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# The Equivalence Theorem in the Generalized Gravity of $f(R)$ -Type and Canonical Quantization

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## 1. Introduction

Since the discovery of the accelerated expansion of the universe (Fadely et al., 2009; Fu et al., 2008; Hicken et al., 2009; Kessler et al., 2009; Massey et al., 2007; Mantz et al., 2009; Percival et al., 2009; Reid et al., 2009; Riess et al., 2009; Schrabbach et al., 2009; Suyu et al., 2009; Vikhlinin et al., 2009), (Bennet et al., 2010; Jarosik et al., 2010; Komatsu et al., 2010; Larson et al., 2010), much attention has been attracted to the generalized gravity theories of the  $f(R)$ -type (Caroll et al., 2004; Sotiriou & Faraoni, 2008; Nojiri & Odintsov, 2006). Before the discovery, such theories have been interested in because of its theoretical advantages: The theory of the graviton is renormalizable (Utiyama & DeWitt, 1962; Stelle, 1977). It seems to be possible to avoid the initial singularity of the universe which is the prediction of the theorem by Hawking (Hawking & Ellis, 1973) (Nariai, 1971; Nariai & Tomita, 1971). And inflationary model without inflaton field is possible (Starobinsky, 1980).

There is a well-known equivalence theorem between this type of theories and Einstein gravity with a scalar field (Barrow & Cotsakis, 1988; Maeda, 1989; Teyssandier & Tourrence, 1983; Wands, 1994; Witt, 1984). The theorem states that two types of theories related by a suitable conformal transformation are equivalent in the sense that the field equations of both theories lead to the same paths. Many investigations have been devoted to this issue (Magnano & Sokolowski, 1994; Sotiriou & Faraoni, 2008). In this work, we first review classical aspects of the theorem by deriving it in a self-contained and pedagogical way. Then we describe the problems of to what extent the equivalence holds. Main problems are: (i) Is the surface term given by Gibbons and Hawking (Gibbons & Hawking, 1977) which is necessary in Einstein gravity also necessary in the  $f(R)$ -type gravity? (ii) Does the equivalence hold also in quantum theory? (iii) Which metric is physical, i.e., which metric should be identified with the observed one? Next we solve the problem of the surface terms or the variational conditions. The surface term is not necessary since we can impose the variational conditions at the time boundaries that the metric and its "time derivative" can be put to be vanishing. This simplicity could be added to the advantages of  $f(R)$ -type gravity. Quantum aspects of the theorem are then summarized when we quantize the theory canonically in the framework of the generalized Ostrogradski formalism (Ezawa et al., 2006) which is a natural generalization to

the system in a curved spacetime. The main result is that if the  $f(R)$ -type theory is quantized canonically, Einstein gravity with a scalar field has to be quantized non-canonically. Brief comments are given on the problem (iii).

In section 2, the Lagrangian density and field equations for the  $f(R)$ -type gravity are summarized. In section 3, the equivalence theorem is derived in a pedagogical way. In section 4, the problems concerning the equivalence theorem are pointed out, especially to what extent the equivalence holds. In section 5, the issue of surface term is clarified. Section 6 is devoted to a description of the canonical formalism of the  $f(R)$ -type gravity and the classically equivalent Einstein gravity with a scalar field. Summary and discussions are given in section 7. Conformal transformations of geometrical quantities are summarized in the appendix.

## 2. Generalized gravity of $f(R)$ -type

Generalized gravity of  $f(R)$ -type is one of the higher curvature gravity(HCG) theories in which the action is given by

$$S = \int d^D x \mathcal{L} = \int d^D x \sqrt{-g} f(R). \quad (2.1)$$

The spacetime is taken to be  $D$ -dimensional. Here  $g \equiv \det g_{\mu\nu}$  and  $R$  is the  $D$ -dimensional scalar curvature. Taking the variational conditions at the hypersurfaces  $\Sigma_{t_1}$  and  $\Sigma_{t_2}$  ( $\Sigma_t$  is the hypersurface  $t = \text{constant}$ ) as

$$\delta g_{\mu\nu} = 0 \quad \text{and} \quad \delta \dot{g}_{\mu\nu} = 0, \quad (2.2)$$

field equations are derived by the variational principle as follows:

$$-\frac{\delta \mathcal{L}}{\delta g_{\mu\nu}(x)} = \sqrt{-g} \left[ f'(R) R^{\mu\nu} - \frac{1}{2} f(R) g^{\mu\nu} - \nabla^\mu \nabla^\nu f'(R) + g^{\mu\nu} \square f'(R) \right] = 0, \quad (2.3a)$$

or

$$G_{\mu\nu} = \frac{1}{f'(R)} \left[ \frac{1}{2} (f(R) - R f'(R)) g_{\mu\nu} - (g_{\mu\nu} \square - \nabla_\mu \nabla_\nu) f'(R) \right], \quad (2.3b)$$

where a prime represents the differentiation with respect to  $R$ ,  $\nabla_\mu$  the covariant derivative with respect to the metric  $g_{\mu\nu}$  and  $G_{\mu\nu}$  is the  $D$ -dimensional Einstein tensor. Equations (2.3a,b) are the 4-th order partial differential equations, so the above variational conditions are allowed. Further discussions on this issue will be given in Section 5.

Here we comment on the dimensionality of  $f(R)$ . Comparing the action  $S$  with the Einstein-Hilbert one

$$S_{E-H} = \frac{1}{2\kappa_D^2} \int d^D x \sqrt{-g} R, \quad (2.4)$$

where  $\kappa_D \equiv \sqrt{8\pi G_D}$  with  $G_D$  the  $D$ -dimensional gravitational constant, we obtain the dimension of  $f'(R)$  to be equal to that of  $\kappa_D^{-2}$ , so that

$$[f'(R)] = [\kappa_D^{-2}] = [L^{2-D}]. \quad (2.5)$$

It is well known that this type of theory is transformed to Einstein gravity with a scalar field by a conformal transformation, which is usually referred to as equivalence theorem. We will review and clarify the content of the theorem.

