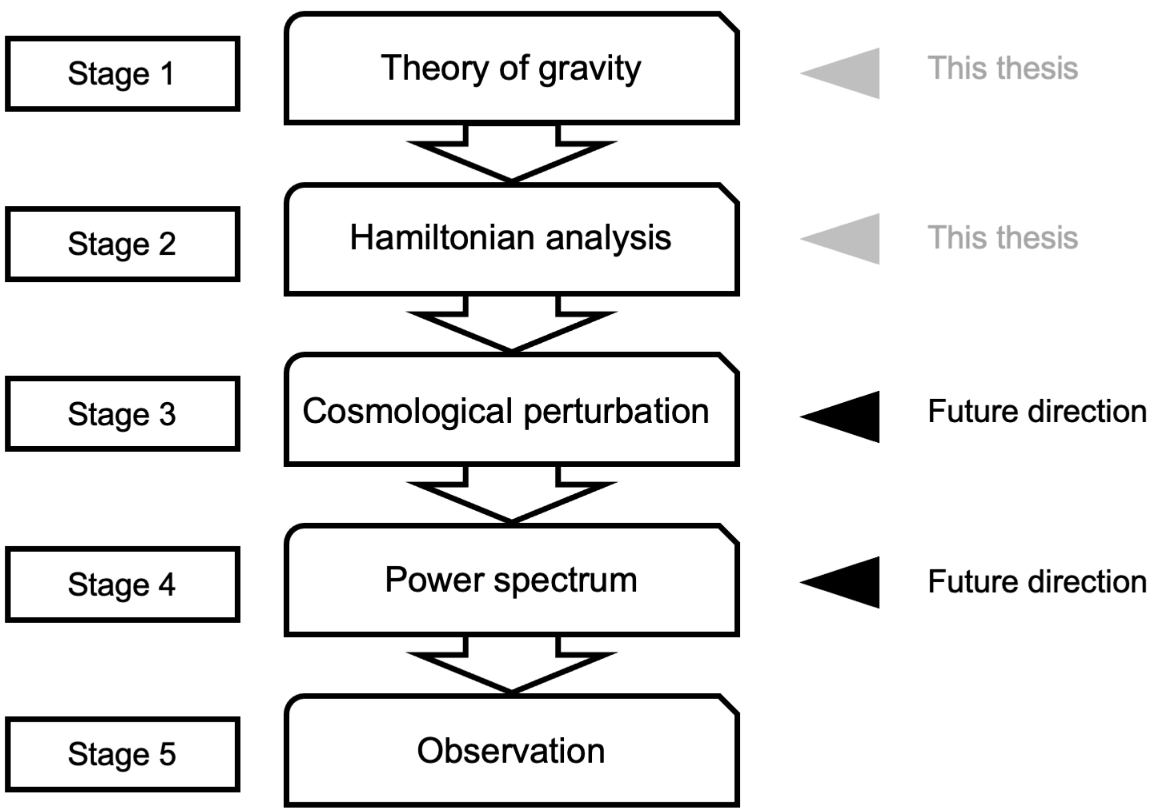

Figure 8.1: Modern framework for cosmology (Future direction)

Appendix A

PB-algebras of coincident $f(Q)$-gravity in $(n+1)$-dimensional spacetime

In the below calculations, all spatial boundary terms are neglected according to Prescription 1 as discussed in Section 7.1. The assumed spatial boundary conditions are $N_i(t\,,\partial\Sigma_t) := 0$ for each leaf Σ_t. In this appendix, the Poisson brackets are denoted as " $\{\cdot\,,\cdot\}$ " (abbreviate " $_{P.b.}$ "). Also, the argument " $(t\,,\mathbf{x})$ " is abbreviated as " x ". We abbreviate the notation of " $_*$ " for the phase space variables.

The PB-algebras among the primary constraint densities $\phi^{(1)}_A$ ($A \in \{0, i, \varphi\}$; $i \in \{1, 2, \cdots, n\}$) and the density $\mathcal{H}_0$:

$$\begin{aligned}
\{\phi^{(1)}_0(x)\,,\mathcal{H}_0(y)\} &= \left[-\mathcal{C}^{f(Q)}_0 - \frac{\sqrt{h}}{N}\frac{N^i}{N} f''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j\varphi\right)\right]\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,\\
\{\phi^{(1)}_i(x)\,,\mathcal{H}_0(y)\} &= \left[-\mathcal{C}^{f(Q)}_i + \frac{1}{n-1}\frac{f''}{f'}\pi\partial_i\varphi\right]\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,\\
\{\phi^{(1)}_\varphi(x)\,,\mathcal{H}_0(y)\} &= \left[-\mathcal{H}'_0 - \frac{1}{n-1}\frac{f''}{f'}\pi\partial_i N^i\right]\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,
\end{aligned} \tag{A.1}$$

where $\mathcal{H}'_0$ is defined by

$$\begin{aligned}
\mathcal{H}'_0 := N\sqrt{h}\Bigg[&-f''\left\{{}^{(n)}Q - \varphi + \frac{1}{h}\left(\frac{1}{f'}\right)^2\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right)\right\} + \mathring{D}_i\left\{f''\left({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i\right)\right\}\\
&-\frac{1}{N}\frac{N^I}{N} f'''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j\varphi\right)\Bigg]\,,
\end{aligned} \tag{A.2}$$

and $\mathcal{C}_0^{f(Q)}$ is computed as follows:

$$\mathcal{C}_0^{f(Q)} := -\sqrt{h}\left[f'^{(n)}Q - \mathring{D}_i\left\{f'\left({}^{(n)}Q^i - {}^{(n)}\bar{Q}^i\right)\right\} + f - \varphi f' - \frac{1}{hf'}\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right)\right]. \tag{A.3}$$

