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Natural Selection of Inflationary Vacuum Required by Infra-Red Regularity and Gauge-Invariance

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It has been an issue of debate whether the inflationary infrared (IR) divergences are physical or not. Our claim is that, at least, in single-field models, the answer is "No", and that the spurious IR divergence is originating from the careless treatment of the gauge modes. In our previous work we have explicitly shown that the IR divergence is absent in the genuine gauge-invariant quantity at the leading order in the slow-roll approximation. We extend our argument to include higher-order slow-roll corrections and the contributions from the gravitational waves. The key issue is to assure the gauge invariance in the choice of the initial vacuum, which is a new concept that has not been considered in conventional calculations.

Subject Index: 440

§1. Introduction

The importance of the gauge-invariant perturbation has been widely recognized since decays ago, but some subtle issues get in the way of its realization particularly in non-linear perturbation theory. During inflation, massless fields are known to yield the scale invariant spectrum $P(k) \propto 1/k^3$ at linear order. These fields contribute to the one-loop diagram with the four point interaction as $\int d^3k/k^3$ in the long wavelength limit, which leads to the logarithmic divergence.[1)–20)] In our previous work,[21)] we pointed out that, at least in single field models, the IR divergences are attributed to the bad treatment of gauge degrees of freedom. The gauge degrees of freedom can be classified into two classes: the local ones and the non-local ones. In the usual calculation only the former is fixed by adapting particular gauge conditions at each space-time point. However, this is not sufficient in order to accomplish the complete gauge fixing because of the presence of the non-local gauge degrees of freedom, which are typically the degrees of freedom to specify boundary conditions in solving the lapse function and the shift vector. These non-local gauge degrees of freedom are formally fixed by imposing the regularity at spatial infinity in the conventional perturbation theory. As a result, however, the time evolution of so-called gauge invariant variables is affected by the information from infinitely large volume outside our observable region. We claimed that this is the origin of IR divergences.[21)]

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Along the line mentioned above, the IR divergence problem reminds us of the importance of maintaining the gauge-invariance in cosmological perturbation. In our previous work,[22] we provide one simple but calculable example of genuine gauge-invariant quantities, and showed its regularity at the leading order in the slow-roll approximation. In order to realize IR regular perturbation theory, one important additional aspect is to guarantee the gauge invariance of the initial quantum state. We found that by choosing the Bunch-Davies vacuum, which yields the scale-invariant spectrum, at the lowest order in slow-roll approximation, the gauge invariance of the initial quantum state is realized. In this paper, we extend our argument about IR regularity of such genuine gauge invariant quantities and the existence of gauge-invariant initial state to the quadratic order in the slow-roll approximation. This extension would be wanted, because the presence of IR divergences that has been reported so far mostly starts with this order (see Ref. 19) for a recent review). We also include the discussion about the contributions from the graviton loops.

To quantify the primordial fluctuations and provide the testable predictions for models of inflation, it is necessary to remedy the singular behaviour of IR corrections as well as the ultraviolet divergence.[23)–25)] The feasibility of the secular growth of IR contributions has also been addressed, motivated as a possible solution to the smallness of the cosmological constant.[26)–29)] (See also Refs. 30) and 31).) Despite the several efforts,[21),32)–43)] the debate regarding the possibility of the IR divergence has not been settled. To put an end to this debate, following the idea presented in our previous works,[21),22)] we explicitly show the absence of the IR divergence, restricting our argument to single field models of inflation.

Our paper is organized as follows. In §2, we give the setup of our problem and briefly review our solution to the IR divergence problem. In §2.2, we clarify the relation between the residual gauge degrees of freedom and the boundary conditions in solving the lapse function and the shift vector. In §3, we give one example of genuine gauge-invariant variables. In §4, we show the regularity of the genuine gauge-invariant variable and study the requirement of the gauge-invariance on the initial quantum state. Our results are summarized in §5.

§2. Brief review of IR divergence problem

In this section, we briefly summarize our solution to the IR divergence problem, proposed in our previous work.[22]

2.1. *Basic equations*

We consider a standard single field inflation model whose action takes the form

$$S = \frac{M_{\rm pl}^2}{2} \int \sqrt{-g}\, [R - g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - 2V(\phi)] d^4x \,, \tag{2·1}$$

where $M_{\rm pl}$ is the Planck mass and the scalar field Φ was rescaled as $\Phi \to \Phi/M_{\rm pl}$ to be dimensionless. The ADM formalism has been utilized to derive the action of the dynamical variables particularly in the non-linear perturbation theory.[44] Using the decomposed metric

$$ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt) \ , \tag{2·2}$$

the action is rewritten as

$$S = \frac{M_{\rm pl}^2}{2} \int \sqrt{h} \Big[N\,{}^sR - 2NV(\phi) + \frac{1}{N}(E_{ij}E^{ij} - E^2) + \frac{1}{N}(\partial_t\phi - N^i\partial_i\phi)^2 - Nh^{ij}\partial_i\phi\partial_j\phi \Big] d^4x \ , \tag{2·3}$$

where ${}^sR$ is the three-dimensional scalar curvature and E_{ij} and E are defined by

$$E_{ij} = \frac{1}{2}\left(\partial_t h_{ij} - D_i N_j - D_j N_i\right), \quad E = h^{ij}E_{ij} \ . \tag{2·4}$$

The spatial index of N_i is raised and lowered by h_{ij}.

In this paper we work both in the comoving gauge and in the flat gauge. We defer the introduction of the latter gauge to §3.2. The comoving gauge is defined by

$$\delta\phi = 0 \ , \tag{2·5}$$

where $\delta\phi$ is the perturbation of the scalar field. We decompose the spatial metric as

$$h_{ij} = e^{2(\rho+\zeta)} \left[e^{\delta\gamma} \right]_{ij} \ , \tag{2·6}$$

where $a := e^\rho$ denotes the background scale factor, and $\mathrm{tr}[\delta\gamma] = 0$. Using the degrees of freedom in the choice of the spatial coordinates, we further impose the gauge conditions $\partial^i\delta\gamma_{ij} = 0$. Here, the indices of spatial derivatives are raised or lowered by using Kronecker's delta as $\partial^i = \delta^{ij}\partial_j$.

Varying the action with respect to N and N^i, we obtain the Hamiltonian and momentum constraints as

$${}^sR - 2V - N^{-2}(E^{ij}E_{ij} - E^2) - N^{-2}\left(\partial_t\phi\right)^2 = 0 \, , \tag{2·7}$$

$$D_j\left[N^{-1}\left(E^j{}_i - \delta^j{}_i E\right)\right] = 0 \, . \tag{2·8}$$

Introducing the perturbed variables as

$$\check{h}_{ij} := e^{-2\rho}h_{ij}, \quad N_i = e^\rho \check{N}_i \, , \quad \check{N}^i := \check{h}^{ij}\check{N}_i = e^\rho N^i \, , \tag{2·9}$$

we factorize the scale factor from the metric as

$$ds^2 = e^{2\rho}[-(N^2 - \check{N}_i\check{N}^i)d\eta^2 + 2\check{N}_i d\eta dx^i + \check{h}_{ij}dx^i dx^j] \, . \tag{2·10}$$

Expanding the perturbations, $\mathcal{Q} = \delta N (:= N-1)$, $\check{N}_i$, ζ, and $\delta\gamma_{ij}$ as $\mathcal{Q} = \mathcal{Q}_1 + \mathcal{Q}_2 + \cdots$, the zeroth-order Hamiltonian constraint equation yields the background Friedmann equation:

$$6\rho'^{\,2} = \phi'^{\,2} + 2e^{2\rho}V(\phi) \ , \tag{2·11}$$

where a prime " $'$ " denotes the differentiation with respect to the conformal time η. The constraint equations at the linear order are obtained as

$$e^{2\rho}V\delta N_1 - 3\rho'\zeta_1' + \partial^2\zeta_1 + \rho'\partial^i\check{N}_{i,1} = 0 \ , \tag{2·12}$$

$$4\partial_i\left(\rho'\delta N_1 - \zeta_1'\right) - \partial^2\check{N}_{i,1} + \partial_i\partial^j\check{N}_{j,1} = 0 \ , \tag{2·13}$$

where $\partial^2 := \partial^i\partial_i$. The higher-order constraints can be obtained similarly.

2.2. *Residual gauge degrees of freedom*

The constraint equations (2·7) and (2·8) allow us to describe the non-dynamical variables N and N_i in terms of ζ. Here we stress that the constraints (2·12) and the divergence of (2·13) are elliptic-type equations, which require boundary conditions to solve. Even though we impose the gauge conditions (2·5) and (2·6) at each spacetime point, N and N_i are not uniquely determined because of the presence of such non-local gauge degrees of freedom. At the first order of perturbation, these degrees of freedom are studied in Ref. 22), where general solutions of δN_1 and $N_{i,1}$ are given in the form:

$$\delta N_1 = \frac{1}{\rho'}\left(\zeta_1' - \frac{1}{4}\partial^i G_i\right) \ , \tag{2·14}$$

$$\check{N}_{i,1} = \partial_i\left(\frac{\phi'^{\,2}}{2\rho'^{\,2}}\partial^{-2}\zeta_1' - \frac{1}{\rho'}\zeta_1\right) - \frac{1}{4}\left(1+\frac{\phi'^{\,2}}{2\rho'^{\,2}}\right)\partial_i\partial^{-2}\partial^j G_j + G_i \ . \tag{2·15}$$

Here, an arbitrary vector function $G_i(x)$ that satisfies the Laplace equation $\partial^2 G_i(x) = 0$ was introduced to make explicit the presence of degrees of freedom corresponding to the boundary conditions. Substituting Eqs. (2·14) and (2·15) into the equations of motion for ζ_1 and $\delta\gamma_{ij,1}$, we find that the introduction of the gauge function $G_i(x)$ modifies their evolution equations as well.[22)]

The ambiguity originating from the choice of the vector $G_i(x)$ is a sign of the presence of residual gauge degrees of freedom. Here, we explicitly show that $G_i(x)$ represents the residual gauge degrees of freedom that remain undetermined even after specifying the gauge by the conditions (2·5) and (2·6). Since the gauge condition $\delta\phi = 0$ completely fixes the temporal gauge, the residual gauge can reside only in changing the spatial coordinates: $x^i \to \tilde{x}^i = x^i + \delta x^i$. The metric perturbations then transform as

$$\tilde{\check{N}}_{i,1}(x) = \check{N}_{i,1}(x) - \delta x_i' \ , \tag{2·16}$$

$$\tilde{\zeta}_1(x) = \zeta_1(x) - \tfrac{1}{3}\partial^i\delta x_i \ , \tag{2·17}$$

$$\delta\tilde{\gamma}_{ij,1}(x) = \delta\gamma_{ij,1}(x) - 2\left\{\partial_{(i}\delta x_{j)} - \tfrac{1}{3}\partial^k\delta x_k\delta_{ij}\right\} \ . \tag{2·18}$$

In this section we associate a tilde "˜" with the perturbed variables in the gauge with $G_i \neq 0$ to discriminate them from the perturbed variables in the gauge with $G_i = 0$.

