Strong restriction on inflationary vacua from the local \textit{gauge} invariance I: Local \textit{gauge} invariance and infrared regularity

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The primordial perturbation is widely accepted to be generated through vacuum fluctuation of the scalar field that drives inflation. It is, however, not completely clear what the natural vacuum in the inflationary universe is, particularly in the presence of non-linear interactions. In this series of papers, we will address this issue, focusing on the condition required for the removal of divergence from the infrared (IR) contribution to loop diagrams. We show that requesting the \textit{gauge} invariance in the local observable universe guarantees the IR regularity of the loop corrections beginning with a simple initial state. In our previous works, the IR regularity condition was discussed using slow-roll expansion, which restricts the background evolution of the inflationary universe. We will show more generally that requesting the \textit{gauge} invariance or IR regularity leads to non-trivial constraints on the allowed quantum states.

1. Introduction

It is widely accepted that primordial curvature perturbations originate from vacuum fluctuation of the inflaton field in the inflationary universe. Different choices of quantum states lead to different statistics for the primordial fluctuation. Among various options of vacuum states, we usually choose the adiabatic vacuum. A free scalar field can be understood as a set of independent harmonic oscillators. Selecting the adiabatic vacuum looks reasonable, because each oscillator tends to have an approximately fixed frequency as the time scale becomes shorter than that of the cosmic expansion. However, once we start to take into account the self-interaction of the field, the reason for choosing the adiabatic vacuum becomes obscure. Therefore it is an interesting question whether some physical requirement prohibits taking an arbitrary quantum state or not. This is the question we address in this series of papers.

The key idea is to focus on fluctuations that we can measure in observations. Since the region we can observe is limited to a portion of the whole universe, we need to take into account the local property of the observable fluctuations. In the case in which we can get access to information only on a portion of the whole universe, there appear additional degrees of freedom to choose boundary conditions in fixing the coordinates. As shown in our recent publications [1–6] and as will be briefly described later, these degrees of freedom in the boundary conditions can be thought of as residual...
degrees of freedom in fixing the coordinates of the local observable universe. The observable fluctuations should be insensitive to the coordinate choice in the local observable universe. We showed that removing this ambiguity significantly affects the infrared (IR) behavior of primordial fluctuations. In the conventional gauge-invariant perturbation, in which this ambiguity is not taken care of, it is widely known that loop corrections of massless fields such as the inflaton diverge because of the IR contributions [7–28]. One may expect that performing the quantization after we remove these residual coordinate degrees of freedom in the local universe can cure the singular behavior of the IR contributions. However, these residual coordinate degrees of freedom are not present if we deal with the whole universe including spatial infinity, since what we call the residual coordinate transformation diverges at spatial infinity. In this sense, if we think of the whole universe, they are not gauge degrees of freedom. In Ref. [1], we imposed the boundary condition at a finite distance to remove the degrees of freedom in choosing coordinates, but the quantization (or equivalently setting the initial quantum state) was performed considering the whole spatial section of the universe. In that analysis we concluded that there is no IR divergence irrespective of the initial quantum state. However, there were several points that were overlooked. After we set the initial quantum state at a finite initial time, we needed to translate it into a language written solely in terms of the local quantities. Namely, the Heisenberg operators corresponding to the perturbation variables should be transformed into the ones that satisfy the given boundary conditions using an appropriate residual spatial coordinate transformation. Since the non-linear part of this transformation is not guaranteed to be IR regular, it can produce IR divergences. (A more detailed discussion can be found in Sect. 1 of Ref. [29].)

If we send the initial time to the past infinity, one may think that this problem may disappear because our observable region in comoving coordinates becomes infinitely large in this limit. However, this argument is not so obvious. If we think of, for instance, the conformal diagram of de Sitter space, the causal past of an observer never covers the whole region of a time-constant slice in the flat chart. Furthermore, in this case we also need to concern ourselves with the secular growth of fluctuation. In Ref. [1], we discussed the absence of secular growth, focusing only on modes beyond the horizon length scale. To complete the discussion, we also need to include the vertices that contain modes that are below the Hubble scale, because these vertices may yield secular growth through correlations between sub-Hubble modes and super-Hubble modes.

Later in Refs. [3,4], leaving the residual coordinate degrees of freedom unfixed, we calculated quantities that are invariant under the residual coordinate transformation in the local universe under the so-called slow-roll approximation. Then, we derived the conditions on the initial states that guarantee IR regularity. These conditions are the ones that guarantee the absence of additional IR divergences originating from the coordinate transformation mentioned above. However, the physical meaning of these conditions is not transparent from the derivation in Refs. [3,4].

In this paper, as in the conventional perturbation theory and also as in Refs. [3,4], we will perform the quantization over the whole universe. Then, calculating observable quantities, which are invariant under the residual coordinate transformation in the local universe, we will derive the necessary conditions for the initial quantum state to be free from IR divergences more generally, removing the limitation to the slow-roll approximation. We will also show that the IR regularity conditions can be thought of as the conditions that request the equivalence between two systems related by means of the dilatation transformation of spatial coordinates, which is one of the residual gauge transformations. In this paper, we will consider a case in which the interaction is turned on at a finite initial time. In the succeeding paper, we will discuss the case when the initial time is sent to the past infinity. This paper is organized as follows. In Sect. 2, we first show the symmetry of the system, which plays an
important role in our discussion. Then, following Refs. [3,4], we construct an operator that remains invariant under the residual coordinate transformation. In Sect. 3, we address the conditions on the initial states. In Sect. 4, we summarize the results of this paper and outline future issues.

2. Preparation

In this section, we will introduce basic ingredients to calculate observable fluctuations. In this paper, we consider a standard single field inflation model whose action takes the form

\[ S = \frac{M_{\text{pl}}^2}{2} \int \sqrt{-g} \left[ R - g^{\mu\nu} \phi_{,\mu} \phi_{,\nu} - 2V(\phi) \right] d^4x, \] (2.1)

where \( M_{\text{pl}} \) is the Planck mass and \( \phi \) is a dimensional scalar field divided by \( M_{\text{pl}} \). In Sect. 2.1, we show the symmetry of this system, which plays a key role in our argument. In Sect. 2.2, after we introduce a variable that preserves invariance regarding the coordinate choice in the local universe, we provide a way of quantizing the system.

2.1. Symmetry of the system

To fix the time slicing, we adopt the uniform field gauge \( \delta \phi = 0 \). Under the (3 + 1)-metric decomposition, which is given by

\[ ds^2 = -N^2 dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt), \] (2.2)

we take the spatial metric \( h_{ij} \) as

\[ h_{ij} = e^{2(\rho + \zeta)} \left[ e^{\delta y} \right]_{ij}, \] (2.3)

where \( e^\rho \) denotes the background scale factor, \( \zeta \) is the so-called curvature perturbation, and \( \delta y_{ij} \) is a traceless tensor:

\[ \delta y_i^i = 0, \] (2.4)

where the spatial index was raised by \( \delta \). As spatial gauge conditions we impose transverse conditions on \( \delta y_{ij} \):

\[ \partial_i \delta y_j^i = 0. \] (2.5)

In this paper, we neglect the vector and tensor perturbations. The tensor perturbation, which is a massless field, can also contribute to the IR divergence of loop corrections. We will address this issue in a future publication.

Solving the Hamiltonian and momentum constraints, we can derive the action that is expressed only in terms of the curvature perturbation [30]. Since the spatial metric is given in the form \( e^{2\rho} e^{2\zeta} dx^2 \), we naively expect that the explicit dependence on the spatial coordinates appears in the action only in the form of the physical distance \( e^\rho e^\zeta dx \). We first examine this property.