$\mathcal{C}_i^{f(Q)}$ does not change from Eq (7.120) excepting the range of summations. The PB-algebras among two of the primary constraint densities $\phi_A^{(1)}$ $(A \in \{0, i, \varphi\};\ i \in \{1, 2, \cdots, n\})$ and the density $\mathcal{H}_0$:

$$\begin{aligned}
\{\{\phi_0^{(1)}, \mathcal{H}_0\}(x), \phi_0^{(1)}(y)\} =& \frac{\sqrt{h}}{N}\frac{N^i}{N}\frac{2}{N}f''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j \varphi\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi_0^{(1)}, \mathcal{H}_0\}(x), \phi_i^{(1)}(y)\} =& \frac{1}{n-1}\frac{1}{N}\frac{f''}{f'}\pi\partial_i\varphi\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi_0^{(1)}, \mathcal{H}_0\}(x), \phi_\varphi^{(1)}(y)\} =& \left[\sqrt{h}f''\left\{{}^{(n)}Q - \varphi + \frac{1}{h}\left(\frac{1}{f'}\right)^2\left(\pi^{ij}\pi_{ij} - \frac{1}{n-1}\pi^2\right)\right\} - \frac{1}{n-1}\frac{1}{N}\frac{f''}{f'}\pi\partial_i N^i\right.\\
&\left. -\frac{\sqrt{h}}{N}\frac{N^i}{N}f'''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j\varphi\right)\right]\delta^{(n)}(\mathbf{x}-\mathbf{y}).
\end{aligned} \tag{A.4}$$

$$\begin{aligned}
\{\{\phi_i^{(1)}, \mathcal{H}_0\}(x), \phi_0^{(1)}(y)\} =& -\frac{1}{N}\frac{\sqrt{h}}{N}f''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j\varphi\right)\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi_i^{(1)}, \mathcal{H}_0\}(x), \phi_j^{(1)}(y)\} =& \frac{n}{2(n-1)}\frac{h}{N}\frac{(f'')^2}{f'}\partial_i\varphi\partial_j\varphi\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi_i^{(1)}, \mathcal{H}_0\}(x), \phi_\varphi^{(1)}(y)\} =& \left[\frac{\sqrt{h}}{N}f'''\left(\partial_j N^j \partial_i\varphi - \partial_i N^j \partial_j\varphi\right) + \frac{1}{n-1}\frac{1}{f'}\pi\partial_i\varphi\left(f''' - \frac{f''}{f'}\right)\right.\\
&\left. -\frac{n}{2(n-1)}\frac{\sqrt{h}}{N}\frac{(f'')^2}{f'}\partial_j N^j \partial_i\varphi\right]\delta^{(n)}(\mathbf{x}-\mathbf{y}).
\end{aligned} \tag{A.5}$$

$$
\begin{aligned}
\{\{\phi^{(1)}_{\varphi}\,,\mathcal{H}_0\}(x)\,,\phi^{(1)}_0(y)\} = \Bigg[&\sqrt{h}f''\left\{{}^{(n)}Q-\varphi+\frac{1}{h}\left(\frac{1}{f'}\right)^2\left(\pi^{ij}\pi_{ij}-\frac{1}{n-1}\pi^2\right)-\frac{f'''}{f''}\partial_i\varphi\left({}^{(n)}Q^i-{}^{(n)}\bar{Q}^i\right)\right\}\\
&-\frac{2\sqrt{h}}{n-1}\frac{f''}{f'}\pi\partial_iN^i+\frac{1}{n-1}\frac{f''}{f'}\frac{1}{N}\pi\partial_iN^i\\
&-\frac{\sqrt{h}}{N}\frac{N^i}{N}f'''\left(\partial_JN^j\partial_i\varphi-\partial_iN^j\partial_j\varphi\right)\Bigg]\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi^{(1)}_{\varphi}\,,\mathcal{H}_0\}(x)\,,\phi^{(1)}_i(y)\} = \Bigg[&-\frac{n}{2(n-1)}\frac{\sqrt{h}}{N}\frac{(f'')^2}{f'}\partial_jN^j\partial_i\varphi-\frac{1}{n-1}\frac{f'''}{(f')^2}\partial_i\varphi\\
&+\frac{\sqrt{h}}{N}f'''\left(\partial_jN^j\partial_i\varphi-\partial_iN^j\partial_j\varphi\right)+\frac{1}{n-1}\frac{\pi}{f'}\left(f'''-\frac{f''}{f'}\right)\partial_i\varphi\Bigg]\delta^{(n)}(\mathbf{x}-\mathbf{y}),\\
\{\{\phi^{(1)}_{\varphi}\,,\mathcal{H}_0\}(x)\,,\phi^{(1)}_{\varphi}(y)\} = \Bigg[&-\mathcal{H}''_0+\frac{1}{n-1}\left(\frac{f''}{f'}\right)^2\pi\partial_iN^i-\frac{1}{n-1}\frac{1}{f'}\left(f''''-\frac{f''}{f'}\right)\partial_iN^i\\
&+\frac{n}{2(n-1)}\sqrt{h}\frac{(f'')^2}{f'}\partial_iN^i\partial_jN^j\Bigg]\delta^{(n)}(\mathbf{x}-\mathbf{y})\,,
\end{aligned}
\tag{A.6}
$$

where $\mathcal{H}''_0$ is defined as follows:

$$
\begin{aligned}
\mathcal{H}''_0 := N\sqrt{h}\Bigg[&-f'''\left({}^{(n)}Q-\varphi\right)+f''-\frac{1}{h}\frac{1}{N}\left(\frac{1}{f'}\right)^2\left(1-\frac{2}{f'}\right)\left(\pi^{ij}\pi_{ij}-\frac{1}{n-1}\pi^2\right)\\
&+\mathring{D}_i\left\{f'''\left({}^{(n)}Q^i-{}^{(n)}\bar{Q}^i\right)\right\}-\frac{1}{N}\frac{N^i}{N}f''''\left(\partial_JN^j\partial_i\varphi-\partial_iN^j\partial_j\varphi\right)\Bigg]\,.
\end{aligned}
\tag{A.7}
$$

The PB-algebras among the primary constraint densities $\phi^{(1)}_A$ ($A\in\{0,i,\varphi\};\ i\in\{1,2,\cdots,n\}$), A_i/B, C_i/B, and the density $\mathcal{H}_0$ are calculated as follows:

$$
\left\{\{\phi^{(1)}_A\,,\mathcal{H}_0\}(x)\,,\left(\frac{A_i}{B}\right)(y)\right\}=0\ ,\quad \left\{\{\phi^{(1)}_A\,,\mathcal{H}_0\}(x)\,,\left(\frac{C_i}{B}\right)(y)\right\}=0\,. \tag{A.8}
$$