Since we have not changed the temporal coordinate, the lapse function remains unchanged at the linear order. Equating δN_1 with $\delta\tilde{N}_1$, given by Eq. (2·14), we find that ζ_1 is related to $\tilde{\zeta}_1$ as

$$\tilde{\zeta}_1' = \zeta_1' + \frac{1}{4}\partial^i G_i \ . \tag{2·19}$$

Comparing Eq. (2·17) with (2·19), we obtain

$$\partial^i\delta x_i' = -\tfrac{3}{4}\partial^i G_i \ . \tag{2·20}$$

Imposing the transverse condition on $\delta\gamma_{ij}$ in Eq. (2·18), we obtain another condition for δx^i as

$$\partial^2 \delta x_i = -\tfrac{1}{3}\partial_i \partial^j \delta x_j \ . \tag{2·21}$$

Then, Eqs. (2·20) and (2·21) are integrated to give

$$\delta x_i = -\int d\eta\, G_i(x) + \frac{1}{4}\int d\eta\, \partial_i \partial^{-2}\partial^j G_j(x) + \int d\eta\, h_i(x) + H_i(\boldsymbol{x}), \tag{2·22}$$

where we introduced vector functions $h_i(x)$ and $H_i(\boldsymbol{x})$ that satisfy

$$\partial^i h_i(x) = \partial^2 h_i(x) = 0 \ , \tag{2·23}$$

$$3\partial^2 H_i(\boldsymbol{x}) + \partial_i \partial^j H_j(\boldsymbol{x}) = 0 \ . \tag{2·24}$$

Using Eqs. (2·17) and (2·20), Eq. (2·15) is recast into

$$\tilde{\check{N}}_{i,1}(x) = \check{N}_{i,1}(x) + \frac{1}{3\rho'}\partial_i\partial^j \delta x_j - \frac{1}{4}\partial_i \partial^{-2}\partial^j G_{j,1}(x) + G_{i,1}(x) \ . \tag{2·25}$$

Comparing Eq. (2·25) with Eq. (2·16), the vector function $h_i(x)$ is determined by

$$h_i(x) = \frac{1}{4\rho'}\int d\eta\, \partial_i \partial^j G_j(x) + \frac{1}{\rho'}\partial^2 H_i(\boldsymbol{x}) \ . \tag{2·26}$$

The degrees of freedom in boundary conditions are then found to represent the change of the spatial coordinates:

$$\begin{aligned}\delta x_i(x) = &-\int d\eta\, G_i(x) + \frac{1}{4}\int d\eta \partial_i \partial^{-2}\partial^j G_j(x)\\ &+ \frac{1}{4}\int \frac{d\eta}{\rho'}\int d\eta\, \partial_i\partial^j G_j(x) + H_i(\boldsymbol{x}) \int \frac{d\eta}{\rho'}\, \partial^2 H_i(\boldsymbol{x}) \ ,\end{aligned} \tag{2·27}$$

which is basically expressed in terms of $G_i(x)$. We note that the time-independent vector $H_i(\boldsymbol{x})$ can be absorbed into the integration constant of the temporal integral, $\int d\eta \,\{-G_i(x) + (1/4)\partial_i\partial^{-2}\partial^j G_j(x)\}$. Substituting Eq. (2·27) into Eqs. (2·17) and (2·18), we find that spatial components of metric perturbation transform as

$$\tilde{\zeta}_1 = \zeta_1 + \frac{1}{4}\int d\eta\, \partial^i G_i - \frac{1}{3}\partial^i H_i \ . \tag{2·28}$$

$$\begin{aligned}\delta\tilde{\gamma}_{ij,1} = \delta\gamma_{ij,1} &+ \int d\eta \left\{ 2\partial_{(i} G_{j)} - \tfrac{1}{2}(\partial_i\partial_j\partial^{-2} + \delta_{ij})\partial^k G_k \right\} - \frac{1}{2}\int \frac{d\eta}{\rho'}\int d\eta \partial_i\partial_j\partial^k G_k\\ &-2\left\{ \partial_{(i} H_{j)} - \tfrac{1}{3}\partial^k H_k \delta_{ij} \right\} - 2\int \frac{d\eta}{\rho'}\partial^2 \partial_{(i} H_{j)}.\end{aligned} \tag{2·29}$$

When we consider the universe with infinite volume and require that all quantities are regular at the spatial infinity, the solution of δN_1 and $\check{N}_{i,1}$ would be specified uniquely. However, in this case, we observe the singular behaviour in the loop corrections of the curvature perturbation ζ.[8)–12),14)–20),42)] This is because the IR fluctuation acausally propagates through the non-physical gauge modes and comes into play. In contrast, if we do not care about any singular behaviors at infinity, that would never be observed by us, a variety of homogeneous solutions G_i can be added to the solution of δN_1 and $\check{N}_{i,1}$. In our previous work,[21)] we have shown that, by choosing the function G_i appropriately, we can guarantee the regularity of fluctuations of ζ in the flat gauge as long as a finite spatial region of our universe is concerned. We think that this is a remarkable progress, but the prescription given in Ref. 21) is not completely satisfactory in that the loop corrections for ζ depend on the choice of the boundary conditions for the lapse function and the shift vector. This fact signifies that the n-point functions for the "so-called" curvature perturbation ζ is not a genuine gauge-invariant quantity, when we take into account the gauge degrees of freedom associated with the choice of boundary conditions. Our discussion here can be extended straightforwardly to the higher-order in perturbations.

§3. Gauge-invariant quantities

In this section, we provide one simple example of genuine gauge-invariant quantities. If we compute genuine gauge-invariant quantities, the results by definition should be unaffected by the choice of the gauge. Hence, they should be IR regular even if we calculate them based on the standard perturbation theory. We demonstrate this in the following two sections.

3.1. *Definitions of scalar curvatures*

One simple way to realize the gauge invariance is to use variables defined in a completely fixed slicing and threading. What is revealed in the previous section is the fact that the genuine gauge-invariant variables cannot be constructed by simply adapting gauge conditions to metric components at each space-time point. In order to fix the gauge completely, we also need to remove the unphysical degrees of freedom associated with the choice of boundary conditions. This cannot be achieved easily due to the difficulties in removing all arbitrariness regarding the choice of space-time coordinates. It is, however, possible to calculate genuine gauge-invariant quantities even if we do not accomplish the complete gauge fixing.

Since the time slicing is uniquely fixed by the gauge condition $\delta\phi = 0$, it is enough if we can arrange quantities so as to be invariant under the transformation of spatial coordinates. In our previous work,[22)] we proposed to calculate n-point functions for the scalar curvature of the induced metric on a $\phi =$ constant surface, ${}^sR$. Although ${}^sR$ itself does not remain invariant but transforms as a scalar quantity under the change of spatial coordinates, the gauge invariance of the n-point functions of ${}^sR$ would be ensured, if we could specify its n arguments in a coordinate-independent manner. The distances of spatial geodesics that connect pairs of n points characterize the configuration in a coordinate independent manner. On the basis of this idea, we specify the n spatial points in terms of the geodesic distances and the directional cosines, measured from a reference point. Although we cannot specify the reference point and frame in a coordinate independent manner, this gauge dependence would not matter as long as we are interested in the correlation functions in a quantum state that respects the spatial homogeneity and isotropy of the universe.

We consider the three-dimensional geodesics whose affine parameter ranges from $\lambda = 0$ to 1 with the initial "velocity" given by

$$\left. \frac{dx^i(\boldsymbol{X}, \lambda)}{d\lambda} \right|_{\lambda=0} = X^i \ .$$

We identify a point in the geodesic normal coordinates X^i with the end point of the geodesic $x^i(\boldsymbol{X}, \lambda = 1)$. Noting that in the absence of the fluctuations X^i coincides with x^i, we expand $x^i(\boldsymbol{X})$ as

$$x^i(\boldsymbol{X}) := X^i + \delta x^i(\boldsymbol{X}) \ .$$

We denote the spatial curvature whose argument is specified by the geodesic normal coordinates X^i as

$${}^g\!R(\eta,\, \boldsymbol{X}) := {}^s\!R(\eta,\, x^i(\boldsymbol{X})) \ . \tag{3·1}$$

Then, ${}^g\!R$ can be expanded as

$${}^g\!R(\eta,\, \boldsymbol{X}) = \sum_{n=0}^{\infty} \frac{\delta x^{i_1} \cdots \delta x^{i_n}}{n!} \partial_{i_1} \cdots \partial_{i_n} {}^s\!R(\eta,\, x^i)|_{x^i = X^{(i)}} \ . \tag{3·2}$$

The n-point functions of ${}^g\!R$ would be surely gauge-invariant, unless the initial quantum state breaks the gauge-invariance.