Using the Lagrangian density in the physical coordinates \( \mathcal{L}_{\text{phys}} \), we express the action as

\[ S = \int dt \int d^3x \mathcal{L}(x) = \int dt \int d^3x e^{3(\rho + \zeta)} \mathcal{L}_{\text{phys}}(x). \] (2.6)

We can confirm that the Lagrangian density \( \mathcal{L}_{\text{phys}} \) is composed of terms that are in a covariant form regarding a spatial coordinate transformation such as \( h_{ij} \partial_i N_j \) and \( h_{ij} N_i \partial_j \zeta \). Using

\[ d\tilde{x}^i = e^{\rho + \zeta} dx^i, \quad \partial / \partial \tilde{x}^i = e^{-(\rho + \zeta)} \partial / \partial x^i, \quad \tilde{N}_i = e^{-(\rho + \zeta)} N_i, \] (2.7)
we can absorb the curvature perturbation \( \zeta \) without differentiation that appears from the spatial metric, for instance, as

\[
h^{ij} \partial_i N_j = \delta^{ij} e^{-2(\rho + \zeta)} \partial_i \tilde{N} j = \delta^{ij} \left( \frac{\partial}{\partial \tilde{x}^i} \tilde{N} j + \tilde{N} j \frac{\partial}{\partial \tilde{x}^i} \zeta \right).
\]  (2.8)

After a straightforward repetition, the Lagrangian density can be recast into

\[
S = \int dt \ d^3x \ e^{3(\rho + \zeta)} L_{\text{phys}}[D\zeta, N, \tilde{N}].
\]  (2.9)

Here, to stress the fact that all \( \zeta \)'s that remain unabsorbed are multiplied by the derivative operators \( \partial_t \) or \( \partial/\partial \tilde{x}^i \), we introduce \( D \), which denotes these derivative operators. Using this expression for the action, the Hamiltonian constraint is given by

\[
\delta L \delta N = e^{3(\rho + \zeta)} \frac{\delta L_{\text{phys}}}{\delta N} = 0,
\]  (2.10)

and the momentum constraints are given by

\[
\delta L \delta N^i = e^{2(\rho + \zeta)} \frac{\delta L_{\text{phys}}}{\delta \tilde{N}^i} = 0.
\]  (2.11)

Perturbing these constraints, we can show that the Lagrange multipliers \( N \) and \( \tilde{N}_i \) are given by solutions of the elliptic-type equations:

\[
\left( \frac{\partial}{\partial \tilde{x}} \right)^2 N = f[D\zeta(x)], \quad \left( \frac{\partial}{\partial \tilde{x}} \right)^2 \tilde{N}_i = f_i[D\zeta(x)].
\]  (2.12)

To address the system of the whole universe, the integration in the action is assumed to be taken over the whole universe. Then, by assuming regularity at spatial infinity, these Poisson equations can be uniquely solved as

\[
N = N[D\zeta(x)], \quad \tilde{N}_i = \tilde{N}_i[D\zeta(x)].
\]  (2.13)

Substituting these expressions for \( N \) and \( \tilde{N}_i \) into the action (2.9), we can show that the action takes the form:

\[
S = \int dt \ d^3\tilde{x} \ L_{\text{phys}}[D\tilde{d}\tilde{x}\zeta(x)].
\]  (2.14)

Here, we put the subscript \( d\tilde{x} \) on \( D \) to specify the spatial coordinates used in \( D \). Equation (2.14) explicitly shows that the action for \( \zeta \) only depends on the physical spatial distance.

Now we are ready to show the dilatation symmetry of the system, which plays a crucial role in discussing the IR regularity. (See also the discussions in Refs. [31–37].) Changing the coordinates in the integral from \( x \) to \( e^{-s}x \) with a constant parameter \( s \), we can rewrite the action (2.14) as

\[
S = \int dt \ d^3x \ e^{3(\rho + \zeta)} L_{\text{phys}}[D_{e^{\rho + \zeta} \tilde{d}x}\zeta(x)] = \int dt \ d^3x \ e^{3(\rho + \zeta - s)} L_{\text{phys}}[D_{e^{\rho + \zeta - s} \tilde{d}x}\zeta(t, e^{-s}x)].
\]  (2.15)

This implies that the action for \( \zeta \) possesses the dilatation symmetry

\[
S = \int dt \ d^3x \ L[\zeta(x)] = \int dt \ d^3x \ L[\zeta(t, e^{-s}x) - s].
\]  (2.16)

We should note that, as long as we consider a theory that preserves the 3D diffeomorphism invariance, the system preserves the dilatation symmetry. This is because the above-mentioned dilatation symmetry can be thought of as one of the spatial coordinate transformations. This symmetry is also discussed in Refs. [38,39].
To make use of the dilatation symmetry, we introduce another set of canonical variables as well as $\zeta(x)$ and its conjugate momentum $\pi(x)$. We can show that

$$\tilde{\zeta}(t, x, \pi(t, e^{-s}x)) = e^{-3s}\pi(t, e^{-s}x)$$

satisfy the canonical commutation relations as well as $\zeta(x) \text{ and } \pi(x)$. Actually, using the commutation relations for $\zeta(x) \text{ and } \pi(x)$, we can verify

$$\{\tilde{\zeta}(t, x), \tilde{\pi}(t, y)\} = \{\zeta(t, e^{-s}x), -e^{-s}\pi(t, e^{-s}y)\} = e^{-3s}i\delta^{(3)}(e^{-s}(x - y)) = i\delta^{(3)}(x - y),$$

and also

$$\{\tilde{\zeta}(t, x), \tilde{\zeta}(t, y)\} = [\tilde{\pi}(t, x), \tilde{\pi}(t, y)] = 0.$$

Using Eq. (2.16), we can show that the Hamiltonian densities expressed in terms of these two sets of canonical variables are related to each other as

$$\int d^3x H[\zeta(x), \pi(x)] = \int d^3x \{\pi(x)\zeta(x) - L[\zeta(x)]\}
= \int d^3x \left\{ e^{-3s}\pi(t, e^{-s}x)\tilde{\zeta}(t, e^{-s}x) - L[\zeta(t, e^{-s}x)] - s \right\}
= \int d^3x H[\tilde{\zeta}(x) - s, \tilde{\pi}(x)] = \int d^3x \tilde{H}[\tilde{\zeta}(x), \tilde{\pi}(x)],$$

where a dot denotes the differentiation $\partial_t$. In the second equality, we again changed the coordinates in the integral as $x \to e^{-s}x$. Note that the Hamiltonian density for $\tilde{\zeta}$ and $\tilde{\pi}$ is given by the same functional as the one for $\zeta$ and $\pi$ with $\tilde{\zeta}$ shifted by $-s$.

We define the non-interacting part of the Hamiltonian density for $\tilde{\zeta}$ and $\tilde{\pi}$ by the quadratic part of $H$ in perturbation, assuming that $s$ is as small as $\tilde{\zeta}$ and $\tilde{\pi}$, as follows:

$$\tilde{H}_0[\tilde{\zeta}(x), \tilde{\pi}(x)] = H_0[\tilde{\zeta}(x) - s, \tilde{\pi}(x)],$$

where $H_0$ is the free part of the Hamiltonian density for $\zeta$ and $\pi$. Using Eq. (2.20) with Eq. (2.21), we can show that the interaction Hamiltonian densities that are defined by $H_I := H - H_0$ for each set of the canonical variables are related as

$$\tilde{H}_I[\tilde{\zeta}(x), \tilde{\pi}(x)] = H_I[\tilde{\zeta}(x) - s, \tilde{\pi}(x)].$$

Note that the Hamiltonian densities $H_I$ and $\tilde{H}_I$ also take the same functional form except for the constant shift of $\tilde{\zeta}$.

2.2. Residual coordinate transformations and quantization

In this subsection, we consider a way to calculate observable fluctuations. First, we begin with the classical theory. To obtain the action for $\zeta$ by eliminating the Lagrange multipliers $N$ and $N_i$, we need to solve the Hamiltonian and momentum constraint equations. As is schematically expressed in Eqs. (2.12), these constraint equations are given by the elliptic-type equations. Here we note that the region that we can observationally access is restricted to the causally connected region whose spatial volume is bounded at a finite past. As we are concerned only with the observable region, boundary conditions for Eqs. (2.12) cannot be restricted from the regularity of spatial infinity, which is far outside the observable region. The degrees of freedom for solutions of $N$ and $N_i$ can be understood as degrees of freedom in choosing coordinates. Since the time slicing is fixed by the gauge condition...
\( \delta \phi = 0 \), there are remaining degrees of freedom only in choosing the spatial coordinates. In the following, we refer to such degrees of freedom that cannot be uniquely specified without knowledge from outside the observable region as residual gauge degrees of freedom in the local universe. We write the term gauge in italics, because changing the boundary conditions for \( N \) and \( N_i \) in the local region modifies the action for \( \zeta \) obtained after solving the constraint equations, while it keeps the action expressed by \( N \), \( N_i \), and \( \zeta \) invariant. In this sense, the change of the boundary condition is distinct from the usual gauge transformation, which keeps the action invariant.