The PB-algebras among the primary constraint densities $\phi^{(1)}_A$ ($A\in\{0,i,\varphi\};\ i\in\{1,2,\cdots,n\}$), A_i/B, and C_i/B are calculated as follows:

$$
\left\{\left(\frac{A_i}{B}\right)(x)\,,\phi^{(1)}_0(y)\right\}=0\ ,\quad \left\{\left(\frac{C_i}{B}\right)(x)\,,\phi^{(1)}_0(y)\right\}=-\frac{1}{f''}\frac{1}{\partial_iN^i}f'''\partial_i\varphi\delta^{(n)}(\mathbf{x}-\mathbf{y})\,. \tag{A.9}
$$

$$\left\{\left(\frac{A_i}{B}\right)(x)\,,\phi_j^{(1)}(y)\right\} = 0\;, \quad \left\{\left(\frac{C_i}{B}\right)(x)\,,\phi_j^{(1)}(y)\right\} = 0\,. \tag{A.10}$$

$$\left\{\left(\frac{A_i}{B}\right)(x)\,,\phi_\varphi^{(1)}(y)\right\} = 0\;, \quad \left\{\left(\frac{C_i}{B}\right)(x)\,,\phi_\varphi^{(1)}(y)\right\} = N\frac{1}{\partial_i N^i}\frac{1}{f''}\left[\frac{(f''')^2}{f''} - f''''\right]\partial_i\varphi\,\delta^{(n)}(\mathbf{x}-\mathbf{y})\,. \tag{A.11}$$

Appendix B

The explicit formulae of α and β^i_j

$$
\begin{aligned}
\alpha :=& \frac{1}{2}\frac{n}{n-1}\frac{h}{N}\frac{(f'')^2}{f'} + \frac{1}{n-1}\frac{1}{N}\frac{f'''}{f'}\frac{1}{\partial_i N^i}\pi \\
&+ \frac{1}{\partial_k N^k}\left[\frac{\sqrt{h}}{N}\partial_k N^k + \frac{1}{n-1}\frac{1}{f'}\pi\left(f''' - \frac{f'''}{f'}\right) - \frac{n}{2(n-1)}\frac{\sqrt{h}}{N}\frac{(f'')^2}{f'}\partial_k N^k\right] \\
&+ \frac{1}{\partial_k N^k}\left[-\frac{n}{2(n-1)}\frac{\sqrt{h}}{N}\frac{(f'')^2}{f'}\partial_k N^k - \frac{1}{n-1}\frac{f''}{(f')^2} + \frac{\sqrt{h}}{N}f'''\partial_k N^k - \frac{1}{n-1}\frac{1}{f'}\left(f'''' - \frac{f''}{f'}\right)\partial_k N^k\right] \\
&- \frac{f'''}{\partial_k N^k}\left[\frac{\sqrt{h}}{N}\partial_k N^k\right] + \left(\frac{1}{\partial_k N^k}\right)^2 N\frac{f''''}{f''}\{\phi_0^{(1)}, \mathcal{H}_0\} \\
&+ \left(\frac{1}{\partial_k N^k}\right)^2\left(\frac{f'''}{f''}\right)^2\{\{\phi_0^{(1)}, \mathcal{H}_0\}, \phi_0^{(1)}\} + \left(\frac{1}{\partial_k N^k}\right)^2\frac{f'''}{f''}N\{\{\phi_0^{(1)}, \mathcal{H}_0\}, \phi_\varphi^{(1)}\} \\
&+ \left(\frac{1}{\partial_k N^k}\right)^2\frac{f'''}{f''}N\{\{\phi_\varphi^{(1)}, \mathcal{H}_0\}, \phi_0^{(1)}\} + \left(\frac{1}{\partial_k N^k}\right)^2\{\{\phi_\varphi^{(1)}, \mathcal{H}_0\}, \phi_\varphi^{(1)}\}
\end{aligned}
\tag{B.1}
$$

$$
\beta^I_J := -\frac{1}{\partial_K N^K}\frac{\sqrt{h}}{N}f'''\partial_J N^I \,. \tag{B.2}
$$

Appendix C

Inönü-Wigner contraction of metric-affine geometry and its extensions

In this Appendix, based on the unified description of curvature, torsion, and non-metricity (or equivalently, dilation and shear) given Section 6.2 and in Ref [Tomonari (2023a)], the relationships between the algebraic structure and geometric quantities of each geometry are scrutinized by using the so-called Inönü-Wigner contraction. The ultimate purpose is to beyond the metric-affine geometry and to pursue a new class of geometry and its gauge theory of gravity. First, the Inönü-Wigner contraction is introduced. Second, the contractions of the metric-affine geometry and its extension are performed. Finally, the de Sitter/anti-de Sitter cases are discussed.

Inönü-Wigner contraction is a method of parametrizing a Lie algebra to decompose it into subalgebras [Segal (1951); Inonu and Wigner (1953); Lord (1985); Weimar-Woods (1995); Khasanov and Kuperstein (2011); Subag et al. (2012)]. The contraction is originally valid not only for Lie algebras but also for those representations, but, in this paper, we discuss only the contraction of Lie algebras.

Let G be a Lie group and $\mathfrak{g}$ be its Lie algebra. Then an element $g = g(\tau_i) \in G$, where τ_i $(i = 1\,, 2\,, \cdots\,, t)$ are the number of t group parameters, leads to an element of the Lie algebra of G as its derivative with respect to the unit element $e \in G$. Let I_i be such elements of the Lie algebra. Then the following commutation relations hold:

$$[I_i\,, I_j] = C^k{}_{ij} I_k\,, \tag{C.1}$$

where $[\,\cdot\,,\cdot\,]$ is the Lie bracket and $C^k{}_{ij}$ are the structure constants of the Lie algebra. For this algebra, a transformation of the elements I_i and the group parameters τ_i is introduced as follows:

$$I'_i = P^j{}_i I_j \,, \quad \tau'_i = P^j{}_i \tau_j \,, \tag{C.2}$$

where $P^j{}_i$ is a parametrization matrix. If the matrix is non-singular then the above transformation is just an automorphism of the Lie algebra. However, if it is singular, the situation gets changed; a subalgebra can be obtained. In particular, it is an intriguing case that the singularity is realized as some limits of the parameters.