Our main purpose of this paper is to demonstrate the absence of IR divergence in the genuine gauge-invariant quantities at one-loop order. At this order, the following three terms contribute to the two-point function:

$$\langle {}^g\!R {}^g\!R \rangle_4 := \langle {}^g\!R_1 {}^g\!R_3 \rangle + \langle {}^g\!R_2 {}^g\!R_2 \rangle + \langle {}^g\!R_3 {}^g\!R_1 \rangle \ , \tag{3·3}$$

where the subscripts $1, 2, 3, 4$ represent the numbers of the contained creation and annihilation operators or equivalently the number of the contained interaction picture field operators. For simplicity, we neglect the terms that do not yield the IR divergence. In the above expression, each term contains two pairs of contraction between creation and annihilation operators. Only when one of these pairs does not contain any differentiation, the term potentially contributes to IR divergence. Since the loop integrals diverge at most logarithmically, one spatial or temporal derivative is sufficient to remedy their divergent behaviors. Noting that the curvature perturbation in the first-order scalar curvature is multiplied by the spatial derivatives as

$${}^g\!R_1 = {}^s\!R_1 \propto \partial^2 \zeta_1 \ , \tag{3·4}$$

the terms in ${}^g\!R_3$ that include more than one interaction picture field operators with spatial or temporal derivatives do not yield divergences. This statement also applies to the terms in ${}^g\!R_2$. Since ${}^g\!R_2$ contains at least one interaction picture field operator that is differentiated, the terms in ${}^g\!R_2$ that include more than one differentiated interaction picture field operators do not yield IR divergences.

The loops of gravitational wave perturbation without derivatives yield the logarithmic divergence, too. However, the gravitational wave perturbation $\delta\gamma_{ij}$ with derivatives no longer contributes to such divergent loop corrections.

Hereafter, we denote an equality which is valid only when we neglect the terms irrelevant to IR divergences by "$\overset{\rm IR}{\approx}$". Then, abbreviating the unimportant pre-factor, we simply denote the scalar curvature ${}^sR$ as

$$ {}^sR \overset{\rm IR}{\approx} e^{-2\zeta}\left[e^{-\delta\gamma}\right]^{ij}\partial_i\partial_j\zeta. \tag{3·5}$$

3.2. *Gauge transformation*

To calculate the non-linear corrections under the slow-roll approximation, it is convenient to temporally work in the flat gauge:

$$\tilde{h}_{ij} = e^{2\rho}\left[e^{\delta\tilde{\gamma}}\right]_{ij}, \quad {\rm tr}[\delta\tilde{\gamma}] = 0, \quad \partial^i\delta\tilde{\gamma}_{ij} = 0, \tag{3·6}$$

because all the interaction vertexes are explicitly suppressed by the slow-roll parameters in this gauge.[21),44)] Here in this section we associate a tilde with the metric perturbations in the flat gauge to discriminate those in the comoving gauge. The action in this gauge is given by

$$\begin{aligned} S \overset{\rm IR}{\approx} \frac{M_{\rm pl}^2}{2}\int e^{2\rho}\Big[&\tilde{N}^{-1}\left(\phi' + \varphi' - \tilde{\tilde{N}}^i\partial_i\varphi\right)^2 - 2\tilde{N}e^{2\rho}\sum_{m=0}\frac{V^{(m)}}{m!}\varphi^m \\ &- \tilde{N}\tilde{\tilde{h}}^{ij}\partial_i\varphi\partial_j\varphi + \tilde{N}^{-1}\left(-\rho'^2 + 4\rho'\partial_i\tilde{\tilde{N}}^i\right)\Big]d\eta d^3\boldsymbol{x}. \end{aligned} \tag{3·7}$$

The transformation formulae between the comoving gauge and the flat gauge are studied in Ref. 44), and we briefly summarize them in Appendix A. The curvature perturbation in the comoving gauge ζ is related to the fluctuation of the dimensionless scalar field (divided by $M_{\rm pl}$) in the flat gauge φ as

$$\zeta \overset{\rm IR}{\approx} \zeta_n + \zeta_n\partial_\rho\zeta_n + \frac{\varepsilon_2}{4}\zeta_n^2 + \frac{\zeta_n^2\partial_\rho^2\zeta_n}{2} + \frac{3\varepsilon_2\zeta_n^2\partial_\rho\zeta_n}{4} + \frac{1}{12}\varepsilon_2(\varepsilon_2 + 2\varepsilon_3)\zeta_n^3, \tag{3·8}$$

where we have introduced $\zeta_n := -(\rho'/\phi')\varphi$, following Ref. 44). We use the horizon flow function:

$$\varepsilon_0 := \frac{H_i}{H}, \quad \varepsilon_{m+1} := \frac{1}{\varepsilon_m}\frac{d\varepsilon_m}{d\rho} \qquad \text{for } m \geq 0, \tag{3·9}$$

where H is the Hubble parameter and H_i is the one at the initial time. The horizon flow function is related to the conventional slow-roll parameters as shown in Ref. 45). Hereafter, assuming that the horizon flow functions ε_m with $m \geq 1$ are all small of $\mathcal{O}(\varepsilon)$, we neglect the terms of $\mathcal{O}(\varepsilon^3)$. In Eq. (3·8), we neglected the cubic terms that include only one graviton field $\delta\tilde{\gamma}_{ij}$, for the following reason. Since ${}^gR_1$ includes only ζ_1, the terms in ${}^gR_3$ that include only one graviton field $\delta\tilde{\gamma}_{ij}$, does not contribute to $\langle {}^gR^gR\rangle_4$ after taking the contraction.

In line with the preceding papers,[21),32)] in order to calculate the n-point functions, we solve the evolution equation (Heisenberg equation) for the operator φ, and we express φ in terms of the interaction picture field φ_I. Variation of the total action with respect to φ yields

$$e^{-2\rho}\partial_\eta\left[\frac{e^{2\rho}}{\tilde{N}}\left(\phi'+\varphi'\right)\right]+\tilde{N}e^{2\rho}\sum_{m=0}\frac{V^{(m+1)}}{m!}\varphi^m \\ -\left(\phi'+\varphi'\right)\frac{1}{\tilde{N}}\partial_i\tilde{\tilde{N}}^i-\tilde{N}\left[e^{-\delta\tilde{\gamma}}\right]^{ij}\partial_i\partial_j\varphi \overset{\rm IR}{\approx} 0\ , \tag{3·10}$$

where $V^{(m)} := d^mV/d\phi^m$. To address the regularity of the graviton loops, we also include the contributions from the gravitational wave perturbation. Variations with respect to the lapse function and the shift vector, respectively, yield the Hamiltonian constraint:

$$(\tilde{N}^2-1)e^{2\rho}V+\tilde{N}^2e^{2\rho}\sum_{m=1}^{\infty}\frac{V^{(m)}}{m!}\varphi^m+2\rho'\partial_i\tilde{\tilde{N}}^i+\phi'\varphi'+\frac{1}{2}\varphi'^2 \overset{\rm IR}{\approx} 0\,, \tag{3·11}$$

and the momentum constraints:

$$2\rho'\partial_i\tilde{N}-\tilde{N}(\phi'\partial_i\varphi+\partial_i\varphi\varphi') \overset{\rm IR}{\approx} 0\,. \tag{3·12}$$

For the calculation of one loop corrections, it is enough to solve the constraint equations up to the quadratic order. These constraint equations are solved to give

$$\delta\tilde{N} \overset{\rm IR}{\approx} -\frac{\phi'^2}{2\rho'^2}\zeta_n+\frac{1}{4\rho'}\varphi\left(\phi'\delta\tilde{N}_1+\varphi'\right) \\ \overset{\rm IR}{\approx} -\varepsilon_1\zeta_n+\frac{\varepsilon_1}{2}\left(\varepsilon_1+\frac{\varepsilon_2}{2}\right)\zeta_n^2, \tag{3·13}$$

$$\partial_i\tilde{\tilde{N}}^i \overset{\rm IR}{\approx} \varepsilon_1\zeta_n'-\frac{1}{2}\varepsilon_1\varepsilon_2\zeta_n\zeta_n'. \tag{3·14}$$

Substituting Eqs. (3·13) and (3·14) into Eq. (3·10), the evolution equation of ζ_n is recast into a rather compact expression,

$$\mathcal{L}\zeta_n \overset{\rm IR}{\approx} \left[-2\varepsilon_1\zeta_n+\frac{1}{2}\varepsilon_1(4\varepsilon_1+\varepsilon_2)\zeta_n^2\right]\frac{1}{\rho'^2}\partial^2\zeta_n-\varepsilon_1\varepsilon_2\zeta_n\partial_\rho\zeta_n \\ -\frac{3}{4}\varepsilon_2\varepsilon_3\zeta_n^2+\left(\left[e^{-\delta\tilde{\gamma}}\right]^{ij}-\delta^{ij}\right)\frac{1}{\rho'^2}\partial_i\partial_j\zeta_n\,, \tag{3·15}$$

where the differential operator $\mathcal{L}$ is defined by

$$\mathcal{L} := \partial_\rho^2+(3-\varepsilon_1+\varepsilon_2)\partial_\rho-\frac{1}{\rho'^2}\partial^2. \tag{3·16}$$

We expand ζ_n as $\zeta_n=\zeta_{n,1}+\zeta_{n,2}+\zeta_{n,3}+\cdots$ and denote $\zeta_{n,1}$ simply as $\psi := \zeta_{n,1}$. The equation of motion (3·15) is expanded as

$$\mathcal{L}\psi = 0\ , \tag{3·17}$$

$$\mathcal{L}\zeta_{n,2} \overset{\text{IR}}{\approx} -\varepsilon_1\varepsilon_2\psi\partial_\rho\psi - \frac{3}{4}\varepsilon_2\varepsilon_3\psi^2 - 2\varepsilon_1\psi\frac{1}{\rho'^2}\partial^2\psi - \frac{1}{\rho'^2}\delta\tilde{\gamma}_1^{ij}\partial_i\partial_j\psi \ , \tag{3·18}$$

$$\begin{aligned}\mathcal{L}\zeta_{n,3} \overset{\text{IR}}{\approx} & -\frac{2}{\rho'^2}\varepsilon_1(\psi\partial^2\zeta_{n,2} + \zeta_{n,2}\partial^2\psi) + \frac{1}{2\rho'^2}\varepsilon_1(4\varepsilon_1+\varepsilon_2)\psi^2\partial^2\psi \\ & - \frac{1}{\rho'^2}\delta\tilde{\gamma}_1^{ij}\partial_i\partial_j\zeta_{n,2} + \frac{1}{2\rho'^2}(\delta\tilde{\gamma}_1^2)^{ij}\partial_i\partial_j\psi \ .\end{aligned} \tag{3·19}$$