### 3. Equivalence theorem

The theorem concerns with the conformal transformation

$$\tilde{g}_{\mu\nu} \equiv \Omega^2 g_{\mu\nu}. \quad (3.1)$$

In terms of the transformed Einstein tensor, field equations (2.3b) are written as

$$\begin{aligned} \tilde{G}_{\mu\nu} = & \frac{1}{f'(R)} \nabla_\mu \nabla_\nu f'(R) - (d-1) \nabla_\mu \nabla_\nu (\ln \Omega) - g_{\mu\nu} \left[ \frac{1}{f'(R)} \square f'(R) - (d-1) \square (\ln \Omega) \right] \\ & + (d-1) \partial_\mu (\ln \Omega) \partial_\nu (\ln \Omega) + g_{\mu\nu} \left[ \frac{f(R) - R f'(R)}{2 f'(R)} + \frac{(d-1)(d-2)}{2} \partial_\lambda (\ln \Omega) \partial^\lambda (\ln \Omega) \right], \end{aligned} \quad (3.2)$$

where we put  $D \equiv 1 + d$  (i.e.  $d$  is the dimension of the space). Eqs.(3.2) are the field equations after the conformal transformation. If they are the equations for Einstein gravity with a scalar field, 2nd order derivatives on the right hand side should vanish. From this requirement,  $\Omega$  is determined to be

$$\Omega^2 = \left[ 2\kappa_D^2 f'(R) \right]^{2/(d-1)}. \quad (3.3)$$

The coefficient of  $f'(R)$  in the square bracket, which can be any constant, was chosen to be  $2\kappa_D^2$  in order to make  $\Omega$  to be dimensionless and equal to unity for Einstein gravity. So, (3.1) takes the following form

$$\tilde{g}_{\mu\nu} = \left[ 2\kappa_D^2 f'(R) \right]^{2/(d-1)} g_{\mu\nu}. \quad (3.4)$$

Scalar field is defined as

$$\kappa_D \tilde{\phi} \equiv \sqrt{d(d-1)} \ln \Omega = \sqrt{d/(d-1)} \ln [2\kappa_D^2 f'(R)], \quad (3.5a)$$

or

$$\begin{aligned} f'(R) &= \frac{1}{2\kappa_D^2} \exp \left( \sqrt{(d-1)/d} \kappa_D \tilde{\phi} \right), \\ \ln \Omega &= \frac{1}{\sqrt{d(d-1)}} \kappa_D \tilde{\phi}. \end{aligned} \quad (3.5b)$$

The coefficient of  $\ln \Omega$ , or equivalently  $\ln [2\kappa_D^2 f'(R)]$ , in (3.5a) was chosen for the right-hand side of (3.2) to take the usual form of scalar field source. Solving (3.5) for  $R$ , we denote the solution as

$$R = r(\tilde{\phi}). \quad (3.6)$$

In terms of  $\tilde{\phi}$ , (3.2) takes the following form

$$\tilde{G}_{\mu\nu} = \kappa_D^2 \left[ \partial_\mu \tilde{\phi} \partial_\nu \tilde{\phi} + \tilde{g}_{\mu\nu} \left( -\frac{1}{2} \partial_\lambda \tilde{\phi} \partial^\lambda \tilde{\phi} - V(\tilde{\phi}) \right) \right], \quad (3.7)$$

where  $\tilde{\partial}\tilde{\phi} \equiv \tilde{g}^{\lambda\rho}\partial_\rho\tilde{\phi}$  and

$$V(\tilde{\phi}) \equiv -f(r(\tilde{\phi})) \exp\left(-\frac{d+1}{\sqrt{d(d-1)}}\kappa_D\tilde{\phi}\right) + \frac{1}{2\kappa_D^2}r(\tilde{\phi}) \exp\left(-\frac{2}{\sqrt{d(d-1)}}\kappa_D\tilde{\phi}\right). \quad (3.8)$$

Field equation for the scalar field is obtained by taking the trace of (3.2) as

$$\tilde{\square}\tilde{\phi} = -\frac{\kappa_D}{\sqrt{d(d-1)}} \exp\left(-\frac{d+1}{\sqrt{d(d-1)}}\kappa_D\tilde{\phi}\right) \left[(d+1)f(r(\tilde{\phi})) - \kappa_D^{-2}r(\tilde{\phi}) \exp\left(\sqrt{(d-1)/d}\kappa_D\tilde{\phi}\right)\right]. \quad (3.9)$$

Equations (3.7) and (3.9) are obtained also by the variational principle with the following Lagrangian density:

$$\tilde{\mathcal{L}} = \tilde{\mathcal{L}}_G + \tilde{\mathcal{L}}_{\tilde{\phi}}, \quad (3.10)$$

where

$$\tilde{\mathcal{L}}_G = \frac{1}{16\pi G_D} \sqrt{-\tilde{g}}\tilde{R}, \quad \tilde{\mathcal{L}}_{\tilde{\phi}} = \sqrt{-\tilde{g}}\left[-\frac{1}{2}\partial_\lambda\tilde{\phi}\tilde{\partial}^\lambda\tilde{\phi} - V(\tilde{\phi})\right]. \quad (3.11)$$

Here

$$\sqrt{-\tilde{g}} = \left[2\kappa_D^2 f'(R)\right]^{(d+1)/(d-1)} \sqrt{-g}, \quad (3.12)$$

and

$$\tilde{R} = \left[2\kappa_D^2 f'(R)\right]^{-2/(d-1)} \left[R - \frac{2d}{d-1} \left(\frac{1}{f'(R)}\square f'(R) - \frac{1}{2} \frac{1}{f'(R)^2} \partial_\lambda f'(R) \partial^\lambda f'(R)\right)\right]. \quad (3.13)$$

$\tilde{\mathcal{L}}_{\tilde{\phi}}$  is given by terms in the parenthesis multiplying  $\tilde{g}_{\mu\nu}$  in (3.7) and  $V(\tilde{\phi})$  is given by (3.8). It is noted that this Lagrangian density  $\tilde{\mathcal{L}}$  is not equal to the Lagrangian density  $\mathcal{L}$  in (2.1) which, in terms of the transformed variables  $\tilde{g}_{\mu\nu}$  and  $\tilde{\phi}$ , is expressed as

$$\mathcal{L} = \sqrt{-g}f(r(\tilde{\phi})) \exp\left(-\frac{d+1}{\sqrt{d(d-1)}}\kappa_D\tilde{\phi}\right).$$

Thus from the field equations (2.3b) for the  $f(R)$ -type gravity, field equations for  $\tilde{g}_{\mu\nu}$  with the source of the scalar field and the field equation for the scalar field are derived. So the equivalence seems to be shown. However, eqs.(2.3b) are 10 4-th order differential equations for 10 component  $g_{\mu\nu}$ , so that, to obtain a unique set of solutions, 40 initial conditions seem to be required. On the other hand eqs.(3.7) are 10 2nd order differential equations for 10 component  $\tilde{g}_{\mu\nu}$ , only 20 initial conditions are required to have a set of unique solution. Similarly, eq.(3.9) requires only 2 initial conditions. Therefore equivalence does not appear to hold if the initial conditions are taken into account. This apparent breakdown comes from the fact that the 40 initial conditions are not independent, which is easily seen in canonical formalism (see section 5).