A simple case is the contraction by the following matrix:

$$P^i{}_j = \begin{bmatrix} 1_{r\times r} & 0_{r\times(n-r)} \\ 0_{(n-r)\times r} & 0_{(n-r)\times(n-r)} \end{bmatrix} + \begin{bmatrix} \epsilon^\alpha{}_\beta & 0_{r\times(n-r)} \\ 0_{(n-r)\times r} & \epsilon^{\bar\alpha}{}_{\bar\beta} \end{bmatrix} \,, \tag{C.3}$$

where $\epsilon^\alpha{}_\beta \in (0\,,1]$, $\epsilon^{\bar\alpha}{}_{\bar\beta} \in (0\,,1]$, $\alpha\,,\beta \in \{1\,,2\,,\cdots\,,t' < t\}$, and $\bar\alpha\,,\bar\beta \in \{t'+1\,,t'+2\,,\cdots\,,t\}$. Then, on one hand, the elements I_i and those algebras are transformed as follows:

$$I'_i = (\delta^\alpha{}_i + \delta^\beta{}_i \epsilon^\alpha{}_\beta) I_\alpha + \delta^{\bar\beta}{}_i \epsilon^{\bar\alpha}{}_{\bar\beta} I_{\bar\alpha} \,, \tag{C.4}$$

and

$$[I'_i\,, I'_j]_\epsilon = \delta^\alpha{}_i \delta^\beta{}_i C^\gamma{}_{\alpha\beta} I_\gamma + \mathcal{O}(\epsilon) \,, \tag{C.5}$$

respectively, where $[\,\cdot\,,\cdot\,]_\epsilon$ denotes the Lie brackets of the transformed elements I'_i. Let $\mathfrak{g}_\epsilon$ and G_ϵ denote a new Lie algebra that is generated by I'_i with satisfying the above algebra and the Lie group of $\mathfrak{g}_\epsilon$, respectively. Notice that $\mathfrak{g}_\epsilon$ and G_ϵ include $\mathfrak{g}$ and G as a special case of $\epsilon^\alpha{}_\beta \to +0$ and $\epsilon^{\bar\alpha}{}_{\bar\beta} \to \delta^{\bar\alpha}{}_{\bar\beta}$, where " $+0$ " means the right-limit to zero in $(0\,,1]$. Therefore, if the limit of the transformation of the above algebras with respect to $\epsilon^\alpha{}_\beta \to +0$

and $\epsilon^{\bar{\alpha}}{}_{\bar{\beta}} \to +0$ exists then the following new algebra is obtained:

$$[I'_\alpha\,, I'_\beta]_{\epsilon\to+0} = C^\gamma{}_{\alpha\beta} I'_\gamma\,. \tag{C.6}$$

That is, a new subalgebra $\mathfrak{g}_0 = \mathfrak{g}_{\epsilon\to+0} = \langle I'_{\bar{\alpha}} \rangle$ is obtained, and $\mathfrak{g}_0$ generates the Lie group $G_0 = G_{\epsilon\to+0}$. On the other hand, the group parameters τ_i are contracted as follows:

$$\begin{aligned} \tau'_\alpha &= \tau_\alpha + \epsilon^\beta{}_\alpha \tau_\beta \to \tau_\alpha \quad (\epsilon^\beta{}_\alpha \to +0)\,, \\ \tau'_{\bar{\alpha}} &= \epsilon^{\bar{\beta}}{}_{\bar{\alpha}} \tau_{\bar{\beta}} \to 0 \quad (\epsilon^{\bar{\beta}}{}_{\bar{\alpha}} \to +0)\,. \end{aligned} \tag{C.7}$$

Notice that the group parameters $\tau'_{\bar{\alpha}}$ of the group G_ϵ converge to zero while remaining the corresponding parameters $\tau_{\bar{\beta}}$ of G. Since G_ϵ includes not only G but also G_0, this means that the parametrization given in Eq (C.2) extended the original group G into a larger group G_ϵ as a topological space.

Now, first of all, let us consider the contraction of the metric-affine group. The Lie algebra of $MA(n+1\,;\mathbb{R})$ is summarized as follows:

$$\begin{aligned} &[P_I\,, P_J] = 0\,, \quad [E^I{}_J\,, P_K] = \delta^I{}_K P_J\,, \quad [E^I{}_J\,, E^K{}_L] = \delta^I{}_L E^K{}_J - \delta^K{}_J E^I{}_L\,, \\ &[D\,, D] = 0\,, \quad [D\,, P_I] = P_I\,, \quad [D\,, E^I{}_J] = 0\,, \\ &[S^I{}_J\,, P_K] = \delta^I{}_K P_J\,, \quad [S^I{}_J\,, E^K{}_L] = 0\,, \quad [S^I{}_J\,, D] = 0\,, \quad [S^I{}_J\,, S^K{}_L] = 0\,. \end{aligned} \tag{C.8}$$

A parametrization for the Inönü-Wigner contraction of the above algebra can be set as follows:

$$P'_I = \epsilon^{(P)} P_I\,, \quad E'^I{}_J = \epsilon^{(E)} E^I{}_J\,, \quad D' = \epsilon^{(D)} D\,, \quad S'^I{}_J = \epsilon^{(S)} S^I{}_J\,, \tag{C.9}$$

where $\epsilon^{(P)}$, $\epsilon^{(E)}$, $\epsilon^{(D)}$, and $\epsilon^{(S)}$ are a set of parameters and belong to the range $(0\,,1]$. Hereinafter, let us denote the parameter space spanned by the above parameters as $\epsilon_{\text{ type of contraction/geometry in MA}} = (\epsilon^{(P)}\,, \epsilon^{(E)}\,, \epsilon^{(D)}\,, \epsilon^{(S)})$, where "type of contraction/geometry in MA" denotes a geometry which is obtained by performing the contraction. Hereinafter, we use this notation. Then the above algebras are parameterized as follows:

$$
\begin{aligned}
&[P'_I\,, P'_J] = 0\,, \quad [E'^I{}_J\,, P'_K] = \epsilon^{(E)}\delta^I{}_K P'_J\,, \quad [E'^I{}_J\,, E'^K{}_L] = \epsilon^{(E)}(\delta^I{}_L E'^K{}_J - \delta^K{}_J E'^I{}_L)\,,\\
&[D'\,, D'] = 0\,, \quad [D'\,, P'_I] = \epsilon^{(D)} P'_I\,, \quad [D'\,, E'^I{}_J] = 0\,,\\
&[S'^I{}_J\,, P'_K] = \epsilon^{(S)}\delta^I{}_K P'_J\,, \quad [S'^I{}_J\,, E'^K{}_L] = 0\,, \quad [S'^I{}_J\,, D'] = 0\,, \quad [S'^I{}_J\,, S'^K{}_L] = 0\,.
\end{aligned}
\tag{C.10}
$$