Here, we neglected $\delta\tilde{\gamma}_{ij,2}$ on the right-hand side of Eq. (3·19), because a particular solution of $\delta\tilde{\gamma}_{ij,2}$ is associated with derivatives, and we set its homogeneous solution to zero. At the second order, Eq. (3·18) is integrated to give

$$\zeta_{n,2} \overset{\text{IR}}{\approx} \breve{\zeta}_{n,2} + \frac{1}{2}\delta\tilde{\gamma}_1^{ij}x_i\partial_j\psi, \tag{3·20}$$

where, for a later use, we have distinguished the part containing the contributions due to gravitational waves from the pure scalar part $\breve{\zeta}_{n,2}$ given by

$$\begin{aligned}\breve{\zeta}_{n,2} \overset{\text{IR}}{\approx} & \left(\frac{\varepsilon_1}{2} + \xi_2\right)\psi^2 + \varepsilon_1\psi\partial_\rho\psi + \varepsilon_1(\varepsilon_1+\varepsilon_2)\psi\partial_\rho\psi \\ & + \delta\zeta_{n,2} + \lambda_2\psi(\partial_\rho - x^i\partial_i)\psi \ .\end{aligned} \tag{3·21}$$

Here, $\breve{\zeta}_{n,2}$ includes the non-local term:

$$\delta\zeta_{n,2} := -\mathcal{L}^{-1}\left[\frac{3}{4}\varepsilon_2(2\varepsilon_1+\varepsilon_3)\psi^2\right] \ . \tag{3·22}$$

It should be emphasized that the homogeneous solutions $\xi_2\psi^2$ and $\lambda_2\psi(\partial_\rho - x^i\partial_i)\psi$ can be added to $\breve{\zeta}_{n,2}$, where the time dependent functions ξ_2 and λ_2 should be of $\mathcal{O}(\varepsilon^2)$ and their derivatives should be of $\mathcal{O}(\varepsilon^3)$. One can easily check that the above solution satisfies Eq. (3·18) to the present order of approximation, using the commutation relations

$$\begin{aligned}[\mathcal{L},\, \partial_\rho] &= -2(1-\varepsilon_1)\frac{1}{\rho'^2}\partial^2 + \mathcal{O}(\varepsilon^2) \ , \\ \left[\mathcal{L},\, x^i\partial_i\right] &= -\frac{2}{\rho'^2}\partial^2 \ , \\ \left[\mathcal{L},\, 1/\rho'^2\right] &= -\frac{2}{\rho'^2}(2\partial_\rho + 1) + \mathcal{O}(\varepsilon) \ .\end{aligned} \tag{3·23}$$

We are also allowed to change the solution of $\breve{\zeta}_{n,2}$ at $\mathcal{O}(\varepsilon)$ by adjusting its solution at $\mathcal{O}(\varepsilon^2)$.*) In the succeeding section, we will explain that the solution of $\breve{\zeta}_{n,2}$ is restricted by the requirement that the canonical commutation relation should be consistently satisfied. This requirement is, however, not enough to determine $\breve{\zeta}_{n,2}$ uniquely. Therefore, in Eq. (3·21), we fixed the terms of $\mathcal{O}(\varepsilon)$, requesting that, in addition to the consistency of the commutation relation, $\breve{\zeta}_{n,2}$ should be kept in the simplest form.

*) Actually, we could add a term of $\mathcal{O}(\varepsilon)$ proportional to $\psi(\partial_\rho - x^i\partial_i)\psi$ to $\breve{\zeta}_{n,2}$.

At the third-order of perturbation, Eq. (3·19) is integrated to give

$$\zeta_{n,3} \overset{\rm IR}{\approx} \breve{\zeta}_{n,3} + \frac{1}{8}\left(\delta\tilde{\gamma}_1\delta\tilde{\gamma}_1\right)^{ij} x_i\partial_j\psi + \frac{1}{8}\delta\tilde{\gamma}_1^{ij}\delta\tilde{\gamma}_1^{kl}x_jx_l\partial_i\partial_k\psi, \tag{3·24}$$

where $\breve{\zeta}_{n,3}$ is the part purely composed of the scalar perturbation as

$$\begin{aligned}\breve{\zeta}_{n,3} \overset{\rm IR}{\approx} \xi_3\psi^3 + \lambda_3\psi^2(\partial_\rho - x^i\partial_i)\psi \\ + \frac{1}{2}\varepsilon_1^2\psi^2\partial_\rho^2\psi + \frac{1}{4}\varepsilon_1(6\varepsilon_1 - \varepsilon_2)\psi^2x^i\partial_i\psi.\end{aligned} \tag{3·25}$$

It is again allowed to add homogeneous solutions whose coefficients ξ_3 and λ_3 are of $\mathcal{O}(\varepsilon^2)$ and their derivatives by ρ is of $\mathcal{O}(\varepsilon^3)$. Here we note that $[\mathcal{L},\, \partial_\rho - x^i\partial_i] = \mathcal{O}(\varepsilon)$.

3.3. *Consistency of commutation relations*

We have to take into account the following additional conditions that determine the choice of the homogeneous solution in ζ_n. Until Eq. (4·13), we will leave ξ_3 unspecified, but the other time dependent functions ξ_2, λ_2 and λ_3 are constrained in principle so as to guarantee the normal commutation relation for ψ, as we will explain soon below.

The evolution of the Heisenberg field ζ_n is usually supposed to be solved with the initial conditions that the Heisenberg field ζ_n is identified with the interaction picture field ψ at the initial time. This procedure guarantees that the operator U that relates ψ to ζ_n by $\psi = U\zeta_nU^\dagger$ is unitary. In this case, the canonical commutation relation for ζ_n

$$[\zeta_n(\eta, \boldsymbol{x}),\, \pi_n(\eta, \boldsymbol{y})] = i\delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}), \tag{3·26}$$

is equivalent to the commutation relation for the interaction picture fields

$$[\psi(\eta, \boldsymbol{x}),\, \pi_\psi(\eta, \boldsymbol{y})] = i\delta^{(3)}(\boldsymbol{x} - \boldsymbol{y}), \tag{3·27}$$

where π_n is the conjugate momentum of ζ_n and π_ψ is its linear truncation. We give a more explicit expression only up to $\mathcal{O}(\varepsilon)$ relative to the leading term here. In this approximation, using Eq. (3·7), we obtain the kinetic term in the action as

$$\begin{aligned}S_{\rm kin} &= \int d\eta \int d^3x \frac{M_{\rm pl}^2 e^{2\rho}}{2\tilde{N}}(\phi' + \varphi')^2 + \cdots \\ &\supset \int d\eta \int d^3x M_{\rm pl}^2 e^{2\rho}\varepsilon_1\zeta_n' \left[(1 + \varepsilon_1\zeta_n)\zeta_n' + \rho'(\varepsilon_2 - 2\varepsilon_1)\zeta_n + \mathcal{O}(\varepsilon^2)\right].\end{aligned}$$

From this expression, we can define the conjugate momentum

$$\pi_n := \frac{\delta S_{\rm kin}}{\delta\zeta_n'} = M_{\rm pl}^2\varepsilon_1 e^{2\rho}\left[2(1 + \varepsilon_1\zeta_n)\zeta_n' + \rho'(\varepsilon_2 - 2\varepsilon_1)\zeta_n + \mathcal{O}(\varepsilon^2)\right].$$

In the preceding subsection, we gave the non-linear solution by integrating the equation of motion without care about its initial conditions. Therefore unitary relation between ψ and ζ_n is not guaranteed. Once we obtain the definite expansions of

ζ_n and π_n in terms of ψ and π_ψ, it would be possible to check whether the commutation relation of ψ and π_ψ is guaranteed from that of ζ_n and π_n or vise versa. We can here check this consistency of these commutation relations to the only limited extent because we have neglected the terms containing more than two interaction picture field operators with space-time differentiation. Under this limitation, we can evaluate the commutator, assuming $[\psi(\eta,\boldsymbol{x}),\, \pi_\psi(\eta,\boldsymbol{y})] = i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})$, as

$$[\zeta_n(\eta,\boldsymbol{x}),\, \pi_n(\eta,\boldsymbol{y})] = i\delta^{(3)}(\boldsymbol{x}-\boldsymbol{y})\Big[1+\left\{4\xi_2-3\lambda_2+\mathcal{O}(\varepsilon^2)\right\}\zeta_n \\ +\left\{6\xi_3+3\lambda_3+\mathcal{O}(\varepsilon^2)\right\}\zeta_n^2+\cdots\Big], \quad (3\cdot28)$$

where the ellipsis represents the terms containing π_ψ and spatial derivatives, which are the beyond the scope of the present paper. In this way we can verify that the solution we gave is consistent with the expected commutation relation at $\mathcal{O}(\varepsilon)$. If we have chosen an inappropriate solution for $\check{\zeta}_{n,2}$ at $\mathcal{O}(\varepsilon)$, the commutation relation would not be satisfied.

At $\mathcal{O}(\varepsilon^2)$ the terms that we could evaluate in (3·28) include the unspecified functions ξ_2, λ_2, and λ_3. From the requirement that the right-hand side of Eq. (3·28) should be equated to Eq. (3·26), λ_2 and λ_3 are related to ξ_2 and ξ_3, respectively.