The above result that the variational equations of both theories coincide is usually stated as "HCG described by the Lagrangian density  $\mathcal{L}$  is equivalent to Einstein gravity with a scalar field described by the Lagrangian density  $\tilde{\mathcal{L}}$ " and is referred to as the equivalence theorem. Note, however, that the variational equations hold on the paths that make the action stationary. Ref.(Magnano & Sokolowski, 1994) is recommended as a good review on the equivalence theorem. For recent investigations, see Ref.(Faraoni & Nadeau, 2007) and

references cited in these references. We use the following usual terminology on this issue:

$$\begin{cases} \text{descriptions with } \mathcal{L} : \text{descriptions in the Jordan frame} \\ \text{descriptions with } \tilde{\mathcal{L}} : \text{descriptions in the Einstein frame} \end{cases}$$

## 4. Problems

We have seen that the equivalence of the two theories hold at least on the classical paths which can be determined by the variational principle. However, there would be problems on the other kinds of equivalence. In order to examine these problems, we note the following:

1. The theories are not conformally invariant.
2. The physical metric is identified with the one determined from observations.

Unsettled problems include the following:

(I) To what extent the equivalence would hold?

(I-1) In the Einstein frame, it is well known that the surface term given by Gibbons and Hawking (GH term) is necessary. It is often argued that, from the equivalence point of view, surface term is necessary also in the Jordan frame (Dyer & Hinterbichler, 2009). However, this equivalence is not taken for granted, but should be examined carefully. The examination is given in the next section.

(I-2) Would the equivalence hold also in quantum theory? If the equivalence holds in the canonical quantum theories, fundamental Poisson brackets should be equivalent. That is, the fundamental Poisson brackets in one frame should be derived from those of the other frame.

(II) Which metric is physical in the sense that should be identified with the observed one?

This problem has been investigated from various aspects (Magnano & Sokolowski, 1994). If the metric in the Einstein frame is physical (Chiba, 2003), HCG has no essential meaning and it appears by the choice of unphysical frame. If the metric in the Jordan frame is physical, the equivalence theorem states that the metric in this frame has one more scalar degrees of freedom which could be observed as non-transverse-traceless polarization of gravitational waves (Alves et al. 2009, 2010) in future observations. Furthermore, equivalence theorem states that, instead of treating the complicated Jordan frame, we can use the simpler and familiar Einstein frame for calculation. However, for comparison with observations, the results should be expressed in the words of Jordan frame. It should be noted only one of the metrics is physical. In the following, assuming that the metric in the Jordan frame is physical, we restrict ourselves to the description of problem (I).

## 5. Surface terms

### 5.1 General considerations

We first consider discrete systems whose Lagrangians contain the time derivatives of the generalized coordinates  $q^i$  up to the  $n$ -th order  $q^{i(n)}$ . If the  $n$ -th order derivatives are contained non-linearly the equations of motion are  $2n$ -th order differential equations. Then  $2n$  conditions are necessary for each  $q^i$  to determine the solution uniquely. These conditions can be given by

$2n$  initial conditions or  $n$  boundary conditions at two times,  $t_1$  and  $t_2$ . The latter conditions can be taken to be the values of the generalized coordinates themselves and their time derivatives up to the  $(n - 1)$ -th order. Then we can take the variational conditions (boundary conditions) as

$$\delta q^{i(k)}(t_1) = \delta q^{i(k)}(t_2) = 0, \quad (k = 0, 1, \dots, n - 1). \quad (5.1)$$

Therefore no boundary terms are necessary.

On the other hand, if the  $n$ -th order derivatives are contained linearly, equations of motion are at most  $(2n - 1)$ -th order differential equations. Then at least one condition in (5.1) does not hold generally. Therefore special solutions are required to satisfy all the conditions in (5.1) and to eliminate generally the corresponding variations at the boundaries, boundary terms are necessary. In other words, in order that the equations of motion and the variational conditions are compatible, boundary terms are required.

For continuous systems, or fields, we can proceed similarly, i.e. if the Lagrangian contains the highest order derivatives linearly, surface terms are required to eliminate some of the variations of derivatives at the boundaries.

## 5.2 $f(R)$ -type gravity

In this theory, the Lagrangian density contains the components of the metric, the generalized coordinates, and their derivatives up to the second order in a non-linear way. So from the general considerations above, no surface terms are necessary. Concrete situations are as follows.

The variational principle leads to the field equations which are 4-th order differential equations, (3.2), so that 40 conditions are formally required to decide the solution for the metric uniquely, although they are not independent. These conditions can be taken to be the initial functions of the components of the metric  $g_{\mu\nu}$  itself and their derivatives up to the 3rd order, or  $g_{\mu\nu}$  and their first order derivatives at 2 times  $t = t_1$  and  $t = t_2$ . The latter conditions correspond to the variational conditions at the time boundaries. That is, at 2 time boundaries  $t = t_1$  and  $t = t_2$ , variational conditions are taken as  $\delta g_{\mu\nu} = 0$  and  $\delta \dot{g}_{\mu\nu} = 0$  given by (2.2). In fact the Lagrangian density contains up to the 2nd order derivatives non-linearly, no surface term is necessary.

