

Quadratic isocurvature cross-correlation, Ward identity, and dark matterDaniel J. H. Chung,^{*} Hojin Yoo,[†] and Peng Zhou[‡]*Department of Physics, University of Wisconsin-Madison, 1150 University Avenue, Madison, Wisconsin 53706, USA*

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Sources of isocurvature perturbations and large non-Gaussianities include field degrees of freedom whose vacuum expectation values are smaller than the expansion rate of inflation. The inhomogeneities in the energy density of such fields are quadratic in the fields to leading order in the inhomogeneity expansion. Although it is often assumed that such isocurvature perturbations and inflaton-driven curvature perturbations are uncorrelated, this is not obvious from a direct computational point of view due to the form of the minimal gravitational interactions. We thus compute the irreducible gravitational contributions to the quadratic isocurvature-curvature cross-correlation. We find a small but nondecaying cross-correlation, which in principle serves as a measurable prediction of this large class of isocurvature perturbations. We apply our cross-correlation result to two dark matter isocurvature perturbation scenarios: QCD axions and wimpzillas. On the technical side, we utilize a gravitational Ward identity in a novel manner to demonstrate the gauge invariance of the computation. Furthermore, the detailed computation is interpreted in terms of a soft- ζ theorem and a gravitational Ward identity. Finally, we also identify explicitly all the counterterms that are necessary for renormalizing the isocurvature perturbation composite operator in inflationary cosmological backgrounds.

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I. INTRODUCTION

As physics beyond the Standard Model is expected to contain many fields in addition to the inflaton; there are many candidates for isocurvature perturbations in the context of inflationary cosmology, including those of the dark matter. Indeed, the current data are consistent with the existence of an $O(5\%)$ isocurvature component [1–8]. Furthermore, it is well known that quadratic isocurvature perturbations [i.e., the vacuum expectation value (VEV) of the field is much smaller than the Hubble expansion rate] are one of the very few ways to generate measurably large local non-Gaussianities [9–40] in the context of the slow-roll inflationary paradigm. The only nontrivial requirement that the isocurvature field degree of freedom must possess is that it be light enough to be excited by the inflationary quasi-de Sitter (dS) background and that it not be conformally invariant. In the literature [41–43], quadratic isocurvature perturbations are often assumed to have negligible cross-correlations with the curvature perturbations (which corresponds to the inflaton field degree of freedom dressed by gravity). However, the gravitational interactions lead to a minimum cross-correlation, which in principle can be observationally important. We present a computation of this minimal gravitational cross-correlation in this paper.

As explained below, the form of the gravitational interaction between the curvature and isocurvature perturbations naively suggests that there can be cross-correlators which do not vanish in the long wavelength limit. If this

were true, the cross-correlation could dominate over the isocurvature two-point function in the observables since the latter vanishes in the long wavelength limit for a massive field. By an explicit rigorous computation, we show that the cross-correlator vanishes in the long wavelength in such a way that the cross-correlation induced by gravity never dominates over the isocurvature two-point function, given that the curvature inhomogeneity perturbation is characterized by a strength of order 10^{-5} . We explain this qualitatively as well using a combination of a soft- ζ theorem [44–61] and a Ward identity associated with a spatial dilatation diffeomorphism. We also check the gauge invariance of our computation using a Ward identity.

Among the possible isocurvature candidates, thermal dark matter is usually produced copiously by the inflaton decay products, which typically leads to a large suppression of isocurvature effects. On the other hand, nonthermal dark matter that is not produced by the inflaton decay can easily generate large isocurvature effects that survive until today. Hence, as an illustration, we apply our computation of the cross-correlation to two different nonthermal dark matter models: QCD axions and wimpzillas. In both cases, we find a cross-correlation characterized by the parameter $|\beta| \sim O(10^{-5})$ [the parameter definition is given in Eq. (29)] which is below the boundary value of $O(10^{-2})$ when the cross-correlation becomes competitive with the isocurvature two-point function. In principle, β can be measured and is a generic prediction of this class of nonthermal dark matter quadratic isocurvature models. Note that even though the nonthermal dark matter fields can be identified with the isocurvature degrees of freedom, this scenario is consistent with the WIMP dark matter scenario since the isocurvature perturbations can be as small as an

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order 10^{-5} fraction of the total dark matter and still leave an isocurvature imprint on the cosmic microwave background (CMB) spectrum.