Notice that this algebra does not explicitly contain the parameter $\epsilon^{(P)}$. Therefore, it is enough to express the parameter space without $\epsilon^{(P)}$ as $\epsilon_{\text{ type of contraction/geometry in MA}} = (\epsilon^{(E)}\,, \epsilon^{(D)}\,, \epsilon^{(S)})$, and there are eight possible contractions. Of course, if all parameters are taken to be unity then the above algebra (C.10) results in the original algebra (C.8). In terms of the parameter space notation, the algebra is expressed as $\epsilon_{\text{ L}_{\text{n+1}}} = (1\,, 1\,, 1)$.

The contraction generated by the parameters $\epsilon_{\text{ Y}_{\text{n+1}}} = (1\,, 1\,, +0)$ derives the following algebras:

$$
\begin{aligned}
&[P'_I\,, P'_J] = 0\,, \quad [E'^I{}_J\,, P'_K] = \delta^I{}_K P'_J\,, \quad [E'^I{}_J\,, E'^K{}_L] = \delta^I{}_L E'^K{}_J - \delta^K{}_J E'^I{}_L\,,\\
&[D'\,, D'] = 0\,, \quad [D'\,, P'_I] = P'_I\,, \quad [D'\,, E'^I{}_J] = 0\,,\\
&[S'^I{}_J\,, P'_K] = 0\,, \quad [S'^I{}_J\,, E'^K{}_L] = 0\,, \quad [S'^I{}_J\,, D'] = 0\,, \quad [S'^I{}_J\,, S'^K{}_L] = 0\,.
\end{aligned}
\tag{C.11}
$$

This is nothing but the algebra of the Weyl geometry. In this algebra, the shear given in Eq (6.53) vanishes, *i.e.*, $\not{\Delta} = 0$, for the metric tensor of the internal space with satisfying the following equations:

$$
g^{IK}\partial_\mu g_{KJ} = \frac{1}{n}\,\delta^I{}_J\, g^{LM}\partial_\mu g_{LM}\,. \tag{C.12}
$$

The contraction generated by the parameters $\epsilon_{\text{ Y}_{\text{n+1}}\text{ with vanishing dilation}} = (1\,, +0\,, 1)$ leads to the following algebras:

$$
\begin{aligned}
&[P'_I\,,P'_J]=0\,,\quad [E'^I{}_J\,,P'_K]=\delta^I{}_K P'_J\,,\quad [E'^I{}_J\,,E'^K{}_L]=\delta^I{}_L E'^K{}_J-\delta^K{}_J E'^I{}_L\,,\\
&[D'\,,D']=0\,,\quad [D'\,,P'_I]=0\,,\quad [D'\,,E'^I{}_J]=0\,,\\
&[S'^I{}_J\,,P'_K]=\delta^I{}_K P'_J\,,\quad [S'^I{}_J\,,E'^K{}_L]=0\,,\quad [S'^I{}_J\,,D']=0\,,\quad [S'^I{}_J\,,S'^K{}_L]=0\,.
\end{aligned}
\tag{C.13}
$$

Then the dilation given in Eq (6.46) vanishes, $i.e.$, $\Delta=0$ for the metric tensor of the internal space with satisfying the following equations:

$$
g^{IJ}\partial_\mu g_{IJ}:=0\,. \tag{C.14}
$$

Therefore, choosing a constant metric tensor, $g_{IJ}=c_{IJ}$, is a possible gauge condition for vanishing non-metricity. That is, a flat internal space does not have non-vanishing non-metricity. Remark that Conditions (C.12) and (C.14) can be independently imposed.

In the same manner, the contraction generated by $\epsilon_{\,\mathrm{U_{n+1}}}=(1\,,+0\,,+0)$ derives the algebra of the Riemann-Cartan geometry as follows:

$$
\begin{aligned}
&[P'_I\,,P'_J]=0\,,\quad [E'^I{}_J\,,P'_K]=\delta^I{}_K P'_J\,,\quad [E'^I{}_J\,,E'^K{}_L]=\delta^I{}_L E'^K{}_J-\delta^K{}_J E'^I{}_L\,,\\
&[D'\,,D']=0\,,\quad [D'\,,P'_I]=0\,,\quad [D'\,,E'^I{}_J]=0\,,\\
&[S'^I{}_J\,,P'_K]=0\,,\quad [S'^I{}_J\,,E'^K{}_L]=0\,,\quad [S'^I{}_J\,,D']=0\,,\quad [S'^I{}_J\,,S'^K{}_L]=0\,.
\end{aligned}
\tag{C.15}
$$

The algebras in the first line above are nothing but the affine algebra. In the same manner as the cases of the dilation and the shear, the full contraction, $i.e.$, $\epsilon_{\,0}=(+0\,,+0\,,+0)$ does not lead directly to the vanishing curvature and/or torsion as follows:

$$
T=d\mathbf{e}^{-1}\,,\quad \Omega^{(E)}=d\omega^{(E)}\,. \tag{C.16}
$$

That is, to vanish the torsion and/or curvature 2-forms, some additional conditions are necessary. Using Eq (6.36), the condition of vanishing torsion is given as follows

$$d\mathbf{e}^{-1} + d^2\zeta = d\mathbf{e}^{-1} := 0\,, \tag{C.17}$$

This is nothing but just imposing $T := 0$. That is, the theory is consistent. In the case of the curvature, the so-called Weitzenböch gauge condition

$$\omega^{(E)} := 0\,, \quad \text{or equivalently}\,, \quad {\omega^{(E)}}^{I}{}_{\mu J} := 0 \tag{C.18}$$

realizes the vanishing curvature. Under the imposition of the above two conditions, the geometry becomes either E_{n+1} or M_{n+1}. In Section 5.4, in particular, the Weitzenböch connection is derived as in Eq (5.40). Under the imposition of Eq (C.18), the connection is given as follows:

$$\tilde{\Gamma}^{\rho}_{\mu\nu} = e_I{}^{\rho}\partial_\mu e^I{}_\nu\,. \tag{C.19}$$

