Review Article

Second-Order Gauge-Invariant Cosmological Perturbation Theory: Current Status

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Received 19 April 2010; Accepted 12 July 2010

Academic Editor: Eiichiro Komatsu

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The current status of the recent developments of the second-order gauge-invariant cosmological perturbation theory is reviewed. To show the essence of this perturbation theory, we concentrate only on the universe filled with a single scalar field. Through this paper, we point out the problems which should be clarified for the further theoretical sophistication of this perturbation theory. We also expect that this theoretical sophistication will be also useful to discuss the theoretical predictions of non-Gaussianity in CMB and comparison with observations.

1. Introduction

The general relativistic cosmological linear perturbation theory has been developed to a high degree of sophistication during the last 30 years [1–3]. One of the motivations of this development was to clarify the relation between the scenarios of the early universe and cosmological data, such as the cosmic microwave background (CMB) anisotropies. Recently, the first-order approximation of our universe from a homogeneous isotropic one was revealed through the observation of the CMB by the Wilkinson Microwave Anisotropy Probe (WMAP) [4, 5], the cosmological parameters are accurately measured, we have obtained the standard cosmological model, and the so-called “precision cosmology” has begun. These developments in observations were also supported by the theoretical sophistication of the linear-order cosmological perturbation theory.

The observational results of CMB also suggest that the fluctuations of our universe are adiabatic and Gaussian at least in the first-order approximation. We are now on the stage to discuss the deviation from this first-order approximation from the observational [5] and theoretical sides [6–21] through the non-Gaussianity, the nonadiabaticity, and so on. These will be goals of future satellite missions. With the increase of precision of the CMB data, the study of relativistic cosmological perturbations beyond linear order is a topical subject. The second-order cosmological perturbation theory is one of such perturbation theories beyond linear order.

Although the second-order perturbation theory in general relativity is an old topic, a general framework of the gauge-invariant formulation of the general relativistic second-order perturbation has been proposed [22, 23]. This general formulation is an extension of the works of Bruni et al. [24] and has also been applied to cosmological perturbations: the derivation of the second-order Einstein equation in a gauge-invariant manner without any gauge fixing [25, 26]; applicability in more generic situations [27]; confirmation of the consistency between all components of the second-order Einstein equations and equations of motions [28]. We also note that the radiation case has recently been discussed by treating the Boltzmann equation up to second order [29, 30] along the gauge-invariant manner of the above series of papers by the present author.

In this paper, we summarize the current status of this development of the second-order gauge-invariant cosmological perturbation theory through the simple system of a scalar field. Through this paper, we point out the problems which should be clarified and directions of the further development of the theoretical sophistication of the general relativistic higher-order perturbation theory, especially in cosmological perturbations. We expect that this sophistication will be also useful to discuss the theoretical predictions...
of non-Gaussianity in CMB and comparison with observations.

The organization of this paper is as follows. In Section 2, we review the general framework of the second-order gauge-invariant perturbation theory developed in [22, 23, 25, 26, 31]. This review also includes additional explanation not given in those papers. In Section 3, we present also the derivations of the second-order perturbation of the Einstein equation and the energy-momentum tensor from general point of view. For simplicity, in this paper, we only consider a single scalar field as a matter content. The ingredients of Sections 2 and 3 will be applicable to perturbation theory in any theory with general covariance, if the decomposition formula (23) for the linear-order metric perturbation is correct. In Section 4, we summarize the Einstein equations in the case of a background homogeneous isotropic universe, which are used in the derivation of the first- and second-order Einstein equations. In Section 5, the first-order perturbation of the Einstein equations and the Klein-Gordon equations are summarized. The derivation of the second-order perturbations of the Einstein equations and the Klein-Gordon equations, and their consistency are reviewed in Section 6. The final section, Section 7, is devoted to a summary and discussions.

## 2. General Framework of the General Relativistic Gauge-Invariant Perturbation Theory

In this section, we review the general framework of the gauge-invariant perturbation theory developed in [22–26, 31–39]. To develop the general relativistic gauge-invariant perturbation theory, we first explain the general arguments of the Taylor expansion on a manifold without introducing an explicit coordinate system in Section 2.1. Further, we also have to clarify the notion of “gauge” in general relativity to develop the gauge-invariant perturbation theory from general point of view, which is explained in Section 2.2. After clarifying the notion of “gauge” in general relativistic perturbations, in Section 2.3, we explain the formulation of the general relativistic gauge-invariant perturbation theory from general point of view. Although our understanding of “gauge” in general relativistic perturbations essentially is different from “degree of freedom of coordinates” as in many literature, “a coordinate transformation” is induced by our understanding of “gauge.” This situation is explained in Section 2.4. To exclude “gauge degree of freedom” which is unphysical degree of freedom in perturbations, we construct “gauge-invariant variables” of perturbations as reviewed in Section 2.5. These “gauge-invariant variables” are regarded as physical quantities.

### 2.1. Taylor Expansion of Tensors on a Manifold

First, we briefly review the issues on the general form of the Taylor expansion of tensors on a manifold \( \mathcal{M} \). The gauge issue of general relativistic perturbation theories which we will discuss is related to the coordinate transformation. Therefore, we have to discuss the general form of the Taylor expansion without the explicit introduction of coordinate systems. Although we only consider the Taylor expansion of a scalar function \( f : \mathcal{M} \to \mathbb{R} \), here, the resulting formula is extended to that for any tensor field on a manifold as in Appendix A. We have to emphasize that the general formula of the Taylor expansion shown here is the starting point of our gauge-invariant formulation of the second-order general relativistic perturbation theory.

The Taylor expansion of a function \( f \) is an approximated form of \( f(q) \) at \( q \in \mathcal{M} \) in terms of the variables at \( p \in \mathcal{M} \), where \( q \) is in the neighborhood of \( p \). To derive the formula for the Taylor expansion of \( f \), we have to compare the values of \( f \) at the different points on the manifold. To accomplish this, we introduce a one-parameter family of diffeomorphisms \( \Phi_{\lambda} : \mathcal{M} \to \mathcal{M} \), where \( \Phi_{\lambda}(p) = q \) and \( \Phi_{0}(p) = p \). One example of a diffeomorphism \( \Phi_{\lambda} \) is an exponential map with a generator. However, we consider a more general class of diffeomorphisms.

The diffeomorphism \( \Phi_{\lambda} \) induces the pull-back \( \Phi_{\lambda}^* f \) of the function \( f \) and this pull-back enables us to compare the values of the function \( f \) at different points. Further, the Taylor expansion of the function \( f(q) \) is given by

\[
f(q) = f(\Phi_{\lambda}(p)) = (\Phi_{\lambda}^* f)(p) = f(p) + \frac{\partial}{\partial \lambda} (\Phi_{\lambda}^* f) \bigg|_p + \frac{1}{2} \frac{\partial^2}{\partial \lambda^2} (\Phi_{\lambda}^* f) \bigg|_p \lambda^2 + O(\lambda^3),
\]

Since this expression hold for an arbitrary smooth function \( f \), the function \( f \) in (1) can be regarded as a dummy. Therefore, we may regard the Taylor expansion (1) to be the expansion of the pull-back \( \Phi_{\lambda}^* \) of the diffeomorphism \( \Phi_{\lambda} \), rather than the expansion of the function \( f \).

According to this point of view, Sonego and Bruni [36] showed that there exist vector fields \( \xi_{\lambda}^1 \) and \( \xi_{\lambda}^2 \) such that the expansion (1) is given by

\[
f(q) = (\Phi_{\lambda}^* f)(p) = f(p) + (\xi_{\lambda} f) \bigg|_p \lambda + \frac{1}{2} \left( \xi_{\lambda}^1 + \xi_{\lambda}^2 \right) f \bigg|_p \lambda^2 + O(\lambda^3),
\]

without loss of generality (see Appendix A). Equation (2) is not only the representation of the Taylor expansion of the function \( f \), but also the definitions of the generators \( \xi_{\lambda}^1 \) and \( \xi_{\lambda}^2 \). These generators of the one-parameter family of diffeomorphisms \( \Phi_{\lambda} \) represent the direction along which the Taylor expansion is carried out. The generator \( \xi_{\lambda}^1 \) is the first-order approximation of the flow of the diffeomorphism \( \Phi_{\lambda} \), and the generator \( \xi_{\lambda}^2 \) is the second-order correction to this flow. We should regard the generators \( \xi_{\lambda}^1 \) and \( \xi_{\lambda}^2 \) to be independent. Further, as shown in Appendix A, the representation of the Taylor expansion of an arbitrary scalar function \( f \) is extended to that for an arbitrary tensor field \( Q \) just through the replacement \( f \to Q \).
We must note that, in general, the representation (2) of the Taylor expansion is different from an usual exponential map which is generated by a vector field. In general,

\[ \Phi_\sigma \circ \Phi_\lambda \neq \Phi_{\sigma \circ \lambda}, \quad \Phi_\lambda^{-1} \neq \Phi_{-\lambda}. \quad (3) \]

As noted in [24], if the second-order generator \( \xi_2 \) in (2) is proportional to the first-order generator \( \xi_1 \) in (2), the diffeomorphism \( \Phi_\lambda \) is reduced to an exponential map. Therefore, one may reasonably doubt that \( \Phi_\lambda \) forms a group except under very special conditions. However, we have to note that the properties (3) do not directly mean that \( \Phi_\lambda \) does not form a group. There will be possibilities that \( \Phi_\lambda \) form a group in a different sense from exponential maps, in which the properties (3) will be maintained.

Now, we give an intuitive explanation of the representation (2) of the Taylor expansion through the case where the scalar function \( f \) in (2) is a coordinate function. When two points \( p, q \in M \) in (2) are in the neighborhood of each other, we can apply a coordinate system \( M \to \mathbb{R}^n (n = \dim M) \), which is denoted by \( \{ x^\mu \} \), to an open set which includes these two points. Then, we can measure the relative position of these two points \( p \) and \( q \) in \( M \) in terms of this coordinate system in \( \mathbb{R}^n \) through the Taylor expansion (2). In this case, we may regard that the scalar function \( f \) in (2) is a coordinate function \( x^\mu \) and (2) yields

\[ x^\nu(q) = (\Phi_\lambda^* x^\mu)(p) \]

\[ = x^\nu(p) + \lambda \xi_1(p) + \frac{1}{2} \lambda^2 (\xi_2 + \lambda \xi_1 \partial_\mu \xi_1) |_p + O(\lambda^3). \quad (4) \]

The second term \( \lambda \xi_1(p) \) in the right-hand side of (4) is familiar. This is regarded as the vector which points from the point \( x^\nu(p) \) to the point \( x^\nu(q) \) in the sense of the first-order correction as shown in Figure 1(a). However, in the sense of the second order, this vector \( \lambda \xi_1(p) \) may fail to point to \( x^\nu(q) \). Therefore, it is necessary to add the second-order correction as shown in Figure 1(b). As a correction of the second order, we may add the term \( (1/2) \lambda^2 \xi_1^\mu(p) \partial_\mu \xi_1^\nu(p) \). This second-order correction corresponds to that coming from the exponential map which is generated by the vector field \( \xi_1^\mu \). However, this correction completely determined by the vector field \( \xi_1^\mu \). Even if we add this correction that comes from the exponential map, there is no guarantee that the corrected vector \( \lambda \xi_1(p) + (1/2) \lambda^2 \xi_1^\mu(p) \partial_\mu \xi_1^\nu(p) \) does point to \( x^\nu(q) \) in the sense of the second order. Thus, we have to add the new correction \( (1/2) \lambda^2 \xi_1^\mu(p) \) of the second order, in general.

Of course, without this correction \( (1/2) \lambda^2 \xi_1^\mu(p) \), the vector which comes only from the exponential map generated by the vector field \( \xi_1 \) might point to the point \( x^\nu(q) \). Actually, this is possible if we carefully choose the vector field \( \xi_1^\mu \) taking into account the deviations at the second order. However, this means that we have to take care of the second-order correction when we determine the first-order correction. This contradicts to the philosophy of the Taylor expansion as a perturbative expansion, in which we can determine everything order-by-order. Therefore, we should regard that the correction \( (1/2) \lambda^2 \xi_1^\mu(p) \) is necessary in general situations.

2.2. Gauge Degree of Freedom in General Relativity. Since we want to explain the gauge-invariant perturbation theory in general relativity, first of all, we have to explain the notion of “gauge” in general relativity [31]. General relativity is a theory with general covariance, which intuitively states that there is no preferred coordinate system in nature. This general covariance also introduces the notion of “gauge” in the theory. In the theory with general covariance, these “gauges” give rise to the unphysical degree of freedom and we have to fix the “gauges” or to extract some invariant quantities to obtain physical result. Therefore, treatments of “gauges” are crucial in general relativity and this situation becomes more delicate in general relativistic perturbation theory as explained below.

In 1964, Sachs [32] pointed out that there are two kinds of “gauges” in general relativity. Sachs called these two “gauges” as the first- and the second-kind of gauges, respectively. Here, we review these concepts of “gauge.”

2.2.1. First-Kind Gauge. The first-kind gauge is a coordinate system on a single manifold \( M \). Although this first-kind gauge is not important in this paper, we explain this to emphasize the “gauge” discuss in this paper is different from this first-kind gauge.

In the standard text book of manifolds (e.g., see [40]), the following property of a manifold is written: on a manifold, we can always introduce a coordinate system as a diffeomorphism \( \psi_\alpha \) from an open set \( O_\alpha \subset M \) to an open set \( \psi_\alpha(O_\alpha) \subset \mathbb{R}^n (n = \dim M) \). This diffeomorphism \( \psi_\alpha \), that is, coordinate system of the open set \( O_\alpha \), is called gauge choice (of the first-kind). If we consider another open set \( O_\beta \subset M \), we have another gauge choice \( \psi_\beta : O_\beta \to \psi_\beta(O_\beta) \subset \mathbb{R}^n \) for \( O_\beta \). If these two open sets \( O_\alpha \) and \( O_\beta \) have the intersection \( O_\alpha \cap O_\beta \neq \emptyset \), we can consider the diffeomorphism \( \psi_\beta \circ \psi_\alpha^{-1} \). This diffeomorphism \( \psi_\beta \circ \psi_\alpha^{-1} \) is just a coordinate transformation: \( \psi_\alpha(O_\alpha \cap O_\beta) \subset \mathbb{R}^n \to \psi_\beta(O_\alpha \cap O_\beta) \subset \mathbb{R}^n \), which is called gauge transformation (of the first-kind) in general relativity.

According to the theory of a manifold, coordinate system are not on a manifold itself but we can always introduce a
coordinate system through a map from an open set in the manifold $\mathcal{M}$ to an open set of $\mathbb{R}^n$. For this reason, general covariance in general relativity is automatically included in the premise that our spacetime is regarded as a single manifold. The first-kind gauge does arise due to this general covariance. The gauge issue of the first-kind is represented on the manifold. This represents the implicit assumption of the existence of a map $\mathcal{M}_0 \rightarrow \mathcal{M} : p \in \mathcal{M}_0 \mapsto "p" \in \mathcal{M}$, which is usually called a gauge choice (of the second-kind) in perturbation theory [33–35].

It is important to note that the second-kind gauge choice between points on $\mathcal{M}_0$ and $\mathcal{M}$, which is established by such a relation as (5), is not unique to the theory with general covariance. Rather, (5) involves the degree of freedom corresponding to the choice of the map $\mathcal{M}_0 \rightarrow \mathcal{M}$. This is called the gauge degree of freedom (of the second-kind). Such a degree of freedom always exists in perturbations of a theory with general covariance. General covariance intuitively means that there is no preferred coordinate system in the theory as mentioned above. If general covariance is not imposed on the theory, there is a preferred coordinate system in the theory, and we naturally introduce this preferred coordinate system onto both $\mathcal{M}_0$ and $\mathcal{M}$. Then, we can choose the identification map $\mathcal{X}$ using this preferred coordinate system. However, there is no such coordinate system in general relativity due to the general covariance, and we have no guiding principle to choose the identification map $\mathcal{X}$. Indeed, we may identify “$p$” $\in$ $\mathcal{M}$ with $q$ $\in$ $\mathcal{M}_0$ ($q \neq p$) instead of $p$ $\in$ $\mathcal{M}_0$. In the above understanding of the concept of “gauge” (of the second-kind) in general relativistic perturbation theory, a gauge transformation is simply a change of the map $\mathcal{X}$.

These are the basic ideas of gauge degree of freedom (of the second-kind) in the general relativistic perturbation theory which are pointed out by Sacks [32] and mathematically clarified by Stewart and Walker [33–35]. Based on these ideas, higher-order perturbation theory has been developed in [22–28, 31, 38, 39, 41].