The observable fluctuations should be free from such residual gauge degrees of freedom. Following Refs. [3,4], we construct a genuine gauge invariant operator, which preserves the gauge invariance in the local observable universe. For the construction, we note that the scalar curvature \( \tilde{R} \), which transforms as a scalar quantity for spatial coordinate transformations, become genuinely gauge invariant if we evaluate it in the geodesic normal coordinates span on each time slice. The geodesic normal coordinates are introduced by solving the spatial 3D geodesic equation:

\[
\frac{d^2 x^i_{gl}}{d\lambda^2} + \Gamma^i_{jk} \frac{dx^j_{gl}}{d\lambda} \frac{dx^k_{gl}}{d\lambda} = 0,
\]  

(2.23)

where \( \Gamma^i_{jk} \) is the Christoffel symbol with respect to the 3D spatial metric on a constant time hypersurface and \( \lambda \) is the affine parameter. We consider the 3D geodesics whose affine parameter ranges from \( \lambda = 0 \) to \( \lambda = 1 \) with the initial “velocity” given by

\[
\left. \frac{dx^i_{gl}(x, \lambda)}{d\lambda} \right|_{\lambda=0} = e^{-\zeta(\lambda=0)}x^i.
\]  

(2.24)

Here we put the index gl on the global coordinates, using the simple notation \( x \) for the geodesic normal coordinates, which will be mainly used in this paper. A point \( x^i \) in the geodesic normal coordinates is identified with the end point of the geodesic, \( x^i_{gl}(x, \lambda = 1) \) in the original coordinates. Using the geodesic normal coordinates \( x^i \), we perturbatively expand \( x^i_{gl} \) as \( x^i_{gl} = x^i + \delta x^i(x) \). Then, we can construct a genuinely gauge invariant variable as

\[
\tilde{R}(t, x) := \tilde{R}(t, x^i_{gl}(x)) = \tilde{R}(t, x^i + \delta x^i(x)).
\]  

(2.25)

As long as the deviation from the homogeneous and isotropic universe is kept perturbatively small, we can foliate the universe by the geodesic normal coordinates.

Next, we quantize the system to calculate quantum correlation functions that become observable. A straightforward and frequently used way to preserve the gauge invariance is to eliminate gauge degrees of freedom by fixing the coordinates completely. In the local observable universe, complete gauge fixing requires us to fix the boundary conditions in solving the constraint equations. However, to quantize the locally restricted system, we need to abandon several properties that are available in the quantization of the whole universe. One is that the quantization restricted to a local system cannot be compatible with the global translation symmetry, at least in a manifest way. Another but related aspect is that basis functions for a mode decomposition (even if it exists) become rather complicated compared to the Fourier modes. To preserve the global translation symmetry manifestly, we take another way of quantization than the quantization in the completely fixed gauge.

In this paper, we perform quantization in the whole universe with infinite spatial volume. The global translation symmetry in spatial directions is then manifestly guaranteed in the sense that a shift of the spatial coordinates \( x \) to \( x + a \) just changes the overall phase factor in the Fourier mode by \( e^{i k \cdot a} \). Based on this idea, we consider and calculate observable quantities. Since the gauge invariant
variable $g_R$ does not include the conjugate momentum of $\zeta$, we can consider products of $g_R$ at an equal time without the problem of operator ordering. The $n$-product of $g_R$, i.e., $g_R(x_1) \cdots g_R(x_n)$, preserves the gauge invariance in the local universe. To calculate the $n$-point functions of $g_R$, we need to specify the quantum state as well. One may think that the quantum state should also be invariant under the residual gauge transformations. However, we cannot directly discuss this invariance as a condition for allowed quantum states in this approach, because the residual gauge degrees of freedom are absent when we quantize fields in the whole universe.

Here we note that, even though the operator $g_R$ is not affected by the residual gauge degrees of freedom, this does not imply that the $n$-point functions of $g_R$ are uncorrelated to the fields in the causally disconnected region. To explain this aspect more clearly, let us consider the $n$-point function of $g_R$ at $t = t_f$, whose vertices are located within the observable region $O_f$. For later use, we refer to the spacetime region that is causally connected to spacetime points in $O_f$ as the observable region $O$. After expanding the operator $g_R$ in terms of $\zeta_I$, the interaction picture field of $\zeta$, even if interaction vertices that affect $g_R(t_f, x)$ are confined within the observable region $O$, the $n$-point functions of $g_R$ have a correlation to the outside of $O$ through the Wightman function of $\zeta_I$, which can be expressed in the Fourier space as

$$G^+(x_1, x_2) = \langle \zeta_I(t, x_1) \zeta_I(t, x_2) \rangle = \int \frac{d^3k}{(2\pi)^3} \epsilon^{ik(x_1-x_2)} |v_k(t)|^2, \quad (2.26)$$

where $v_k$ is the mode function for $\zeta_I$. Since all the vertices are confined within $O$, the spatial distance $|x_1 - x_2|$ is bounded from above. However, the IR modes with $k \leq |x_1 - x_2|^{-1}$ are not suppressed and let the Wightman function $G^+$ diverge for scale-invariant or red-tilted spectra.

This long-range correlation becomes the origin of the IR divergence of loop contributions. Since the observable quantities should take a finite value, we request the IR regularity of observable fluctuations, which is achieved only when the quantum state is selected so that the long-range correlation is properly isolated from the observable quantities. In the following section, we will show that requesting the absence of IR divergence in fact constrains the quantum state of the inflationary universe.

3. **IR regularity condition and the residual gauge invariance**

A simple way to address the evolution of a non-linear system is to solve the Heisenberg equation perturbatively by assuming that the interaction is turned on at the initial time. In this section, taking this setup, we calculate the correlation function of $g_R$ up to one-loop order and investigate the IR behavior.

3.1. **Specifying the iteration scheme**

For notational convenience, we introduce the horizon flow functions as

$$\varepsilon_0 := \frac{\dot{\rho}}{\rho}, \quad \varepsilon_n := \frac{1}{\varepsilon_{n-1}} \frac{d}{d\rho} \varepsilon_{n-1}, \quad (3.1)$$

with $n \geq 1$, but without assuming that these functions are small we leave the background inflation model unconstrained. The assumption that the interaction is turned on at the initial time $t_i$ requests

$$\zeta(t_i, x) = \zeta_I(t_i, x), \quad (3.2)$$

and

$$\pi(t_i, x) = \pi_I(t_i, x), \quad (3.3)$$
where \(\pi_I\) is the conjugate momentum defined from the non-interacting action:

\[
S_0 = M_{pl}^2 \int dt \, d^3x \, e^{3\rho} \rho^2 \varepsilon_1 \left[ \left( \partial_\rho \xi \right)^2 - \frac{e^{-2\rho}}{\rho^2} \partial_\rho^2 \left( \partial_\rho \xi \right)^2 \right],
\]  

as \(\pi_I := 2M_{pl}^2 e^{3\rho} \varepsilon_1 \xi_I\).

Employing the initial condition (3.2), we can relate the Heisenberg picture field \(\xi\) to the interaction picture field \(\xi_I\) as

\[
\xi(t, x) = U_I^\dagger(t, t_i) \xi_I(t, x) U_I(t, t_i),
\]  

where \(U_I\) is the unitary operator given by

\[
U_I(t_1, t_2) = T \exp \left[ -i \int_{t_1}^{t_2} dt \, d^3x \, H_I(t, x) \right].
\]

Since the Heisenberg fields are related to the interaction picture fields by the unitary operator, the canonical commutation relations for the canonical variables \(\xi\) and \(\pi\) guarantee those for \(\xi_I\) and \(\pi_I\) as

\[
[\xi_I(t, x), \pi_I(t, y)] = i \delta^{(3)}(x - y), \quad [\xi_I(t, x), \xi_I(t, y)] = [\pi_I(t, x), \pi_I(t, y)] = 0.
\]

As we show in Appendix A, the n-point functions for \(\xi\) given in Eq. (3.5) agree with those given by the solution of \(\xi\) written in terms of the retarded Green function. We express the equation of motion for \(\xi\) schematically as

\[
\mathcal{L} \xi = S_{NL},
\]  

where \(\mathcal{L}\) denotes the differential operator

\[
\mathcal{L} := \partial^2_\rho + (3 - \varepsilon_1 + \varepsilon_2) \partial_\rho - \frac{\partial^2}{e^{2\rho} \rho^2},
\]  

and the left-hand side of Eq. (3.8) is the same equation of motion as is derived from the non-interacting part of the action (3.4).