Using Eq (6.8) in a coordinate/holonomic basis, the vanishing torsion is equivalent to the existence of the so-called Stükelberg fields, denoted by $\eta = \eta^I\xi_I$, as follows:

$$e^I{}_\mu = \partial_\mu \eta^I\,, \quad \text{or equivalently,} \quad \mathbf{e}^{-1} = e^I \otimes \xi_I = d\eta^I \otimes \xi_I\,. \tag{C.20}$$

This, of course, satisfies Eq (C.17). Therefore, even if the flat geometries E_{n+1} or M_{n+1}, the internal space still has the degrees of freedom of the Stükelberg fields. Furthermore, the imposition of the so-called coincident gauge condition [Beltrán Jiménez et al. (2018); Beltrán Jiménez and Koivisto (2022)], $\eta^I = A^I{}_\mu x^\mu + B^I$, where x^μ are the coordinates of a point in the base space $\mathcal{M}$, $A^I{}_\mu \in G(n+1\,;\mathbb{R})$ (it is a global symmetry), and $B = \xi_I B^I$ is a constant vector with respect to the global symmetry, then the Weitzenböch connection given in Eq (C.19) vanishes.

Finally, let us consider the contraction generated by $\epsilon_{\text{ abelian MA}} = (+0\,,1\,,1)$. The algebra is given as follows:

$$\begin{aligned}
&[P'_I\,,P'_J] = 0\,, \quad [E'^I{}_J\,,P'_K] = 0\,, \quad [E'^I{}_J\,,E'^K{}_L] = 0\,,\\
&[D'\,,D'] = 0\,, \quad [D'\,,P'_I] = P'_I\,, \quad [D'\,,E'^I{}_J] = 0\,,\\
&[S'^I{}_J\,,P'_K] = \delta^I{}_K P'_J\,, \quad [S'^I{}_J\,,E'^K{}_L] = 0\,, \quad [S'^I{}_J\,,D'] = 0\,, \quad [S'^I{}_J\,,S'^K{}_L] = 0\,,
\end{aligned} \tag{C.21}$$

where "abelian" in the subscript of the parameter space means that the algebras in the first line above, which was the Poincare algebra before performing the contraction, turn now to be a set of commutative algebras. Hereinafter, we use this notation. Imposing Eqs (C.17) and (C.18), the curvature and the torsion vanish; the geometry turns into the symmetric teleparallel geometry, S_{n+1}, which is described only by the dilation and shear, or equivalently, the non-metricity. Notice that Eq (C.19) and Eq (C.20) hold for the contraction generated by $\epsilon_{\text{ abelian MA}} = (+0\,,1\,,1)$. The dilation-free case, $\epsilon_{\text{ abelian MA with dilation}-\text{free}} = (+0\,,+0\,,1)$, and the shear-free case, $\epsilon_{\text{ abelian MA with shear}-\text{free}} = (0+\,,1\,,+0)$, can be constituted in the same manner.

Second, let us consider an extension of the metric-affine group. An extension of the Lie algebra of $MA(n+1\,;\mathbb{R})$, let us denote $EMA(n+1\,;\mathbb{R})$, can be given follows:

$$\begin{aligned}
&[P_I\,,P_J] = 0\,, \quad [E^I{}_J\,,P_K] = C^{(A3)}{}^{IL}{}_{JK}P_L\,, \quad [E^I{}_J\,,E^K{}_L] = C^{(A6)}{}^{IKN}{}_{JLM}E^M{}_N\,,\\
&[D\,,D] = 0\,, \quad [D\,,P_I] = C^{(W4)}{}^J{}_I P_J\,, \quad [D\,,E^I{}_J] = C^{(W9)}{}^I{}_J D\,,\\
&[S^I{}_J\,,P_K] = C^{(MA1)}{}^{IL}{}_{JK}P_L\,, \quad [S^I{}_J\,,E^K{}_L] = C^{(MA16)}{}^{IKM}{}_{JLN}S^N{}_M\,,\\
&[S^I{}_J\,,D] = 0\,, \quad [S^I{}_J\,,S^K{}_L] = 0\,.
\end{aligned} \tag{C.22}$$

If $C^{(A3)}{}^{IL}{}_{JK} = \delta^I{}_K\delta^L{}_J$, $C^{(A6)}{}^{IKN}{}_{JLM} = \delta^I{}_L\delta^K{}_M\delta^N{}_J - \delta^I{}_M\delta^K{}_J\delta^N{}_L$, $C^{(W4)}{}^J{}_I = \delta^J{}_I$, $C^{(MA1)}{}^{IL}{}_{JK} = \delta^I{}_K\delta^L{}_J$, and otherwise vanish then the Lie algebra $\mathfrak{ema}(n+1\,;\mathbb{R})$ of $EMA(n+1\,;\mathbb{R})$ turns into that of $MA(n+1\,;\mathbb{R})$. Therefore, the algebra of Eq (C.22) is an extension of the algebra of Eq (C.8). Another important algebra, which includes the Poincare algebra as a subalgebra, is obtained under the following structure constants: ${C^{(A3)}}^{IL}{}_{JK} = \delta^I{}_K \delta^L{}_J - g^{IL} g_{JK}$, ${C^{(A6)}}^{IKN}{}_{JLM} = g^{IK} g_{JM} \delta^N{}_L - g^{KN} g_{JM} \delta^I{}_L - \delta^K{}_J \delta^I{}_M \delta^N{}_L + g^{KN} g_{JL} \delta^I{}_M$, ${C^{(W4)}}^J{}_I = \delta^J{}_I$, ${C^{(MA1)}}^{IL}{}_{JK} = \delta^I{}_K \delta^L{}_J$, and otherwise vanish. Then $\mathfrak{ema}(n\,;\mathbb{R})$ is an extension of the Poincare algebra with the dilation and the shear. Hereinafter, however, we treat the algebra (C.22) without specifying the structure constants: after obtaining a contraction, we specify a set of structure constants and then develop a theory of gravity, although constructing physical theories is out of scope of the current thesis.