## 5.3 Einstein gravity with a scalar field

In this theory, the gravity theory is the Einstein one and if we start from the Lagrangian density  $\tilde{\mathcal{L}}$ , (3.10), whose gravitational part  $\tilde{\mathcal{L}}_G$  contains the second order derivatives of the metric linearly, surface term e.g. the GH term, is necessary from the above considerations. Some arguments exist that if we require the equivalence also in the boundary terms, surface term is necessary also in the  $f(R)$ -type gravity (Dyer & Hinterbichler, 2009). This is not the case. This equivalence should be examined carefully. The situation can be seen by examining the variation. If the theory is obtained from the  $f(R)$ -type theory by the conformal transformation,  $\tilde{g}_{\mu\nu} = [2\kappa_D^2 f'(R)]^{2/(d-1)} g_{\mu\nu}$  and if we express the variation of this quantity and  $\tilde{\phi}$  in terms of



the variations in the Jordan frame, we have the following relations:

$$\begin{cases} \delta \tilde{g}_{\mu\nu} = \left[ 2\kappa_D^2 f'(R) \right]^{2/(d-1)} \delta g_{\mu\nu} + \frac{4\kappa_D^2}{d-1} \left[ 2\kappa_D^2 f'(R) \right]^{-(d-3)/(d-1)} g_{\mu\nu} \delta f'(R), \\ \delta \tilde{\phi} = \kappa_D^{-1} \sqrt{d/(d-1)} \frac{1}{f'(R)} \delta f'(R), \end{cases} \quad (5.2)$$

where

$$\delta f'(R) = \frac{\partial f'}{\partial g_{\alpha\beta}} \delta g_{\alpha\beta} + \frac{\partial f'}{\partial (\partial_\lambda g_{\alpha\beta})} \delta (\partial_\lambda g_{\alpha\beta}) + \frac{\partial f'}{\partial (\partial_\lambda \partial_\rho g_{\alpha\beta})} \delta (\partial_\lambda \partial_\rho g_{\alpha\beta}). \quad (5.3)$$

Therefore, if both sets of the variational conditions

$$\delta \tilde{g}_{\mu\nu} = \delta \tilde{\phi} = 0, \quad (5.4)$$

which are usually taken for  $\tilde{\mathcal{L}}$  and (2.2),  $\delta g_{\mu\nu} = \delta \dot{g}_{\mu\nu} = 0$ , are imposed, we have

$$\delta \ddot{g}_{\mu\nu} = 0, \quad (5.5)$$

at the boundary. However, this is not generally possible, but would require specific solutions as noted above. That is, the variational conditions, which require the GH term in the Einstein gravity with a scalar field, are different from those in the  $f(R)$ -type theory. To compare the surface terms, the variational conditions have to be carefully treated.

The above situation is related to the fact that the conformal transformation is not the transformation of the generalized coordinates,  $g_{\mu\nu}$ , but the transformation depending on the 2nd order derivatives of them. Comparison of the surface terms is made as follows. When  $\tilde{\mathcal{L}}$  is expressed in terms of the metric in the Jordan frame,  $g_{\mu\nu}$ , it is written as follows:

$$\tilde{\mathcal{L}} = \mathcal{L} - \partial_\lambda \left( \frac{2d}{d-1} \sqrt{-g} \partial^\lambda f'(R) \right). \quad (5.6)$$

Since  $\mathcal{L}$  requires no surface term when the variational condition (2.2) are taken, the second term on the right-hand side is the surface term which is different from the GH term. This is an example that surface terms depend on the boundary conditions.

## 6. Canonical formalism

The canonical formalism belongs to classical physics. However, most quantum theory is obtained by canonical quantization which requires that commutation relations among the fundamental quantities are proportional to the corresponding Poisson brackets, e.g. for one dimensional system

$$[\hat{q}, \hat{p}] = i\hbar \{q, p\}_{PB},$$

where a hat represents an operator. It is noted that one of the proportional factor  $i$  assures that the observables are Hermitian operators and the other  $\hbar$  adjusts the dimensionality, a very natural proportional factors.

Canonical quantum theories are very successful and only well-known failure is the theory of gravitons in general relativity. On the other hand, the canonical quantum theory of gravitons



in  $f(R)$ -type gravity is known to be renormalizable (Utiyama & DeWitt, 1962; Stelle, 1977). This suggests a possibility that the equivalence theorem would be violated in quantum theory. The violation might come from the fact that classical equivalence means the equivalence along the classical paths. While, the Poisson brackets require derivatives in all directions in the phase space. The laws of usual canonical quantum theory describe the dynamics of matter and radiation which have duality of waves and particles assured by experiments. On the other hand, gravity describes the dynamics of spacetime. However, no nature of spacetime similar to the duality has been observed. Investigation of quantum gravity arises from various motivations. For example, since the gravity mediates interactions of elementary particles, it would be natural that the gravity is also described quantum mechanically. A preferable possibility that fundamental laws of nature would take forms of quantum theory is also one of them. The canonical quantum theory would be the first candidate for quantum gravity. Therefore a canonical formalism of gravity is very important. In this section results on a canonical formalism, a generalization of the Ostrogradski formalism, are reviewed. In the following, we use a unit for which  $2\kappa_D^2 = 1$ .

### 6.1 Canonical formalism in the Einstein frame

We adopt the ADM method for the gravitational field (Arnowitt et al., 2006), so the procedure is well known.

#### (1) Gravitational field

The spacetime is supposed to be constructed from the hypersurfaces  $\Sigma_t$  with  $t = \text{constant}$  (foliation of spacetime). The dynamics of the spacetime determines the evolution of the hypersurface. So the generalized coordinates are the metric of the  $d$ -dimensional hypersurface  $\tilde{h}_{ij}(\mathbf{x}, t)$ .

Since  $\tilde{R}$  contains 2nd order time derivatives linearly, we first make a partial integration to transform the Lagrangian density of the gravitational part in (3.11) to the following GH form:

$$\tilde{\mathcal{L}}_h = \sqrt{\tilde{h}} \tilde{N} [\tilde{K}_{ij} \tilde{K}^{ij} - \tilde{K}^2 + \tilde{\mathbf{R}}], \quad (6.1)$$

where  $\tilde{K}$  is the trace of the extrinsic curvature  $\tilde{K}_{ij}$  ( $\tilde{K} \equiv \tilde{h}^{ij} \tilde{K}_{ij}$ ) and  $\tilde{\mathbf{R}}$  is the scalar curvature constructed from  $\tilde{h}_{ij}$ .