3.4. *Calculations of scalar curvature*

In this subsection, we give the expansion of the scalar curvature of a $\phi=$ constant hypersurface ${}^gR$ in terms of ψ, which is the interaction picture field of ζ_n. Using Eqs. (3·20) and (3·24), we first perturb the scalar curvature ${}^sR$, given by Eq. (3·5), to obtain

$${}^sR_1 = {}^s\check{R}_1 = \partial^2\psi, \quad (3\cdot29)$$

$${}^sR_2 \overset{\rm IR}{\approx} {}^s\check{R}_2 + \frac{1}{2}\delta\gamma_1^{ij}x_i\partial_j\partial^2\psi, \quad (3\cdot30)$$

$${}^sR_3 \overset{\rm IR}{\approx} {}^s\check{R}_3 + \frac{1}{8}\delta\gamma_1^{ij}\delta\gamma_1^{kl}x_jx_l\partial_i\partial_k\partial^2\psi + \frac{1}{8}(\delta\gamma_1^2)^{ij}x_i\partial_j\partial^2\psi, \quad (3\cdot31)$$

where ${}^s\check{R}_2$ and ${}^s\check{R}_3$ are defined by

$${}^s\check{R}_2 \overset{\rm IR}{\approx} \partial^2\check{\zeta}_{n,2} + \psi\,\partial^2(\partial_\rho - 2 + \varepsilon_2/2)\,\psi, \quad (3\cdot32)$$

$${}^s\check{R}_3 \overset{\rm IR}{\approx} \partial^2\check{\zeta}_{n,3} + \check{\zeta}_{n,2}\partial^2\left(\partial_\rho - 2 + \varepsilon_2/2\right)\partial^2\psi \\ + \psi\left(\partial_\rho - 2 + \varepsilon_2/2\right)\partial^2\check{\zeta}_{n,2} + \partial^2\psi\partial_\rho\check{\zeta}_{n,2} \\ + \frac{\psi^2}{2}\,\partial^2\Big[\partial_\rho^2 - 4(\partial_\rho - 1) + \frac{3}{2}\varepsilon_2\partial_\rho - 3\varepsilon_2 + \frac{1}{2}\varepsilon_2(\varepsilon_2+\varepsilon_3)\Big]\psi. \quad (3\cdot33)$$

To derive Eqs. (3·30) and (3·31), we have used the fact that, as presented in Eq. (A·8), the gravitational wave perturbation in the comoving gauge $\delta\gamma_{ij}$ is identical to that in the flat gauge $\delta\tilde{\gamma}_{ij}$, besides the terms irrelevant to IR divergences.

Noting that the spatial metric after removing the common scale factor is given by

$$d\lambda^2 = e^{2\zeta}\left[e^{\delta\gamma}\right]_{ij} dx^i dx^j\ , \quad (3\cdot34)$$

the geodesic normal coordinates X^i is given by

$$x^i(\boldsymbol{X}) \overset{\text{IR}}{\approx} e^{-\zeta}\left[e^{-\delta\gamma/2}\right]^i_{\ j} X^j, \tag{3·35}$$

where we again abbreviated the terms that include space-time derivatives. The difference between the global coordinates and the geodesic normal ones is given by

$$\delta x^i := x^i(\boldsymbol{X}) - X^i = \delta x^i_1 + \delta x^i_2 + \cdots, \tag{3·36}$$

where

$$\delta x^i_1 \overset{\text{IR}}{\approx} -\psi X^i - \frac{1}{2}\delta\gamma_1^{ij} X_j , \tag{3·37}$$

$$\delta x^i_2 \overset{\text{IR}}{\approx} -\zeta_2 X^i + \frac{1}{2}\psi^2 X^i + \frac{1}{8}(\delta\gamma_1^2)^{ij} X_j . \tag{3·38}$$

Now, we are ready to calculate the scalar curvature ${}^gR$. Substituting Eqs. (3·30) and (3·37) into Eq. (3·2), we obtain

$${}^gR_2 = {}^sR_2 + \delta x^i_1 \partial_i {}^sR_1 \overset{\text{IR}}{\approx} {}^s\breve{R}_2 - \psi X^i \partial_i {}^s\breve{R}_1 , \tag{3·39}$$

and substituting Eqs. (3·31) and (3·38) into Eq. (3·2), we obtain

$$\begin{aligned} {}^gR_3 &= {}^sR_3 + \delta x^i_1 \partial_i {}^sR_2 + \delta x^i_2 \partial_i {}^sR_1 + \frac{1}{2}\delta x^i_1 \delta x^j_1 \partial_i \partial_j {}^sR_1 \\ &\overset{\text{IR}}{\approx} {}^s\breve{R}_3 - \psi X^i \partial_i {}^s\breve{R}_2 - \left(\breve{\zeta}_{n,2} + \frac{\varepsilon_2}{4}\psi^2\right) X^i \partial_i {}^s\breve{R}_1 + \frac{1}{2}\psi^2 (X^i\partial_i)^2 {}^s\breve{R}_1. \end{aligned} \tag{3·40}$$

It would be appropriate to emphasize that, in contrast to the contributions from ζ, the contribution from the gravitational wave perturbation $\delta\gamma_{ij}$ completely cancels with each other in ${}^gR$. This clearly shows that the graviton loop does not lead to IR divergence at the one-loop order. This is essentially because the effect on ${}^sR$ from IR modes of gravitational wave perturbation is simply caused by the associated deformation of the spatial coordinates. Such gauge artifacts should completely disappear when we consider coordinate independent quantities like ${}^gR$.

§4. IR regularity and gauge-invariant vacuum

This section is devoted to show how the possibly divergent terms are cancelled in the n-point functions of ${}^gR$. As described in §3.1, in the standard cosmological perturbation the Hilbert space has not been reduced to the one that is composed only of the physical degrees of freedom. Namely, a part of gauge degrees of freedom are left unfixed. Hence, an arbitrary quantum state defined in this Hilbert space can be non-invariant along the gauge orbit of these residual gauge degrees of freedom. To ensure the gauge-invariance of the n-point functions of ${}^gR$, it turns out to be crucial to set the initial quantum state to be gauge invariant as well. Otherwise, the n-point functions fail to be regular due to the gauge artifacts. In this section, we reveal how the gauge-invariance condition(= regularity condition for the n-point functions) restricts the initial vacuum, particularly considering the one-loop correction to the two-point function.

4.1. *Proof of IR regularity*

In the previous section, we expanded the scalar curvature ${}^gR$ in terms of the interaction picture field ψ. We expand ψ as

$$\psi = \int \frac{d^3\boldsymbol{k}}{(2\pi)^{3/2}} \left(\psi_{\boldsymbol{k}} a_{\boldsymbol{k}} + \psi^*_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}\right), \tag{4·1}$$

where the creation and annihilation operators satisfy $[a_{\boldsymbol{k}},\, a^\dagger_{\boldsymbol{k}'}] = \delta^{(3)}(\boldsymbol{k}-\boldsymbol{k}')$. Focusing on the contribution from each Fourier mode $\psi_{\boldsymbol{k}} = v_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{x}}$, the derivative operator $x^i\partial_i$ is rewritten as

$$x^i\partial_i\psi_{\boldsymbol{k}} = v_{\boldsymbol{k}}\partial_{\log k} e^{i\boldsymbol{k}\boldsymbol{x}} = \partial_{\log k}\psi - e^{i\boldsymbol{k}\boldsymbol{x}}\partial_{\log k} v_{\boldsymbol{k}}. \tag{4·2}$$

For illustrative purpose, we first consider the leading order in the slow-roll approximation.[22] For the Bunch-Davies vacuum, the mode function v_k is given by

$$v_k(\eta) = -\frac{\rho'^2 e^{-\rho}}{\phi'}\frac{1}{k^{3/2}}\frac{i}{\sqrt{2}} e^{-ik\eta}(1+ik\eta)\ , \tag{4·3}$$

and is easily checked to satisfy

$$(\partial_\rho - x^i\partial_i)\psi_{\boldsymbol{k}} = -D_k\psi_{\boldsymbol{k}}\ , \tag{4·4}$$

where the operator D_k is defined by

$$D_k := \partial_{\log k} + \frac{3}{2}\ . \tag{4·5}$$

Using Eq. (4·4), ${}^gR_2$ and ${}^gR_3$ could be compactly written as

$${}^gR_2 \overset{\rm IR}{\approx} -\psi\partial^2 D_k\psi_{\boldsymbol{k}}\ , \qquad {}^gR_3 \overset{\rm IR}{\approx} \frac{1}{2}\psi^2\partial^2 D_k\psi_{\boldsymbol{k}}\ . \tag{4·6}$$