The order of presentation is as follows. In Sec. II, we present our assumptions about the inflationary cosmology, review gauge invariant variables in the perturbation theory, and summarize the observational constraints on the isocurvature scenario relevant to our paper. One of the most important aspects of this section is our review of features of the β variable that we compute. In Sec. III, we first explain two naive estimates, one leading to the wrong observationally large result, and the other leading to the correct suppressed result. In explaining the correct estimate (which requires assumptions that cannot be known without the justification of a full computation), we present the interpretation in terms of a soft- ζ theorem and a Ward identity. The rigorous explicit computation at one loop is then presented, demonstrating how the correct naive estimate result is achieved. We also present in this section how gauge invariance is achieved for these quadratic isocurvature computations using a gravitational Ward identity. Next, we apply these results to the axion and the wimpzilla scenarios in Sec. IV. This section contains a detailed explanation for choosing nonthermal dark matter to illustrate the computations of our paper instead of thermal dark matter. Finally, we summarize our results in Sec. V. In the Appendixes, we collect technical details and also supplementary computational results: the radiation transfer functions are derived in Appendix A, a brief review of the gravitational Ward identity used for the gauge invariance computation is given in Appendix B, the Arnowitt-Deser-Misner (ADM) formalism is reviewed in Appendix C, the details about the Pauli-Villars regulator is explained in Appendix D, and the two-point function computation in the uniform curvature gauge is presented in Appendix E.

II. A CLASS OF CURVATURE AND ISOCURVATURE PERTURBATIONS

Inflation through quantum correlator dynamics generates “classical” initial conditions for superhorizon cosmological fluid perturbations [62–65]. The resulting initial conditions for the classical equations governing classical fluid variables (which are set during radiation domination before the CMB last scattering time) are categorized into two types: adiabatic and isocurvature [66–69]. An adiabatic initial condition is intuitively characterized by all species composing the fluid having the same initial number overdensities. In the context of inflation, if there is a *single dynamical degree of freedom* ϕ during inflation such that after a few e-folds of inflation, the quantum vacuum boundary can be approximated as Bunch-Davies initial conditions (for a discussion of the number of e-folds requirement see, e.g., [70]), and if all the degrees of freedom during radiation domination come from the inflaton decay, then this adiabatic condition is the resulting

approximate classical boundary condition during the radiation domination era of the Universe. An isocurvature initial condition intuitively corresponds to setting nonzero the initial difference of the number overdensities of at least one pair of fluid element species while setting to zero the total energy density inhomogeneity on long wavelength scales. Because these two types of initial conditions are linearly independent, a generic initial condition to the linearized perturbation equations can be written as a linear combination of them.

In this paper, we are concerned with the following physical system which is generic for isocurvature scenarios. One real scalar slow-roll inflaton degree of freedom ϕ dominates the energy density during inflation. During this time period, there exists also another light degree of freedom σ which has no coupling to ϕ stronger than gravity. We assume that this system carries an approximately conserved discrete charge (such as \mathbb{Z}_2 broken at most by a model dependent nonrenormalizable operator) such that the one particle states are stable and can act as dark matter. Note that since we do not require all of the dark matter to come from σ , this system is consistent with the existence of the weakly interacting massive particle (WIMP) dark matter. If WIMP dark matter exists, the parameter $\omega_\sigma \equiv \Omega_\sigma/\Omega_{\text{CDM}} < 1$ will play a role, and this scenario can yield interesting isocurvature signatures for ω_σ as small as 10^{-5} [30]. The action of this system can thus be written as

$$S[\phi, \sigma, \{\psi\}] = \int (dx) \left\{ \frac{1}{2} M_p^2 R + \left[-\frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - V(\phi) \right] + \left[-\frac{1}{2} g^{\mu\nu} \partial_\mu \sigma \partial_\nu \sigma - U(\sigma) \right] \right\} + S_{\text{rh}}[\phi, \{\psi\}], \quad (1)$$

where R is the Ricci scalar, $M_p^2 = \frac{1}{8\pi G}$, $(dx) = d^4x \sqrt{|\det(g_{\mu\nu})|}$, and S_{rh} corresponds to the action of the reheating degrees of freedom $\{\psi\}$. We assume that $\{\psi\}$ is heavy during inflation such that it can be integrated out or if $\{\psi\}$ are light, they are conformal such that they are not excited during inflation. After inflation ends, we assume $\{\psi\}$ fields are light, leading to a successful reheating scenario. The only special initial condition dependent assumption that we make in this isocurvature scenario is that $\langle \sigma \rangle \ll H/(2\pi)$ during inflation even when $\partial^2 U(\sigma)/\partial \sigma^2 \ll H$.¹ Because $\langle \sigma \rangle = 0$ during inflation, σ by itself