2.3. Formulation of Perturbation Theory. To formulate the above understanding in more detail, we introduce an infinitesimal parameter $\lambda$ for the perturbation. Further, we consider the $4 + 1$-dimensional manifold $\mathcal{N} = \mathcal{M} \times \mathbb{R}$, where $4 = \dim \mathcal{M}$ and $\lambda \in \mathbb{R}$. The background spacetime $\mathcal{M}_0 = \mathcal{N}_{|\lambda=0}$ and the physical spacetime $\mathcal{M} = \mathcal{M}_\lambda = \mathcal{N}_{|\lambda=1}$ are also submanifolds embedded in the extended manifold $\mathcal{N}$. Each point on $\mathcal{N}$ is identified by a pair $(p, \lambda)$, where $p \in \mathcal{M}_\lambda$, and each point in $\mathcal{M}_0 \subset \mathcal{N}$ is identified by $\lambda = 0$.

Through this construction, the manifold $\mathcal{N}$ is foliated by four-dimensional submanifolds $\mathcal{M}_\lambda$ of each $\lambda$, and these are diffeomorphic to $\mathcal{M}$ and $\mathcal{M}_0$. The manifold $\mathcal{N}$ has a natural differentiable structure consisting of the direct product of $\mathcal{M}$ and $\mathbb{R}$. Further, the perturbed spacetimes $\mathcal{M}_\lambda$ for each $\lambda$ must have the same differential structure with this construction. In other words, we require that perturbations be continuous in the sense that $\mathcal{M}$ and $\mathcal{M}_0$ are connected by a continuous curve within the extended manifold $\mathcal{N}$. Hence, the changes of the differential structure resulting from the perturbation, for example, the formation of singularities and singular perturbations in the sense of fluid mechanics, are excluded from consideration.

Let us consider the set of field equations

$$\mathcal{E}[Q_\lambda] = 0$$

(6)
by simplicity. We denote the generator of this exponential map equation for the metric on \( M \) is given, the first- and the second-order perturbations \( Q \).

Thus, we have extended an arbitrary tensor field and the field equations (6) on each \( M \) to those on the extended manifold \( N \).

Tensor fields on \( N \) obtained through the above construction are necessarily "tangent" to each \( M \). To consider the basis of the tangent space of \( N \), we introduce the normal form and its dual, which are normal to each \( M \) in \( N \).

These are denoted by \((d\lambda)_a\) and \((\partial/\partial \lambda)^a\), respectively, and they satisfy \((d\lambda)_a(\partial/\partial \lambda)^a = 1\). The form \((d\lambda)_a\) and its dual, \((\partial/\partial \lambda)^a\), are normal to any tensor field extended from the tangent space on each \( M \) through the above construction. The set consisting of \((d\lambda)_a\), \((\partial/\partial \lambda)^a\), and the basis of the tangent space on each \( M \) is regarded as the basis of the tangent space of \( N \).

Now, we define the perturbation of an arbitrary tensor field \( Q \). We compare \( Q \) on \( M \) with \( Q_0 \) on \( M_0 \), and it is necessary to identify the points of \( M \) with those of \( M_0 \) as mentioned above. This point identification map is the gauge choice of the second-kind as mentioned above. The gauge choice is made by assigning a diffeomorphism \( \chi_\lambda : N \rightarrow N \) such that \( \chi_\lambda : M_0 \rightarrow M \). Following the paper of Bruni et al. [24], we introduce a gauge choice \( \chi_\lambda \) as an one-parameter groups of diffeomorphisms, that is, an exponential map, for simplicity. We denote the generator of this exponential map by \( \chi_{\eta} \). This generator \( \chi_{\eta} \) is decomposed by the basis on \( N \) which are constructed above. Although the generator \( \chi_{\eta} \) should satisfy some appropriate properties [22], the arbitrariness of the gauge choice \( \chi_\lambda \) is represented by the tangential component of the generator \( \chi_{\eta} \) to \( M \).

The pull-back \( \chi_\lambda^* Q \), which is induced by the exponential map \( \chi_\lambda \), maps a tensor field \( Q \) on the physical manifold \( M \) to a tensor field \( \chi_\lambda^* Q \) on the background spacetime. In terms of this generator \( \chi_{\eta} \), the pull-back \( \chi_\lambda^* Q \) is represented by the Taylor expansion

\[
Q(r) = Q(\chi_\lambda(p)) = \chi_\lambda^* Q(p) = Q(p) + \lambda \xi_{\chi_\eta} Q|_p + \frac{1}{2} \lambda^2 \xi_{\chi_{\eta}}^2 Q|_p + O(\lambda^3),
\]

where \( r = \chi_\lambda(p) \in M \). Because \( p \in M_0 \), we may regard the equation

\[
\chi_\lambda^* Q(p) = Q_0(p) + \lambda \xi_{\chi_\eta} Q|_{M_0}(p) + \frac{1}{2} \lambda^2 \xi_{\chi_{\eta}}^2 Q|_{M_0}(p) + O(\lambda^3)
\]

as an equation on the background spacetime \( M_0 \), where \( Q_0 = Q|_{M_0} \) is the background value of the physical variable \( Q \). Once the definition of the pull-back of the gauge choice \( \chi_\lambda \) is given, the first- and the second-order perturbations \( Q_\lambda^{(1)} \) and \( Q_\lambda^{(2)} \) of a tensor field \( Q \) under the gauge choice \( \chi_\lambda \) are given by the expansion

\[
\chi_\lambda^{(1)} \equiv Q_\lambda^{(1)} Q|_{M_0} = Q_0 + \lambda \xi_{\chi_\eta} Q|_{M_0} + \frac{1}{2} \lambda^2 \xi_{\chi_{\eta}}^2 Q|_{M_0} + O(\lambda^3),
\]

\[
\chi_\lambda^{(2)} \equiv Q_\lambda^{(2)} Q|_{M_0} = 2 \xi_{\chi_{\eta}} \xi_{\chi_{\eta}} Q|_{M_0} + O(\lambda^3)
\]

with respect to the infinitesimal parameter \( \lambda \). Comparing (8) and (9), we define the first- and the second-order perturbations of a physical variable \( Q \) under the gauge choice \( \chi_\lambda \) by

\[
\chi_\lambda^{(1)} \equiv Q_\lambda^{(1)} Q|_{M_0} \equiv \xi_{\chi_{\eta}} Q|_{M_0},
\]

\[
\chi_\lambda^{(2)} \equiv Q_\lambda^{(2)} Q|_{M_0} \equiv 2 \xi_{\chi_{\eta}} Q|_{M_0}.
\]

We note that all variables in (9) are defined on \( M_0 \).

Now, we consider two different gauge choices based on the above understanding of the second-kind gauge choice. Suppose that \( \chi_\lambda \) and \( \chi_\lambda' \) are two exponential maps with the generators \( \chi_\eta \) and \( \chi'_{\eta} \) on \( N \), respectively. In other words, \( \chi_\lambda \) and \( \chi_\lambda' \) are two gauge choices (see Figure 2). Then, the integral curves of each \( \chi_\eta \) and \( \chi'_{\eta} \) in \( N \) are the orbits of the actions of the gauge choices \( \chi_\lambda \) and \( \chi_\lambda' \), respectively. Since we choose the generators \( \chi_\eta \) and \( \chi'_{\eta} \) so that these are transverse to each \( M \) everywhere on \( N \), the integral curves of these vector fields intersect each \( M \). Therefore, points lying on the same integral curve of either of the two are to be regarded as the same point within the respective gauges. When these curves are not identical, that is, the tangential components to each \( M \) of \( \chi_{\eta} \) and \( \chi'_{\eta} \) are different, these point identification maps \( \chi_\lambda \) and \( \chi_\lambda' \) are regarded as two different gauge choices.

We next introduce the concept of gauge invariance. In particular, in this paper, we consider the concept of order-by-order gauge invariance [27]. Suppose that \( \chi_\lambda \) and \( \chi_\lambda' \) are two different gauge choices which are generated by the vector...
fields $x\eta^a$ and $y\eta^a$, respectively. These gauge choices also pull back a generic tensor field $Q$ on $\mathcal{N}$ to two other tensor fields, $\mathcal{X}^*_f Q$ and $Y^*_f Q$, for any given value of $\lambda$. In particular, on $\mathcal{M}_0$, we now have three tensor fields associated with a tensor field $Q$; one is the background value $Q_0$ of $Q$, and the other two are the pulled-back variables of $Q$ from $\mathcal{M}_1$ to $\mathcal{M}_0$ by the two different gauge choices

$$
\begin{align*}
x Q_1 &:= \mathcal{X}^*_f Q \big|_{\mathcal{M}_0} \\
&= Q_0 + \lambda^{(1)}_x Q + \frac{1}{2} \lambda^{(2)}_x Q + O(\lambda^3), \\
y Q_1 &:= Y^*_f Q \big|_{\mathcal{M}_0} \\
&= Q_0 + \lambda^{(1)}_y Q + \frac{1}{2} \lambda^{(2)}_y Q + O(\lambda^3).
\end{align*}
$$

(11)

(12)

Here, we have used (9). Because $\mathcal{X}_1$ and $Y_1$ are gauge choices which map from $\mathcal{M}_0$ to $\mathcal{M}_1$, $x Q_1$ and $y Q_1$ are the different representations on $\mathcal{M}_0$ in the two different gauges of the same perturbed tensor field $Q$ on $\mathcal{M}_1$. The quantities $x Q_1$ and $y Q_1$ in (11) and (12) are the perturbations of $O(\lambda)$ in the gauges $\mathcal{X}_1$ and $Y_1$, respectively. We say that the $k$th-order perturbation $x Q_1$ of $Q$ is order-by-order gauge-invariant if and only if for any two gauges $\mathcal{X}_1$ and $Y_1$ the following holds:

$$
x Q_1^{(k)} = y Q_1^{(k)}. \tag{13}
$$

Now, we consider the gauge transformation rules between different gauge choices. In general, the representation $x Q_1$ on $\mathcal{M}_0$ of the perturbed variable $Q$ on $\mathcal{M}_1$ depends on the gauge choice $x Q_1$. If we employ a different gauge choice, the representation of $Q_1$ on $\mathcal{M}_0$ may change. Suppose that $x Q_1$ and $y Q_1$ are different gauge choices, which are the point identification maps from $\mathcal{M}_0$ to $\mathcal{M}_1$, and the generators of these gauge choices are given by $x \eta^a$ and $y \eta^a$, respectively. Then, the change of the gauge choice from $x Q_1$ to $y Q_1$ is represented by the diffeomorphism

$$
\Phi_1 := (x Q_1)^{-1} \circ y Q_1. \tag{14}
$$

This diffeomorphism $\Phi_1$ is the map $\Phi_1 : \mathcal{M}_0 \to \mathcal{M}_0$ for each value of $\lambda \in \mathbb{R}$. The diffeomorphism $\Phi_1$ does change the point identification, as expected from the understanding of the gauge choice discussed above. Therefore, the diffeomorphism $\Phi_1$ is regarded as the gauge transformation $\Phi_1$.

The gauge transformation $\Phi_1$ induces a pull-back from the representation $x Q_1$ of the perturbed tensor field $Q$ in the gauge choice $\mathcal{X}_1$ to the representation $y Q_1$ in the gauge choice $Y_1$. Actually, the tensor fields $x Q_1$ and $y Q_1$, which are defined on $\mathcal{M}_0$, are connected by the linear map $\Phi_1^*$ as

$$
y Q_1 = y Q_1^* \big|_{\mathcal{M}_0} = \left( x Q_1^* \left( \mathcal{X}_1 \mathcal{X}^{-1}_1 \right)^* Q \right) \big|_{\mathcal{M}_0} = \Phi_1^* \mathcal{X}^*_1 Q_1. \tag{15}
$$

According to generic arguments concerning the Taylor expansion of the pull-back of a tensor field on the same manifold, given in Section 2.1, it should be possible to express the gauge transformation $\Phi_1^* \mathcal{X}^*_1 Q_1$ in the form

$$
\Phi_1^* \mathcal{X}^*_1 Q = x Q + \lambda \mathcal{X}^*_e \mathcal{X}^*_e Q + \frac{\lambda^2}{2} \left\{ \mathcal{X}^*_e + \mathcal{X}^*_e \right\} \mathcal{X} Q + O(\lambda^3), \tag{16}
$$

where the vector fields $\mathcal{X}^*_e$ are the generators of the gauge transformation $\Phi_1$ (see (2)).

Comparing the representation (16) of the Taylor expansion in terms of the generators $\mathcal{X}^*_e$ and $\mathcal{X}^*_e$ of the pull-back $\mathcal{X}^*_e \mathcal{X}^*_e Q$ and that in terms of the generators $x \eta^a$ and $y \eta^a$ of the pull-back $y Q_1^* \circ (\mathcal{X}^{-1}_1)^* x Q = (\Phi_1^* x Q)$, we readily obtain explicit expressions for the generators $\mathcal{X}^*_e$ and $\mathcal{X}^*_e$ of the gauge transformation $\Phi = (\mathcal{X}^{-1}_1)^* \circ y Q_1$ in terms of the generators $x \eta^a$ and $y \eta^a$ of each gauge choices as follows:

$$
\begin{align*}
\mathcal{X}^*_e &= y \eta^a - x \eta^a, \\
\mathcal{X}^*_e &= \left[ y \eta^a \cdot x \eta^a \right]. \tag{17}
\end{align*}
$$

Further, because the gauge transformation $\Phi_1$ is a map with the background spacetime $\mathcal{M}_0$, the generator should consist of vector fields on $\mathcal{M}_0$. This can be satisfied by imposing some appropriate conditions on the generators $x \eta^a$ and $x \eta^a$.

We can now derive the relation between the perturbations in the two different gauges. Up to second order, these relations are derived by substituting (11) and (12) into (16):

$$
\begin{align*}
y Q_1^{(1)} - x Q_1^{(1)} &= \mathcal{X}^*_e Q_0, \\
y Q_1^{(2)} - x Q_1^{(2)} &= 2 \mathcal{X}^*_e Q_1 + \left\{ \mathcal{X}^*_e + \mathcal{X}^*_e \right\} Q_0. \tag{18}
\end{align*}
$$

Here, we should comment on the gauge choice in the above explanation. We have introduced an exponential map $\mathcal{X}_1$ (or $Y_1$) as the gauge choice, for simplicity. However, this simplified introduction of $\mathcal{X}_1$ as an exponential map is not essential to the gauge transformation rules (18) and (19). Actually, we can generalize the diffeomorphism $\mathcal{X}_1$ from an exponential map. For example, the diffeomorphism whose pull-back is represented by the Taylor expansion (2) is a candidate of the generalization. If we generalize the diffeomorphism $\mathcal{X}_1$, the representation (8) of the pulled-back variable $\mathcal{X}_1^* Q(p)$, the representations of the perturbations (10), and the relations (17) between generators of $\Phi_1$, $\mathcal{X}_1$, and $Y_1$ will be changed. However, the gauge transformation rules (18) and (19) are direct consequences of the generic Taylor expansion (16) of $\Phi_1$. Generality of the representation of the Taylor expansion (16) of $\Phi_1$ implies that the gauge transformation rules (18) and (19) will not be changed, even if we generalize the each gauge choice $\mathcal{X}_1$. Further, the relations (17) between generators also imply that, even if we employ simple exponential maps as gauge choices, both of the generators $\mathcal{X}^*_e$ and $\mathcal{X}^*_e$ are naturally induced by the generators of the original gauge choices. Hence, we conclude that the gauge transformation rules (18) and (19) are quite general and irreducible. In this paper, we review the development of a second-order gauge-invariant cosmological perturbation theory based on
the above understanding of the gauge degree of freedom only through the gauge transformation rules (18) and (19). Hence, the developments of the cosmological perturbation theory presented below will not be changed even if we generalize the gauge choice $X_\lambda$ from a simple exponential map.

We also have to emphasize the physical implication of the gauge transformation rules (18) and (19). According to the above construction of the perturbation theory, gauge degree of freedom, which induces the transformation rules (18) and (19), is unphysical degree of freedom. As emphasized above, the physical spacetime $M_\lambda$ is our nature itself, while there is no background spacetime $M_0$ in our nature. The background spacetime $M_0$ is a fictitious spacetime and it has nothing to do with our nature. Since the gauge choice $X_\lambda$ just gives a relation between $M_\lambda$ and $M_0$, the gauge choice $X_\lambda$ also has nothing to do with our nature. On the other hand, any observations and experiments are carried out only on the physical spacetime $M_\lambda$ through the physical processes on the physical spacetime $M_\lambda$. Therefore, any direct observables in any observations and experiments should be independent of the gauge choice $X_\lambda$, that is, should be gauge-invariant. Keeping this fact in our mind, the gauge transformation rules (18) and (19) imply that the perturbations $^{(1)}XQ$ and $^{(2)}XQ$ include unphysical degree of freedom, that is, gauge degree of freedom, if these perturbations are transformed as (18) or (19) under the gauge transformation $X_\lambda \rightarrow Y_\lambda$. If the perturbations $^{(1)}XQ$ and $^{(2)}XQ$ are independent of the gauge choice, these variables are order-by-order gauge-invariant. Therefore, order-by-order gauge-invariant variables does not include unphysical degree of freedom and should be related to the physics on the physical spacetime $M_\lambda$.