By using the retarded Green function:

\[
G_R(x, x') = -i \theta(t - t') \left[ \xi_I(x), \xi_I(x') \right],
\]

which satisfies

\[
\mathcal{L} G_R(x, x') = -\frac{1}{2M_{pl}^2} \varepsilon_1 e^{3\rho} \rho^2 \delta^{(4)}(x - x'),
\]

with \(\delta^{(4)}(x - x') := \delta(t - t') \delta^{(3)}(x - x')\), the solution of the equation of motion with the initial conditions (3.2) and (3.3) is given by

\[
\xi(x) = \xi_I(x) + \mathcal{L}_R^{-1} S_{NL}(x),
\]  

where the non-linear terms are given by

\[
\mathcal{L}_R^{-1} S_{NL}(t, x) := -2M_{pl}^2 \int dt' \int d^3x' \varepsilon_1(t') e^{3\rho(t')} \dot{\rho}(t')^2 \rho(t')^2 G_R(x, x') S_{NL}(x').
\]

We expand the interaction picture field \(\xi_I\), which satisfies

\[
\mathcal{L} \xi_I(x) = 0,
\]

as follows:

\[
\xi_I(x) = \int \frac{d^3k}{(2\pi)^3/2} \left( a_k v_k e^{ikx} + \text{h.c.} \right).
\]
The mode function $v_k$ satisfies $L_k v_k = 0$ where

$$L_k := \partial^2_\rho + (3 - \varepsilon_1 + \varepsilon_2)\partial_\rho + \frac{k^2}{\rho^2 e^{2\rho}}. \quad (3.16)$$

The mode function is normalized as

$$\left(v_k e^{ik\cdot x}, v_\rho e^{ip\cdot x}\right) = (2\pi)^3 \delta^{(3)}(k - p), \quad (3.17)$$

where the Klein–Gordon inner product is defined by

$$\langle f_1, f_2 \rangle := -2i M^2 \int \frac{d^3 x e^{3\rho}}{\varepsilon_1} \{ f_1 \partial_t f_2^* - (\partial_t f_1) f_2^* \}. \quad (3.18)$$

With this normalization, we obtain the commutation relations for the creation and annihilation operators as

$$[a_k, a_p^\dagger] = \delta^{(3)}(k - p), \quad [a_k, a_p] = 0. \quad (3.19)$$

Inserting Eq. (3.15) into Eq. (3.10), we can rewrite the retarded Green function as

$$G_R(x, x') = -i\theta(t - t') \int \frac{d^3 k}{(2\pi)^3} e^{ik\cdot(x - x')} R_k(t, t'), \quad (3.20)$$

where $R_k(t, t')$ is given by

$$R_k(t, t') := v_k(t)v_k^*(t') - v_k^*(t)v_k(t'). \quad (3.21)$$

We calculate the $n$-point function of $\delta R$, setting the initial state to the vacuum defined by

$$a_k|0\rangle = 0. \quad (3.22)$$

Next, we explicitly calculate non-linear corrections. Since we are interested in the IR divergence, employing the iteration scheme of $L_R^{-1}$, we pick up only the terms that can contribute to the IR divergences. For convenience, we here introduce the symbol $\langle \rangle_{IR}$ as in Ref. [4] to denote an equality, neglecting the terms unrelated to the IR divergences. The IR divergences mean the appearance of the factor $\langle \xi^2_I \rangle$. For the scale invariant spectrum, this variance diverges logarithmically. Once a temporal or spatial differentiation acts on one of two $\xi$'s in $\langle \xi^2_I \rangle$, the variance no longer diverges. In this sense we keep only terms that can yield $\langle \xi^2_I \rangle$. When we write down the Heisenberg operator $\xi$ in terms of the interaction picture field $\xi_I$, at the one-loop level, this is equivalent to keeping only the terms without temporal and/or spatial differentiations and the terms containing only one interaction picture field with differentiation.

A further comment regarding the IR divergence is in order. Using Eq. (3.15), we can express the variance $\langle (\xi_I(x))^2 \rangle$ as

$$\langle (\xi_I(x))^2 \rangle = \int \frac{d^3 k}{(2\pi)^3} |v_k(t)|^2. \quad (3.23)$$

The singular contribution from the IR modes in the variance can be removed by introducing the comoving IR cutoff $k_{IR}$. We should discriminate the singular contribution due to the modes $k \lesssim k_{IR}$ from the remaining IR contribution due to the modes $k_{IR} \lesssim k \lesssim e^\rho$, which cannot be eliminated by the introduction of the comoving IR cutoff. The latter is known to lead to secular growth with $\ln(e^\rho/k_{IR}) \sim \rho$. In this paper, we focus on the former. The regularization of secular growth is discussed for instance in Refs. [1,29].
In this paper, we refer to a term that does (not) contribute to the IR divergences simply as an IR (ir)relevant term. In the following, we will use

\[ \mathcal{L}_R^{-1} \mathcal{R}_I \xi_I \approx \xi_I \mathcal{L}_R^{-1} \mathcal{R}_I, \]  

(3.23)

where \( \mathcal{R} \) is a derivative operator that suppresses the IR modes of \( \xi_I \) such as \( \partial_\rho \) and \( \delta^i / \rho \epsilon^0 \).

Equation (3.23) can be shown as follows. The Fourier transformation of \( \mathcal{L}_R^{-1} \xi_I D \xi_I \) is proportional to

\[ \int d^3p \int_{t_i}^t dt' \epsilon_1(t') e^{3p(t')} \rho^2(t') \mathcal{R}_k(t, t') \xi_I p(t') (\mathcal{R}_k t_k) (t') \),

where \( \xi_I k \) and \( (\mathcal{R}_k t_k) \) denote the Fourier modes of \( \xi_I \) and \( \mathcal{R}_k t_k \). Since \( (\mathcal{R}_k t_k) - (\mathcal{R}_k t_k) \) is suppressed and \( \xi_I p \) becomes time independent in the limit \( p \to 0 \), the IR relevant piece in the momentum integral can be recast into

\[ \xi_I p \int_{t_i}^t dt' \epsilon_1(t') e^{3p(t')} \rho^2(t') \mathcal{R}_k(t, t') (\mathcal{R}_k t_k) (t'). \]  

(3.24)

We will also use

\[ \mathcal{L}_R^{-1} f(x) \approx 0 \quad \text{for } f(x) \approx 0. \]  

(3.25)

Keeping only the IR relevant terms, the action for \( \xi \) is simply given by

\[ S \approx M_{pl}^2 \int dt d^3x e^{3(\rho + \xi)} \rho^2 \epsilon_1 [ (\partial_\rho \xi)^2 - \frac{2}{\rho^2} (\partial \xi)^2], \]  

where we use the lapse function \( N \) and the shift vector \( N_i \), given by solving the constraint equations as follows:

\[ N \approx 1 + \partial_\rho \xi, \]  

(3.27)

\[ \frac{1}{\rho} \partial_i N^i \approx - \frac{2}{\rho^2} \partial^2 \xi + e_1 \partial_\rho \xi. \]  

(3.28)

The action (3.26) can be easily derived from the action for the non-interacting theory. Extending the action (3.4) to a non-linear expression that preserves the dilatation symmetry, we obtain

\[ S = M_{pl}^2 \int dt d^3x e^{3(\rho + \xi)} \rho^2 \epsilon_1 [ (\partial_\rho \xi)^2 - \frac{2}{\rho^2} (\partial \xi)^2 + \cdots], \]  

where the abbreviated terms do not appear in the non-interacting action. Since the abbreviated terms should have more than two fields with differentiation, such terms are IR irrelevant up to one-loop order. Thus, we obtain Eq. (3.26).

In this paper, as a simple setup, which is consistent with the initial conditions (3.2) and (3.3), we turn on the interaction at \( t = t_i \), assuming that the action is given as

\[ S \approx S_0 + M_{pl}^2 \int dt d^3x \theta(t - t_i) e^{3\rho} \rho^2 \epsilon_1 \left[ (e^3 - 1)(\partial_\rho \xi)^2 - \frac{2}{\rho^2} (e^3 - 1)(\partial \xi)^2 \right]. \]  

(3.30)

Then, the conjugate momentum and the Hamiltonian density are given by

\[ \pi(x) := \frac{\delta S}{\delta \xi(x)} \approx 2M_{pl}^2 [1 + \theta(t - t_i)(e^3 - 1)] e^{3\rho} \rho \epsilon_1 \partial_\rho \xi(x), \]  

(3.31)
Combining Heisenberg’s equations for $\zeta$ and $\pi$, we obtain the equation of motion for $t \geq t_i$ as

$$
\frac{1}{e^{3\rho}} \frac{\partial}{\partial \rho} \left( e^{3\rho} \rho \epsilon_1 \frac{\partial}{\partial \rho} \right) - \frac{e^{-2(\rho + \zeta)}}{\rho^2} \frac{\partial^2 \zeta}{\partial \rho^2} + \delta(\rho - \rho_i)(e^{3\zeta} - 1) \frac{\partial}{\partial \rho} \zeta \approx 0,
$$