The parametrization given in Eq (C.9) is also taken for the above algebra (C.22) to perform the contraction. Then the parametrized algebra of Eq (C.22) is given as follows:

$$
\begin{aligned}
&[P'_I\,, P'_J] = 0\,, \quad [E'^I{}_J\,, P'_K] = \epsilon^{(E)} {C^{(A3)}}^{IL}{}_{JK} P'_L\,, \quad [E'^I{}_J\,, E'^K{}_L] = \epsilon^{(E)} {C^{(A6)}}^{IKN}{}_{JLM} E'^M{}_N\,,\\
&[D'\,, D'] = 0\,, \quad [D'\,, P'_I] = \epsilon^{(D)} {C^{(W4)}}^J{}_I P'_J\,, \quad [D'\,, E'^I{}_J] = \frac{\epsilon^{(D)}\epsilon^{(E)}}{\epsilon^{(P)}} {C^{(W9)}}^{IK}{}_J P'_K\,,\\
&[S'^I{}_J\,, P'_K] = \epsilon^{(S)} {C^{(MA1)}}^{IL}{}_{JK} P'_L\,, \quad [S'^I{}_J\,, E'^K{}_L] = \frac{\epsilon^{(S)}\epsilon^{(E)}}{\epsilon^{(P)}} {C^{(MA16)}}^{IKM}{}_{JL} P'_M\,,\\
&[S'^I{}_J\,, D'] = 0\,, \quad [S'^I{}_J\,, S'^K{}_L] = 0\,.
\end{aligned}
\tag{C.23}
$$

Notice that this algebra explicitly contains the parameter $\epsilon^{(P)}$. Therefore, we use the parameter space $\epsilon_{\text{ type of contraction/geometry in EMA}} = (\epsilon^{(P)}\,, \epsilon^{(E)}\,, \epsilon^{(D)}\,, \epsilon^{(S)})$. This is a different situation from the contraction of the metric-affine algebra. The geometric quantities of the contraction generated by $\epsilon_{\ 0} = (1\,, +0\,, +0\,, +0)$, $\epsilon_{\text{ abelian EMA}} = (1\,, +0\,, 1\,, 1)$, $\epsilon_{\text{ abelian EMA with dilation−free}} = (1\,, +0\,, +0\,, 1)$, and $\epsilon_{\text{ abelian EMA with shear−free}} = (1\,, +0\,, 1\,, +0)$ are constructed in the same manner as the metric-affine case up to the difference of structure constants (local symmetry). That is, the departures from the metric-affine case are caused by the non-vanishing parameter $\epsilon^{(E)}$.

Let us consider the geometric quantities in the contraction generated by $\epsilon_{\text{ EMA}} = (1\,, 1\,, 1\,, 1)$.

Then the curvature and torsion 2-forms are given as Eq (6.39). The dilation and shear 2-forms, which are given as Eq (6.46) and Eq (6.53), respectively, are changed as follows:

$$\Delta = \frac{1}{n}\,\mathrm{Tr}\,(\,Q\,)\,\mathbf{e}^{-1} + \omega^{(E)} \wedge \omega^{(D)} \tag{C.24}$$

and

$$\not\Delta = \left(Q - \frac{1}{n}\,\mathrm{Tr}\,(\,Q\,) \right)\,\mathbf{e}^{-1} + \omega^{(E)} \wedge \omega^{(S)}\,, \tag{C.25}$$

respectively. These changes are caused by the violation of the commutativity of D and $E^I{}_J$, and, $S^I{}_J$ and $E^I{}_J$. Of course, the contraction generated by $\epsilon_{\text{ EMA with dilation−free}} = (1\,,1\,,+0\,,1)$ and $\epsilon_{\text{ EMA with shear−free}} = (1\,,1\,,1\,,+0)$ leads to $\Delta = 0$ and $\not\Delta = 0$ under the imposition of the gauge conditions given in Eq (C.14) and Eq (C.12), respectively.

The parameter space $\epsilon_{\text{ type of contraction/geometry in EMA}} = (0+\,,\epsilon^{(E)}\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ provides a set of new sort of geometric quantities. The coefficients of the third algebra of the second line and that of the second algebra of the third line in the algebra (C.23) diverge unless an appropriate set of the parameters $\epsilon^{(E)}$, $\epsilon^{(D)}$, and $\epsilon^{(S)}$ converges to zero simultaneously. The case of $\epsilon_{\text{ abelian EMA}} = (+0\,,+0\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ is the same situation as that of $\epsilon_{\text{ abelian MA}} = (+0\,,1\,,1)$ in the metric-affine case up to the difference of structure constants (local symmetry). Therefore, the intriguing cases are those of parameter spaces given by $\epsilon_{\text{ type of contraction/geometry in EMA}} = (+0\,,1\,,\epsilon^{(D)}\,,\epsilon^{(S)})$. If the contraction is performed by the parameters $\epsilon_{\text{ EMA with shear−free}} = (+0\,,1\,,1\,,+0)$ under the imposition of the gauge conditions (C.12) and (C.14) then the dilation given in Eq (C.24) remains but the shear given in Eq (C.25) turns into $\not\Delta = \omega^{(E)} \wedge \omega^{(S)}$. In the case of $\epsilon_{\text{ EMA with dilation−free}} = (+0\,,1\,,+0\,,1)$ under the same gauge conditions (C.12) and (C.14), the shear given in Eq (C.25) remains but the dilation given in Eq (C.24) turns into $\Delta = \omega^{(E)} \wedge \omega^{(D)}$. Remark, here, that the limitations of $\epsilon^{(D)} \to +0$ and $\epsilon^{(S)} \to +0$ are taken in the same order magnitude as $\epsilon^{(P)} \to +0$. The important point here is that these two algebras provide new geometric quantities, which are different from the dilation, the shear, or the non-metricity while holding the richness of the curvature and torsion 2-forms. This richness together with new geometric quantities would beyond the metric-affine geometry and yield a new class of gauge theories of gravity.