2.4. Coordinate Transformations Induced by the Second Kind Gauge Transformation. In many literature, gauge degree of freedom is regarded as the degree of freedom of the coordinate transformation. In the linear-order perturbation theory, these two degree of freedom are equivalent with each other. However, in the higher-order perturbations, we should regard that these two degree of freedom are different. Although the essential understanding of the gauge degree of freedom (of the second-kind) is as that explained above, the gauge transformation (of the second-kind) also induces the infinitesimal coordinate transformation on the physical spacetime $M_\lambda$ as a result. In many cases, the understanding of “gauge” in perturbations based on coordinate transformations leads mistakes. Therefore, we did not use any ingredient of this subsection in our series of papers [22, 23, 25–28] concerning about higher-order general relativistic gauge-invariant perturbation theory. However, we comment on the relations between the coordinate transformation, briefly. Details can be seen in [22, 37, 38].

To see that the gauge transformation of the second-kind induces the coordinate transformation, we introduce the coordinate system $\{O_\alpha, \psi_\alpha\}$ on the “background spacetime” $M_0$, where $O_\alpha$ are open sets on the background spacetime and $\psi_\alpha$ are diffeomorphisms from $O_\alpha$ to $\mathbb{R}^4$ ($4 = \dim M_0$). The coordinate system $\{O_\alpha, \psi_\alpha\}$ is the set of the collection of the pair of open sets $O_\alpha$ and diffeomorphism $O_\alpha \rightarrow \mathbb{R}^4$. If we employ a gauge choice $X_\lambda$, we have the correspondence of $M_\lambda$ and $M_0$. Together with the coordinate system $\psi_\alpha$ on $M_0$, this correspondence between $M_\lambda$ and $M_0$ induces the coordinate system on $M_\lambda$. Actually, $X_\lambda (O_\alpha)$ for each $\alpha$ is an open set of $M_\lambda$. Then, $\psi_\alpha \circ X_\lambda^{-1}$ becomes a diffeomorphism from an open set $X_\lambda (O_\alpha) \subset M_\lambda$ to $\mathbb{R}^4$. This diffeomorphism $\psi_\alpha \circ X_\lambda^{-1}$ induces a coordinate system of an open set on $M_\lambda$.

When we have two different gauge choices $X_\lambda$ and $Y_\lambda$, the coordinate system $\{O_\alpha, \psi_\alpha \circ X_\lambda^{-1}\}$ and $\{O_\alpha, \psi_\alpha \circ Y_\lambda^{-1}\}$ become different coordinate systems on $M_\lambda$. We can also consider the coordinate transformation from the coordinate system $\psi_\alpha \circ X_\lambda^{-1}$ to another coordinate system $\psi_\alpha \circ Y_\lambda^{-1}$. Since the gauge transformation $X_\lambda \rightarrow Y_\lambda$ is induced by the diffeomorphism $\Phi_1$ defined by (14), the induced coordinate transformation is given by

$$y^\mu (q) := x^\mu (p) = ((\Phi_1^{-1})^* x^\nu) (q)$$

in the passive point of view [22, 37, 38]. If we represent this coordinate transformation in terms of the Taylor expansion in Section 2.1, up to third order, we have the coordinate transformation

$$y^\mu (q) = x^\mu (q) - \lambda \xi^\mu_1 (q) + \frac{\lambda^2}{2} \left\{ - \xi^\nu_2 (q) + \xi^\nu_1 (q) \partial_\nu \xi^\mu_1 (q) \right\} + O (\lambda^3).$$

2.5. Gauge-Invariant Variables. Here, inspecting the gauge transformation rules (18) and (19), we define the gauge-invariant variables for a metric perturbation and for arbitrary matter fields (tensor fields). Employing the idea of order-by-order gauge invariance for perturbations [27], we proposed a procedure to construct gauge-invariant variables of higher-order perturbations [22]. This proposal is as follows. First, we decompose a linear-order metric perturbation into its gauge-invariant and variant parts. The procedure for decomposing linear-order metric perturbations is extended to second-order metric perturbations, and we can decompose the second-order metric perturbation into gauge-invariant and variant parts. Then, we can define the gauge-invariant variables for the first- and second-order perturbations of an arbitrary field other than the metric by using the gauge variant parts of the first- and second-order metric perturbations. Although the procedure for finding gauge-invariant variables for linear-order metric perturbations is highly nontrivial, once we know this procedure, we can easily define the gauge-invariant variables of a higher-order perturbation through a simple extension of the procedure for the linear-order perturbations.

Now, we review the above strategy to construct gauge-invariant variables. To consider a metric perturbation, we expand the metric on the physical spacetime $M_\lambda$, which is pulled back to the background spacetime $M_0$ using a gauge choice in the form given in (9):

$$X_\lambda^a \overline{g}_{ab} = g_{ab} + \lambda \chi h_{ab} + \frac{\lambda^2}{2} \chi l_{ab} + O (\lambda),$$

(22)

where $g_{ab}$ is the metric on $M_0$. Of course, the expansion (22) of the metric depends entirely on the gauge choice $X_\lambda$. 

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Nevertheless, henceforth, we do not explicitly express the index of the gauge choice \( X_\lambda \) in an expression if there is no possibility of confusion.

Our starting point to construct gauge-invariant variables is the assumption that we already know the procedure for finding gauge-invariant variables for the linear metric perturbations. Then, a linear metric perturbation \( h_{ab} \) is decomposed as

\[
h_{ab} =: H_{ab} + \xi a g_{ab}, \tag{23}
\]

where \( H_{ab} \) and \( X^a \) are the gauge-invariant and variant parts of the linear-order metric perturbations, that is, under the gauge transformation (18), these are transformed as

\[
y H_{ab} - \chi H_{ab} = 0, \quad y X^a - \chi X^a = \xi \tag{24}
\]

The first-order metric perturbation (23) together with the gauge transformation rule (18) for the first-order metric perturbation, that is,

\[
\frac{1}{y} H_{ab} - \chi H_{ab} = \xi a g_{ab}. \tag{25}
\]

As emphasized in our series of papers [22, 23, 25–28], the above assumption is quite non-trivial and it is not simple to carry out the systematic decomposition (23) on an arbitrary background spacetime, since this procedure depends completely on the background spacetime \( (\mathcal{M}_0, g_{ab}) \). However, as we will show below, this procedure exists at least in the case of cosmological perturbations of a homogeneous and isotropic universe in Section 5.1.

Once we accept this assumption for linear-order metric perturbations, we can always find gauge-invariant variables for higher-order perturbations [22]. According to the gauge transformation rule (19), the second-order metric perturbation \( l_{ab} \) is transformed as

\[
\frac{1}{y} l_{ab} - \chi l_{ab} = 2 \xi a X h_{ab} + \left\{ \xi a + \xi a \right\} g_{ab} \tag{26}
\]

under the gauge transformation \( \Phi_l = (X\lambda)^{-1} \circ \chi \lambda : \chi \lambda \rightarrow \chi \lambda \). Although this gauge transformation rule is slightly complicated, inspecting this gauge transformation rule, we first introduce the variable \( L_{ab} \) defined by

\[
\tilde{L}_{ab} := l_{ab} - 2 \xi a X h_{ab} + \xi a g_{ab}. \tag{27}
\]

Under the gauge transformation \( \Phi_l = (X\lambda)^{-1} \circ \chi \lambda : \chi \lambda \rightarrow \chi \lambda \), the variable \( L_{ab} \) is transformed as

\[
y \tilde{L}_{ab} - \chi \tilde{L}_{ab} = \xi a g_{ab}, \tag{28}
\]

\[
\sigma a := \xi a + \xi 1, X a = \xi 1. \tag{29}
\]

The gauge transformation rule (28) is identical to that for a linear metric perturbation. Therefore, we may apply the above procedure to decompose \( h_{ab} \) into \( H_{ab} \) and \( X^a \) when we decompose of the components of the variable \( \tilde{L}_{ab} \). Then, \( \tilde{L}_{ab} \) can be decomposed as

\[
\tilde{L}_{ab} = \mathcal{L}_{ab} + \sigma a g_{ab}, \tag{30}
\]

where \( \mathcal{L}_{ab} \) is the gauge-invariant part of the variable \( \tilde{L}_{ab} \), or equivalently, of the second-order metric perturbation \( l_{ab} \), and \( Y^a \) is the gauge variant part of \( l_{ab} \), that is, the gauge variant part of \( l_{ab} \). Under the gauge transformation \( \Phi_l = (X\lambda)^{-1} \circ \chi \lambda \), the variables \( L_{ab} \) and \( Y^a \) are transformed as

\[
y \mathcal{L}_{ab} - \chi \mathcal{L}_{ab} = 0, \quad y Y^a - \chi Y^a = \sigma a, \tag{31}
\]

respectively. Thus, once we accept the assumption (23), the second-order metric perturbations are decomposed as

\[
l_{ab} =: \mathcal{L}_{ab} + 2 \xi a X h_{ab} + (\xi Y - \xi X) g_{ab}, \tag{32}
\]

where \( \mathcal{L}_{ab} \) and \( Y^a \) are the gauge-invariant and variant parts of the second-order metric perturbations, that is,

\[
y \mathcal{L}_{ab} - \chi \mathcal{L}_{ab} = 0, \quad y Y^a - \chi Y^a = \xi a + \xi 1, X a. \tag{33}
\]

Furthermore, as shown in [22], using the first- and second-order gauge variant parts, \( X^a \) and \( Y^a \), of the metric perturbations, the gauge-invariant variables for an arbitrary field \( Q \) other than the metric are given by

\[
(1) Q := \frac{1}{y} Q - \xi a Q_0, \tag{34}
\]

\[
(2) Q := \frac{1}{y} Q - 2 \xi a \frac{1}{y} Q - \left\{ \xi Y - \xi X \right\} Q_0. \tag{35}
\]

It is straightforward to confirm that the variables \( pQ \) defined by (34) and (35) are gauge-invariant under the gauge transformation rules (18) and (19), respectively.

Equations (34) and (35) have very important implications. To see this, we represent these equations as

\[
(1) Q = \frac{1}{y} Q + \xi a Q_0, \tag{36}
\]

\[
(2) Q = \frac{1}{y} Q + 2 \xi a \frac{1}{y} Q + \left\{ \xi Y - \xi X \right\} Q_0. \tag{37}
\]

These equations imply that any perturbation of first and second order can always be decomposed into gauge-invariant and gauge-variant parts as (36) and (37), respectively. These decomposition formulae (36) and (37) are important ingredients in the general framework of the second-order general relativistic gauge-invariant perturbation theory.

### 3. Perturbations of the Field Equations

In terms of the gauge-invariant variables defined last section, we derive the field equations, that is, Einstein equations and the equation for a matter field. To derive the perturbation of the Einstein equations and the equation for a matter field (Klein-Gordon equation), first of all, we have to derive the perturbative expressions of the Einstein tensor [23]. This is reviewed in Section 3.1. We also derive the first and the second order perturbations of the energy momentum tensor for a scalar field and the Klein-Gordon equation [27] in Section 3.2. Finally, we consider the first- and the second-order the Einstein equations in Section 3.3.
3.1. Perturbations of the Einstein Curvature. The relation between the curvatures associated with the metrics on the physical spacetime $\mathcal{M}_A$ and the background spacetime $\mathcal{M}_0$ is given by the relation between the pulled-back operator $\mathcal{X}_a^* \nabla_a (\mathcal{X}_1^{-1})^* \delta$ of the covariant derivative $\nabla_a$ associated with the metric $\bar{g}_{ab}$ on $\mathcal{M}_A$ and the covariant derivative $\nabla_a$ associated with the metric $g_{ab}$ on $\mathcal{M}_0$. The pulled-back covariant derivative $\mathcal{X}_a^* \nabla_a (\mathcal{X}_1^{-1})^*$ depends on the gauge choice $\mathcal{X}_1$. The property of the derivative operator $\mathcal{X}_a^* \nabla_a (\mathcal{X}_1^{-1})^*$ as the covariant derivative on $\mathcal{M}_A$ is given by

$$\mathcal{X}_A^* \nabla_a \left((\mathcal{X}_1^{-1})^* \mathcal{X}_A^* \bar{g}_{ab}\right) = 0,$$  \hspace{1cm} (38)

where $\mathcal{X}_A^* \bar{g}_{ab}$ is the pull-back of the metric on $\mathcal{M}_A$, which is expanded as (22). In spite of the gauge dependence of the operator $\mathcal{X}_A^* \nabla_a (\mathcal{X}_1^{-1})^*$, we simply denote this operator by $\nabla_a$, because our calculations are carried out only on $\mathcal{M}_0$ in the same gauge choice $\mathcal{X}_1$. Further, we denote the pulled-back metric $\mathcal{X}_A^* \bar{g}_{ab}$ on $\mathcal{M}_A$ by $\bar{g}_{ab}$ as mentioned above.

Since the derivative operator $\nabla_a := \mathcal{X}_A^* \nabla_a (\mathcal{X}_1^{-1})^*$ may be regarded as a derivative operator on $\mathcal{M}_0$ that satisfies the property (38), there exists a tensor field $\mathcal{C}^a_{bc}$ on $\mathcal{M}_0$ such that

$$\nabla_a \omega_b = \nabla_a \omega_b - \mathcal{C}^a_{bc} \omega_c,$$  \hspace{1cm} (39)

where $\omega_a$ is an arbitrary one-form on $\mathcal{M}_0$. From the property (38) of the covariant derivative operator $\nabla_a$ on $\mathcal{M}_A$, the tensor field $\mathcal{C}^a_{bc}$ on $\mathcal{M}_0$ is given by

$$\mathcal{C}^a_{bc} = \frac{1}{2} \bar{g}^{cd} \left(\nabla_a \bar{g}_{db} + \nabla_b \bar{g}_{da} - \nabla_d \bar{g}_{ab}\right),$$  \hspace{1cm} (40)

where $\bar{g}^{ab}$ is the inverse of $\bar{g}_{ab}$ (see Appendix B). We note that the gauge dependence of the covariant derivative $\nabla_a$ appears only through $\mathcal{C}^a_{bc}$. The Riemann curvature $\mathcal{R}^d_{abc}$ on $\mathcal{M}_A$, which is also pulled back to $\mathcal{M}_0$, is given by [42]

$$\mathcal{R}^d_{abc} = R^d_{abc} - 2 \nabla_a \mathcal{C}^d_{bc} + 2 \mathcal{C}^e_{cl} \mathcal{C}^d_{eb},$$  \hspace{1cm} (41)

where $R^d_{abc}$ is the Riemann curvature on $\mathcal{M}_0$. The perturbative expression for the curvatures are obtained from the expansion of (41) through the expansion of $\mathcal{C}^a_{bc}$.

The first- and the second-order perturbations of the Riemann, the Ricci, the scalar, the Weyl curvatures, and the Einstein tensors on the general background spacetime are summarized in [23]. We also derived the perturbative form of the divergence of an arbitrary tensor field of second rank to check the perturbative Bianchi identities in [23]. In this paper, we only present the perturbative expression for the Einstein tensor, and its derivations in Appendix B.

We expand the Einstein tensor $\bar{G}^a_{b} := \bar{R}^a_{b} - (1/2) \delta^a_{b} \bar{R}$ on $\mathcal{M}_A$ as

$$\bar{G}^a_{b} = G^a_{b} + \lambda^{(1)} G^a_{b} + \frac{1}{2} \lambda^{(2)} G^a_{b} + O(\lambda^3).$$  \hspace{1cm} (42)

As shown in Appendix B, each order perturbation of the Einstein tensor is given by

$$(1) \overline{G}^{a}_{b} := (1) \delta^{a}_{b} \left[H + X \delta^{a}_{b}\right],$$  \hspace{1cm} (43)

$$(2) \overline{G}^{a}_{b} := (2) \delta^{a}_{b} \left[H + \delta^{a}_{b}\right] + (2) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right],$$  \hspace{1cm} (44)

where

$$(1) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right] := (1) \Sigma^a_{b} \left[H, \delta^{a}_{b}\right],$$  \hspace{1cm} (45)

$$(2) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right] := (2) \Sigma^a_{b} \left[H, \delta^{a}_{b}\right],$$  \hspace{1cm} (46)

and

$$(1) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right] := (1) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right] = (1) \Sigma^a_{b} \left[H, \delta^{a}_{b}\right],$$  \hspace{1cm} (47)

We note that $(1) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right]$ and $(2) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right]$ in (43) and (44) are the gauge-invariant parts of the perturbative Einstein tensors, and (43) and (44) have the same forms as (34) and (37), respectively. The expression of $(2) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right]$ in (46) with (47) is derived by the consideration of the general relativistic gauge-invariant perturbation theory with two infinitesimal parameters in [22, 23].