(3.33)

where we use $\rho_i := \rho(t_i)$.\(^1\) By expanding $\zeta$ as $\zeta = \zeta_1 + \zeta_2 + \zeta_3 \cdots$, we solve the equation of motion (3.33). After some manipulation, which is summarized in Appendix B, we obtain a solution of $\zeta$ that satisfies the initial conditions (3.2) and (3.3) as

$$
\zeta_2 \approx -\zeta_1 L^{-1}_R \left[ 2\Delta + 3\delta(\rho - \rho_i) \frac{\partial}{\partial \rho} \right] \zeta_1,
$$

(3.36)

$$
\zeta_3 \approx \frac{1}{2} \zeta_2^2 \left[ 4L^{-1}_R \Delta L^{-1}_R (2\Delta + 3\delta(\rho - \rho_i) \frac{\partial}{\partial \rho}) + 4L^{-1}_R \Delta + 9L^{-1}_R \delta(\rho - \rho_i) \frac{\partial}{\partial \rho} \right] \zeta_1,
$$

(3.37)

where we define

$$
\nabla_i := \frac{e^{-\rho}}{\rho} \partial_i, \quad \Delta := \delta^{ij} \nabla_i \nabla_j.
$$

(3.38)

In solving the equation of motion for $\zeta$, we used the properties of $L^{-1}_R$ given in Eqs. (3.23) and (3.25).

### 3.2. Calculating the gauge invariant operator

Solving the 3D geodesic equations, we obtain the relation between the global coordinates $x^i_{gl}$ and the geodesic normal coordinates $x^i$ as

$$
x^i_{gl} \approx e^{-\zeta(x)} x^i.
$$

(3.39)

Using the geodesic normal coordinates, the gauge-invariant curvature $sR$ is expressed as

$$
sR(t, x) \approx sR(t, e^{-\zeta(t,x)} x).
$$

(3.40)

Here, we introduce the spatial average of $\zeta$ at the local observable region whose spatial scale is $L_i$ in the geodesic normal coordinates as

$$
\bar{sR}_i(t) := \frac{\int d^3 x W_{L_i}(x) \zeta(t, e^{-\zeta x})}{\int d^3 x W_{L_i}(x)}.
$$

(3.41)

\(^1\) Here, we consider a setup where we can use the same solution of $\zeta$ as the one given in Eqs. (3.12) and (3.13), accepting the presence of the discontinuity in the interaction. By contrast, if we modify the solution of $\zeta$, adding the homogeneous solution:

$$
2iM^2_{pl} \int d^3 x' \epsilon_1(t') e^{3\rho(t')} \left[ \zeta_1(t, x), \zeta_1(t, x') \right] \left( e^{-3\zeta(t, x')} - 1 \right) \partial_t \zeta_1(t, x'),
$$

(3.34)

we can construct a solution that satisfies the initial conditions (3.2) and (3.3) in the system without discontinuity whose equation of motion is given by

$$
\frac{1}{e^{3\rho}} \frac{\partial}{\partial \rho} \left( e^{3\rho} \rho \epsilon_1 \frac{\partial}{\partial \rho} \right) - \frac{e^{-2(\rho + \zeta)}}{\rho^2} \frac{\partial^2 \zeta}{\partial \rho^2} \approx 0.
$$

(3.35)

Thus, the constructed solution $\zeta$ turns out to agree with the one we constructed in Eqs. (3.36) and (3.37). This setup will give another realization of the solution, allowing us to avoid explicit introduction of the discontinuity. (For a more detailed explanation about the solution with the homogeneous solution (3.34), see for instance Ref. [40]).

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where $W_L(x)$ is the window function that vanishes far out of our observable region. We approximate this averaging scale at each time $t$ by the horizon scale, i.e., $L_t \simeq \{e^{\rho(t)} \dot{\rho}(t)\}^{-1}$. Using $g^\zeta(t)$, we decompose the spatial coordinates as
\[
^g R(t, x) \overset{\text{IR}}{\approx} ^s R(t, x) e^{-[\zeta(t, x) - \bar{\zeta}(t)]} e^{-\bar{\zeta}(t) x}.
\] (3.42)
Using the window function $W_L(x)$, we define the local average of an operator $O(t, x)$ as
\[
\bar{O}(t) := \frac{\int d^3 x W_L(x) O(t, x)}{\int d^3 x W_L(x)}.
\] (3.43)
We note that the factor $e^{-[\zeta(t, x) - \bar{\zeta}(t)]}$, which can be expanded in perturbation as
\[
e^{-[\zeta(t, x) - \bar{\zeta}(t)]}
= 1 - \{\zeta_t - \bar{\zeta}_t\} + \{\zeta_2 - \bar{\zeta}_2\} - (\zeta_t x \cdot \delta_x \zeta_t - \bar{\zeta}_t x \cdot \delta_x \bar{\zeta}_t)\right\} + \frac{1}{2} (\zeta_t - \bar{\zeta}_t)^2 + \cdots,
\] (3.44)
yields only IR regular contributions up to one-loop order, such as $\langle (\zeta_t - \bar{\zeta}_t) \zeta_t \rangle$ and $(\zeta_t x \cdot \delta_x \zeta_t)$. The latter also becomes finite because of the derivative suppression and the finiteness of $|x|^2$.\footnote{One may think that interaction vertices located outside the past light cone can appear from the inverse Laplacian $\partial^{-2}$ that is included in the lapse function and shift vector. In that case, $|x|$ becomes unbounded. However, tuning the boundary condition of the constraint equations, which are the elliptic-type equations, we can manifestly shut off the influences from outside the observable region $\mathcal{O}$. Since this change can be thought of as a change in the residual gauge degrees of freedom, it does not influence the gauge invariant operator $^g R$. A detailed explanation of this is given in the Appendix of Ref. [29].} For the reason mentioned above, neglecting the factor $e^{-[\zeta(t, x) - \bar{\zeta}(t)]}$, we rewrite the gauge invariant operator $^g R$ as
\[
^g R(x) \overset{\text{IR}}{\approx} ^s R(t, x) e^{-\bar{\zeta}(t) x}.
\] (3.45)
Since the spatial curvature $^s R$ is given by
\[
^s R(x) \overset{\text{IR}}{\approx} -4 e^{-2 \rho} e^{-2 \zeta(x)} \partial^2 \zeta(x),
\]
using the curvature perturbation in the geodesic normal coordinates:
\[
^g \zeta(t, x) := \zeta(t, x) e^{-\bar{\zeta}(t) x},
\] (3.46)
we can describe the gauge-invariant spatial curvature $^g R$ as
\[
^g R(t, x) \overset{\text{IR}}{\approx} -4 e^{-2 \rho} e^{-2 (\zeta - \bar{\zeta})} \partial^2 \zeta(t, x) e^{-\bar{\zeta}(t) x}
\approx -4 e^{-2 \rho} \partial^2 g \zeta(t, x)
\] (3.47)
at least up to third order in perturbation. At the second equality, we again used the fact that the exponential factor $e^{-(\zeta - \bar{\zeta})}$ does not give IR relevant contributions. As is pointed out by Tsamis and Woodard in Ref. [41] (see also Ref. [42]), using the geodesic normal coordinates can introduce an additional origin of UV divergence. We suppose that replacing $\zeta$ in the geodesic normal coordinates with $^g \zeta$, which is smoothed by the window function, can moderate the singular behavior.
Inserting the solution of $\xi$ given in Eq. (3.36) into Eq. (3.46), we obtain $\xi_2$ as

$$\xi_2 = \xi_2 - \xi_1 x \cdot \partial_x \xi_1 \approx -\xi_1 D_x \xi_1,$$

(3.48)

where we introduce

$$D_x := 2L_R^{-1} \Delta + 3L_R^{-1} \delta(\rho - \rho_i)\partial_\rho + x \cdot \partial_x.$$  

(3.49)

The computation of $\xi_3$ is messier, but we can show that $\xi_3$ can be summarized in the compact form:

$$\xi_3 \approx \frac{1}{2} \xi_1^2 D_x^2 \xi_1.$$  

(3.50)

The detailed computation is shown in Appendix B.