¹Note that even with Gaussian distributed values of $\langle \sigma \rangle$ on an inflationary patch with a Gaussian width $H/(2\pi)$, there is about a 2/3 probability that such initial condition configurations can be found. Also, an unbroken discrete symmetry such as $\mathbb{Z}_2: \sigma \rightarrow -\sigma$ can stabilize the VEV. In the context of supergravity, generic terms in the effective potential however can appear leading to $\langle \sigma \rangle \neq 0$ during inflation. In the end, whether or not $\langle \sigma \rangle = 0$ is model dependent, it is not fine-tuned.

does not spontaneously break time translation invariance and therefore does not mix with $\delta\phi$ in forming the gauged time translation Nambu-Goldstone boson ζ . Hence, we can treat the scalar fluid variable $\zeta(\delta g_{\mu\nu}, \delta\phi)$ as the curvature degree of freedom and $\delta_S(\sigma, \zeta)$ as the isocurvature degree of freedom. (As we will show in detail below, the isocurvature degree of freedom δ_S will be quadratic in σ and will involve ζ as a difference).

Thus, the basic physics picture of the classical fluid that we are concerned with in this paper is the following. To predict CMB temperature fluctuation $\langle\Delta T\Delta T\rangle$, we must compute the cross-correlation $\langle\delta_S\zeta\rangle$ since at the linearized level, Einstein-Boltzmann equations give the relationship $\Delta T/T \sim c_1\zeta + c_2\delta_S$ for computable order unity (for long wavelengths) coefficients c_i . Up until this paper, there has never been an explicit computation of the $\langle\delta_S\zeta\rangle/\sqrt{\langle\zeta\zeta\rangle\langle\delta_S\delta_S\rangle}$ coming from irreducible gravitational interactions.² What will emerge is a clean universal result that applies to a wide range of isocurvature models including those of the QCD axions (in a particular initial condition regime) and wimpzillas. We find that $\langle\delta_S\zeta\rangle$ contribution is generically subdominant to $\langle\delta_S\delta_S\rangle$ in the case of pure gravitational interactions.

In the following, we establish our conventions in describing this isocurvature degree of freedom carrying the nonadiabatic initial condition information. In the process, we review the gauge invariant construction of these cosmological perturbations and the current CMB observational constraint, which represents the strongest constraint on the isocurvature initial condition derived from inflation.

A. Gauge invariant construction

The cosmological inhomogeneity perturbation variables are generally spacetime coordinate gauge dependent because of the coordinate dependent definition of fictitious background metric slices. From the perspective of matching classical equation initial conditions to inflationary quantum correlator computations, identifying gauge invariant combinations is helpful [71–73]. On the other hand, the gauge freedom involved in computing gauge invariant quantities facilitates the quantum computation. Hence, understanding the gauge dependences of the correlation computations is helpful. In this subsection, we review the gauge invariant variable construction and establish our notation. For a more general discussion, see for example [71,72,74–84].

In (t, \vec{x}) coordinates, we parametrize the metric as $g_{\mu\nu} = \bar{g}_{\mu\nu} + \delta g_{\mu\nu}^{(S)}$ where the scalar metric perturbation is

$$\delta g_{\mu\nu}^{(S)} = \begin{pmatrix} -E & aF_{,i} \\ aF_{,i} & a^2[A\delta_{ij} + B_{,ij}] \end{pmatrix}, \quad (2)$$

the background metric is $\bar{g}_{\mu\nu} \equiv \text{diag}\{-1, a^2(t), a^2(t), a^2(t)\}$, and derivatives are denoted as usual as $X_{,i} \equiv \partial X/\partial x^i$. Under the diffeomorphism $x \rightarrow x + \epsilon$ where

$$\epsilon^\mu = (\epsilon^0, a^{-2}\partial_i(\epsilon^S)), \quad (3)$$

the scalar metric perturbation components transform as

$$\Delta A = -2H\epsilon^0, \quad \Delta B = -\frac{2}{a^2}\epsilon^S, \quad (4)$$

$$\Delta E = -2\dot{\epsilon}^0, \quad \Delta F = \frac{1}{a}(\epsilon^0 - \dot{\epsilon}^S + 2H\epsilon^S), \quad (5)$$

which is obtained from $\delta g_{\mu\nu}^{(S)} \rightarrow \delta g_{\mu\nu}^{(S)} + \Delta(\delta g_{\mu\nu}^{(S)})$ with $\Delta(\delta g_{\mu\nu}^{(S)}) = -\mathcal{L}_{\epsilon^\mu \partial_\mu} \bar{g}_{\mu\nu}$.