We also note that $(1) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right]$ and $(2) \delta^{a}_{b} \left[H, \delta^{a}_{b}\right]$ defined by (45)–(47) satisfy the identities

$$\nabla_a \delta^{a}_{b} \left[H, \delta^{a}_{b}\right] = -H_{a}^{c} \left[H, G^{c}_{b}\right] + H_{b}^{c} \left[H, G^{c}_{a}\right],$$  \hspace{1cm} (50)

$$\nabla_a \delta^{a}_{b} \left[H, \delta^{a}_{c}\right] \left[H, \delta^{a}_{c}\right] = H_{a}^{c} \left[H, \delta^{a}_{c}\right] \left[H, \delta^{a}_{c}\right] - \left[H, \delta^{a}_{c}\right] \left[H, \delta^{a}_{c}\right] G^{c}_{a},$$  \hspace{1cm} (51)

for arbitrary tensor fields $\Lambda_{ab}$ and $\Lambda_{bc}$, respectively. We can directly confirm these identities without specifying arbitrary tensors $\Lambda_{ab}$ and $\Lambda_{bc}$ of the second rank, respectively. This implies that our general framework of the second-order gauge-invariant perturbation theory discussed here gives a self-consistent formulation of the second-order perturbation theory. These identities (50) and (51) guarantee the first- and
second-order perturbations of the Bianchi identity $\nabla_b \varepsilon^b_a = 0$ and are also useful when we check whether the derived components of (45) and (46) are correct.

3.2. Perturbations of the Energy Momentum Tensor and Klein-Gordon Equation. Here, we consider the perturbations of the energy momentum tensor of the equation of motion. As a model of the matter field, we only consider the scalar field, for simplicity. Then, equation of motion for a scalar field is the Klein-Gordon equation.

The energy momentum tensor for a scalar field $\varphi$ is given by

$$\mathcal{T}^a_b = \nabla_a \varphi \nabla^b \varphi - \frac{1}{2} \delta_a^b \left( \nabla_c \varphi \nabla^c \varphi + 2V(\varphi) \right),$$  \hspace{1cm} (52)

where $V(\varphi)$ is the potential of the scalar field $\varphi$. We expand the scalar field $\varphi$ as

$$\varphi = \phi + \lambda \phi_1 + \frac{1}{2} \lambda^2 \phi_2 + O(\lambda^3),$$ \hspace{1cm} (53)

where $\phi$ is the background value of the scalar field $\varphi$. Further, following to the decomposition formulae (34) and (35), each order perturbation of the scalar field $\varphi$ is decomposed as

$$\phi_1 =: \phi_1 + \varepsilon_\chi \phi,$$

$$\phi_2 =: \phi_2 + 2\varepsilon_\chi \phi_1 + (\varepsilon_\gamma - \varepsilon_\delta) \phi,$$

where $\phi_1$ and $\phi_2$ are the first- and the second-order gauge-invariant perturbations of the scalar field, respectively.

Through the perturbative expansions (53) and (22) of the scalar field $\varphi$ and the inverse metric, the energy momentum tensor (52) is also expanded as

$$\mathcal{T}^a_b = T^a_b + \lambda (1) (T^a_b) + \frac{1}{2} \lambda^2 (2) (T^a_b) + O(\lambda^3).$$ \hspace{1cm} (55)

The background energy momentum tensor $T^a_b$ is given by the replacement $\varphi \rightarrow \phi$ in (52). Further, through the decompositions (23), (32), (54), the perturbations of the energy momentum tensor $(1)(T^a_b)$ and $(2)(T^a_b)$ are also decomposed as

$$\begin{align*}
(1) (T^a_b) &= : (1) T^a_b + \varepsilon_\chi T^a_b, \\
(2) (T^a_b) &= : (2) T^a_b + 2\varepsilon_\chi (1) (T^a_b) + (\varepsilon_\gamma - \varepsilon_\delta) (1) (T^a_b),
\end{align*}$$ \hspace{1cm} (56)

where the gauge-invariant parts $(1)T^a_b$ and $(2)T^a_b$ of the first and the second order are given by

$$\begin{align*}
(1) T^a_b &= \nabla_a \varphi \nabla^b \varphi_1 - \nabla_a \varphi \mathcal{H}^{bc} \nabla_b \varphi + \nabla_a \varphi_1 \nabla^b \varphi \\
&- \delta_a^b \left( \nabla_c \varphi \nabla^c \varphi_1 - \frac{1}{2} \nabla_c \varphi \mathcal{H}^{cd} \nabla_d \varphi + \phi_1 \frac{\partial V}{\partial \varphi} \right), \\
(2) T^a_b &= \nabla_a \varphi \nabla^b \varphi_2 - \nabla_a \varphi \mathcal{H}^{bc} \nabla_b \varphi - \nabla_a \varphi_1 \nabla^b \varphi \\
&- 2\nabla_a \varphi \mathcal{H}^{bc} \nabla_b \varphi_1 + 2\nabla_a \varphi \mathcal{H}^{bd} \mathcal{H}_{dc} \nabla^c \varphi \\
&+ 2\nabla_a \varphi_1 \nabla^b \varphi_2 - 2\nabla_a \varphi_1 \mathcal{H}^{bd} \nabla_c \varphi \\
&- \delta_a^b \left( \nabla_c \varphi \nabla^c \varphi_2 - \frac{1}{2} \nabla_c \varphi \mathcal{H}^{cd} \nabla_d \varphi + \phi_2 \frac{\partial^2 V}{\partial^2 \varphi} \right). \\
\end{align*}$$ \hspace{1cm} (58)

We note that (56) and (57) have the same form as (36) and (37), respectively.

Next, we consider the perturbation of the Klein-Gordon equation

$$\mathcal{C}_{(K)} := \nabla^a \nabla_a \varphi - \frac{\partial V}{\partial \varphi} (\varphi) = 0.$$ \hspace{1cm} (60)

Through the perturbative expansions (53) and (22), the Klein-Gordon equation (60) is expanded as

$$\mathcal{C}_{(K)} =: C_{(K)} + \lambda C_{(K)}^{(1)} + \frac{1}{2} \lambda^2 C_{(K)}^{(2)} + O(\lambda^3).$$ \hspace{1cm} (61)

$C_{(K)}$ is the background Klein-Gordon equation

$$C_{(K)} := \nabla^a \nabla_a \varphi - \frac{\partial V}{\partial \varphi} (\varphi) = 0.$$ \hspace{1cm} (62)

The first- and the second-order perturbations $C_{(K)}^{(1)}$ and $C_{(K)}^{(2)}$ are also decomposed into the gauge-invariant and the gauge-variant parts as

$$\begin{align*}
C_{(K)}^{(1)} &= C_{(K)}^{(1)} + \varepsilon_\chi C_{(K)}^{(1)}, \\
C_{(K)}^{(2)} &= C_{(K)}^{(2)} + 2\varepsilon_\chi (1) C_{(K)}^{(1)} + (\varepsilon_\gamma - \varepsilon_\delta) C_{(K)}^{(1)},
\end{align*}$$ \hspace{1cm} (63)

where

$$\begin{align*}
C_{(K)}^{(1)} &= \nabla^a \nabla_a \varphi_1 - \mathcal{H}^{ac} \nabla_a \varphi - \mathcal{H}^{bc} \nabla_b \varphi - \varphi_1 \frac{\partial^2 V}{\partial \varphi^2} (\varphi), \\
C_{(K)}^{(2)} &= \nabla^a \nabla_a \varphi_2 - \mathcal{H}^{ac} \nabla_a \varphi - 2\mathcal{H}_d^{ab} \mathcal{H}_c^d \nabla^c \varphi \nabla_a \varphi_1 \\
&- \mathcal{H}_d^{ab} \nabla_d \nabla_b \varphi - 2\mathcal{H}_d^{ab} \nabla_d \varphi_1 \nabla_b \varphi - 2\mathcal{H}_d^{ab} \nabla_d \varphi \varphi_1 \\
&- \varphi_2 \frac{\partial^2 V}{\partial^2 \varphi} (\varphi) - \varphi_1 \varphi_2 \frac{\partial^2 V}{\partial \varphi^2} (\varphi). \\
\end{align*}$$ \hspace{1cm} (64)

Here, we note that (63) have the same form as (36) and (37).
By virtue of the order-by-order evaluations of the Klein-Gordon equation, the first- and the second-order perturbation of the Klein-Gordon equation are necessarily given in gauge-invariant form as
\[
C^{(1)}_{(K)} = 0, \quad C^{(2)}_{(K)} = 0. \tag{66}
\]

We should note that, in [27], we summarized the formulae of the energy momentum tensors for an perfect fluid, an imperfect fluid, and a scalar field. Further, we also summarized the equations of motion of these three matter fields, that is, the energy continuity equation and the Euler equation for a perfect fluid; the energy continuity equation and the Navier-Stokes equation for an imperfect fluid; the Klein-Gordon equation for a scalar field. All these formulae also have the same form as the decomposition formulae (36) and (37). In this sense, we may say that the decomposition formulae (36) and (37) are universal.

3.3. Perturbations of the Einstein Equation. Finally, we impose the perturbed Einstein equation of each order,
\[
(G_a^b = 8\pi G^{(1)} T_a^b, \quad (2) G_a^b = 8\pi G^{(2)} T_a^b. \tag{67}
\]
Then, the perturbative Einstein equation is given by
\[
(1) g_a^b [\mathcal{H}] = 8\pi G^{(1)} \gamma_a^b \tag{68}
\]
at linear order and
\[
(1) g_a^b [L] + (2) g_a^b [\mathcal{H}, \mathcal{H}] = 8\pi G^{(2)} \gamma_a^b \tag{69}
\]
at second order. These explicitly show that, order-by-order, the Einstein equations are necessarily given in terms of gauge-invariant variables only.

Together with (66), we have seen that the first- and the second-order perturbations of the Einstein equations and the Klein-Gordon equation are necessarily given in gauge-invariant form. This implies that we do not have to consider the gauge degree of freedom, at least in the level where we concentrate only on the equations of the system.

We have reviewed the general outline of the second-order gauge-invariant perturbation theory. We also note that the ingredients of this section are independent of the explicit form of the background metric $g_{ab}$, except for the decomposition assumption (23) for the linear-order metric perturbations and are valid not only in cosmological perturbation case but also the other generic situations if (23) is correct. Within this general framework, we develop a second-order cosmological perturbation theory in terms of the gauge-invariant variables.

4. Cosmological Background Spacetime and Equations

The background spacetime $\mathcal{M}_b$ considered in cosmological perturbation theory is a homogeneous, isotropic universe that is foliated by the three-dimensional hypersurface $\Sigma(\eta)$, which is parametrized by $\eta$. Each hypersurface of $\Sigma(\eta)$ is a maximally symmetric three-space [43], and the spacetime metric of this universe is given by
\[
g_{ab} = a^2(\eta) \left( -(d\eta)_a (d\eta)_b + \gamma_{ij}(dx^i)_a (dx^j)_b \right), \tag{70}
\]
where $a = a(\eta)$ is the scale factor, $\gamma_{ij}$ is the metric on the maximally symmetric 3-space with curvature constant $K$, and the indices $i, j, k, \ldots$ for the spatial components run from 1 to 3.

To study the Einstein equation for this background spacetime, we introduce the energy-momentum tensor for a scalar field, which is given by
\[
T_a^b = \nabla_a \phi \nabla^b \phi - \frac{1}{2} \delta_a^b \left( \nabla_i \phi \nabla^i \phi + 2V(\phi) \right) = \left( \frac{1}{2a^2} \left( \partial_\eta \phi \right)^2 + V(\phi) \right) (d\eta)_a \left( \frac{\partial}{\partial \eta} \right)^b + \left( \frac{1}{2a^2} \left( \partial_\eta \phi \right)^2 - V(\phi) \right) \gamma_a^b,
\]
where we assumed that the scalar field $\phi$ is homogeneous
\[
\phi = \phi(\eta) \tag{72}
\]
and $\gamma_a^b$ are defined as
\[
\gamma_{ab} := \gamma_{ij}(dx^i)_a (dx^j)_b, \quad \gamma_a^b := \gamma_{ij} (dx^i)_a \left( \frac{\partial}{\partial x^j} \right)^b \tag{73}
\]
The background Einstein equations $G_a^b = 8\pi GT_a^b$ for this background spacetime filled with the single scalar field are given by
\[
\mathcal{H}^2 + K = \frac{8\pi G}{3} a^2 \left( \frac{1}{2a^2} \left( \partial_\eta \phi \right)^2 + V(\phi) \right),
\]
\[
2\partial_\eta \mathcal{H} + \mathcal{H}^2 + K = 8\pi G \left( -\frac{1}{2} \left( \partial_\eta \phi \right)^2 + a^2 V(\phi) \right). \tag{74}
\]
We also note that (74) lead to
\[
\mathcal{H}^2 + K - \partial_\eta \mathcal{H} = 4\pi G \left( \partial_\eta \phi \right)^2. \tag{75}
\]
Equation (75) is also useful when we derive the perturbative Einstein equations.

Next, we consider the background Klein-Gordon equation which is the equation of motion $\nabla_a T_a^b = 0$ for the scalar field
\[
\partial_\eta^2 \phi + 2\mathcal{H} \partial_\eta \phi + a^2 \frac{\partial V}{\partial \phi} = 0. \tag{76}
\]

The Klein-Gordon equation (76) is also derived from the Einstein equations (74). This is a well known fact and is just due to the Bianchi identity of the background spacetime. However, these types of relation are useful to check whether the derived system of equations is consistent.
5. Equations for the First-Order Cosmological Perturbations

On the cosmological background spacetime in the last section, we develop the perturbation theory in the gauge-invariant manner. In this section, we summarize the first-order perturbation of the Einstein equation and the Klein-Gordon equations. In Section 5.1, we show that the assumption on the decomposition (23) of the linear-order metric perturbation is correct. In Section 5.2, we summarize the first-order perturbation of the Einstein equation. Finally, in Section 5.3, we show the first-order perturbation of the Klein-Gordon equation.

5.1. Gauge-Invariant Metric Perturbations. Here, we consider the first-order metric perturbation $h_{ab}$ and show the assumption on the decomposition (23) is correct in the background metric (70). To accomplish the decomposition (23), first, we assume the existence of the Green functions $\Delta^{-1} := (D^iD_j)^{-1}$, $(\Delta + 2K)^{-1}$, and $(\Delta + 3K)^{-1}$, where $D_i$ is the covariant derivative associated with the metric $g_{ij}$ and $K$ is the curvature constant of the maximally symmetric three space. Next, we consider the decomposition of the linear-order metric perturbation $h_{ab}$ as

$$ h_{ab} = h_{\eta\eta}(d\eta)_a(d\eta)_b + 2(Dh_{(V)L} + h_{(V)_i})(d\eta)_a(dx^i)_b + a^2 \left\{ \frac{1}{2} \left( h_{(L)}y_{ij} + \frac{1}{2} D_iD_j - \frac{1}{2} \gamma_{ij}\Delta \right) h_{(TL)} \right\} d\eta d\eta $$

(77)

where $h_{(V)L}$, $h_{(V)_i}$, and $h_{(TT)ij}$ satisfy the properties

$$ D^i h_{(V)L} = 0, \quad D^i h_{(TV)_i} = 0, \quad h_{(TT)ij} = h_{(TT)ji}, \quad h_{(T)_i} := \gamma^{ij} h_{(T)ij} = 0, $$

(78)

$$ D^i h_{(TT)ij} = 0. $$

The gauge-transformation rules for the variables $h_{\eta\eta}$, $h_{(V)L}$, $h_{(V)_i}$, $h_{(L)}$, $h_{(TT)ij}$ and $h_{(TT)ij}$ are derived from (25). Inspecting these gauge-transformation rules, we define the gauge-invariant part $X_a$ in (23):

$$ X_a := \left( h_{(V)L} - \frac{1}{2} a^2 \partial_\eta h_{(TL)} \right) (d\eta)_a + a^2 \left\{ (h_{(TV)_i} + \frac{1}{2} D_i h_{(TL)}) (dx^i)_a \right\}. $$

(79)

We can easily check this vector field $X_a$ satisfies (24). Subtracting gauge-invariant part $\Delta X_{ab}$ from $h_{ab}$, we have the gauge-invariant part $\mathcal{H}_{ab}$ in (23):

$$ \mathcal{H}_{ab} = a^2 \left\{ -2 \Phi \left( (d\eta)_a (d\eta)_b + 2 (d\eta)_a (dx^i)_b \right) + \left\{ -2 \Psi y_{ij} + \chi_{ij} \right\} \left( dx^i \right)_a \left( dx^j \right)_b \right\}, $$

(80)

where the properties $D^i \chi_{ij} := \gamma^{ij} D_i \psi = \chi_{ij}$ and $D^i \gamma_{ij} = 0$ are satisfied as consequences of (78).