Canonical formalism is obtained by the Legendre transformation as usual. The momenta  $\tilde{\pi}^{ij}$  canonically conjugate to  $\tilde{h}_{ij}$  are defined as

$$\tilde{\pi}^{ij} \equiv \frac{\partial \tilde{\mathcal{L}}_h}{\partial (\partial_0 \tilde{h}_{ij})} = \sqrt{\tilde{h}} [\tilde{K}^{ij} - \tilde{h}^{ij} \tilde{K}], \quad (6.2)$$

where  $\tilde{h} \equiv \det \tilde{h}_{ij}$  and  $\tilde{N}$  is the lapse function. The extrinsic curvature  $\tilde{K}_{ij}$  with respect to  $\tilde{h}_{ij}$  is defined as

$$\tilde{K}_{ij} \equiv \frac{1}{2} \tilde{N}^{-1} (\partial_0 \tilde{h}_{ij} - \tilde{N}_{ij} - \tilde{N}_{ji}), \quad (6.3)$$

$\tilde{N}_i$  is the shift vector. A semicolon ; represents a covariant derivative with respect to  $\tilde{h}_{ij}$ . Solving (6.3) for  $\tilde{K}_{ij}$ , we have

$$\tilde{K}^{ij} = \frac{1}{\sqrt{\tilde{h}}} \left[ \tilde{\pi}^{ij} - \frac{1}{d-1} \tilde{h}^{ij} \tilde{\pi} \right] \quad \text{and} \quad \tilde{K} = -\frac{\tilde{\pi}}{(d-1)\sqrt{\tilde{h}}}. \quad (6.4)$$

Hamiltonian density is given as

$$\begin{aligned} \tilde{\mathcal{H}}_h &= \tilde{\pi}^{ij} \dot{\tilde{h}}_{ij} - \tilde{\mathcal{L}}_h \\ &= \tilde{N} \left[ G_{ijkl} \tilde{\pi}^{ij} \tilde{\pi}^{kl} - \sqrt{\tilde{h}} \tilde{\mathbf{R}} \right] + 2(\tilde{\pi}^{ij} \tilde{N}_i)_{;j} - 2\tilde{\pi}^{ij}_{;j} \tilde{N}_i. \end{aligned} \quad (6.5)$$

where

$$G_{ijkl} \equiv \frac{1}{2\sqrt{\tilde{h}}} \left( \tilde{h}^{ik} \tilde{h}^{jl} + \tilde{h}^{il} \tilde{h}^{jk} - \frac{2}{d-1} \tilde{h}^{ij} \tilde{h}^{kl} \right), \quad (6.6)$$

is sometimes referred to as supermetric. In deriving (6.5), we used the expression for  $\tilde{\mathcal{L}}_h$ , expressed in terms of canonical variables, as follows

$$\tilde{\mathcal{L}}_h = \frac{\tilde{N}}{\sqrt{\tilde{h}}} \left[ \tilde{\pi}^{ij} \tilde{\pi}_{ij} - \frac{1}{d-1} \tilde{\pi}^2 + \tilde{h} \tilde{\mathbf{R}} \right]. \quad (6.7)$$

## (2) Scalar field

The generalized coordinate is  $\tilde{\phi}(\mathbf{x}, t)$ . Momenta canonically conjugate to  $\tilde{\phi}$  is defined as usual by

$$\tilde{\pi}(\mathbf{x}, t) \equiv \frac{\partial \tilde{\mathcal{L}}_\phi}{\partial(\partial_0 \tilde{\phi}(\mathbf{x}, t))} = -\sqrt{\tilde{g}} \tilde{g}^{0\mu} \partial_\mu \tilde{\phi} = \tilde{N}^{-1} \sqrt{\tilde{h}} \left[ \partial_0 \tilde{\phi} - \tilde{N}^i \partial_i \tilde{\phi} \right], \quad (6.8a)$$

so

$$\partial_0 \tilde{\phi} = \frac{\tilde{N}}{\sqrt{\tilde{h}}} \left[ \tilde{\pi} + \tilde{N}^{-1} \sqrt{\tilde{h}} \tilde{N}^i \partial_i \tilde{\phi} \right] = \frac{\tilde{N}}{\sqrt{\tilde{h}}} \tilde{\pi} + \tilde{N}^i \partial_i \tilde{\phi}. \quad (6.8b)$$

In terms of canonical variables,  $\tilde{\mathcal{L}}_\phi$  is expressed as follows

$$\tilde{\mathcal{L}}_\phi = \tilde{N} \left[ \frac{1}{2\sqrt{\tilde{h}}} \tilde{\pi}^2 - \frac{1}{2} \sqrt{\tilde{h}} \tilde{h}^{ij} \partial_i \tilde{\phi} \partial_j \tilde{\phi} - V(\tilde{\phi}) \right].$$

Using this, we have the following expression for the Hamiltonian density

$$\tilde{\mathcal{H}}_\phi = \tilde{\pi} \dot{\tilde{\phi}} - \tilde{\mathcal{L}}_\phi = \frac{\tilde{N}}{2\sqrt{\tilde{h}}} \tilde{\pi}^2 + \tilde{N}^i \partial_i \tilde{\phi} \tilde{\pi} + \frac{1}{2} \tilde{N} \sqrt{\tilde{h}} \tilde{h}^{ij} \partial_i \tilde{\phi} \partial_j \tilde{\phi} + V(\tilde{\phi}). \quad (6.9)$$

## (3) Fundamental Poisson brackets

Nonvanishing fundamental Poisson brackets in the Einstein frame are given as

$$\{\tilde{h}_{ij}(\mathbf{x}, t), \tilde{\pi}^{kl}(\mathbf{y}, t)\}_{PB} = \delta_{(ij)}^{kl} \delta(\mathbf{x} - \mathbf{y}) \quad \text{and} \quad \{\tilde{\phi}(\mathbf{x}, t), \tilde{\pi}(\mathbf{y}, t)\}_{PB} = \delta(\mathbf{x} - \mathbf{y}), \quad (6.10)$$

where  $(ij)$  expresses the symmetrization and not the symmetric part.