Similarly, we parametrize the perfect fluid stress tensor for a fluid element a as

$$T_{\mu\nu}^{(a)} = \bar{T}_{\mu\nu}^{(a)} + \delta T_{\mu\nu}^{(a)}, \quad (6)$$

where $\bar{T}_{\mu\nu}^{(a)} \equiv \text{diag}\{\bar{\rho}_a, \bar{P}_a, \bar{P}_a, \bar{P}_a\}$ contains the average energy density and pressure seen by a comoving observer, $\delta T_{ij}^{(a)} = \bar{P}_a \delta g_{ij}^{(S)} + a^2 \delta_{ij} \delta P_a$, $\delta T_{i0}^{(a)} = \bar{P}_{(a)} \delta g_{i0}^{(S)} - (\bar{\rho}_a + \bar{P}_a) \delta U_i^{(a)}$ [where $\delta U_i^{(a)}$ is the velocity perturbation], and $\delta T_{00}^{(a)} = -\bar{\rho}_a \delta g_{00}^{(S)} + \delta \rho_a$. Under the diffeomorphism of Eq. (3), the energy density perturbation transforms as

$$\Delta \delta \rho_a = -\epsilon^0 \dot{\bar{\rho}}_a. \quad (7)$$

In practice, gauge invariant variables are constructed by combining metric perturbations and other perturbations, such as densities. A popular choice is

$$\zeta_a \equiv \frac{A}{2} - H \frac{\delta \rho_a}{\dot{\bar{\rho}}_a}. \quad (8)$$

For example, the first-order gauge invariant perturbation associated with the inflaton ϕ is usually defined as

$$\zeta_\phi \equiv \frac{A}{2} - H \frac{\delta \rho_\phi}{\dot{\bar{\rho}}_\phi} \quad (9)$$

(see for example Ref. [73] and references therein). Now, one can form a quantity that is conserved through reheating by defining

$$\zeta_{\text{tot}} \equiv \sum_i r_i \zeta_i, \quad (10)$$

where

$$r_i \equiv \frac{\bar{\rho}_i + \bar{P}_i}{\sum_n \bar{\rho}_n + \bar{P}_n}. \quad (11)$$

Because there must be reheating dynamical degrees of freedom, ζ_{tot} must involve at least two degrees of freedom by the end of inflation of any single field slow-roll model.

²As we will later explain, we do not compute $\langle\delta_S\zeta\rangle$ analytically fully beyond the time of the end of inflation. However, the importance of the isocurvature cross-correlation can be generically predicted by $\langle\delta_S\zeta\rangle/\sqrt{\langle\zeta\zeta\rangle\langle\delta_S\delta_S\rangle}$ which is insensitive to the postinflationary evolution for superhorizon modes.

In single field slow-roll scenarios, what is done in practice is to argue that the reheating degrees of freedom are integrated out during inflation and then integrated back in at the end of inflation due to the different location of the inflaton VEV at the end of inflation. Alternatively, another often-used assumption is that the main reheating degrees of freedom are conformal such that no isocurvature fluctuations are appreciably excited during inflation. This means that in single field models, we have

$$\zeta_{\text{tot}} \approx \zeta_\phi \quad (12)$$

up to ambiguities in how one hides the reheating degrees of freedom.

One reason why the combination of Eq. (10) is convenient is because the superhorizon mode of this is approximately conserved through reheating if this mode object can be shown to obtain initial conditions of what is sometimes referred to as the adiabatic solution [45,73] and there are no nonadiabatic processes that mix superhorizon modes of isocurvature degrees of freedom with ζ_{tot} . Such classical adiabatic solution initial conditions are generated by the Bunch-Davies quantum fluctuations for ζ_ϕ , and we will restrict the couplings of the isocurvature degrees of freedom (discussed below) such as to avoid nonadiabatic mixing. This means that Eq. (12) ensures that ζ_{tot} is approximately conserved if $\bar{\rho}_\phi + \bar{P}_\phi$ dominates over others. More explicitly, as discussed in the introduction to this section, suppose there exists only one isocurvature field degree of freedom which we call σ during the inflationary period.³ The total curvature perturbation can be written as