Thus, we may say that our assumption for the decomposition (23) in linear-order metric perturbation is correct in the case of cosmological perturbations. However, we have to note that to accomplish (23), we assumed the existence of the Green functions $\Delta^{-1}$, $(\Delta + 2K)^{-1}$, and $(\Delta + 3K)^{-1}$. As shown in [25, 26], this assumption is necessary to guarantee the one to one correspondence between the variables $\{h_{\eta\eta}, h_{ij}, h_{ij}\}$ and $\{h_{\eta\eta}, h_{(V)L}, h_{(V)_i}, h_{(TT)_i}, h_{(TV)_i}, h_{(TT)ij}\}$, but excludes some perturbative modes of the metric perturbations which belong to the kernel of the operator $\Delta$, $(\Delta + 2K)$, and $(\Delta + 3K)$ from our consideration. For example, homogeneous modes belong to the kernel of the operator $\Delta$ and are excluded from our consideration. If we have to treat these modes, the separate treatments are necessary. In this paper, we ignore these modes, for simplicity.

We also note the fact that the definition (23) of the gauge-invariant variables is not unique. This comes from the fact that we can always construct new gauge-invariant quantities by the combination of the gauge-invariant variables. For example, using the gauge-invariant variables $\Phi$ and $\Psi$ of the first-order metric perturbation, we can define a vector field $Z_a := -a \phi (d\eta)_a + a \Psi (dx^i)_a$, which is gauge invariant. Then, we can rewrite the decomposition formula (23) for the linear-order metric perturbation as

$$ h_{ab} = \mathcal{H}_{ab} - \Delta X_{ab} + \Delta X_{ab} + \Delta Z_{ab}, $$

(81)

where we have defined new gauge invariant variable $K_{ab}$ by

$$ K_{ab} := \mathcal{H}_{ab} - \Delta X_{ab}. $$

Clearly, $K_{ab}$ is gauge-invariant and the vector field $X^a + Z^a$ satisfies (24). In spite of this nonuniqueness, we specify the components of the tensor $h_{ab}$ as (80), which is the gauge-invariant part of the linear-order metric perturbation associated with the longitudinal gauge.

The non-uniqueness of the definitions of gauge-invariant variables is related to the “gauge-fixing” for the linear-order metric perturbations. Due to this non-uniqueness, we can consider the gauge-fixing in the first-order metric perturbation from two different points of view. The first point of view is that the gauge-fixing is to specify the gauge-variant part $X^a$. For example, the longitudinal gauge is realized by the gauge fixing $X^a = 0$. Due to this gauge fixing $X^a = 0$, we can regard the fact that perturbative variables in the longitudinal gauge are the completely gauge fixed variables. On the other hand, we may also regard that the gauge fixing is the specification of the gauge-invariant vector field $Z^a$ in (81). In this point of view, we do not specify the vector field $X^a$. Instead, we have to specify the gauge-invariant vector $Z^a$ or equivalently to specify the gauge-invariant metric perturbation $\mathcal{K}_{ab}$ without specifying $X^a$ so that the first-order metric perturbation $h_{ab}$ coincides with the gauge-invariant variables $\mathcal{K}_{ab}$ when we fix the gauge $X^a$ so that $X^a + Z^a = 0$. These two different point of view of “gauge fixing” is equivalent with each other due to the non-uniqueness of the definition (81) of the gauge-invariant variables.
5.2. First-Order Einstein Equations. Here, we derive the linear-order Einstein equation (68). To derive the components of the gauge-invariant part of the linearized Einstein tensor $^{(1)}\mathcal{G}_a^b[\mathcal{H}]$, which is defined by (45), we first derive the components of the tensor $\mathcal{H}_{ab}[\mathcal{H}]$, which is defined in (48) with $A_{ab} = \mathcal{H}_{ab}$ and its component (80). These components are summarized in [25, 26].

From (45), the component of $^{(1)}\mathcal{G}_a^b[\mathcal{H}]$ are summarized as

\[
^{(1)}\mathcal{G}_\eta^\eta[\mathcal{H}] = -\frac{1}{a^2} \left[ \left( -6H\partial_\eta + 2\Delta + 6K \right) \left( \frac{1}{\Psi} \right)^{(1)} - 6H^2 \left( \frac{1}{\Phi} \right) \right],
\]

\[
^{(1)}\mathcal{G}_\eta^i[\mathcal{H}] = -\frac{1}{a^2} \left[ 2\partial_\eta D_i \left( \frac{1}{\Psi} \right) + 2\mathcal{H} D_i \left( \frac{1}{\Phi} \right) - \frac{1}{2}(\Delta + 2K) \eta_i \right],
\]

\[
^{(1)}\mathcal{G}_i^i[\mathcal{H}] = \frac{1}{a^2} \left[ 2\partial_i D_j \left( \frac{1}{\Psi} \right) + 2\mathcal{H} D_i \left( \frac{1}{\Phi} \right) \eta_j \right.
\]

\[
+ \left\{ \left( -\Delta + 2\partial_i^2 + 4\mathcal{H}\partial_\eta - 2K \right) \left( \frac{1}{\Psi} \right)
\]

\[+ \left( 2\partial_\eta \partial_i + 4\partial_i \mathcal{H} + 2\mathcal{H}^2 + \Delta \right) \left( \frac{1}{\Phi} \right) \right\} \eta_i,
\]

\[\left. \right. - \frac{1}{2a^2} \partial_i \left( a^2 \left( D_i \left( \frac{1}{\Psi} \right) + D_j \left( \frac{1}{\Phi} \right) \eta_j \right) \right),\]

\[+ \frac{1}{2} \left( \partial_i^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta \right) \chi_i, \]

(82)

Straightforward calculations show that these components of the first-order gauge-invariant perturbation $^{(1)}\mathcal{G}_a^b[\mathcal{H}]$ of the Einstein tensor satisfies the identity (50). Although this confirmation is also possible without specification of the tensor $\mathcal{H}_{ab}$, the confirmation of (50) through the explicit components (82) implies that we have derived the components of $^{(1)}\mathcal{G}_a^b[\mathcal{H}]$ consistently.

Next, we summarize the first-order perturbation of the energy momentum tensor for a scalar field. Since, at the background level, we assume that the scalar field $\phi$ is homogeneous as (72), the components of the gauge-invariant part of the first-order energy-momentum tensor $^{(1)}T_a^b$ are given by

\[
^{(1)}T_\eta^\eta = -\frac{1}{a^2} \left( \partial_\eta \phi_1 \partial_\eta \phi - \Phi \left( \frac{1}{\partial_\eta \phi} \right)^2 + a^2 \frac{dV}{d\phi} \phi_1 \right),
\]

\[
^{(1)}T_i^i = -\frac{1}{a^2} D_i \phi_1 \partial_\eta \phi,
\]

(83)

The second equation in (84) shows that there is no anisotropic stress in the energy-momentum tensor of the single scalar field. Then, we obtain that

\[
\frac{1}{\Psi} \phi = \Phi.
\]

From (82)–(84) and (85), the components of scalar parts of the linearized Einstein equation (68) are given as [3]

\[
\left( \mathcal{H} - 3\partial_\eta + 4K - \partial_\eta \mathcal{H} - 2\mathcal{H}^2 \right) \phi = 4\pi G \left( \partial_\eta \phi_1 \partial_\eta \phi + a^2 \frac{dV}{d\phi} \phi_1 \right),
\]

(86)

\[
\partial_\eta \phi_1 + \mathcal{H} \phi = 4\pi G \phi_1 \partial_\eta \phi,
\]

(87)

\[
\left( \partial_\eta^2 + 3\mathcal{H}\partial_\eta + \partial_\eta \mathcal{H} + 2\mathcal{H}^2 \right) \phi = 4\pi G \left( \partial_\eta \phi_1 \partial_\eta \phi - a^2 \frac{dV}{d\phi} \phi_1 \right).
\]

(88)

In the derivation of (86)–(88), we have used (75). We also note that only two of these equations are independent. Further, the vector part of the component $^{(1)}\mathcal{G}_i^i[\mathcal{H}] = 8\pi G^{(1)}T_i^i$ shows that

\[
\frac{1}{\Psi} \gamma_i = 0.
\]

(89)

The equation for the tensor mode $\chi_{ij}$ is given by

\[
\left( \partial_\eta^2 + 2\mathcal{H}\partial_\eta + 2K - \Delta \right) \chi_{ij} = 0.
\]

(90)

Combining (86) and (88), we eliminate the potential term of the scalar field and thereby obtain that

\[
\left( \partial_\eta^2 + \Delta + 4K \right) \phi = 8\pi G \partial_\eta \phi_1 \partial_\eta \phi.
\]

(91)

Further, using (87) to express $\partial_\eta \phi_1$ in terms of $\partial_\eta \phi_1$ and $\Phi$, we also eliminate $\partial_\eta \phi_1$ in (91). Hence, we have

\[
\left\{ \partial_\eta^2 + 2 \left( \mathcal{H} - 2\partial_\eta \phi \frac{d\mathcal{H}}{d\phi} \right) \partial_\eta - \Delta - 4K + 2 \left( \partial_\eta \mathcal{H} - \frac{\partial_\eta \mathcal{H}^2}{\partial_\eta \phi} \right) \right\} \Phi = 0.
\]

(92)

This is the master equation for the scalar mode perturbation of the cosmological perturbation in universe filled with a single scalar field. It is also known that (92) reduces to a simple equation through a change of variables [3].
5.3. First-Order Klein–Gordon Equations. Next, we consider the first-order perturbation of the Klein–Gordon equation (64). By the straightforward calculations using (70), (80), (72), (76), and the components $H_{a}^{\mu\nu}$ summarized in [25, 26], the gauge-invariant part $C_{i}^{(1)}$ of the first-order Klein–Gordon equation defined by (64) is given by

\[-a^{2} C_{i}^{(1)} = \partial_{\eta}^{2} \phi_{1} + 2 \mathcal{H} \partial_{\eta} \phi_{1} - \Delta \phi_{1} - \left( \partial_{\eta}^{2} \Phi + 3 \partial_{\eta} \Psi \right) \partial_{\eta} \phi \]
\[+ 2 a^{2} ( \Phi \frac{dV}{d\phi} (\phi) + a^{2} \phi_{1} \frac{d^{2} V}{d\phi_{1}^{2}} (\phi) \]
\[= 0. \]  

(93)

Through the background Einstein equations (74) and the first-order perturbations (87) and (92) of the Einstein equation, we can easily derive the first-order perturbation of the Klein–Gordon equation (93) [28]. Hence, the first-order perturbation of the Klein–Gordon equation is not independent of the background and the first-order perturbation of the Einstein equation. Therefore, from the viewpoint of the Cauchy problem, any information obtained from the first-order perturbation of the Klein–Gordon equation should also be obtained from the set of the background and the first-order the Einstein equation, in principle.

6. Equations for the Second-Order Cosmological Perturbations

Now, we develop the second-order perturbation theory on the cosmological background spacetime in Section 4 within the general framework of the gauge-invariant perturbation theory reviewed in Section 2. Since we have already confirmed the important step of our general framework, that is, the assumption for the decomposition (23) of the linear-order metric perturbation is correct. Hence, the general framework reviewed in Section 2 is applicable. Applying this framework, we define the second-order gauge-invariant variables of the metric perturbation in Section 6.1. In Section 6.2, we summarize the explicit components of the gauge-invariant parts of the second-order perturbation of the Einstein tensor. In Section 6.3, we summarize the explicit components of the second-order perturbation of the energy-momentum tensor and the Klein–Gordon equations. Then, in Section 6.4, we derive the second-order Einstein equations in terms of gauge-invariant variables. The resulting equations have the source terms which constitute of the quadratic terms of the linear-order perturbations. Although these source terms have complicated forms, we give identities which comes from the consistency of all the second-order perturbations of the Einstein equation and the Klein–Gordon equation in Section 6.5.

6.1. Gauge-Invariant Metric Perturbations. First, we consider the components of the gauge-invariant variables for the metric perturbation of second order. The variable $\tilde{L}_{a}^{\mu\nu}$ defined by (27) is transformed as (28) under the gauge transformation and we may regard the generator $\sigma_{a}$ defined by (29) as an arbitrary vector field on $\mathcal{M}_{0}$ from the fact that the generator $\tilde{\xi}^{a}_{1}$ in (29) is arbitrary. We can apply the procedure to find gauge-invariant variables for the first-order metric perturbations (80) in Section 5.1. Then, we can accomplish the decomposition (30). Following to the same argument as in the linear case, we may choose the components of the gauge-invariant variables $L_{ab}$ in (32) as

\[L_{ab} = -2 a^{2} \Phi (d\eta)_{a} (d\eta)_{b} + 2 a^{2} \phi_{1} (d\eta)_{a} (d\xi^{c})_{b} \]
\[+ a^{2} (2 \Psi_{ij} + \phi_{ij} (d\xi^{i})_{a} (d\xi^{j})_{b} \]
\[where \ \phi_{ij} \ and \ \chi_{ij} \ satisfy \ the \ equations \]
\[D^{i} \phi_{ij} = 0, \quad D^{i} \chi_{ij} = 0. \]  

(94)

(95)

The gauge-invariant variables $\phi_{i}$ and $\Psi$ are the scalar mode perturbations of second order, and $\phi_{ij}$ and $\chi_{ij}$ are the second-order vector and tensor modes of the metric perturbations, respectively.

Here, we also note the fact that the decomposition (32) is not unique. This situation is similar to the case of the linear order, but more complicated. In the definition of the gauge-invariant variables of the second-order metric perturbation, we may replace

\[X^{a} = X^{a} - Z^{a}, \]  

(96)

where $Z^{a}$ is gauge invariant and $X^{a}$ is transformed as

\[yX^{a} - \chi X^{a} = \xi^{a}_{1} \]  

(97)

under the gauge transformation $X_{1} = \chi_{1}$. This $Z^{a}$ may be different from the vector $Z^{a}$ in (81). By the replacement (96), the second-order metric perturbation (32) is given in the form

\[L_{ab} : = L_{ab} + 2 \xi^{X}_{ab} h_{ab} + (\xi^{V}_{ab} - \xi^{X}_{ab}) g_{ab}, \]  

(98)

where we defined

\[J_{ab} := L_{ab} - \xi^{W}_{ab} g_{ab} - 2 \xi^{Z}_{ab} \mathcal{K}_{ab} \]
\[+ 2 \xi^{Z}_{ab} \xi^{X}_{ab} g_{ab}, \]
\[Y^{a} := Y^{a} + W^{a} + [X^{i}, Z^{j}]^{a}. \]  

(99)

(100)

Here, the vector field $W^{a}$ in (100) constitute of some components of gauge-invariant second-order metric perturbation $L_{ab}$ like $Z^{a}$ in (81). The tensor field $J_{ab}$ is manifestly gauge invariant. The gauge transformation rule of the new gauge-invariant part $Y^{a}$ of the second-order metric perturbation is given by

\[yY^{a} - \chi Y^{a} = \xi^{a}_{(2)} + \xi^{a}_{(1)} X^{a}. \]  

(101)
Although (98) is similar to (32), the tensor fields $L_{ab}$ and $\mathcal{J}_{ab}$ are different from each other. Thus, the definition of the gauge-invariant variables for the second-order metric perturbation is not unique in a more complicated way than the linear order. This nonuniqueness of gauge-invariant variables for the metric perturbations propagates to the definition (34) and (35) of the gauge-invariant variables for matter fields.

In spite of the existence of infinitely many definitions of the gauge-invariant variables, in this paper, we consider the components of $L_{ab}$ given by (94). Equation (94) corresponds to the second-order extension of the longitudinal gauge, which is called Poisson gauge $X^a = Y^a = 0$.

6.2. Einstein Tensor. Here, we evaluate the second-order perturbation of the Einstein tensor (44) with the cosmological background (70). We evaluate the term $(1)^{a}_{b} [L]$ and $(2)^{a}_{b} [\mathcal{H}, \mathcal{H}]$ in the Einstein equation (69).

First, we evaluate the term $(1)^{a}_{b} [L]$ in the Einstein equation (69). Because the components (94) of $L_{ab}$ are obtained through the replacements

$$(1) \rightarrow (2), \quad (i) \rightarrow (2), \quad \Psi \rightarrow \Psi, \quad (i) \rightarrow (2), \quad (i) \rightarrow (2)$$

in the components (80) of $\mathcal{H}_{ab}$, we easily obtain the components of $(1)^{a}_{b} [L]$ through the replacements (102) in (82).