## 6.2 Canonical formalism in the Jordan frame

There are several canonical formalisms for generalized gravity theories in the Jordan frame. Among them formalism given by Buchbinder and Lyakhovich (Buchbinder & Lyakhovich, 1987) is logically very simple. However, concrete calculation is somewhat cumbersome partly due to arbitrariness although it allows a wide application. In addition, the Hamiltonian is generally transformed under the transformation of generalized coordinates that does not depend on time explicitly. Here we use the formalism which is a generalization of the well-known one given by Ostrogradski (Ezawa et al., 2010). For comparison of typical formalisms, see (Deruelle et al., 2009).

### (1) Generalized coordinates

In this frame, we also use the foliation of the spacetime. Since the  $f(R)$ -type gravity is a higher-derivative theory, we follow the modified Ostrogradski formalism in which the time derivatives in the Ostrogradski formalism is replaced by Lie derivatives along the timelike normal  $n$  to the hypersurface  $\Sigma_t$  in the ADM formalism (Ezawa et al., 2006, 2010). So the generalized coordinates are

$$h_{ij}(\mathbf{x}, t) \quad \text{and} \quad K_{ij}(\mathbf{x}, t) = \frac{1}{2} \mathcal{L}_n h_{ij}(\mathbf{x}, t) \equiv Q_{ij}(\mathbf{x}, t). \quad (6.11)$$

Here contravariant and covariant components of  $n$  are given as follows:

$$n^\mu = N^{-1}(1, -N^i) \quad \text{and} \quad n_\mu = N(-1, 0, 0, 0). \quad (6.12)$$

### (2) Conjugate momenta

Denoting the momenta canonically conjugate to these generalized coordinates as  $\pi^{ij}$  and  $\Pi^{ij}$  respectively, we have from the modified Ostrogradski transformation

$$\begin{cases} \pi^{ij} = -\sqrt{h} \left[ f'(R) Q^{ij} + h^{ij} f''(R) \mathcal{L}_n R \right], \\ \Pi^{ij} = 2\sqrt{h} f'(R) h^{ij}. \end{cases} \quad (6.13)$$

From (6.13), it is seen that  $\Pi^{ij}$  has only the trace part, so it is expressed as

$$\Pi^{ij} = \frac{1}{d} \Pi h^{ij} \quad \text{and} \quad \Pi = 2d\sqrt{h} f'(R). \quad (6.14)$$

From the second equation, we have

$$f'(R) = \frac{\Pi}{2d\sqrt{h}} \quad \text{or} \quad R = f'^{-1}(\Pi/2d\sqrt{h}) \equiv \psi(\Pi/2d\sqrt{h}). \quad (6.15)$$

Correspondingly, it is also seen from (6.13) that the traceless part of  $Q_{ij}$  is related to that of  $\pi^{ij}$ , and we have

$$Q^{ij} = -\frac{2}{P} \pi^{ij} + \frac{1}{d} h^{ij} Q, \quad (6.16)$$

where

$$P \equiv \frac{\Pi}{d}, \quad (6.17)$$

and

$$\pi^{\dagger ij} \equiv \pi^{ij} - \frac{1}{d} h^{ij} \pi \quad (6.18)$$

is the traceless part. A dagger is used to represent the traceless part.  $(Q, P)$  is one of the canonical pairs. In terms of these variables, the scalar curvature is expressed as follows

$$R = 2h^{ij} \mathcal{L}_n Q_{ij} + Q^2 - 3Q_{ij} Q^{ij} + \mathbf{R} - 2\Delta(\ln N). \quad (6.19)$$

### (3) Hamiltonian density

In the modified Ostrogradski formalism, Hamiltonian density is defined as

$$\mathcal{H} \equiv \pi^{ij} \dot{h}_{ij} + \Pi^{ij} \dot{Q}_{ij} - \mathcal{L}. \quad (6.20)$$

Using

$$\mathcal{L}_n Q_{ij} = N^{-1} (\partial_0 Q_{ij} - N^k Q_{ij;k} - N^k_{;i} Q_{kj} - N^k_{;j} Q_{ik} - N^{-1} \partial_i N \partial_j N) \quad (6.21)$$

and eqs. (6.14)–(6.19), we have an explicit expression for  $\mathcal{H}$  as follows:

$$\begin{aligned} \mathcal{H} = N & \left[ \frac{2}{P} \pi^{\dagger ij} \pi^{\dagger}_{ij} + \frac{2}{d} Q \pi + \frac{1}{2} P \psi(P/2\sqrt{h}) - \frac{d-3}{2d} Q^2 P - \frac{1}{2} \mathbf{R} P + \Delta P - \sqrt{h} f(\psi(P/2\sqrt{h})) \right] \\ & + N^k \left[ 2\pi^{\dagger}_{kj}{}^{;j} - \frac{2}{d} \pi_{;k} + P \partial_k Q - \frac{2}{d} (QP)_{;k} \right] \\ & + \left[ -2N_j \pi^{\dagger ij} + \frac{2}{d} N^i (\pi + QP) + \partial^i NP - NP^{;i} \right]_{;i}. \end{aligned} \quad (6.22)$$

### (4) Fundamental Poisson brackets

Non-vanishing fundamental Poisson brackets are the following:

$$\{h_{ij}(\mathbf{x}, t), \pi^{kl}(\mathbf{y}, t)\}_{PB} = \delta^i_{(k} \delta^j_{l)} \delta(\mathbf{x} - \mathbf{y}), \quad (6.23a)$$

and

$$\{Q_{ij}(\mathbf{x}, t), \Pi^{kl}(\mathbf{y}, t)\}_{PB} = \delta^i_{(k} \delta^j_{l)} \delta(\mathbf{x} - \mathbf{y}). \quad (6.23b)$$