$$\zeta_{\text{tot}} = \zeta_\phi + r_\sigma(\zeta_\sigma - \zeta_\phi) \quad (13)$$

with the sum over n runs over ϕ and σ (assuming that ψ has been integrated out during inflation). However, one can estimate that the coefficient of ζ_σ during inflation is

$$r_\sigma \approx \frac{1}{(2\pi)^2} \Delta_\zeta^2 \sim 10^{-11}, \quad (14)$$

which makes the approximation of $\zeta_{\text{tot}} \approx \zeta_\phi$ accurate, just as in the single field case of Eq. (12). Thus just as in the single field scenarios without σ , ζ_{tot} acquires an approximately adiabatic boundary condition from the Bunch-Davies vacuum field fluctuations.

To complete the examination of how ζ_{tot} is used in the scenario of concern in this paper, let us look at the time period surrounding the reheating transition when the Universe reaches radiation domination. Near the time of the completion of the reheating, the variable ζ_{tot} is approximately

$$\zeta_{\text{tot}} \approx r_\phi \zeta_\phi + \sum_i r_{\psi_i} \zeta_{\psi_i} \quad (15)$$

³The species σ will later be identified as dark matter candidates such as the axions and wimpzillas.

such that after the inflaton decays, we have $r_\phi = 0$ and⁴

$$\zeta_{\text{tot}} \approx \sum_i r_{\psi_i} \zeta_{\psi_i}. \quad (16)$$

[The approximation used in Eq. (15) neglects the r_σ contribution because of Eq. (14).] It is also a standard assumption that

$$\zeta_{\psi_i} = \zeta_{\text{tot}}, \quad (17)$$

which is rigorously true if one relativistic species dominates the fluid (e.g., $r_{\psi_1} \approx 1$) or if the decay process does not redistribute the spatial inhomogeneities of ψ_i in a distinct configuration from that of ϕ .⁵ This justifies the usual statement in the literature that ζ_{tot} defined in Eq. (10) is primarily useful for arguing how a combination of quantities involving the inflaton and the reheating decay products remain unchanged through the reheating phase transition. Here, we have merely described how this argument is not changed by the presence of σ because of the smallness of r_σ in Eq. (14) during the primordial periods of interest.

In summary, as long as boundary conditions for the classical fluid equation are evaluated at a time when r_σ is small (compared to the accuracy desired), we can neglect the r_σ contribution from ζ_{tot} both through reheating and until the time that boundary conditions for the classical fluid equations are imposed. Hence, if ζ_{tot} remains constant on long wavelengths (due to the initial conditions set by the Bunch-Davies vacuum), Eqs. (13) and (14) imply that the effective curvature perturbation during this early primordial epoch is given by Eq. (12). Hence, in the discussion below, we will drop the ϕ subscript and write

$$\zeta \equiv \zeta_\phi \approx \zeta_{\text{tot}}. \quad (18)$$

During this radiation dominated early primordial time t_p , the relationship between superhorizon $A(t_p, \vec{k})$ and the value of $\zeta(t_e, \vec{k})$ evaluated at the end of inflation time t_e is

$$\frac{A(t_p, \vec{k})}{2} \approx \frac{2}{3} \zeta(t_e, \vec{k}) \quad (19)$$

in the Newtonian gauge ($B = F = 0$) and the presence of ζ_σ gives a small error controlled by r_σ .

At the same radiation dominated era⁶ when the initial condition is set by $\zeta_{\text{tot}} \approx \zeta$, the inhomogeneity of the small mixture of dark matter component σ can be related to the isocurvature perturbation ζ_σ . Conventionally, this information is parametrized by the gauge invariant isocurvature perturbation [67,69,76]

⁴In the case that ψ_i is integrated back in at the end of inflation, we have made the assumption that this does not change ζ_{tot} .

⁵However this need not be true for more general reheating scenarios.