From (80), we can derive the components of $(2)^{a}_{b} [\mathcal{H}, \mathcal{H}]$ defined by (46)–(49) in a straightforward manner. Here, we use the results (85) and (89) of the first-order Einstein equations, for simplicity. Then the explicit components $(2)^{a}_{b} = (2)^{a}_{b} [\mathcal{H}, \mathcal{H}]$ are summarized as

$$(2)^{a}_{b} = \frac{2}{a^2} \left[ -3 D_k \left( \begin{array}{c} \Phi \\ \Phi \end{array} \right) + 8 \left( \begin{array}{c} \Phi \\ \Phi \end{array} \right) - 3 \left( \begin{array}{c} \partial_\eta \Phi \\ \Phi \end{array} \right)^2 - 12 \left( \begin{array}{c} \partial_\eta \Phi \\ \Phi \end{array} \right)^2 + D_k \left( \begin{array}{c} \Phi \\ \Phi \end{array} \right)^2 \right]

+ \frac{1}{8} \partial_\eta \chi^{ij} \left( \partial_\eta + 8 \mathcal{H} \right) \chi_{klm} + \frac{1}{2} D_k \chi_{lm} D^l \chi^{klm}

- \frac{1}{8} D_k \chi_{lm} \left( \begin{array}{c} \chi^{kl} \\ \chi^{kl} \end{array} \right) - \frac{1}{2} \chi_{lm} \left( \begin{array}{c} \chi^{ij} \\ \chi^{ij} \end{array} \right)

+ \left( \begin{array}{c} \partial_\eta \Phi \\ \Phi \end{array} \right) + 2 \mathcal{H} D_j \Phi \right] \chi^{ij}

+ \frac{1}{4} \partial_\eta \chi^{ij} D^l \chi^{|j|} + \chi^{ij} \partial_\eta D^l \chi^{|j|}

\right],

where we have checked the identity (51) through (103), Then, we may say that the expressions (103) are self-consistent.
6.3. Energy-Momentum Tensor and Klein-Gordon Equation. Here, we summarize the explicit components of the gauge-invariant variables. Through (72), (80), and (94), the components of (59) are derived by the straightforward calculations. In this paper, we just summarize the components of (2) in the situation where the first-order Einstein equations (85) and (89) are satisfied:

\begin{align*}
a^2 (2)T_{\eta}^\eta &= -\partial_\eta \varphi \partial_\eta \varphi + \frac{1}{2} \left( \partial_\eta \varphi \right)^2 - 2 \partial_\eta \varphi \frac{\partial V}{\partial \varphi} \\
&+ 4 \partial_\eta \varphi \frac{\partial V}{\partial \varphi} - 4 \left( \partial_\eta \varphi \right)^2 - \left( \partial_\eta \varphi \right)^2 \\
&- G_1 i \eta \partial_\eta \varphi \partial_\eta \varphi - a^2 (\partial_\eta \varphi)^2 2 \partial V \partial \varphi \\
&- D_1 i \eta \partial_\eta \varphi \partial_\eta \varphi - a^2 (\partial_\eta \varphi)^2 2 \partial V \partial \varphi \\
&+ 2 \partial_\eta \varphi \frac{\partial V}{\partial \varphi} - a^2 (\partial_\eta \varphi)^2 2 \partial V \partial \varphi. 
\end{align*}

where we defined

\[ \Xi_{(K)} := 8 \partial_\eta ( \frac{1}{2} \partial_\eta \varphi + 8 \varphi \Delta \varphi - 4a^2 \varphi \frac{\partial^2 V}{\partial \varphi^2} (\varphi) \]

\[ - a^2 (\varphi)^2 \frac{\partial^2 V}{\partial \varphi^2} (\varphi) + 8 \left( \frac{1}{2} \partial_\eta \varphi \partial_\eta \varphi \right) \]

\[ - 2 \chi_{ij} D_1 D_1 \varphi \partial_\eta \varphi \partial_\eta \varphi \chi_{ij} \]

In (105), \( \Xi_{(K)} \) is the source term which is the collection of the quadratic terms of the linear-order perturbations in the second-order perturbation of the Klein-Gordon equation. If we ignore this source term, (105) coincides with the first-order perturbation of the Klein-Gordon equation. From this source term (106) of the Klein-Gordon equation, we can see that the mode-mode coupling due to the nonlinear effects appear in the second-order Klein-Gordon equation.

We cannot discuss solutions to (105) only through this equation, since this includes metric perturbations. To determine the behavior of the metric perturbations, we have to treat the Einstein equations simultaneously. The second-order Einstein equation is shown in Section 6.4.

6.4. Einstein Equations. Here, we show all the components of the second-order Einstein equation (69). All components of (69) are summarized as

\[ \left\{ \begin{array}{c} -3H \partial_\eta + \Delta + 3K \right\} (2) \Psi + \left( - \partial_\eta H - 2H^2 + K \right) (2) \Phi \\
- 4 \pi G \left( \partial_\eta \varphi \partial_\eta \varphi + a^2 \varphi \frac{\partial V}{\partial \varphi} \right) = \Gamma_0 \\
2 \partial_\eta D_1 (2) \Psi + 2H \partial_\eta (2) \Phi - \frac{1}{2} (\Delta + 2K) \frac{\partial V}{\partial \varphi} \\
- 8 \pi G D_1 \partial_\eta \varphi = \Gamma_1 \\
D_1 D_1 \left( \frac{\partial V}{\partial \varphi} \right) - \Phi \\
+ \left\{ \begin{array}{c} - \Delta + 2 \partial_\eta^2 + 4H \partial_\eta - 2K \\
+ \left( 2H \partial_\eta + 2H \partial_\eta + 4H^2 + \Delta + 2K \right) \right\} \chi_{ij} \\
- \frac{1}{2} \partial_\eta \varphi \left( a^2 D_1 \chi_{ij} \right) + \frac{1}{2} \left( \partial_\eta^2 + 2H \partial_\eta + 2K - \Delta \right) \chi_{ij} \\
- 8 \pi G \left( \partial_\eta \varphi \partial_\eta \varphi - a^2 \varphi \frac{\partial V}{\partial \varphi} \right) \chi_{ij} = \Gamma_{ij}. \end{array} \right. \]

More generic formulae for the components of (2)\( T_{\mu}^b \) are given in [27].

Next, we show the gauge-invariant second-order the Klein-Gordon equation. We only consider the simple situation where (85) and (89) are satisfied. The formulae for more generic situation is given in [27]. Through (80), (94), and (72), the second-order perturbation of the Klein-Gordon equation (65) is given by

\begin{align*}
-a^2 \tilde{C}_{(K)} &= \tilde{C}_{(K)}^2 + 2H \partial_\eta \varphi - \Delta \varphi \\
- \left( \partial_\eta \Phi + 3 \partial_\eta \Psi \right) \partial_\eta \varphi \\
+ 2 \partial_\eta \Phi \frac{\partial V}{\partial \varphi} (\varphi) + a^2 \varphi \frac{\partial^2 V}{\partial \varphi^2} (\varphi) - \Xi_{(K)} \\
= 0,
\end{align*}

where \( \Gamma_0, \Gamma_1 \) and \( \Gamma_{ij} \) are the collection of the quadratic term of the first-order perturbations as follows:
\[ \Gamma_0 := 4\pi G \left( \partial_\eta \varphi_1 \right)^2 + D_i \varphi_1 D^i \varphi_1 + a^2 (\varphi_1)^2 \frac{\partial^2 V}{\partial \varphi^2} \]
\[-4\partial_\eta \mathcal{H} \left( \varphi_1 \right)^2 - 2 \varphi_1 \partial_\eta \varphi_1 \]
\[-4D_k \partial_\eta \left( \varphi_1 \right) \partial_\eta \varphi_k - 10 \partial_\eta \varphi \]
\[-3 \partial_\eta \left( \varphi_1 \right)^2 - 16 \left( \varphi_1 \right)^2 - 8 \mathcal{H}^2 \left( \varphi_1 \right)^2 \]
\[+ D_i D_k \Phi X^{ik} + \frac{1}{8} \partial_\eta \eta \partial_\eta \Phi X^{ik} + \mathcal{H} \left( \eta \right) \partial_\eta \Phi X^{ik} \]
\[-\frac{3}{8} D_k \chi_{lm} D^k \chi^{lm} + \frac{1}{4} D_k \chi_{lm} D^l \chi^{mk} \]
\[= \frac{1}{2} \chi_{lm} \Delta \chi^{lm} + \frac{1}{2} \chi^{lm} \Delta \chi_{lm}, \]
\[\Gamma_i := 16\pi G \partial_\eta \varphi_1 D_i \varphi_1 - 4\partial_\eta \left( \varphi_1 \right) \Phi D_i \Phi + \mathcal{H} \Phi D_i \Phi \]
\[-8 \Phi \partial_\eta \Phi D_i \Phi + 2D_k \Phi \partial_\eta \phi X_{ij} - 2\partial_\eta \phi X^{ij} \]
\[\frac{1}{2} \partial_\eta \chi^{ik} D_k \chi^{ij} - \chi^{ik} \partial_\eta D_k \chi^{ij} + \chi^{ij} \partial_\eta D_k \chi^{ik}, \]
\[\Gamma_{ij} := 16\pi G D_i \varphi_1 D_j \varphi_1 \]
\[+ 8\pi G \left( \partial_\eta \varphi_1 \right)^2 - D_i \varphi_1 D^i \varphi_1 - a^2 \left( \varphi_1 \right) \frac{\partial^2 V}{\partial \varphi^2} \]
\[-4D_i \left( \varphi_1 \right) \Phi D_j \left( \varphi_1 \right) - 8 \left( \varphi_1 \right) \Phi D_i \Phi \Phi \]
\[+ 6D_k \Phi \left( \varphi_1 \right) D^k \Phi + 2 \left( \varphi_1 \right) \Delta \Phi + 2 \left( \partial_\eta \left( \varphi_1 \right) \right)^2 + 8\partial_\eta \mathcal{H} \left( \varphi_1 \right)^2 \]
\[+ 16 \mathcal{H}^2 \left( \varphi_1 \right)^2 + 16 \mathcal{H} \left( \varphi_1 \right) \partial_\eta \left( \varphi_1 \right) - 4 \left( \partial_\eta \left( \varphi_1 \right) \right)^2 \]
\[-4 \mathcal{H} \partial_\eta \Phi \chi^{ij} - 2\partial_\eta \left( \chi^{ij} \right) - 4D^k \left( \chi^{ij} \right) D_k \varphi_1 \]
\[+ 4 \Phi \Delta \chi^{ij} - 4D^k \Phi D_k \varphi_1 \]
\[+ 2\Delta \Phi \chi^{ij} + 2D_i D_k \Phi \chi^{ij} + \partial_\eta \chi^{ik} \partial_\eta \chi^{ij} \]
\[-D_k \chi_{lm} D^k \chi^{ij} + D^k \chi_{lm} D^l \chi^{jk} - \frac{1}{2} D^k \chi_{lm} D^l \chi^{jk} \]
\[-\chi_{lm} D_i \chi_{jk} + 2 \chi_{lm} D_i \chi_{jk} - \chi_{lm} D_m D_l \chi_{ij} \]
\[\frac{1}{4} \left( 3\partial_\eta \chi^{ik} \partial_\eta \chi^{kl} - 3 \partial_\eta \chi_{lm} D^k \chi^{lm} \right) \]
\[+ 2D_k \chi_{lm} D^l \chi^{mk} - 4K \chi_{lm} \chi^{mk} \]
\[\gamma^{ij}_{(112)} \]

Here, we used (75), (85), (87), (89), and (91).

The tensor part of (109) is given by
\[\left( \frac{\partial^2 \gamma}{\partial \varphi^2} + 2 \mathcal{H} \partial_\eta + 2K - \Delta \right) \gamma^{ij}_{(2)} \]
\[= 2\Gamma_{ij} - \frac{2}{3} \gamma_{ij} \Gamma_k \frac{1}{3} \gamma_{ij} \Delta \left( \Delta + 3K \right)^{-1} \]
\[\times \left( \Delta^{-1} D^k \Gamma_k^{-1} \frac{1}{3} \Gamma_k \right) \]
\[+ 4 \left( \Gamma_{ij} \left( \Delta + 2K \right)^{-1} D^l \Gamma_l \Gamma_k \right) \]
\[\left( \Delta + 2K \right)^{-1} D^k \Gamma_{jk} \right]. \]

This tensor mode is also called the second-order gravitational waves.

Further, the vector part of (108) yields the initial value constraint and the evolution equation of the vector mode (2): \[\gamma^{ij}_{(2)} = \frac{2}{\Delta + 2K} \left( \Delta^{-1} D^k \Gamma_k - \Gamma_i \right), \]
\[\partial_\eta \left( a^2 \gamma^{ij}_{(2)} \right) = \frac{2a^2}{\Delta + 2K} \left( \Delta^{-1} D^k \Gamma_k - \Gamma_i \right). \]

Finally, scalar part of (108) are summarized as \[2\partial_\eta \Psi + 2\mathcal{H} \Phi - 8\pi G \Phi \eta \Phi = \Delta^{-1} D^k \Gamma_k, \]
\[2 \Psi + \Phi = \frac{3}{2} (\Delta + 3K)^{-1} \left( \Delta^{-1} D^l \Gamma_l - \frac{1}{3} \Gamma_k \Gamma_k \right), \]
\[\left( \frac{\partial^2 \Psi}{\partial \varphi^2} - 4\frac{\Delta}{\Delta + 4K} \Phi \right) \Psi \]
\[= \left( 2\partial_\eta \mathcal{H} + \mathcal{H} \partial_\eta + 4 \mathcal{H}^2 + \frac{4}{3} \right) \Phi - 8\pi G \frac{a^2}{\partial \varphi^2} \frac{\partial V}{\partial \varphi}, \]
\[= \Gamma_0 - \frac{1}{6} \Gamma_k \Delta \]
\[\left\{ \begin{array}{l}
\partial_\eta \left( \partial_\eta \Psi - \partial_\eta \mathcal{H} \Phi \right) - \Delta - 4K + 2 \left( \partial_\eta \mathcal{H} - \frac{\partial_\eta \mathcal{H}}{\partial \varphi} \Phi \right) \\
\partial_\eta \left( 2 \partial_\eta \Psi - \mathcal{H} \partial_\eta \Phi \right) - \Delta - 4K + 2 \left( \partial_\eta \mathcal{H} - \frac{\partial_\eta \mathcal{H}}{\partial \varphi} \Phi \right)
\end{array} \right\} \Phi \]
\[-\Delta^{-1} D^k \Gamma_k \]
\[-\frac{3}{2} \left( \partial_\eta \mathcal{H} - \frac{2 \partial_\eta \mathcal{H}}{\partial \varphi} \Phi \right) \partial_\eta \Phi \left( \Delta + 3K \right)^{-1} \]
\[\times \left( \Delta^{-1} D^k \Gamma_k - \frac{1}{3} \Gamma_k \right). \]

where \(\Gamma_i^j := \gamma^{ij}_{(2)} \Gamma_{ik}^j\) and \(\Gamma_k^j := \gamma^{ij}_{(2)} \Gamma_{ik}^j\). Equation (118) is the second-order extension of (92), which is the master equation of scalar mode of the second-order cosmological perturbation in a universe filled with a single scalar field.

Thus, we have a set of ten equations for the second-order perturbations of a universe filled with a single scalar field, (113)–(118). To solve this system of equations of the second-order Einstein equation, first of all, we have to solve...
the linear-order system. This is accomplished by solving (92) to obtain the potential \( \Phi^1 \), \( \varphi_1 \) is given through (87), and the tensor mode \( \chi_{ij}^{(1)} \) is given by solving (90). Next, we evaluate the quadratic terms \( \Gamma_0, \Gamma_i, \) and \( \Gamma_{ij} \) of the linear-order perturbations, which are defined by (110)–(112). Then, using the information of (110)–(112), we estimate the source term in (118). If we know the two independent solutions to the linear-order master equation (92), we can solve (118) through the method using the Green functions. After constructing the solution \( \Phi \) to (118), we can obtain the second-order metric perturbation \( \Psi \) through (116). Thus, we have obtained the second-order gauge-invariant perturbation \( \varphi_2 \) of the scalar field through (115). Thus, the all scalar modes \( \varphi_1, \varphi_2 \), and \( \varphi_{12} \) are obtained. Equation (117) is then used to check the consistency of the second-order perturbation of the Klein Gordon equation (105) as in Section 6.5.

For the vector-mode, \( \nu_i \) of the first-order identically vanishes due to the momentum constraint (89) for the linear-order metric perturbations. On the other hand, in the second-order, we have evolution equation (114) of the vector mode \( \nu_i^{(2)} \) with the initial value constraint. This evolution equation of the second-order vector mode should be consistent with the initial value constraint, which is confirmed in Section 6.5. Equations (114) also imply that the second-order vector-mode perturbation may be generated by the mode couplings of the linear-order perturbations. As the simple situations, the generation of the second-order vector mode due to the scalar-scalar mode coupling is discussed in [44–47].