### 3.3. Conditions for the absence of IR divergence

We next discuss the condition that IR divergence does not arise in the two-point function of the gauge invariant variable $gR$. Then, using the above expression, the two-point function of $gR$ up to one-loop order is obtained as

$$\langle g(x_1)^R g(x_2)^R \rangle \approx 8e^{-\rho(\xi_1^2)}\partial_{x_1}\partial_{x_2}\left(2D_{x_1}\xi_1(x_1)D_{x_2}\xi_1(x_2) + D_{x_1}^2\xi_1(x_1)\xi_1(x_2) + \xi_1(x_1)D_{x_2}^2\xi_1(x_2)\right).$$  

(3.51)

As we mentioned at the end of the preceding section, the correlation function of $gR$ can contain IR divergences. One may think that the IR regularity is guaranteed if

$$D_x \xi_1(x) = 0$$  

(3.52)

is imposed. However, this condition is in conflict with the use of the ordinary retarded integral in the iteration process. In fact, one can calculate $D_x \xi_1(x)$ as

$$D_x \xi_1(x) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{ik \cdot x} a_k \left[ L_{-1}^{-1}_{R,k} \left( -\frac{k^2}{2\varepsilon^2\rho^2} + 3\delta(\rho - \rho_i)\partial_\rho + ik \cdot k \right) v_k + \text{h.c.} \right].$$  

(3.53)

where $L_{-1}^{-1}_{R,k}$ is the Fourier mode of $L_{-1}^{-1}$. The requirement that this expression should identically vanish leads to

$$\left[ L_{-1}^{-1}_{R,k} \left( -\frac{k^2}{2\varepsilon^2\rho^2} + 3\delta(\rho - \rho_i)\partial_\rho + ik \cdot k \right) v_k = 0. $$  

(3.54)

The first term is independent of $x$, while the second one manifestly depends on $x$. This shows that the condition (3.52) is incompatible with the use of the retarded integral.

In place of this naive condition, an alternative possibility one can think of is to impose

$$D_x \xi_1(x) = \int \frac{d^3k}{(2\pi)^{3/2}} \left( a_k D e^{ik \cdot x} v_k + \text{h.c.} \right)$$  

(3.55)

with

$$D := k^{-3/2} e^{-i\phi(k)} k \cdot \partial_k k^{3/2} e^{i\phi(k)},$$  

(3.56)

where $\phi(k)$ is an arbitrary real function. The condition can be rewritten as a condition on mode functions

$$L_{-1}^{-1}_{R,k} \left( -\frac{k^2}{2\varepsilon^2\rho^2} + 3\delta(\rho - \rho_i)\partial_\rho \right) v_k = D v_k.$$  

(3.57)

which can avoid the problem in Eq. (3.54). We employ an initial condition, requesting that the mode function $v_k$ satisfies Eq. (3.57) and its time derivative at $t = t_i + \epsilon$, where $\epsilon$ is a constant parameter.
with $0 < \epsilon \ll 1$. Then, the condition (3.57) continues to hold also for $t > t_i + \epsilon$, because both sides of this equation vanish under the operation of the second-order differential operator $\mathcal{L}$. With these conditions, for $t \geq t_i + \epsilon$, the expectation value in Eq. (3.51) can be summarized in total derivative form as

$$\langle \delta R(x_1) \delta R(x_2) \rangle_{\text{IR}} \approx 8e^{-4\rho(\zeta)} \frac{\sum_{k} r_k^2}{(2\pi)^3} \int \frac{d\Omega_k}{\ln k} \left\{ k^2 |v_k|^2 e^{i k (x_1 - x_2)} \right\},$$

where we use $k^{3/2} D = e^{-i\phi(k)} k \cdot \partial_k k^{3/2} e^{i\phi(k)}$ and $\int d\Omega_k$ denotes the integration over the angular directions of $k$. Since this total derivative integral vanishes, the IR divergence disappears.

Although requesting the condition (3.57) can make the IR divergence vanish, a little more careful thought rules out this possibility. Since the left-hand side of (3.57) vanishes at $t \simeq t_i$, leaving aside the terms of order $\epsilon$, the condition (3.57) yields $Dv_k(t_i) \simeq 0$, requesting the scale invariant spectrum with $v_k(t_i) \propto 1/k^{3/2}$ for all wavenumbers. This spectrum is not compatible with the vacuum in the flat spacetime in the UV limit and therefore cannot provide a physically natural initial condition.

Even though the IR regularity condition (3.57) cannot be naturally compatible with the initial conditions, particularly Eq. (3.2), it is still instructive to give an alternative interpretation of the condition (3.57). We adopted the initial conditions (3.2) and (3.3) for $\{\zeta, \pi\}$, which identify the Heisenberg fields with the corresponding interaction picture fields at the initial time and select the vacuum state for the free field at the initial time. We denote a set of operations that specify the interacting quantum state by an iteration scheme. In the canonical system of $\{\zeta, \pi\}$, we fixed the iteration scheme by Eqs. (3.2), (3.3), and (3.22). Then, when we take the same iteration scheme in the canonical system $\{\tilde{\zeta}, \tilde{\pi}\}$, it is not obvious whether the same vacuum state as the one in the canonical system $\{\zeta, \pi\}$ is picked up or not. Before closing this section, we show that the condition (3.57) is identical to the condition that these two vacua are equivalent.

Since the transformation from $\{\zeta, \pi\}$ to $\{\tilde{\zeta}, \tilde{\pi}\}$ is a canonical transformation, the correlation functions for the same initial state calculated in these two canonical systems should agree with each other, i.e.,

$$\langle \zeta(x_1) \zeta(x_2) \rangle = \langle \tilde{\zeta}(t, e^x x_1) \tilde{\zeta}(t, e^x x_2) \rangle. \quad (3.58)$$

To employ the same iteration scheme, we request that both $\zeta$ and $\tilde{\zeta}$ are solved with $\mathcal{L}^{-1}_R$ by identifying the Heisenberg fields with the interaction picture fields at the initial time. We expand the interaction picture fields for $\zeta$ and $\tilde{\zeta}$, which we denote as $\zeta_I$ and $\tilde{\zeta}_I$, respectively, in terms of the same mode function $v_k$ as

$$\zeta_I(x) = \int \frac{d^3k}{(2\pi)^3/2} a_k v_k e^{ikx} + \text{h.c.}, \quad (3.59)$$
$$\tilde{\zeta}_I(x) = \int \frac{d^3k}{(2\pi)^3/2} \tilde{a}_k v_k e^{ikx} + \text{h.c.}. \quad (3.60)$$

Further, we select the vacuum states that are erased under the action of $a_k$ and $\tilde{a}_k$ in the respective systems. We denote these vacuum states specified by $a_k$ and $\tilde{a}_k$ as $|0\rangle$ and $|\tilde{0}\rangle$, respectively. Now we show that the equivalence between the two-point functions, i.e.,

$$\langle 0 | \zeta(x_1) \zeta(x_2) | 0 \rangle = \langle \tilde{0} | \tilde{\zeta}(t, e^x x_1) \tilde{\zeta}(t, e^x x_2) | \tilde{0} \rangle, \quad (3.61)$$

Using the Wronskian condition $\partial_t R_k(t, t')|_{t=t_i} = (2i M_p^2 \epsilon_1 e^{\gamma_0})^{-1}$, we can see that the first derivative of the condition (3.57) yields $(D - 3)\dot{v}_k(t_i) \simeq 0$. Then, the IR regularity condition requests $v_k(t_i) \propto k^{-3/2}$ and $\dot{v}_k(t_i) \propto k^{3/2}$ for all $k$s.
yields the condition (3.57). We expand \( \tilde{\zeta}(t, e^s x^i) \) as

\[
\tilde{\zeta}(t, e^s x^i) = \tilde{\zeta}(x) + s x \cdot \partial_x \tilde{\zeta}(x) + \frac{1}{2} s^2 (x \cdot \partial_x)^2 \tilde{\zeta}(x) + O(s^3)
\]

\[
\overset{\text{IR}}{\approx} \tilde{\zeta}_I - \tilde{\zeta}_I \mathcal{L}^{-1}_R \left( 2\Delta + 3\delta(\rho - \rho_i)\partial_\rho \right) \tilde{\zeta}_I + s \mathcal{D}_x \tilde{\zeta}_I + \cdots,
\]

(3.62)

taking into account that the interaction Hamiltonian is shifted by \(-s\). Here, \(\cdots\) denotes higher-order terms in perturbation. Then, the right-hand side of Eq. (3.61) gives

\[
\langle 0 | \tilde{\zeta}(t, e^s x_1) \tilde{\zeta}(t, e^s x_2) | 0 \rangle \overset{\text{IR}}{\approx} \langle 0 | [\tilde{\zeta}_I(x_1) - \tilde{\zeta}_I(x_1) \mathcal{L}^{-1}_R \left( 2\Delta(1) + 3\delta(\rho - \rho_i)\partial_\rho \right) \tilde{\zeta}_I(x_1) + \cdots] \tilde{\zeta}_I(x_2) + \cdots | 0 \rangle \\
\times \langle 0 | \mathcal{D}_x \tilde{\zeta}_I(x_1) \tilde{\zeta}_I(x_2) \tilde{\zeta}_I(x_2) + \cdots | 0 \rangle + s \langle 0 | \mathcal{D}_x \tilde{\zeta}_I(x_1) \tilde{\zeta}_I(x_2) + \cdots | 0 \rangle + O(s^2).
\]