### (5) Wheeler-DeWitt equation

A primary application of the canonical formalism is the Wheeler-DeWitt (WDW) equation (DeWitt, 1967). Before writing down the WDW equation, we make a canonical transformation

$$(Q, P) \rightarrow (\tilde{Q}, \tilde{P}) \equiv (P, -Q), \quad (6.24)$$

which removes the negative powers of the momentum  $P$ . The resulting Hamiltonian is expressed as follows:

$$\mathcal{H} = N \mathcal{H}_0 + N^k \mathcal{H}_k + \text{divergent term}, \quad (6.25)$$

where

$$\left\{ \begin{array}{l} \mathcal{H}_0 = \frac{2}{Q} \pi^{+ij} \pi_{ij}^+ - \frac{2}{d} P \pi + \frac{1}{2} Q \psi(Q/2\sqrt{h}) - \frac{d-3}{2d} Q P^2 - \frac{1}{2} \mathbf{R} Q \\ \quad - \sqrt{h} f(\psi(Q/2\sqrt{h})) + \Delta Q, \\ \mathcal{H}_k = 2\pi_{kj}^{+ij} - \frac{2}{d} \pi_{;k} - Q P_{;k} + \frac{2}{d} (QP)_{;k}. \end{array} \right. \quad (6.26)$$

The WDW equation is written as

$$\hat{\mathcal{H}}_0 \Psi = 0, \quad (6.27)$$

where  $\hat{\mathcal{H}}_0$  is obtained from  $\mathcal{H}_0$  by replacing  $\pi^{ij}$  and  $P$  with  $-i\partial/\partial h_{ij}$  and  $-i\partial/\partial Q$ , respectively. However, in order to apply (6.27) to the observed universe after compactification, we first carry out the dimensional reduction and then we should take into account the cosmological principle. Such procedures were done using the formalism of Buchbinder and Lyakhovich which, although is generally different from the one described above, is very similar in the case of gravity (Ezawa et al., 1994). It was shown by the semiclassical approximation method that the internal space could be stabilized.

### 6.3 Compatibility of the two sets of fundamental Poisson brackets

#### (1) Compatibility conditions

The canonical variables in the Einstein frame can be expressed in terms of those in the Jordan frame. So we can calculate the left hand sides of (6.10) using (6.23a,b). The compatibility conditions are that the results are the right hand sides of (6.10), i.e. the following relations should be satisfied:

$$\begin{aligned} \{\tilde{h}_{ij}(\mathbf{x}, t), \tilde{\pi}^{kl}(\mathbf{y}, t)\}_{PB} &= \sum_{m,n} \int d^d \mathbf{z} \left[ \left\{ \frac{\partial \tilde{h}_{ij}(\mathbf{x}, t)}{\partial h_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\pi}^{kl}(\mathbf{y}, t)}{\partial \pi^{mn}(\mathbf{z}, t)} - \frac{\partial \tilde{\pi}^{kl}(\mathbf{y}, t)}{\partial h_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{h}_{ij}(\mathbf{x}, t)}{\partial \pi^{mn}(\mathbf{z}, t)} \right\} \right. \\ &\quad \left. + \left\{ \frac{\partial \tilde{h}_{ij}(\mathbf{x}, t)}{\partial Q_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\pi}^{kl}(\mathbf{y}, t)}{\partial \Pi^{mn}(\mathbf{z}, t)} - \frac{\partial \tilde{\pi}^{kl}(\mathbf{y}, t)}{\partial Q_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{h}_{ij}(\mathbf{x}, t)}{\partial \Pi^{mn}(\mathbf{z}, t)} \right\} \right] \\ &= \delta_{(k}^i \delta_{l)}^j \delta(\mathbf{x} - \mathbf{y}), \end{aligned} \quad (6.28)$$

and

$$\begin{aligned} \{\tilde{\phi}(\mathbf{x}, t), \tilde{\pi}(\mathbf{y}, t)\}_{PB} &= \sum_{m,n} \int d^d \mathbf{z} \left[ \left\{ \frac{\partial \tilde{\phi}(\mathbf{x}, t)}{\partial h_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\pi}(\mathbf{y}, t)}{\partial \pi^{mn}(\mathbf{z}, t)} - \frac{\partial \tilde{\pi}(\mathbf{y}, t)}{\partial h_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\phi}(\mathbf{x}, t)}{\partial \pi^{mn}(\mathbf{z}, t)} \right\} \right. \\ &\quad \left. + \left\{ \frac{\partial \tilde{\phi}(\mathbf{x}, t)}{\partial Q_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\pi}(\mathbf{y}, t)}{\partial \Pi^{mn}(\mathbf{z}, t)} - \frac{\partial \tilde{\pi}(\mathbf{y}, t)}{\partial Q_{mn}(\mathbf{z}, t)} \frac{\partial \tilde{\phi}(\mathbf{x}, t)}{\partial \Pi^{mn}(\mathbf{z}, t)} \right\} \right] \\ &= \delta(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (6.29)$$

Other fundamental Poisson brackets should vanish. These conditions may lead to some restrictions on  $f(R)$ .

## (2) Expression of the conformal transformation in terms of canonical variables

Using (3.4), (6.2), (6.3) and (6.8a,b), we obtain the following form of the conformal transformation expressing the canonical variables in the Einstein frame in terms of those in the Jordan frame:

$$\left\{ \begin{array}{l} \tilde{h}_{ij} = f'(R)^{2/(d-1)} h_{ij} = \left( P/2\sqrt{h} \right)^{2/(d-1)} h_{ij}, \\ \tilde{\phi} = \sqrt{d/(d-1)} \ln \left( P/2\sqrt{h} \right), \\ \tilde{\pi} = \sqrt{d/2(d-1)} N^{-1} \left[ \partial_0 P - P(NQ + N^i_{;i}) - N^i P_{;i} \right], \\ \tilde{N} = \left( P/2\sqrt{h} \right)^{1/(d-1)} N, \quad \tilde{N}^i = N^i, \\ \tilde{\pi}^{ij} = \left( P/2\sqrt{h} \right)^{(d-3)/(d-1)} \sqrt{h} \left[ -\frac{2}{P} \pi^{ij} + h^{ij} \left\{ \frac{1}{d} Q - (NP)^{-1} \left( \partial_0 P - N^k P_{;k} \right) - N^{-1} N^k_{;k} \right\} \right]. \end{array} \right. \quad (6.30)$$

## (3) Calculation of the Poisson brackets

It may seem that the calculations are carried out easily. However, the evaluations of the brackets involving the time derivatives of the momenta are difficult. It is noted that it is impossible to use the field equations. Since, in that case, changes of variables are restricted to those along the paths of motions, which does not fit to Poisson brackets which use changes in any direction. Nevertheless, we can show, using (6.30), that assumption that all of the equations (6.10), (6.23a,b) hold leads to contradiction (Ezawa et al., 2006, 2010). In other words, two frames are not related by a canonical transformation.