The second-order tensor mode is also generated by the mode-coupling of the linear-order perturbations through the source term in (113). Note that (113) is almost same as (90) for the linear-order tensor mode, except for the existence of the source term in (113). If we know the solution to the linear-order Einstein equations (90) and (92), we can evaluate the source term in (113). Further, we can solve (113) through the Green function method. This leads the generation of the gravitational wave of the second order. Actually, in the simple situation where the first-order tensor mode neglected, the generation of the second-order gravitational waves discussed in some literature [48–54].

6.5. Consistency of Equations for Second-Order Perturbations
Now, we consider the consistency of the second-order perturbations of the Einstein equations (115)–(118) for the scalar modes, (114) for vector mode, and the Klein-Gordon equation (105). The consistency check of these equations are necessary to guarantee that the derived equations are correct, since the second-order Einstein equations have complicated forms owing to the quadratic terms of the linear-order perturbations that arise from the nonlinear effects of the Einstein equations.

Since the first equation in (114) is the initial value constraint for the vector mode \( \nu_i^{(2)} \) and it should be consistent with the evolution equation, that is, the second equation of (114). these equations should be consistent with each other from the general arguments of the Einstein equation. Explicitly, these equations are consistent with each other if the equation

\[
\partial_\eta \Gamma_k + 2\mathcal{H} \Gamma_k - D^i D^j \Gamma_{ij} = 0
\]

is satisfied. Actually, through the first-order perturbative Einstein equations (87), (92), and (90), we can confirm (119). This is a trivial result from a general viewpoint, because the Einstein equation is the first class constrained system. However, this trivial result implies that we have derived the source terms \( \Gamma_i \) and \( \Gamma_{ij} \) of the second-order Einstein equations consistently.

Next, we consider (117). Through the second-order Einstein equations (115), (116), (118), and the background Klein-Gordon equation (76), we can confirm that (117) is consistent with the set of the background, first-order and other second-order Einstein equation if the equation

\[
\left\{ \partial_\eta + 2\mathcal{H} \right\} D^k \Gamma_k - D^i D^j \Gamma_{ij} = 0
\]

is satisfied under the background and first-order Einstein equations. Actually, we have already seen that (119) is satisfied under the background and first-order Einstein equations. Taking the divergence of (119), we can immediately confirm (120). Then, (117) gives no information.

Thus, we have seen that the derived Einstein equations of the second-order (114)–(118) are consistent with each other through (119). This fact implies that the derived source terms \( \Gamma_i \) and \( \Gamma_{ij} \) of the second-order perturbations of the Einstein equations, which are defined by (111) and (112), are correct source terms of the second-order Einstein equations. On the other hand, for \( \Gamma_0 \), we have to consider the consistency between the perturbative Einstein equations and the perturbative Klein-Gordon equation as seen below.

Now, we consider the consistency of the second-order perturbation of the Klein-Gordon equation and the Einstein equations. The second-order perturbation of the Klein-Gordon equation is given by (105) with the source term (2) (106). Since the vector mode \( \nu_i \) and tensor mode \( \chi_{ij}^{(2)} \) of the second-order do not appear in the expressions (105) of the second-order perturbation of the Klein-Gordon equation, we may concentrate on the Einstein equations for scalar mode of the second order, that is, (115), (116), and (118) with the definitions (110)–(112) of the source terms. As in the linear case, the second-order perturbation of the Klein-Gordon equation should also be derived from the set of equations consisting of the second-order perturbations of the Einstein equations (115), (116), (118), the first-order perturbations of the Einstein equations (85), (87), (92), and the background Einstein equations (74). Actually, from these equations, we can show that the second-order perturbation of the Klein-Gordon equation is consistent with the background and the second-order Einstein equations if the equation

\[
2 \left( \partial_\eta + H \right) \Gamma_0 - D^k \Gamma_k + \mathcal{H} \Gamma_k + 8\pi G \partial_\eta \varphi \mathcal{E}_{(k)} = 0
\]
is satisfied under the background and the first-order Einstein equations. Further, we can also confirm (121) through the background Einstein equations (74), the scalar part of the first-order perturbation of the momentum constraint (87), and the evolution equations (92) and (90) for the first-order scalar and tensor modes in the Einstein equation.

As shown in [28], the first-order perturbation of the Klein-Gordon equation is derived from the background and the first-order perturbations of the Einstein equation. In the case of the second-order perturbation, the Klein-Gordon equation (105) can be also derived from the background, the first-order, and the second-order Einstein equations. The first-order perturbations of the Einstein equation and the Klein-Gordon equation include the source terms $\Gamma_0$, $\Gamma_i$, $\Gamma_{ij}$, and $\Xi_{(K)}$ due to the mode-coupling of the linear-order perturbations. The second-order perturbation of the Klein-Gordon equation gives the relation (121) between the source terms $\Gamma_0$, $\Gamma_i$, $\Gamma_{ij}$, and $\Xi_{(K)}$, and we have also confirmed that (121) is satisfied due to the background, the first-order perturbation of the Einstein equations, and the Klein-Gordon equation. Thus, the second-order perturbation of the Klein-Gordon equation is not independent of the set of the background, the first-order, and the second-order Einstein equations if we impose on the Einstein equation at any conformal time $\eta$. This also implies that the derived formulae of the source terms $\Gamma_0$, $\Gamma_i$, $\Gamma_{ij}$, and $\Xi_{(K)}$ are consistent with each other. In this sense, we may say that the formulae (110)–(112) and (106) for these source terms are correct.

7. Summary and Discussions

In this paper, we summarized the current status of the formulation of the gauge-invariant second-order cosmological perturbations. Although the presentation in this paper is restricted to the case of the universe filled by a single scalar field, the essence of the general framework of the gauge-invariant perturbation theory is transparent through this simple case. The general framework of the general relativistic higher-order gauge-invariant perturbation theory can be separated into three parts. First one is the general formulation to derive the gauge-transformation rules (18) and (19). Second one is the construction of the gauge-invariant variables for the perturbations on the generic background spacetime inspecting gauge-transformation rules (18) and (19) and the decomposition formula (36) and (37) for perturbations of any tensor field. Third one is the application of the above general framework of the gauge-invariant perturbation theory to the cosmological situations.

To derive the gauge-transformation rules (18) and (19), we considered the general arguments on the Taylor expansion of an arbitrary tensor field on a manifold, the general class of the diffeomorphism which is wider than the usual exponential map, and the general formulation of the perturbation theory. This general class of diffeomorphism is represented in terms of the Taylor expansion (2) of its pull-back. As commented in Section 2.1, this general class of diffeomorphism does not form a one-parameter group of diffeomorphism as shown through (3). However, the properties (3) do not directly mean that this general class of diffeomorphism does not form a group. One of the key points of the properties of this diffeomorphism is the noncommutativity of generators $\xi^a$ and $\xi^b$ of each order. Although the expression of the nth-order Taylor expansion of the pull-back of this general class is discussed in [41], when we consider the situation of the nth-order perturbation, this noncommutativity becomes important [22]. Therefore, to clarify the properties of this general class of diffeomorphism, we have to take care of this noncommutativity of generators. Thus, there is a room to clarify the properties of this general class of diffeomorphism.

Further, in Section 2.3, we introduced a gauge choice $\mathcal{X}_\lambda$ as an exponential map, for simplicity. On the other hand, we have the concept of the general class of diffeomorphism which is wider than the class of the exponential map. Therefore, we may introduce a gauge choice as one of the element of this general class of diffeomorphism. However, the gauge-transformation rules (18) and (19) will not be changed even if we generalize the definition of a each gauge choice as emphasized in Section 2.3. Although there is a room to sophisticate in logical arguments to derive the gauge-transformation rules (18) and (19), these are harmless to the development of the general framework of the gauge-invariant perturbation theory shown in Sections 2.3, 2.5, 3, and their application to cosmological perturbations in Section 4.

As emphasized in Section 2.5, our starting point to construct gauge-invariant variables is the assumption that we already know the procedure for finding gauge-invariant variables for the linear metric perturbations as (23). This is highly nontrivial assumption on a generic background spacetime. The procedure to accomplish the decomposition (23) completely depends on the details of the background spacetime. In spite of this nontriviality, this assumption is almost correct in some background spacetime [55–59]. Further, once we accept this assumption, we can develop the higher-order perturbation theory in an independent manner of the details of the background spacetime. We also expect that this general framework of the gauge-invariant perturbation theory is extensible to nth-order perturbation theory, since our procedure to construct gauge-invariant variables can be extended to the third-order perturbation theory with two-parameter [22]. Due to this situation, in [27], we propose the conjecture which states that the above assumption for the decomposition of the linear-order metric perturbation is correct for any background spacetime. We may also say that the most nontrivial part of our general framework of higher-order gauge-invariant perturbation theory is in the above assumption. Further, as emphasized in Section 5.1, we assumed the existence of some Green functions to accomplish the decomposition (23) and this assumption exclude some perturbative modes of the metric perturbations from our consideration, even in the case of cosmological perturbations. For example, homogeneous modes of perturbations are excluded in our current arguments of the cosmological perturbation theory. These homogeneous modes will be necessary to discuss
the comparison with the arguments based on the long-wavelength approximation. Therefore, we have to say that there is a room to clarify even in the cosmological perturbation theory.

Even if the assumption is correct on any background spacetime, the other problem is in the interpretations of the gauge-invariant variables. We have commented on the nonuniqueness in the definitions of the gauge-invariant variables through (81) and (98). This nonuniqueness in the definition of gauge-invariant variables also leads some ambiguities in the interpretations of gauge-invariant variables. On the other hand, as emphasized in Section 2.3, any observations and experiments should be independent of the gauge choice. Further, the nonuniqueness in the definitions the gauge-invariant variables expressed by (81) and (98) have the same form as the decomposition formulae (36) and (37). Therefore, if the statement that any direct observables in any observations and experiments is independent of the gauge choice is really true, this also confirms that the nonuniqueness of the definition of the gauge-invariant variables also have nothing to do with the direct observables in observations and experiments. These will be confirmed by the clarification of the relations between gauge-invariant variables and observables in experiments and observations. To accomplish this, we have to specify the concrete process of experiments and observations and clarify the problem of what are the direct observables in the experiments and observations and derive the relations between the gauge-invariant variables and observables in concrete observations and experiments. If these arguments are completed, we will be able to show that the gauge degree of freedom is just an unphysical degree of freedom and the nonuniqueness of the gauge-invariant variables has nothing to do with the direct observables in the concrete observation or experiment, and then, we will be able to clarify the precise physical interpretation of the gauge-invariant variables.

For example, in the case of the CMB physics, we can easily see that the first-order perturbation of the CMB temperature is automatically gauge invariant from (36), because the background temperature of CMB is homogeneous. On the other hand, the decomposition formula (37) of the second order yields that the theoretical prediction of the second-order perturbation of the CMB temperature may depend on gauge choice, since we do know the existence of the first-order fluctuations as the temperature anisotropy in CMB. However, as emphasized above, the direct observables in observations should be gauge invariant and the gauge-variant term in (37) should be disappear in the direct observables. Therefore, we have to clarify how the gauge-invariant variables are related to the observed temperature fluctuations and the gauge-variant term disappears in the observable.

Although there are some rooms to accomplish the complete formulation of the second-order cosmological perturbation theory, we derived all the components of the second-order perturbation of the Einstein equation without ignoring any types modes (scalar-, vector-, tensor-types) of perturbations in the case of a scalar field system. In our formulation, any gauge fixing is not necessary and we can obtain all equations in the gauge-invariant form, which are equivalent to the complete gauge fixing. In other words, our formulation gives complete gauge-fixed equations without any gauge fixing. Therefore, equations obtained in a gauge-invariant manner cannot be reduced without physical restrictions any more. In this sense, the equations shown here are irreducible. This is one of the advantages of the gauge-invariant perturbation theory.

The resulting Einstein equations of the second order show that any type of mode-coupling appears as the quadratic terms of the linear-order perturbations owing to the nonlinear effect of the Einstein equations, in principle. Perturbations in cosmological situations are classified into three types: scalar, vector, and tensor. In the second-order perturbations, we also have these three types of perturbations as in the case of the first-order perturbations. Furthermore, in the equations for the second-order perturbations, there are many quadratic terms of linear-order perturbations owing to the nonlinear effects of the system. Owing to these nonlinear effects, the above three types of perturbations couple with each other. In the scalar field system shown in this paper, the first-order vector mode does not appear due to the momentum constraint of the first-order perturbation of the Einstein equation. Therefore, we have seen that three types of mode-coupling appear in the second-order Einstein equations, that is, scalar-scalar, scalar-tensor, and tensor-tensor type of mode coupling. In general, all types of mode-coupling may appear in the second-order Einstein equations. Actually, in [28], we also derived all the components of the Einstein equations for a perfect fluid system and we can see all types of mode-coupling, that is, scalar-scalar, scalar-vector, scalar-tensor, vector-vector, vector-tensor, and tensor-tensor types mode-coupling, appear in the second-order Einstein equation, in general. Of course, in the some realistic situations of cosmology, we may neglect some modes. In this case, we may neglect some mode-coupling. However, even in this case, we should keep in mind the fact that all types of mode-couplings may appear in principle when we discuss the realistic situations of cosmology. We cannot deny the possibility that the mode-couplings of any type produces observable effects when the quite high accuracy of observations is accomplished.

Even in the case of the single scalar field discussed in this paper, the source terms of the second-order Einstein equation show the mode-coupling of scalar-scalar, scalar-tensor, and the tensor-tensor types as mentioned above. Since the tensor mode of the linear order is also generated due to quantum fluctuations during the inflationary phase, the mode-couplings of the scalar-tensor and tensor-tensor types may appear in the inflation. If these mode-couplings occur during the inflationary phase, these effects will depend on the scalar-tensor ratio r. If so, there is a possibility that the accurate observations of the second-order effects in the fluctuations of the scalar type in our universe also restrict the scalar-tensor ratio r or give some consistency relations between the other observations such as the measurements
of the B-mode of the polarization of CMB. This will be a new effect that gives some information on the scalar-tensor ratio $r$.

Furthermore, we have also checked the consistency between the second-order perturbations of the equations of motion of matter field and the Einstein equations. In the case of a scalar field, we checked the consistency between the second-order perturbations of the Klein-Gordon equation and the Einstein equations. Due to this consistency check, we also showed that these relations between the source terms are satisfied through the background and the first-order perturbation of the Einstein equations in [28]. This implies that the set of all equations are self-consistent and the derived source terms are given by (119) and (121). We note that the relation (119) comes from the consistency in the Einstein equations of the second order by itself, while the relation (121) comes from the consistency between the second-order perturbation of the Klein-Gordon equation and the Einstein equation. Moreover, we have also checked the consistency in the Einstein equations of the second order by itself as mentioned above. After complete the problem of homogeneous modes, we have to clarify the physical behaviors of the second-order cosmological perturbation in the single scalar field system in the context of the inflationary model. This is the preliminary step to clarify the quantum behaviors of second-order perturbations in the inflationary universe. Further, we also have to extend our arguments to the Klein-Gordon equation and the Einstein equation. We also showed that these relations are independent of the details of the potential of the scalar field.

Thus, we have derived the self-consistent set of equations of the second-order perturbation of the Einstein equations and the evolution equations of matter fields in terms of gauge-invariant variables. As the current status of the second-order gauge-invariant cosmological perturbation theory, we may say that the curvature terms in the second-order Einstein tensor (69), that is, the second-order perturbations of the Einstein tensor, are almost completely derived although there remains the problem of homogeneous modes as mentioned above. After complete the problem of homogeneous modes, we have to clarify the physical behaviors of the second-order cosmological perturbation in the single scalar field system in the context of the inflationary scenario. This is the preliminary step to clarify the quantum behaviors of second-order perturbations in the inflationary universe. Further, we also have to carry out the comparison with the result by long-wavelength approximations. If these issues are completed, we may say that we have completely understood the properties of the second-order perturbation of the Einstein tensor. The next task is to clarify the nature of the second-order perturbation of the energy-momentum tensor through the extension to multi-fluid or multi-field systems. Further, we also have to extend our arguments to the Einstein Boltzmann system to discuss CMB physics, since we have to treat photon and neutrinos through the Boltzmann distribution functions. This issue is also discussed in some literature [13–21, 29, 30]. If we accomplish these extension, we will be able to clarify the Non-linear effects in CMB physics.

Finally, readers might think that the ingredients of this paper is too mathematical as Astronomy. However, we have to emphasize that a high degree of the theoretical sophistication leads unambiguous theoretical predictions in many cases. As in the case of the linear-order cosmological perturbation theory, the developments in observations are also supported by the theoretical sophistication and the theoretical sophistication are accomplished motivated by observations. In this sense, now, we have an opportunity to develop the general relativistic second-order perturbation theory to a high degree of sophistication which is motivated by observations. We also expect that this theoretical sophistication will be also useful to discuss the theoretical predictions of non-Gaussianity in CMB and comparison with observations. Therefore, I think that this opportunity is opened not only for observational cosmologists but also for theoretical and mathematical physicists.