Taking the contractions of ${}^gR$, we obtain

$$\begin{aligned}
&\langle {}^gR_3(X_1)\,{}^gR_1(X_2)\rangle \\
&\overset{\rm IR}{\approx} \frac{1}{2}\langle\psi^2\rangle\left[\prod_{i=1,2}\int\frac{d^3\boldsymbol{k}_i}{(2\pi)^{3/2}}\right]\left(D^2_{k_1}k_1^2\psi_{\boldsymbol{k}_1}(X_1)\right)k_2^2\psi^*_{\boldsymbol{k}_2}(X_2)\delta^{(3)}\left(\boldsymbol{k}_1-\boldsymbol{k}_2\right) \\
&= \frac{1}{2}\langle\psi^2\rangle\int\frac{d(\log k)}{2\pi^2}\partial^2_{\log k}\left\{k^{7/2}\psi_{\boldsymbol{k}}(X_1)\right\}k^{7/2}\psi^*_{\boldsymbol{k}}(X_2),
\end{aligned}$$

and

$$\begin{aligned}
&\langle {}^gR_2(X_1)\,{}^gR_2(X_2)\rangle \\
&\overset{\rm IR}{\approx} \langle\psi^2\rangle\left[\prod_{i=1,2}\int\frac{d^3\boldsymbol{k}_i}{(2\pi)^{3/2}}\right]\left(D_{k_1}k_1^2\psi_{\boldsymbol{k}_1}(X_1)\right)\left(D_{k_2}k_2^2\psi^*_{\boldsymbol{k}_2}(X_2)\right)\delta^{(3)}\left(\boldsymbol{k}_1-\boldsymbol{k}_2\right) \\
&= \langle\psi^2\rangle\int\frac{d(\log k)}{2\pi^2}\partial_{\log k}\left\{k^{7/2}\psi_{\boldsymbol{k}}(X_1)\right\}\partial_{\log k}\left\{k^{7/2}\psi_{\boldsymbol{k}}(X_2)\right\},
\end{aligned}$$

where using the geodesic normal coordinate we defined $X_m := (\eta,\, \boldsymbol{X}_m)$ for $m = 1, 2$. Gathering the three terms on the right-hand side of Eq. (3·3), the two-point function at one-loop order is summarized as

$$\begin{aligned}&\langle\{{}^g\!R(X_1),\, {}^g\!R(X_2)\}\rangle_4 \\ &\quad\overset{\text{IR}}{\approx} \frac{1}{2}\langle\psi^2\rangle \int \frac{d(\log k)}{2\pi^2}\Big[\partial^2_{\log k}\left\{k^7 \psi_{\boldsymbol{k}}(X_1)\psi^*_{\boldsymbol{k}}(X_2)\right\} + (\text{c.c.})\Big],\end{aligned} \tag{4·7}$$

where we symmetrized about X_1 and X_2. This indicates that all the potentially divergent pieces become the total derivative with respect to k and hence they vanish.[*)]

At the leading order in the slow-roll approximation, the condition (4·4), satisfied in the scale-invariant/Bunch Davies vacuum, was crucial to remove the IR divergences. If we do not choose this vacuum, the quantum state is not invariant under the residual gauge transformation, and hence the two-point function diverges. We think that this possible divergence is attributed to infinitely large fluctuation in the residual gauge degree of freedom corresponding to the overall rescaling of the spatial coordinates. This unphysical degree of freedom can be tamed if and probably only if we set the initial state to be invariant under this residual gauge transformation, as we have anticipated earlier.

Now, we extend our argument to $\mathcal{O}(\varepsilon^2)$. Once we include the slow-roll corrections, the condition (4·4) no longer ensures the gauge invariance of the initial state. Using Eqs. (3·32), (3·37), and (3·39), the second-order scalar curvature is summarized as

$$\begin{aligned}{}^g\!R_2 \overset{\text{IR}}{\approx} \psi\partial^2\bigg[&\left(1+\varepsilon_1+\varepsilon_1^2+\varepsilon_1\varepsilon_2+\lambda_2\right)\partial_\rho\psi - (1+\lambda_2)x^i\partial_i\psi \\ &+\left(\varepsilon_1+\frac{\varepsilon_2}{2}+2\xi_2\right)\psi - \frac{3}{2}\mathcal{L}^{-1}\varepsilon_2(2\varepsilon_1+\varepsilon_3)\psi\bigg].\end{aligned} \tag{4·8}$$

Here we used

$$\partial^2\delta\zeta_{n,2} \overset{\text{IR}}{\approx} -\frac{3}{2}\left[\psi\partial^2\mathcal{L}^{-1}\varepsilon_2(2\varepsilon_1+\varepsilon_3)\psi\right], \tag{4·9}$$

which follows from

$$\mathcal{L}\partial^2\delta\zeta_{n,2} \overset{\text{IR}}{\approx} -\frac{3}{2}\mathcal{L}\left[\psi\partial^2\mathcal{L}^{-1}\varepsilon_2(2\varepsilon_1+\varepsilon_3)\psi\right] .$$

As a natural extension of the condition (4·4), we assume that there is a set of mode functions which satisfies

$$\begin{aligned}&\left(1+\varepsilon_1+\varepsilon_1^2+\varepsilon_1\varepsilon_2\right)\partial_\rho v_k + \left(\varepsilon_1+\frac{\varepsilon_2}{2}+2\xi_2\right)v_k \\ &\qquad - \frac{3}{2}\mathcal{L}_k^{-1}\varepsilon_2(2\varepsilon_1+\varepsilon_3)v_k = -D_k v_k + \mathcal{O}(\varepsilon^3)\,,\end{aligned} \tag{4·10}$$

*) Here, we assumed that the ultraviolet contribution has already been regularized appropriately, say, by dimensional regularization. (See Ref. 25).)

where we replaced $\mathcal{L}$ with $\mathcal{L}_k$:

$$\mathcal{L}_k := \partial_\rho^2 + (3 - \varepsilon_1 + \varepsilon_2)\partial_\rho + \frac{1}{{\rho'}^2}k^2. \tag{4·11}$$

We will show the presence of such mode function in the succeeding subsection.

For such mode functions, the second-order scalar curvature ${}^gR_2$ is then simply rewritten as

$${}^gR_2 \overset{\text{IR}}{\approx} -(1+\lambda_2)\psi\partial^2 D_k\psi$$

as in the leading-order of the slow-roll approximation. Using Eqs. (3·33), (3·38), and (3·40) together with Eq. (4·10), the straight-forward but lengthy calculation leads to ${}^gR_3$ in a rather simple expression:

$$\begin{aligned}{}^gR_3 \overset{\text{IR}}{\approx} \frac{1}{2}\psi^2\partial^2\Big[&(1+2\lambda_2)D_k^2\psi - \mu D_k\psi \\ &+ \left(-2\varepsilon_1^2 + \tfrac{3}{2}\varepsilon_1\varepsilon_2 + \tfrac{1}{2}\varepsilon_2\varepsilon_3 + 6\xi_3\right)\psi\Big] - \delta\zeta_{n,2}\partial^2 D_k\psi\ ,\end{aligned} \tag{4·12}$$

where we defined $\mu := \varepsilon_1 + \frac{1}{2}\varepsilon_2 - 3\varepsilon_1^2 + \frac{1}{2}\varepsilon_1\varepsilon_2 + 2(\xi_2 + \lambda_3)$. To ensure the absence of the IR divergences, the arbitrary time-dependent function ξ_3 should be chosen as

$$\xi_3 := \frac{1}{3}\varepsilon_1^2 - \frac{1}{12}\varepsilon_2(3\varepsilon_1 + \varepsilon_3)\ , \tag{4·13}$$

to find

$${}^gR_3 \overset{\text{IR}}{\approx} \frac{1}{2}\psi^2\partial^2\left[(1+2\lambda_2)D_k^2\psi - \mu D_k\psi\right] - \delta\zeta_{n,2}\partial^2 D_k\psi\ . \tag{4·14}$$

The possibly divergent terms are then summarized as

$$\begin{aligned}&\langle\{{}^gR(X_1),\, {}^gR(X_2)\}\rangle_4 \\ &\overset{\text{IR}}{\approx} \frac{1}{2}\langle\psi^2\rangle\int\frac{d(\log k)}{2\pi^2}\left\{(1+2\lambda_2)\partial_{\log k}^2 - \mu\partial_{\log k}\right\}\left\{\left(k^7\psi_{\boldsymbol{k}}(X_1)\psi_{\boldsymbol{k}}^*(X_2)\right) + (\text{c.c.})\right\} \\ &\qquad - \langle\delta\zeta_{n,2}\rangle\int\frac{d(\log k)}{2\pi^2}\partial_{\log k}\left\{\left(k^7\psi_{\boldsymbol{k}}(X_1)\psi_{\boldsymbol{k}}^*(X_2)\right) + (\text{c.c.})\right\}\ ,\end{aligned} \tag{4·15}$$

indicating that they are completely cancelled. The conditions on the initial vacuum state are derived by requesting the regularity of the IR corrections. Since the IR divergence is, in single field models of inflation, originating from the residual gauge degrees of freedom,[21),22)] the regularity conditions can be considered as the necessary condition for the gauge invariance.

4.2. *Gauge-invariant initial vacuum*

The requirement of the gauge invariance in the initial vacuum leads to the condition (4·10) on the mode function v_k. Taking the mode function v_k in a similar form to Eq. (4·3) as

$$v_k(\bar\rho) = \frac{{\rho'}^2 e^{-\rho}}{\phi'}\frac{1}{k^{3/2}}f_k(\bar\rho)\ , \tag{4·16}$$

the condition (4·10) can be recast into a rather simple form:

$$\begin{aligned}(\partial_{\bar\rho}+\partial_{\log k})\, f_k(\bar\rho)+\left(2\xi_2-\varepsilon_1^2-\frac{1}{2}\varepsilon_1\varepsilon_2\right) f_k(\bar\rho)\\ -\frac{3}{2}\mathcal{L}_k^{-1}\varepsilon_2(2\varepsilon_1+\varepsilon_3)f_k(\bar\rho)=0\ ,\end{aligned}\qquad (4·17)$$

where we changed the time variable ρ into

$$\bar\rho=\log\rho'-\varepsilon_1+\mathcal{O}(\varepsilon^2)\ . \qquad (4·18)$$

Note that $\bar\rho$ is approximately identical to ρ in the sense $d\bar\rho/d\rho=1+\mathcal{O}(\varepsilon)$.