Therefore, in the framework of the canonical formalism used here, we cannot quantize the theory canonically in both frames. That is, if the  $f(R)$ -type theory is quantized canonically, corresponding Einstein gravity with a scalar field has to be quantized non-canonically, e.g. in the non-commutative geometric way.

## 7. Summary and discussions

In this work, we reviewed the equivalence theorem in the  $f(R)$ -type gravity by deriving it in a pedagogical and self-contained way. Equivalence of this theory with Einstein gravity with a scalar field, related by a conformal transformation, holds on the classical paths. Strictly speaking, description in the physical frame is equivalent to the description in the unphysical frame, since only one frame is physical. If the description in the unphysical frame is simpler, calculations could be done in the frame.

Concerning the surface term in the  $f(R)$ -type gravity, it is not necessary in the Jordan frame. Necessity of the surface term in the Einstein frame comes from the structure of the Lagrangian density that it contains the 2nd order derivatives linearly. A concrete example of the surface term is obtained that shows the dependence of it on the variational conditions. The usual variational conditions in the Einstein frame leads to the GH term. On the other hand, if the

variational conditions are taken as in the Jordan frame, the surface term is different and is given by (5.6).

In the canonical formalism, the conformal transformation is not a canonical one. So the fundamental Poisson brackets are not equivalent in the sense that the sets of fundamental Poisson brackets in both frames are not compatible. Thus if the theory is quantized canonically in the Jordan frame, quantization in the Einstein frame has to be non-canonical, e.g. in the non-commutative geometric way (Kempf, 1994). It is pointed out that similar situation occurs in the inflation model in multidimensional Einstein gravity (Ezawa et al., 1996). In this model, the  $n$ -dimensional internal space continues to shrink during inflation and loses its gravitational potential energy which is transferred to the inflating space. The potential energy behaves as  $-a_I^{-(n-2)}$ , which is expected by the Gauss law in  $n$ -dimensional space, so that the shrinkage of the internal space leads classically to the collapse of the internal space similar to the situation in the case of atoms. However if  $n > 3$ , the canonical quantum theory cannot prevent the collapse of the internal space contrary to the case of atoms, so that non-canonical quantum theory is required. Recently, in the noncommutative geometric multidimensional cosmology, it is shown that stabilization of the internal space is possible (Khosravi et al., 2007). This suggests that in the multidimensional  $f(R)$ -type gravity, extra-dimensional space would be stable. This result is in conformity with that obtained by the semiclassical approximation to the WDW equation noted above.

Thus, considering the renormalizability of the graviton theory and stabilization of the internal space in the semiclassical approximation to WDW equation, it is plausible that  $f(R)$ -type gravity can be quantized canonically in the Jordan frame. In addition, similar stabilization is possible in Einstein gravity if the noncommutative geometry is used, so quantization in the Einstein frame would be non-canonical.

## 8. Appendix: Conformal transformations of geometrical quantities

We consider a conformal transformation given as

$$\tilde{g}_{\mu\nu} \equiv \Omega^2 g_{\mu\nu}. \quad (\text{A.1})$$

Transformations of geometrical quantities are given as follows.

### Christoffel symbols

$$\tilde{\Gamma}_{\mu\nu}^{\lambda} = \Gamma_{\mu\nu}^{\lambda} + \delta_{\mu}^{\lambda} \partial_{\nu}(\ln \Omega) + \delta_{\nu}^{\lambda} \partial_{\mu}(\ln \Omega) - g_{\mu\nu} \partial^{\lambda}(\ln \Omega). \quad (\text{A.2})$$

### Covariant derivatives

For a scalar field, we have

$$\tilde{\nabla}_{\mu} \tilde{\nabla}_{\nu} \phi = \nabla_{\mu} \nabla_{\nu} \phi - \left[ \partial_{\mu}(\ln \Omega) \partial_{\nu} \phi + \partial_{\nu}(\ln \Omega) \partial_{\mu} \phi - g_{\mu\nu} \partial^{\lambda}(\ln \Omega) \partial_{\lambda} \phi \right], \quad (\text{A.3a})$$

or

$$\tilde{\square} \phi = \Omega^{-2} \left[ \square \phi + (D - 2) \partial^{\lambda}(\ln \Omega) \partial_{\lambda} \phi \right], \quad (\text{A.3b})$$



**Ricci tensor**

$$\tilde{R}_{\mu\nu} = R_{\mu\nu} - (D-2)[\nabla_\mu \nabla_\nu (\ln \Omega) - \partial_\mu (\ln \Omega) \partial_\nu (\ln \Omega)] - g_{\mu\nu}[\square(\ln \Omega) + (D-2)\partial_\lambda (\ln \Omega) \partial^\lambda (\ln \Omega)] \quad (\text{A.4})$$

**scalar curvature**

$$\tilde{R} = \Omega^{-2} \left[ R - 2(D-1)\square(\ln \Omega) - (D-1)(D-2)\partial_\lambda (\ln \Omega) \partial^\lambda (\ln \Omega) \right] \quad (\text{A.5})$$

**Einstein tensor**

$$\tilde{G}_{\mu\nu} = G_{\mu\nu} - (D-2) \left[ \nabla_\mu \nabla_\nu (\ln \Omega) - g_{\mu\nu} \square(\ln \Omega) - \partial_\mu (\ln \Omega) \partial_\nu (\ln \Omega) - \frac{D-3}{2} g_{\mu\nu} \partial_\lambda \partial^\lambda (\ln \Omega) \right] \quad (\text{A.6})$$

**9. References**

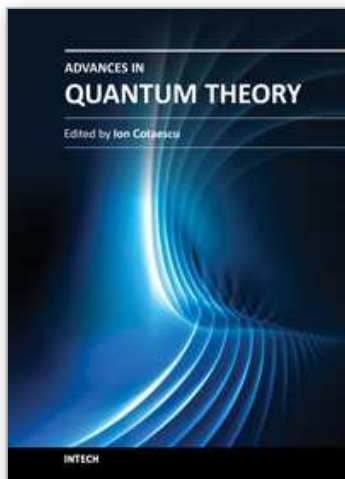
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