Finally, let us consider the following extended dS/AdS Lie algebra:

$$\begin{aligned}
&[P_I\,,P_J] = {C^{(A2)}}^K{}_{IJL}E^L{}_K\,,\quad [E^I{}_J\,,P_K] = {C^{(A3)}}^{IL}{}_{JK}P_L\,,\\
&[E^I{}_J\,,E^K{}_L] = {C^{(A6)}}^{IKN}{}_{JLM}E^M{}_N\,,\\
&[D\,,D] = 0\,,\quad [D\,,P_I] = P_I\,,\quad [D\,,E^I{}_J] = 0\,,\\
&[S^I{}_J\,,P_K] = \delta^I{}_K P_J\,,\quad [S^I{}_J\,,E^K{}_L] = 0\,,\quad [S^I{}_J\,,D] = 0\,,\quad [S^I{}_J\,,S^K{}_L] = 0\,,
\end{aligned} \tag{C.26}$$

where ${C^{(A2)}}^K{}_{IJL} = \epsilon\delta^K{}_J g_{IL}$, ${C^{(A3)}}^{IL}{}_{JK} = \delta^I{}_K\delta^L{}_J - g^{IL}g_{JK}$, and ${C^{(A6)}}^{IKN}{}_{JLM} = g^{IK}g_{JM}\delta^N{}_L - g^{KN}g_{JM}\delta^I{}_L - \delta^K{}_J\delta^I{}_M\delta^N{}_L + g^{KN}g_{JL}\delta^I{}_M$. If $\epsilon = +1\,,-1$ then the algebras of the first line become that of the de Sitter space and anti-de Sitter space, respectively [de Sitter (1917); Wise (2010); Blagojevic and Hehl (2012); Blagojević and Hehl (2013)]. The case of $\epsilon = 0$ is contained as a special case of the extended metric-affine algebra in the previous section 7.3. In order to perform the contraction, the generators P_I, $E^I{}_J$, D, and $S^I{}_J$ are parametrized by Eq (C.9). Then the following parametrized Lie algebras are derived:

$$\begin{aligned}
&[P'_I\,,P'_J] = \frac{(\epsilon^{(P)})^2}{\epsilon^{(E)}}{C^{(A2)}}^K{}_{IJL}E'^L{}_K\,,\quad [E'^I{}_J\,,P'_K] = \epsilon^{(E)}{C^{(A3)}}^{IL}{}_{JK}P'_L\,,\\
&[E'^I{}_J\,,E'^K{}_L] = \epsilon^{(E)}{C^{(A6)}}^{IKN}{}_{JLM}E'^M{}_N\,,\\
&[D'\,,D'] = 0\,,\quad [D'\,,P'_I] = \epsilon^{(D)}P'_I\,,\quad [D'\,,E'^I{}_J] = 0\,,\\
&[S'^I{}_J\,,P'_K] = \epsilon^{(S)}\delta^I{}_K P'_J\,,\quad [S'^I{}_J\,,E'^K{}_L] = 0\,,\quad [S'^I{}_J\,,D] = 0\,,\quad [S'^I{}_J\,,S'^K{}_L] = 0\,.
\end{aligned} \tag{C.27}$$

The contraction of the above algebra generated by $\epsilon_{\text{ Poincare in extended dS/AdS}} = (+0\,,1\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ results in that of the algebra $\mathfrak{ema}(n+1\,,\mathbb{R})$ generated by $\epsilon_{\text{ Poincare in EMA}} = (\epsilon^{(P)}\,,1\,,\epsilon^{(D)}\,,\epsilon^{(S)})$, where $\epsilon^{(P)}$, $\epsilon^{(D)}$, and $\epsilon^{(S)}$ can be taken as an arbitrary value in $(0\,,1]$. So is for the contraction of algebras between that generated by $\epsilon_{\text{ abelian Poincare in extended dS/AdS}} = (+0\,,+0\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ in the extended dS/AdS algebra and that generated by $\epsilon_{\text{ abelian Poincare in EMA}} = (\epsilon^{(P)}\,,+0\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ in the extended metric-affine algebra under the choice of the structure constants as the Poincare algebra. Remark, here, that the contractions generated by $\epsilon_{\text{ type of contraction/geometry in extended dS/AdS}} = (1\,,+0\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ do not exist due to the divergence of the factor $(\epsilon^{(P)})^2/\epsilon^{(E)}$ of the first algebra in the first line. Therefore, it is enough to consider the case of $\epsilon_{\text{ type of contraction/geometry in extended dS/AdS}} = (1\,,1\,,\epsilon^{(D)}\,,\epsilon^{(S)})$.

The contraction generated by $\epsilon_{\text{ type of contraction/geometry in extended dS/AdS}} = (1\,,1\,,\epsilon^{(D)}\,,\epsilon^{(S)})$ alternates the curvature 2-form given in Eq (6.39) as follows

$$\Omega^{(E)} = d_\nabla \omega^{(E)} = d\omega^{(E)} + \omega^{(E)} \wedge \omega^{(E)} + \mathbf{e}^{-1} \wedge \mathbf{e}^{-1}\,. \tag{C.28}$$

The torsion 2-form given in Eq (6.39) does not change. So are the dilation and shear 2-forms, which are given in Eq (6.46) and Eq (6.53), respectively. Notice that a new geometrical quantity arises; the above quantity is not the curvature 2-form in the sense of the metric-affine geometry due to the existence of the third term. That is, this departure in Eq (C.28) from the metric-affine geometry would yield a new class of gauge theories of gravity. In addition, this geometry is not just the (anti-)de Sitter geometry due to the existence of the dilation and the shear (, or equivalently, the non-metricity).

Finally, it is known that the third term in Eq (C.28) relates to the so-called cosmological constant in general relativity if the torsion, the dilation, and the shear vanish [MacDowell and Mansouri (1977); Wise (2010)]. In order to realize this, of course, it is enough to perform further contraction generated by $\epsilon_{\text{ dS/AdS}} = (1\,,1\,,+0\,,+0)$ and to impose the torsion-free condition given in Eq (C.17) and the gauge conditions (C.12) and (C.14). In addition, the contraction generated by $\epsilon_{\text{ V}_{\text{n+1}}} = (+0\,,1\,,+0\,,+0)$ removes out the third term in Eq (C.28), and the geometry results in the (semi-)Riemann geometry; this is nothing but the contraction of the metric-affine geometry generated by $\epsilon_{\,\mathrm{V_{n+1}}} = (1\,,+0\,,+0)$.

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