The mode equation $\mathcal{L}_k v_k=0$ yields the evolution equation of f_k as

$$\bar{\mathcal{L}}_k f_k(\bar\rho)=0\ , \qquad (4·19)$$

where

$$\bar{\mathcal{L}}_k=\partial_{\bar\rho}^2+3\partial_{\bar\rho}+e^{-2(\bar\rho-\log k)}-3(\varepsilon_1+\varepsilon_2/2)+\mathcal{O}\left(\varepsilon^2\right). \qquad (4·20)$$

This operator $\bar{\mathcal{L}}_k$ is identical to $\mathcal{L}_k$ at the leading order in the slow roll approximation. To fix the form of the terms written as $\mathcal{O}(\varepsilon^2)$ in the above equation, we need to specify the form of $\bar\rho$ up to $\mathcal{O}(\varepsilon^2)$. Since the explicit forms of the terms of $\mathcal{O}(\varepsilon^2)$ in Eq. (4·20) are not necessary for the following discussion, we leave the higher order corrections to $\bar\rho$ unspecified here. Operating $\partial_{\bar\rho}+\partial_{\log k}$ on Eq. (4·19), the solution of the mode equation (4·19) is found to satisfy

$$\bar{\mathcal{L}}_k\left(\partial_{\bar\rho}+\partial_{\log k}\right) f_k=\frac{3}{2}\varepsilon_2(2\varepsilon_1+\varepsilon_3)f_k\ , \qquad (4·21)$$

where we used $[\partial_{\bar\rho}+\partial_{\log k},\bar{\mathcal{L}}_k]=-3\varepsilon_2(\varepsilon_1+\varepsilon_3/2)$. Multiplying the inverse of $\mathcal{L}_k$ on Eq. (4·21), Eq. (4·21) reproduces the gauge-invariance condition (4·17), where the second term of Eq. (4·17) appears as a homogeneous solution of $\bar{\mathcal{L}}_k$. This indicates that the solution of the mode equation (4·19) consistently satisfies the gauge-invariance condition.

It is also possible to show that the gauge-invariance condition (4·17) is sufficient to ensure that the mode equation is satisfied for all wavenumbers, if it is satisfied for a particular wavenumber k_0: $\mathcal{L}_{k_0}f_{k_0}(\bar\rho)=0$. In fact, by using the gauge-invariance condition, one can show

$$\begin{aligned}\partial_{\log k}\bar{\mathcal{L}}_k f_k|_{k=k_0}&=\left(\partial_{\bar\rho}+\partial_{\log k}\right)\bar{\mathcal{L}}_k f_k|_{k=k_0}\\ &=\bar{\mathcal{L}}_k\left(\partial_{\bar\rho}+\partial_{\log k}\right) f_k|_{k=k_0}-\frac{3\varepsilon_2}{2}\left(2\varepsilon_1+\varepsilon_3\right)f_{k_0}+\mathcal{O}(\varepsilon^3)=\mathcal{O}(\varepsilon^3)\ ,\end{aligned}\qquad (4·22)$$

which proves that thanks to the gauge-invariance condition, the mode function for another wavenumber is guaranteed from that for k_0.

As was anticipated in §4.1, the commutation relation for ψ is now verified. This commutation relation is equivalent to the normalization condition for v_k given by

$$\mathcal{N}_k:=\frac{ie^{3\bar\rho}\left(f_k\partial_{\bar\rho}f_k^*-f_k^*\partial_{\bar\rho}f_k\right)}{k^3\left\{1-2\varepsilon_1+\mathcal{O}(\varepsilon^2)\right\}}=1\ .$$

As in the case of mode equation, we assume that the normalization condition is satisfied for a particular wavelength k_0 as $\mathcal{N}_{k_0} = 1$. Then, using the gauge-invariance condition (4·17), we obtain

$$\partial_{\log k}\mathcal{N}_k|_{k=k_0} = (\partial_{\bar{\rho}} + \partial_{\log k})\,\mathcal{N}_k|_{k=k_0} = B - 4\xi_2 \ . \qquad (4{\cdot}23)$$

where the first term B is of $\mathcal{O}(\varepsilon^2)$ and its explicit form is not necessary in the current discussion. An important fact is

$$\partial_{\bar{\rho}}\partial_{\log k}\mathcal{N}_k|_{k=k_0} = 0, \qquad (4{\cdot}24)$$

holds exactly, because $\partial_{\bar{\rho}}$ and $\partial_{\log k}$ commute with each other and the normalization condition $\mathcal{N}_k$ is conserved. Therefore the right hand side of Eq. (4·23) is guaranteed to be constant in time. Then, by choosing ξ_2 appropriately, we can always set

$$\partial_{\log k}\mathcal{N}_k|_{k=k_0} = \mathcal{O}\left(\varepsilon^3\right) \ . \qquad (4{\cdot}25)$$

This proves that one can extend the mode function by the gauge-invariance condition (4·17) to the other wavenumbers keeping the normalization condition satisfied.

We summarize how the time dependent functions ξ_2, ξ_3, λ_2 and λ_3 are determined uniquely and consistently. ξ_2 was fixed by requesting the normalization condition to be consistent with the gauge invariance of the initial state, while ξ_3 was fixed from the IR regularity of the two point function. As presented in Eq. (3·28), to ensure the consistent commutation relations, λ_2 and λ_3 are also fixed once ξ_2 and ξ_3 are given. In this paper, we have not derived the gauge-invariance condition (4·17) but we just postulated it. The above discussions, however, have proven that this condition can be imposed consistently by choosing the homogeneous solution appropriately in ζ_n.

§5. Conclusion

We presented, in the standard single field inflation model, one example of the calculation of a genuine gauge-invariant quantity, i.e., the two-point function of ${}^g\!R$, which is the spatial curvature perturbation on a $\phi =$ constant hypersurface with its arguments specified in terms of the geodesic normal coordinates. We showed that, taking an appropriate initial vacuum, the two-point function for ${}^g\!R$ no longer yields IR divergences at one-loop order. It would be also possible to extend our argument to higher orders in loops and also to the general n-point functions. The quantities that are compared with actual observations like the fluctuation in the Cosmic Microwave Background should also be such genuine gauge-invariant quantities. Hence, our result strongly indicates that such quantities are also IR regular for the standard single field inflation model.

In the global gauge that we used in this paper the residual gauge degrees of freedom were not fixed. The residual gauge degrees of freedom include the overall spatial scale transformation corresponding to a constant shift of ζ in the $\delta\phi = 0$ gauge, which is the origin of the IR divergences. To remove IR divergences, hence, we had to impose the invariance of quantum states in the direction of the residual gauge, which requests additional gauge invariance conditions, such as Eqs. (4·10) and (4·13), on the choice of the initial quantum state. The condition (4·10) restricts the mode function for the interaction picture field and the condition (4·13) restricts the relation between the Heisenberg field and the interaction picture field. In the present paper, we derived these conditions, requiring, instead of the gauge-invariance itself, that the possibly divergent terms should be written in the form of total derivatives under the momentum integral. While the adopted iterative solution to the Heisenberg equation, that is used to obtain these gauge invariance conditions, may not be general enough. In this sense, it may be possible to find other vacua that are regular against IR contributions. Namely, the gauge-invariance condition (= regularity condition) may not uniquely determine the vacuum state in the inflationary universe. Therefore what we have derived is not a necessary condition but a sufficient condition for the IR regularity. We also expect one can specify the initial quantum state directly from requirement of the gauge-invariance, but this point has not been clarified yet at all. We leave these issues for future work. At the leading order in the slow-roll approximation, the condition (4·10) is automatically satisfied in the scale-invariant (Bunch-Davies) vacuum. However, at the higher order in the slow-roll approximation, this condition looks quite non-trivial. Our preliminary analysis tells that this vacuum state seems to coincide with the one naturally obtained by using the usual $i\epsilon$ prescription. We would like to report on this point in our forthcoming publication.[46)]

In contrast to the case of the global gauge, if we fix all the residual gauge degrees of freedom and quantize only physical degrees of freedom, we need not to restrict the initial quantum state by imposing additional gauge invariance conditions. This would provide another way of quantization that also yields no artificial divergences. In our previous work,[21)] following this direction, we tried to fix the residual gauge degrees of freedom, including the overall scaling of spatial coordinates, by imposing appropriate conditions. (We refer to this gauge as the local gauge.[21)]) If we perform the canonical quantization in the local gauge and give the initial state there, the local gauge conditions ensure the regularity of the IR corrections, without restricting the initial quantum state. It is, however, not so trivial to perform canonical quantization in the local gauge, because of additional conditions to fix the residual gauge degrees of freedom. Furthermore, if we set initial vacuum in the local gauge, it would be in general breaks the invariance under spatial translation. In our previous work,[21)] We therefore chose the initial vacuum state in the global gauge and then linearly transformed the interaction picture field from the global gauge to the local one. The truth is that in this gauge transformation there appear the non-linear contributions that can cause IR divergence. These contributions were not taken into account in Ref. 21) and the expression in the local gauge was still including the divergent terms. One can say that this is due to the lack of the gauge invariance in choosing the initial state, because the IR divergence actually disappears at the leading order in the slow-roll approximation if we take the Bunch-Davies vacuum, which is invariant under the scale transformation. To guarantee the IR regularity also at higher orders in this approximation, we need to adapt the gauge-invariance condition as is done in this paper.*)

In this paper we have solved the Heisenberg equation to the second order in the slow roll approximation. Up to this order, we showed the presence of a gauge invariant initial quantum state that is free from IR divergences. But it looks quite non-trivial to extend our results to the higher order in the slow roll approximation. For the complete understanding of IR issue in the standard single field inflation model, it is also definitely necessary to prove the existence of such an initial quantum state without relying on the slow roll approximation.

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Appendix A
—— *Third-Order Gauge Transformation* ——

In this appendix, we study the change of variables between the flat gauge with ${}^sR = 0$ and the comoving gauge with $\delta\phi = 0$. We denote the gauge transformation from the flat gauge to the comoving gauge as $\tilde{x}^\mu = e^{\mathcal{L}_\xi} x^\mu$ where ξ^μ is the vector field $\xi^\mu = (\alpha, \beta^i)$. In the present paper it is not strictly necessary to transform the spatial coordinates, but we do this for future application. For the same reason, we also leave the terms that do not yield IR divergences here.