(3.63)

where we use the abbreviated notation \( \Delta_\omega := (e^\rho \dot{\rho})^{-2} \delta^2 \chi_\omega \) for \(\omega = 1, 2\). Since the terms in the second and third lines of Eq. (3.63) agree with the left-hand side of Eq. (3.61), the other terms on the right-hand side of Eq. (3.63) should vanish to satisfy Eq. (3.61). The remaining terms of \(s\) at the leading order in \(\tilde{\zeta}_I\) in Eq. (3.63) are given by

\[
s \int \frac{d^3k}{(2\pi)^3} \left[ v_k e^{-ik \cdot x_1} \mathcal{D}_{x_1} v_k e^{-ik \cdot x_2} + v_k e^{ik \cdot x_1} D_{x_2} v_k e^{-ik \cdot x_2} \right] \\
= -s \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot (x_1 - x_2)} \left[ v_k \left( C^{-1}_{R,k} \left( \frac{k^2}{e^{2\rho \rho^2}} - 3\delta(\rho - \rho_i)\partial_\rho \right) v_k + k^{-3/2} k \cdot \partial_k (k^{3/2} v_k) \right) + \text{c.c.} \right].
\]

(3.64)

where we perform integration by parts. Now it is clear that requesting Eq. (3.61) gives the same condition as requesting the IR regularity (3.57), except for the unimportant \(k\)-dependence of the phase of the mode functions.

4. Summary and discussions

We have focused on observable quantities that are invariant under the residual gauge transformations. The residual gauge degrees of freedom are left unfixed in the ordinary discussion of cosmological perturbation. The key issue for the correlation functions of the gauge invariant operator to be IR regular is shutting off the long-range correlation between observable quantities and the fluctuation outside the observable region. This is a matter of how we choose the initial quantum state. The leading effect of the long-range correlation on local observables is the constant shift of the so-called curvature perturbation (i.e., the trace part of spatial metric perturbation). The constant shift of the curvature perturbation can be absorbed by the dilatation transformation of the spatial coordinates. Assuming that the interactions are shut off before the initial time, we investigated the conditions that guarantee the equivalence between two systems mutually related by the dilatation, and found that these conditions also guarantee the IR regularity of observable quantities. Therefore, we can think of the IR regularity condition (3.57) as requesting the invariance under the dilatation, which is one of the residual gauge transformations.

We also found that these conditions cannot be naturally satisfied when we abruptly switch on the interaction at a finite initial time \(t = t_1\). In this setup, which we chose to simplify our illustration, the initial time is a very particular time, at which the Heisenberg picture fields agree with the interaction...
picture fields. Then, the curvature scale at the initial time becomes distinguishable from other scales. It is, therefore, natural that, unless we choose the fully scale invariant spectrum, which cannot provide a physically natural ultra-violet behavior, the presence of a particular initial time breaks the invariance under the scale transformation. One possibility to avoid breaking the dilatation symmetry is to send the initial time to the infinite past. When we send the initial time to the past infinity, the IR regularity no longer requests the condition \((3.57)\), because Eq. \((3.23)\) does not hold in this limit. At Eq. \((3.24)\), we took \(\zeta_p\) out of the time integration, because \(\zeta_p\) becomes constant in time in the limit \(p/\epsilon \rho \dot{\rho} \ll 1\). However, since all the modes become sub-Hubble modes at the distant past, the same argument does not follow when we send the initial time to the past infinity. Thus, when we keep the interaction turned on from the past infinity, our claim in this paper does not prohibit the presence of acceptable initial states that guarantee the IR regularity.

Then, the question is whether there is an initial state (or an iteration scheme) that guarantees the IR regularity or the gauge invariance in the local observable universe. In our previous papers \([3,4]\), we found that, when we specify the relation between the Heisenberg picture field \(\zeta\) and the interaction picture field \(\zeta_I\) in a non-trivial way and choose the adiabatic vacuum as the vacuum state for the non-interacting theory, the IR contributions in the two-point functions of \(\delta R\) are regularized. The result of the present paper shows that the relation between the Heisenberg picture field and the interaction picture field imposed in Refs. \([3,4]\) is different from the relation fixed by the initial conditions \((3.2)\) and \((3.3)\), because the mode equation for the adiabatic vacuum does not satisfy Eq. \((3.57)\). We naturally expect that the IR regular vacuum that we found in Refs. \([3,4]\) corresponds to the iteration scheme where the interaction has been active from the past infinity.

In general, when we keep the interaction turned on from the past infinity, the time integration at each interaction vertex does not converge. The \(i\epsilon\) prescription provides a noble way to make the time integration converge. The adiabatic vacuum is the vacuum state that is selected by the \(i\epsilon\) prescription. There is another advantage to fixing the iteration scheme by the \(i\epsilon\) prescription. The correspondence between the IR regularity and the gauge invariance provides an important clue to proving the IR regularity. The result of the present paper in the simple iteration scheme suggests that the IR regularity of the loop corrections may be ensured, if we employ an iteration scheme that satisfies

\[
\langle \Omega | \zeta(x_1) \zeta(x_2) \cdots \zeta(x_n) | \Omega \rangle = \langle \tilde{\Omega} | \tilde{\zeta}(t_1, e^{-\delta} x_1) \tilde{\zeta}(t_1, e^{-\delta} x_2) \cdots \tilde{\zeta}(t_1, e^{-\delta} x_n) | \tilde{\Omega} \rangle, \tag{4.1}
\]

where \(|\Omega\rangle\) and \(|\tilde{\Omega}\rangle\) are the initial states selected by the same iteration scheme in the two canonical systems \(\{\zeta, \pi\}\) and \(\{\tilde{\zeta}, \tilde{\pi}\}\), respectively. Since the \(i\epsilon\) prescription can be shown to select the unique state, which becomes the ground state when the Hamiltonian is conserved in time, we expect that the condition \((4.1)\) can be satisfied if we fix the integration scheme by the \(i\epsilon\) prescription. In our succeeding paper \([29]\), we will verify this expectation and will show that the IR regularity and the absence of secular growth can be ensured if we fix the iteration scheme by the \(i\epsilon\) prescription.

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Appendix A. Solutions with the retarded Green function and the in–in formalism

In this appendix, we discuss the relation between the n-point functions obtained from the solution written in terms of the retarded Green function $G_R$ and those obtained in the in–in formalism. We formally show that these n-point functions agree with each other. In the in–in formalism, the Heisenberg fields $\zeta(x)$ and $\pi(x)$ are related to the interaction picture fields $\zeta_I(x)$ and $\pi_I(x)$ by the unitary operator given by

$$ U_I(t_1, t_2) = T \exp \left[ -i \int_{t_2}^{t_1} dt \ H_I(t) \right] \quad (A1) $$

as follows:

$$ \zeta(t, x) = U_I(t, t_i) \zeta_I(t, x) U_I(t, t_i), \quad \pi(t, x) = U_I(t, t_i) \pi_I(t, x) U_I(t, t_i). \quad (A2) $$

Here, we keep the initial time $t_i$ finite. Because of the unitarity of $U(t_1, t_2)$, the commutation relation for $\zeta$ and its conjugate momentum $\pi$ automatically ensures the commutation relation for $\zeta_I$ and its conjugate momentum $\pi_I$. Using Eq. (A2), the n-point function for the curvature perturbation $\zeta$ is given as

$$ \langle \zeta(t, x_1) \cdots \zeta(t, x_n) \rangle = \left\{ U_I(t, t_i) \zeta_I(t, x_1) \cdots \zeta_I(t, x_n) U_I(t, t_i) \right\}. \quad (A3) $$

Using the mathematical induction, we can rewrite the n-point functions (A3) as

$$ \langle \zeta(t, x_1) \cdots \zeta(t, x_n) \rangle = \sum_{i=0}^{\infty} i^N \int_{t_i}^{t_1} dt_N \cdots \int_{t_i}^{t_2} dt_1 \times \langle [H_I(t_1), \cdots [H_I(t_N), \zeta_I(t, x_1) \cdots \zeta_I(t, x_n)] \cdots] \rangle. \quad (A4) $$