**Appendices**

**A. Derivation of the Generic Representation of the Taylor Expansion of Tensors on a Manifold**

In this section, we derive the representation of the coefficients of the formal Taylor expansion (2) of the pull-back of a diffeomorphism in terms of the suitable derivative operators. The guide principle of our arguments is the following theorem [38, 40].

**Theorem A.** Let $\mathcal{D}$ be a derivative operator acting on the set of all the tensor fields defined on a differentiable manifold $\mathcal{M}$ and satisfying the following conditions: (i) it is linear and satisfies the Leibniz rule; (ii) it is tensor-type preserving; (iii) it commutes with every contraction of a tensor field; and (iv) it commutes with the exterior differentiation $d$. Then, $\mathcal{D}$ is equivalent to the Lie derivative operator with respect to some vector field $\xi$, that is, $\mathcal{D} = \mathcal{L}_\xi$.

The proof of the assertion of Theorem A is given in [38] as follows. When acting on functions, the derivative operator $\mathcal{D}$ defines a vector field $\xi$ through the relation

$$\mathcal{D} f =: \xi(f) = \xi f, \quad \forall f \in \mathcal{F}(\mathcal{M}). \quad (A.1)$$

The assertion of the theorem for an arbitrary tensor field holds if and only if the assertions for an arbitrary scalar function and for an arbitrary vector field $V$ hold. To do this, we consider the scalar function $V(f)$ and we obtain that

$$\mathcal{D}(V(f)) = \xi(V(f)) \quad (A.2)$$

through (A.1). Through the conditions (i)–(iv) of $\mathcal{D}$, $\mathcal{D}(V(f))$ is also given by

$$\mathcal{D}(V(f)) = \mathcal{D}(df(V)) = \mathcal{D}[C(df \otimes V)] = C[\mathcal{D}(df \otimes V)] = C[d(df) \otimes V + df \otimes \mathcal{D}V] = C[d(df)] \otimes V + df \otimes \mathcal{D}V = d(\mathcal{D}f)(V) + df(\mathcal{D}V) = V(\mathcal{D}f) + (\mathcal{D}V)(f). \quad (A.3)$$
Then we obtain that
\[
(\mathcal{D} V)(f) = \xi(V(f)) - V(\xi(f)) = [\xi, V](f) = (\xi V)(f)
\] (A.4)
for an arbitrary \( f \), that is,
\[
\mathcal{D} V = \xi V.
\] (A.5)
Through (A.1) and (A.5), we can recursively show that
\[
\mathcal{D} Q = \xi Q
\] (A.6)
for an arbitrary tensor field \( Q \) \([40]\).

Now, we consider the derivation of the Taylor expansion (1). As in the main text, we first consider the representation of the Taylor expansion of \( \Phi^*_f \) for an arbitrary scalar function \( f \in \mathcal{F}(\mathcal{M}) \):
\[
\{ \Phi^*_f (p) \} = f(p) + \lambda \frac{\partial}{\partial \lambda} \{ \Phi^*_f (p) \} \bigg|_{\lambda=0} + \frac{1}{2} \lambda^2 \frac{\partial^2}{\partial \lambda^2} \{ \Phi^*_f (p) \} \bigg|_{\lambda=0} + O(\lambda^3),
\] (A.7)
where \( \mathcal{F}(\mathcal{M}) \) denotes the algebra of \( C^\infty \) functions on \( \mathcal{M} \). Although the operator \( \partial/\partial \lambda \) in the bracket \{(\star)\}_{\lambda=0} \) of (A.7) are simply symbolic notation, we stipulate the properties
\[
\left\{ \frac{\partial^2}{\partial \lambda^2} \{ \Phi^*_f (p) \} \right\} \bigg|_{\lambda=0} = \left\{ \frac{\partial}{\partial \lambda} \left( \frac{\partial}{\partial \lambda} \{ \Phi^*_f (p) \} \right) \right\} \bigg|_{\lambda=0}, \quad (A.8)
\]
\[
\left\{ \frac{\partial}{\partial \lambda} \{ \Phi^*_f (p) \} \right\} \bigg|_{\lambda=0} = \left\{ 2 \Phi^*_f \frac{\partial}{\partial \lambda} \{ \Phi^*_f (p) \} \right\} \bigg|_{\lambda=0}, \quad (A.9)
\]
for all \( f \in \mathcal{F}(\mathcal{M}) \), where \( n \) is an arbitrary finite integer. These properties imply that the operator \( \partial/\partial \lambda \) in fact is not simply symbolic notation but indeed the usual partial differential operator on \( \mathbb{R} \). We note that the property (A.9) is the Leibniz rule, which plays important roles when we derive the representation of the Taylor expansion (A.7) in terms of suitable Lie derivatives.

Together with the property (A.9), Theorem A yields that there exists a vector field \( \xi_2 \), so that
\[
\left\{ \frac{\partial}{\partial \lambda} \{ \Phi^*_f (p) \} \right\} \bigg|_{\lambda=0} = :\xi_2 f.
\] (A.10)
Actually, the conditions (ii)–(iv) in Theorem A are satisfied from the fact that \( \Phi^*_f \) is the pull-back of a diffeomorphism \( \Phi_1 \) and (i) is satisfied due to the property (A.9).

Next, we consider the second-order term in (A.7). Since we easily expect that the second-order term in (A.7) may includes \( \mathcal{L}_2 \xi_1 \), we define the derivative operator \( \mathcal{L}_2 \) by
\[
\left\{ \frac{\partial^2}{\partial \lambda^2} \{ \Phi^*_f (p) \} \right\} \bigg|_{\lambda=0} = :\left( \mathcal{L}_2 + a \xi_2 \right) f,
\] (A.11)
where \( a \) is determined so that \( \mathcal{L}_2 \) satisfies the conditions of Theorem A. The conditions (ii)–(iv) in Theorem A for \( \mathcal{L}_2 \) are satisfied from the fact that \( \Phi^*_f \) is the pull-back of a diffeomorphism \( \Phi_1 \). Further, \( \mathcal{L}_2 \) is obviously linear but we have to check \( \mathcal{L}_2 \) satisfy the Leibniz rule, that is,
\[
\mathcal{L}_2 (f^2) = 2 f \mathcal{L}_2 f,
\] (A.12)
for all \( f \in \mathcal{F}(\mathcal{M}) \). To do this, we use the properties (A.8) and (A.9), then we can easily see that the Leibniz rule (A.12) is satisfied if and only if \( a = 1 \) and we may regard \( \mathcal{L}_2 \) as the Lie derivative with respect to some vector field. Then, when and only when \( a = 1 \), there exists a vector field \( \xi_2 \) such that
\[
\mathcal{L}_2 f = \xi_2 f,
\] (A.13)
Thus, we have seen that the Taylor expansion (A.7) for an arbitrary scalar function \( f \) is given by (2).

Although the formula (2) of the Taylor expansion is for an arbitrary scalar function, we can easily extend this formula to that for an arbitrary tensor field \( Q \) as the assertion of Theorem A. The proof of the extension of the formula (2) to an arbitrary tensor field \( Q \) is completely parallel to the proof of the formula (2) for an arbitrary scalar function if we stipulate the properties
\[
\left\{ \frac{\partial}{\partial \lambda} \{ \Phi^*_f Q \} \right\} \bigg|_{\lambda=0} = \left\{ \frac{\partial}{\partial \lambda} \left( \frac{\partial}{\partial \lambda} \{ \Phi^*_f Q \} \right) \right\} \bigg|_{\lambda=0}, \quad (A.14)
\]
\[
\left\{ \frac{\partial}{\partial \lambda} \{ Q \} \right\} \bigg|_{\lambda=0} = \left\{ 2 \Phi^*_f \frac{\partial}{\partial \lambda} \{ Q \} \right\} \bigg|_{\lambda=0}, \quad (A.9)
\]
instead of (A.8) and (A.9). As the result, we obtain the representation of the Taylor expansion for an arbitrary tensor field \( Q \).

\section*{B. Derivation of the Perturbative Einstein Tensors}

Following the outline of the calculations explained in Section 3.1, we first calculate the perturbative expansion of the inverse metric. The perturbative expansion of the inverse metric can be easily derived from (22) and the definition of the inverse metric
\[
\tilde{g}^{ab} \tilde{g}_{bc} = \delta^a_c.
\] (B.1)
We also expand the inverse metric \( \tilde{g}^{ab} \) in the form
\[
\tilde{g}^{ab} = g^{ab} + \lambda \{ \tilde{g}^{ab} \} + \lambda^2 \{ \tilde{g}^{ab} \} + \ldots.
\] (B.2)
Then, each term of the expansion of the inverse metric is given by
\[
\{ \tilde{g}^{ab} \} = - h^{ab} \quad \text{(1)}
\]
\[
\{ \tilde{g}^{ab} \} = 2 h^{ac} h_c^b - p^{ab} \quad \text{(2)}
\] (B.3)
To derive the formulae for the perturbative expansion of the Riemann curvature, we have to derive the formulae for the perturbative expansion of the tensor \( C^{ab} \) given by (40).
The tensor $C_{ab}^c$ is also expanded in the same form as (11). The first-order perturbations of $C_{ab}^c$ have the well-known form [42]

$$(1) C_{ab}^c = \nabla (a h_b)^c - \frac{1}{2} \nabla h_a =: H_{ab}^c[h],$$

where $H_{ab}^c[A]$ is defined by (48) for an arbitrary tensor field $A_{ab}$ defined on the background spacetime $\mathcal{M}_0$. In terms of the tensor field $H_{ab}^c$ defined by (48) the second-order perturbation (2) of $C_{ab}^c$ of the tensor field $C_{ab}^c$ is given by

$$(2) C_{ab}^c = H_{ab}^c[l] - 2h^d H_{abcd}[h].$$

The first- and the second-order perturbation of the Riemann curvature are given by

$$(1) R_{abc}^d = -2\nabla [a (1) C_{bd}^c],$$

$$(2) R_{abc}^d = -2\nabla [a (2) C_{bd}^c] + 4(1) C_{e}^c [a (1) C_{bd}^c].$$

Substituting (B.4) and (B.5) into (B.7), we obtain the perturbative form of the Riemann curvature in terms of the variables defined by (48) and (49):

$$(1) R_{abc}^d = -2\nabla [a H_b]^c [h],$$

$$(2) R_{abc}^d = -2\nabla [a H_b]^c [l] + 4H_{[a}^d [h] H_b] + 4 \nabla [a H_b]^c [h].$$

To write down the perturbative curvatures (B.8) and (B.9) in terms of the gauge invariant and variant variables defined by (23) and (32), we first derive an expression for the tensor field $H_{ab}^c[h]$ in terms of the gauge-invariant variables, and then, we derive a perturbative expression for the Riemann curvature.

First, we consider the linear-order perturbation (B.8) of the Riemann curvature. Using the decomposition (23) and the identity $R_{ab}^c [d] = 0$, we can easily derive the relation

$$(1) R_{abc}^d = -2\nabla [a H_b]^c [\mathcal{H}] + \xi X R_{abc}^d,$$

where the variable $H_{ab}^c[\mathcal{H}]$ is defined by (48) and (49) with $A_{ab} = \mathcal{H}_{ab}$. Clearly, the variable $H_{ab}^c[\mathcal{H}]$ is gauge invariant. Taking the derivative and using the Bianchi identity $\nabla [a R_{bc}^d] = 0$, we obtain that

$$(2) R_{abc}^d = -2\nabla [a H_b]^c [\mathcal{H}] + \xi X R_{abc}^d.$$

Similar but some cumbersome calculations yield

$$(2) R_{abc}^d = -2\nabla [a H_b]^c [\mathcal{L}] + 4H_{[a}^d [\mathcal{H}] H_b] + 4 \nabla [a H_b]^c [\mathcal{H}]$$

$$+ 4 \nabla [a H_b]^c [\mathcal{H}]$$

$$+ 2\xi X R_{abc}^d.$$

Equations (B.11) and (B.12) have the same for as the decomposition formulæ (36) and (37), respectively.

Contracting the indices $b$ and $d$ in (B.11) and (B.12) of the perturbative Riemann curvature, we can directly derive the formulae for the perturbative expansion of the Ricci curvature: expanding the Ricci curvature

$$(1) R_{ab} = -2\nabla [a H_b] [\mathcal{H}] + \xi X R_{ab},$$

and we obtain the first-order Ricci curvature as

$$(1) R_{ab} = -2\nabla [a H_b] [\mathcal{L}] + \xi X R_{ab}.$$

The scalar curvature on the physical spacetime $\mathcal{M}$ is given by $\mathcal{R} = \nabla R_{ab}$. To obtain the perturbative form of the scalar curvature, we expand the $\mathcal{R}$ in the form (11), that is,

$$(1) \mathcal{R} = -2\nabla [a H_b] [\mathcal{L}] + \xi X \mathcal{R},$$

$$+ 2\xi X \mathcal{R} = R + \xi X \mathcal{R} + 2\xi X \mathcal{R}.$$

and $\nabla \mathcal{R}$ is expanded through the Leibniz rule. Then, the perturbative formula for the scalar curvature at each order is derived from perturbative form of the inverse metric (B.3) and the Ricci curvature (B.14) and (B.15). Straightforward calculations lead to the expansion of the scalar curvature as

$$(1) \mathcal{R} = -2\nabla [a H_b] [\mathcal{L}] - R_{ab} \mathcal{H}^{ab} + \xi X \mathcal{R},$$

$$+ 2\xi X \mathcal{R} = R + \xi X \mathcal{R} + 2\xi X \mathcal{R}.$$

We also note that the expansion formulæ (B.17) and (B.18) have the same for as the decomposition formulæ (36) and (37), respectively.
Next, we consider the perturbative form of the Einstein tensor $\mathcal{G}_{ab} := R_{ab} - (1/2)g_{ab}R$ and we expand $\mathcal{G}_{ab}$ as in the form (11):

$$\mathcal{G}_{ab} =: G_{ab} + \lambda^{(1)}(G_{ab}) + \frac{1}{2}\lambda^{(2)}(G_{ab}) + O(\lambda^3). \quad (B.19)$$

As in the case of the scalar curvature, straightforward calculations lead to

$$\begin{align*}
(1)(G_{ab}) &= -2\nabla_{[a}H_{b]}\epsilon^d[\mathcal{H}] + g_{ab}\nabla_{[c}H_{d]}\epsilon^{cd}[\mathcal{H}]
+ \frac{1}{2}R_{ab} + \frac{1}{2}g_{ab}R_{cd}\mathcal{H}^{cd} + \epsilon_X G_{ab}, \\
(2)(G_{ab}) &= -2\nabla_{[a}H_{c]}\epsilon^d[\mathcal{L}] + 4H_{[a}^{\cd} \mathcal{H} H_{c]b]} [\epsilon][\mathcal{H}]
+ 4\mathcal{H}_{e}^{d}\nabla_{[a}H_{d]}\epsilon^c[\mathcal{H}]
- \frac{1}{2}g_{ab}\left(-2\nabla_{[c}H_{d]}\epsilon^{cd}[\mathcal{L}] + 2R_{de}\mathcal{H}_{c}^{d}\mathcal{H}^{ce}
- R_{de}\mathcal{L}^{ce} + 4H_{[c}^{de} \mathcal{H}^{f]}H_{d]}\epsilon^{ce}[\mathcal{H}]
+ 4\mathcal{H}_{e}^{d}\nabla_{[c}H_{d]}\epsilon^{ce}[\mathcal{H}]
+ 4\mathcal{H}^{ce}\nabla_{[c}H_{de]}\epsilon^{[e}[\mathcal{H}]
+ 2\mathcal{H}_{ab}\nabla_{[c}H_{d]}\epsilon^{cd}[\mathcal{H}]
+ \mathcal{H}_{ab}\mathcal{H}^{cd}R_{cd} - \frac{1}{2}R_{ab}\mathcal{L}
+ 2\epsilon_X (1)(G_{ab}) + (\epsilon_Y - \epsilon_X\epsilon)G_{ab}. \quad (B.20)
\end{align*}$$

We note again that (B.20) and (B.21) have the same form as the decomposition formulae (36) and (37), respectively.

The perturbative formulae for the perturbation of the Einstein tensor

$$G_{ab} = g^{bc}G_{ac} \quad (B.22)$$

is derived by the similar manner to the case of the perturbations of the scalar curvature. Through these formulae summarized previously, straightforward calculations leads (43)–(47). We have to note that to derive the formulae (46) with (47), we have to consider the general relativistic gauge-invariant perturbation theory with two infinitesimal parameters which is developed in [22, 23], as commented in the main text.

Acknowledgments

The author thanks participants in the GCOE/YITP workshop YITP-W-0901 on “Non-linear cosmological perturbations,” which was held at YITP in Kyoto, Japan in April, 2009, for valuable discussions, in particular, professor M. Bruni, professor R. Maartens, professor M. Sasaki, professor T. Tanaka, and professor K. Tomita. This paper is an extension of the contribution to this workshop by the author.

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