In accordance with Ref. 44), we use the cosmic time t and denote its derivative by a dot. From the condition that this transformation makes the scalar field perturbation to vanish, we obtain

$$0 = \varphi + \mathcal{L}_\xi(\phi + \varphi) + \frac{1}{2!}\mathcal{L}_\xi^2(\phi + \varphi) + \frac{1}{3!}\mathcal{L}_\xi^3(\phi + \varphi) + \cdots \ , \tag{A·1}$$

It is enough to calculate the perturbed expansion up to the third order. Using Eq. (A·1), the time shift α is solved at each order as

$$\dot{\rho}\alpha_1 = -\frac{\dot{\rho}}{\dot{\phi}}\varphi =: \zeta_n \ , \tag{A·2}$$

$$\dot{\rho}\alpha_2 = \frac{\dot{\rho}}{2\dot{\phi}^2}\varphi\dot{\varphi} = \frac{1}{4}(\partial_\rho + \varepsilon_2)\zeta_n^2 \ , \tag{A·3}$$

$$\dot{\rho}\alpha_3 = \frac{1}{12}\zeta_n^2\partial_\rho^2\zeta_n + \frac{1}{3}\zeta_n\left(\partial_\rho\zeta_n\right)^2$$

*) These points will be clarified in the errata of 21).

$$+\frac{3}{16}\varepsilon_2\zeta_n\partial_\rho\zeta_n^2+\frac{1}{24}\varepsilon_2(2\varepsilon_2+\varepsilon_3)\zeta_n^3+\frac{1}{2}\beta_2^i\partial_i\zeta_n\ , \qquad (A\cdot 4)$$

where, $\beta_1=0$ is presumed. In both flat and comoving gauges, the traceless part of the spatial metric g_{ij} is requested to satisfy the transverse conditions. To maintain these transverse conditions, we also need to change the spatial coordinates at second order. The spatial component of the metric then transforms as

$$\begin{aligned} e^{2\zeta}\left[e^{\delta\gamma}\right]_{ij} &= \left[e^{\delta\tilde\gamma}\right]_{ij}+(\alpha_1+\alpha_2+\alpha_3)e^{-2\rho}\partial_t\left(e^{2\rho}\left[e^{\delta\tilde\gamma}\right]_{ij}\right)+\beta_2^k\partial_k\left[e^{\delta\tilde\gamma}\right]_{ij}\\ &+2\left\{\partial_{(i}\beta_2^k+\partial_{(i}\beta_3^k\right\}\left[e^{\delta\tilde\gamma}\right]_{j)k}+\frac{1}{2}e^{-2\rho}(\alpha_1+\alpha_2)\partial_t\left\{(\alpha_1+\alpha_2)\partial_t\left(e^{2\rho}\left[e^{\delta\tilde\gamma}\right]_{ij}\right)\right\}\\ &+\frac{1}{3}e^{-2\rho}\alpha_1\partial_t\left\{\alpha_1\partial_t(\alpha_1\dot\rho e^{2\rho})\right\}\delta_{ij}+\mathcal{H}_{ij}, \end{aligned} \qquad (A\cdot 5)$$

where $\mathcal{H}_{ij}$ is defined as

$$\begin{aligned} \mathcal{H}_{ij} := {} & 2e^{-2\rho}\left\{\partial_{(i}\alpha_1+\partial_{(i}\alpha_2\right\}N_{j)}+\alpha_1e^{-2\rho}\partial_t\left\{\partial_{(i}\alpha_1N_{j)}+e^{2\rho}\partial_{(i}\beta_{j),2}\right\}\\ &+\beta_2^k\partial_k\dot\rho\alpha_1\delta_{ij}+2\dot\rho\alpha_1\partial_{(i}\beta_{j),2}\\ &+e^{-2\rho}\partial_{(i}\alpha_1\left\{-\partial_{j)}\alpha_1-2\partial_{j)}\alpha_2-2\partial_{j)}\alpha_1\delta N+\alpha_1\dot N_{j)}+\dot\alpha_1N_{j)}+e^{2\rho}\dot\beta_{j),2}\right\}\\ &-\alpha_1\partial_{(i}\alpha_1\partial_{j)}\dot\alpha_1-\dot\alpha_1\partial_i\alpha_1\partial_j\alpha_1\ . \end{aligned} \qquad (A\cdot 6)$$

Taking the trace part of Eq. (A·5), we obtain

$$\begin{aligned} \zeta &= \dot\rho\left(\alpha_1+\alpha_2+\alpha_3\right)+\left\{\dot\rho(\alpha_1+\alpha_2)\right\}^2+\frac{1}{2}(\alpha_1+\alpha_2)\partial_t\left\{\dot\rho(\alpha_1+\alpha_2)\right\}\\ &+\frac{1}{6}e^{-2\rho}\alpha_1\partial_t\left\{\alpha_1\partial_t(\dot\rho\alpha_1e^{2\rho})\right\}-(\dot\rho\alpha_1)^2+\frac{4}{3}(\dot\rho\alpha_1)^3\\ &-\frac{1}{6}\delta^{ij}\left\{\left[e^{\delta\gamma}\right]_{ij}-\left[e^{\delta\tilde\gamma}\right]_{ij}\right\}+\frac{1}{6}\alpha_1\partial_t\,\delta^{ij}\left[e^{\delta\tilde\gamma}\right]_{ij}+\frac{1}{6}\mathcal{H}+\frac{1}{3}(\partial^i\beta_2^j+\partial^i\beta_3^j)\left[e^{\delta\tilde\gamma}\right]_{ij}\\ &-\dot\rho\alpha_1\left\{2\dot\rho\alpha_2+\frac{2}{3}\partial^i\beta_{i,2}+\alpha_1e^{-2\rho}\partial_t(\dot\rho\alpha_1e^{2\rho})+\frac{1}{3}\mathcal{H}\right\}\ , \end{aligned} \qquad (A\cdot 7)$$

where we defined $\mathcal{H}:=\delta^{ij}\mathcal{H}_{ij}$. For our purpose, it is sufficient to consider the gravitational wave perturbation up to the second order. Neglecting the third-order terms, the transformation of the transverse traceless tensor is given by

$$\begin{aligned} \delta\gamma_{ij} = \delta\tilde\gamma_{ij}+\zeta_n\partial_\rho\delta\tilde\gamma_{ij}+&\left(\delta_i{}^k\delta_j{}^l+\delta_j{}^k\delta_i{}^l-\frac{2}{3}\delta_{ij}\delta^{kl}\right)\\ &\times\left(\partial_k\zeta_n\frac{e^{-2\rho}}{\dot\rho}N_l+\partial_k\beta_{l,2}-\frac{1}{2}\frac{e^{-2\rho}}{\dot\rho^2}\partial_k\zeta_n\partial_l\zeta_n\right)\ . \end{aligned} \qquad (A\cdot 8)$$

Now, it is clear that $\delta\gamma_{ij}$ agrees with $\delta\tilde\gamma_{ij}$, after we neglect the terms that are irrelevant to IR divergences. Using Eqs. (A·2)–(A·4) and Eq. (A·8), Eq. (A·7) is rewritten as

$$\begin{aligned} \zeta &= \zeta_n+\frac{1}{2}\partial_\rho\zeta_n^2+\frac{1}{4}\varepsilon_2\zeta_n^2+\frac{1}{2}\zeta_n^2\partial_\rho^2\zeta_n+\frac{3}{8}\varepsilon_2\zeta_n\partial_\rho\zeta_n^2+\frac{1}{12}\varepsilon_2(\varepsilon_2+2\varepsilon_3)\zeta_n^3+\zeta_n(\partial_\rho\zeta_n)^2\\ &+\frac{1}{2}\beta_2^i\partial_i\zeta_n-\frac{2}{3}\zeta_n\partial^i\beta_{i,2}+\frac{1}{3}(\partial_i\beta_2^i+\partial_i\beta_3^i)-\frac{1}{3}\delta\tilde\gamma^{ij}\partial_i\zeta_n\frac{e^{-2\rho}}{\dot\rho^2}N_j \end{aligned}$$

$$+\frac{1}{6}\frac{e^{-2\rho}}{\dot{\rho}^2}\delta\tilde{\gamma}^{ij}\partial_i\zeta_n\partial_j\zeta_n+\frac{1}{6}(1-2\zeta_n)\mathcal{H}\,. \tag{A·9}$$

Multiplying the spatial derivative ∂^i on Eq. (A·5), $\beta_{i,2}$ is given as a solution of the Poisson equation:

$$\begin{aligned}\partial^2\beta_{i,2}=&-\partial^j\zeta_n\partial_\rho\delta\tilde{\gamma}_{ij}-\partial^j\mathcal{H}_{ij,2}+\frac{1}{3}\partial_i\mathcal{H}_2\\&+\frac{1}{4}\partial_i\partial^{-2}\left[\partial^k\partial^l\zeta_n\partial_\rho\delta\tilde{\gamma}_{kl}+\left(\partial^k\partial^l-\frac{1}{3}\delta^{kl}\partial^2\right)\mathcal{H}_{kl,2}\right]\,,\end{aligned} \tag{A·10}$$

where we used $\partial^i\beta_{i,2}$, given by operating $\partial^i\partial^j$ on Eq. (A·5). At the third order, $\beta_{i,3}$ is obtained in a similar manner. It is notable that $\beta_{i,n}\,(n=2,3,\cdots)$ is multiplied by at least one wavenumber vector in the momentum representation. Neglecting the terms that are irrelevant to the IR divergences, the curvature perturbation ζ is related to ζ_n as

$$\begin{aligned}\zeta=&\zeta_n+\frac{1}{2}\partial_\rho\zeta_n^2+\frac{\varepsilon_2}{4}\zeta_n^2+\frac{1}{2}\zeta_n^2\partial_\rho^2\zeta_n\\&+\frac{3}{8}\varepsilon_2\zeta_n\partial_\rho\zeta_n^2+\frac{1}{12}\varepsilon_2(\varepsilon_2+2\varepsilon_3)\zeta_n^3+\cdots\,.\end{aligned} \tag{A·11}$$

Here, we also neglected the cubic-order terms with only one graviton field $\delta\gamma_{ij}$, since its contribution vanishes in $\langle{}^gR{}^gR\rangle_4$.

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