As a simple example, let us consider the two-point function in the case where the action is given by

$$ S = 2M^2_{pl} \int dt \ d^3x \ e^{3\rho} \rho^2 \varepsilon_1 \left\{ \frac{1}{2} (\partial_\rho \zeta)^2 - \frac{e^{-2\rho}}{2\rho^2} (\partial_\zeta)^2 - \frac{c_p}{p} \zeta^p \right\}, \quad (A5) $$

where $\rho$ is a natural number that is larger than 2 and $c_p$ is a time-dependent function. In this case, the equation of motion for $\zeta$ is simply given by

$$ \mathcal{L} \zeta = -c_p \zeta^{p-1}, \quad (A6) $$

and the interaction Hamiltonian is given by

$$ H_I[\zeta_I](t) = 2M^2_{pl} e^{3\rho} \rho^2 \varepsilon_1 \int d^3x \frac{c_p}{p} \zeta_I^p(t, x). \quad (A7) $$

Noting the fact that the retarded Green function is expressed as

$$ G_R(x, x') = -i\theta(t - t') \left[ \zeta_I(x), \zeta_I(x') \right], \quad (A8) $$

we first calculate the innermost commutation relation in Eq. (A4) as

$$ i \int_{t_i}^{t} dt_N \ [H_I(t_N), \zeta_I(x_1) \cdots \zeta_I(x_n)] $$

$$ = -2M^2_{pl} \int_{t_i}^{t} dt_N \int d^3x e^{3\rho} \rho^2 \varepsilon_1 \frac{c_p}{p} \left\{ \zeta_I^{p-1}(x_N) + \zeta_I(x_N) \zeta_I^{p-2}(x_N) + \cdots + \zeta_I^{p-1}(x_N) \right\}. \quad (A9) $$
where we use the abbreviated notation \( x_N := (t_N, \mathbf{x}) \) and \( x_\alpha := (t, \mathbf{x}_\alpha) \) for \( \alpha = 1, \cdots n \). We define the operator \( \mathcal{C} \) as

\[
\mathcal{C} := -i \theta(t - t_N) [\xi_I(x_N), \xi_I(x_1) \cdots \xi_I(x_n)] \\
= - \sum_{\alpha=1}^n G_R(x_\alpha, x_N) \prod_{m=1, m \neq \alpha}^n \xi_I(x_m). \tag{A10}
\]

Comparing this expression to Eqs. (3.12) and (3.13), for instance, the first term in the curly brackets of Eq. (A9) is recast into

\[
- \sum_{\alpha=1}^n \prod_{m=1, m \neq \alpha}^n \xi_I(x_m) \mathcal{L}_R^{-1} \frac{c_p}{p} \delta_{p-1}(x_\alpha). \tag{A11}
\]

Repeating this procedure, we can show that the \( n \)-point functions (A4) agree with the \( n \)-point functions for \( \xi(x) \), which is iteratively solved by using the retarded Green function. Here, for illustrative purposes, we have considered a simple case, but this argument can be generalized in a straightforward manner.

**Appendix B. The computation of \( ^8\xi \)**

We first solve the equation of motion (3.33), employing the initial conditions (3.2) and (3.3). By expanding \( \xi = \xi_I + \xi_2 + \xi_3 + \cdots \), the equation of motion is recast into

\[
\mathcal{L} \xi_I = 0, \tag{B1}
\]

\[
\mathcal{L} \xi_2 \approx -2 \xi_I \Delta \xi_I - 3 \delta(\rho - \rho_I) \xi_I \partial_\rho \xi_I, \tag{B2}
\]

\[
\mathcal{L} \xi_3 \approx -2 \left( \xi_2 \Delta \xi_I + \xi_I \Delta \xi_2 - \xi_I^2 \Delta \xi_I \right) - 3 \delta(\rho - \rho_I)(\xi_2 \partial_\rho \xi_I + \xi_I \partial_\rho \xi_2) - \frac{9}{2} \delta(\rho - \rho_I) \xi_I^2 \partial_\rho \xi_I. \tag{B3}
\]

Using the initial conditions (3.2) and (3.3), we can express \( \partial_\rho \xi(t, \mathbf{x}) \) in terms of the interaction picture field at the initial time as

\[
\partial_\rho \xi(t, \mathbf{x}) \approx e^{-3 \xi_I(t, \mathbf{x})} \partial_\rho \xi_I(t, \mathbf{x}). \tag{B4}
\]

Using this expression, we can rewrite the equation of motion for \( \xi_3 \) as

\[
\mathcal{L} \xi_3 \approx -2 \left( \xi_2 \Delta \xi_I + \xi_I \Delta \xi_2 - \xi_I^2 \Delta \xi_I \right) + \frac{9}{2} \delta(\rho - \rho_I) \xi_I^2 \partial_\rho \xi_I. \tag{B5}
\]

Solving Eqs. (B2) and (B5), we obtain

\[
\xi_2 \approx -\xi_I \mathcal{L}_R^{-1} \left[ 2 \Delta + 3 \delta(\rho - \rho_I) \partial_\rho \right] \xi_I, \tag{B6}
\]

\[
\xi_3 \approx \frac{1}{2} \xi_I^2 \left[ 4 \mathcal{L}_R^{-1} \Delta \mathcal{L}_R^{-1} (2 \Delta + 3 \delta(\rho - \rho_I) \partial_\rho) + 4 \mathcal{L}_R^{-1} \Delta + 9 \mathcal{L}_R^{-1} \delta(\rho - \rho_I) \partial_\rho \right] \xi_I, \tag{B7}
\]

where we note the properties of the retarded integration \( \mathcal{L}_R^{-1} \) given in Eqs. (3.23) and (3.25).

Next, using Eqs. (B6) and (B7), we express \( ^8\xi \), defined in Eq. (3.46). Inserting Eq. (B6) into Eq. (3.46), we can easily obtain \( ^8\xi_2 \) as given in Eq. (3.48). The computation of \( ^8\xi_3 \) is slightly lengthier.
By using Eqs. (B6) and (3.46), $\xi_3$ is expressed as

$$\xi_3 \approx \xi_3 + \frac{2}{\xi_I} \left( 2L^\perp \Delta + 3L^\perp \delta(\rho - \rho_i) \partial_\rho + x \cdot \partial_x \right) \xi_I + \frac{1}{2} \xi^2_I (x \cdot \partial_x)^2 \xi_I. \quad (B8)$$

To rewrite the terms with $x \cdot \partial_x L^\perp$ in $\xi_3$ into a more desirable form, we use

$$x \cdot \partial_x L^\perp = \frac{1}{2} \left( x \cdot \partial_x L^\perp + L^\perp L x \cdot \partial_x L^\perp \right), \quad (B9)$$

which can be obtained by replacing $L^\perp L$ with 1. To verify this replacement, let us consider a term in the form

$$\delta_R := (1 - L^\perp L) x \cdot \partial_x L^\perp (\cdots).$$

Note that $\delta_R$ can be eliminated by operating $L$, and hence $\delta_R$ is a homogeneous solution of the second-order derivative equation, i.e., $L \delta_R = 0$. Since $\delta_R$ and its first time derivative are both zero at the initial time, which is automatically satisfied by the definition of the retarded integral $L^\perp$, we can confirm that $\delta_R$ vanishes for all times $t \geq t_i$. Using $[L, x \cdot \partial_x] = -2\Delta$ with the operation of $L^\perp$ from the left- and right-hand sides, we can further rewrite the right-hand side of Eq. (B9) as

$$x \cdot \partial_x L^\perp = \frac{1}{2} \left( x \cdot \partial_x L^\perp + L^\perp x \cdot \partial_x \right) - L^\perp \Delta L^\perp. \quad (B10)$$

Using Eqs. (B7), (B8), and (B10), we obtain

$$\xi_3 \approx \frac{1}{2} \xi^2_I \left( 2L^\perp \Delta + 3L^\perp \delta(\rho - \rho_i) \partial_\rho + x \cdot \partial_x \right)^2 \xi_I - 3\xi^2_I L^\perp \delta(\rho - \rho_i) \partial_\rho L^\perp \Delta \xi_I + \frac{9}{2} \xi^2_I (L^\perp \delta(\rho - \rho_i) \partial_\rho - (L^\perp \delta(\rho - \rho_i) \partial_\rho)^2) \xi_I. \quad (B11)$$

Noting the fact that the definition of $L^\perp$ implies

$$L^\perp \delta(\rho - \rho_i) \partial_\rho L^\perp \Delta \xi_I = 0, \quad (L^\perp \delta(\rho - \rho_i) \partial_\rho - (L^\perp \delta(\rho - \rho_i) \partial_\rho)^2) \xi_I = 0, \quad (B12)$$

we arrive at the compact expression given in Eq. (3.50).

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