⁶During this time period, there is possibly a population of thermal dark matter components such as thermal WIMPs.

$$\delta_S(t, \vec{k}) \equiv 3(\zeta_\sigma(t, \vec{k}) - \zeta_{\text{tot}}(t, \vec{k})). \quad (20)$$

The physical interpretation of this quantity can be seen by noting that when σ particles are dominantly nonrelativistic and the Universe is radiation dominated, this expression becomes

$$\delta_S(t, \vec{k}) = \frac{\delta\rho_\sigma(t, \vec{k})}{\bar{\rho}_\sigma} - \frac{3}{4} \frac{\delta\rho_\gamma(t, \vec{k})}{\bar{\rho}_\gamma}, \quad (21)$$

where ρ_γ represents the photon energy densities. This clearly represents the difference in number densities of σ and γ .⁷ Assuming that the radiation inhomogeneity is characterized by ζ as explained in Eqs. (17) and (18) during radiation domination, we have

$$\delta_S(t, \vec{k}) \approx 3(\zeta_\sigma(t, \vec{k}) - \zeta(t_e, \vec{k})). \quad (22)$$

Similarly to the case of ζ_{tot} , long wavelength limits of ζ_σ generated from Bunch-Davies initial conditions simplify (partly because of causality) in the absence of nonadiabatic processes mixing ζ_σ with other superhorizon degrees of freedom. The ζ_σ mode for a comoving wave vector \vec{k} becomes constant once $|\vec{k}/a| \ll H$ and $m_\sigma \ll H$ because the mode functions involved in ζ_σ are governed by the Hubble friction once these conditions are satisfied.

Although the key correlator computation result of this paper involving β evaluated at the end of inflation is independent of the transfer function evolving the isocurvature degrees of freedom after the end of inflation, because its immediate phenomenological application to CMB requires a transfer function describing this postinflationary evolution, we will restrict our illustration in Sec. IV to the situation when the chemical reaction rates that mix σ and the radiation components are negligible. We will discuss in more detail the cross section constraint for this condition in Appendix D 1.

B. Observational constraints on isocurvature perturbation

The current observational data show that the CMB power spectrum is consistent with the adiabatic initial conditions. However, it does not rule out mixed boundary condition contributions from cold dark matter (CDM) isocurvature perturbations. Schematically, the temperature fluctuations depend linearly on ζ and δ_S initial conditions as

$$\frac{\Delta T}{T} = c_1 \zeta + c_2 \delta_S, \quad (23)$$

⁷It is interesting to note that since number densities can diverge while gravitational physics does not care about number densities (in favor of energy densities), this choice of variables is unfortunate in situations when there are IR divergences. In this paper, we stick to this convention which is prevalent in literature.

where $c_i \sim O(1)$. Hence, the CMB temperature correlation data constrain⁸

$$\begin{aligned} & \frac{k^3}{2\pi^2} \int \frac{d^3 p}{(2\pi)^3} \left\langle \frac{\Delta T(\vec{p})}{T} \frac{\Delta T^*(\vec{k})}{T} \right\rangle \\ &= \Delta_\zeta^2(k) \left[|c_1|^2 + |c_2|^2 \frac{\alpha}{1-\alpha} - 2\Re\left(c_1^* c_2 \beta \sqrt{\frac{\alpha}{1-\alpha}}\right) \right], \end{aligned} \quad (24)$$

where [2]

$$\int \frac{d^3 p}{(2\pi)^3} \langle \zeta(\vec{p}) \zeta^*(\vec{k}) \rangle = \Delta_\zeta^2(k) \frac{2\pi^2}{k^3} \quad (25)$$

$$\int \frac{d^3 p}{(2\pi)^3} \langle \delta_S(\vec{p}) \delta_S^*(\vec{k}) \rangle = \Delta_{\delta_S}^2(k) \frac{2\pi^2}{k^3} \quad (26)$$

$$\int \frac{d^3 p}{(2\pi)^3} \langle \delta_S(\vec{p}) \zeta^*(\vec{k}) \rangle = \Delta_{\zeta\delta_S}^2(k) \frac{2\pi^2}{k^3} \quad (27)$$

$$\alpha \equiv \frac{\Delta_{\delta_S}^2(k)}{\Delta_\zeta^2(k) + \Delta_{\delta_S}^2(k)}, \quad (28)$$

$$\beta \equiv -\frac{\Delta_{\zeta\delta_S}^2(k)}{\sqrt{\Delta_\zeta^2(k) \Delta_{\delta_S}^2(k)}}, \quad (29)$$

which are customarily evaluated in the primordial epoch when k corresponds to a far superhorizon scale such that the $\Delta_X^2(k)$ objects are constant in time.⁹ Typically the data constraints are parametrized by evaluating α and β at a pivot scale $k = k_0$ [3,6]. An important utility of this parametrization is the following fact: a necessary and sufficient condition for the cross-correlation to be a significant part of the isocurvature contribution is to have $|\beta| \geq |c_2/c_1| \sqrt{\alpha}$ for $\alpha < 1$. For example, in order to have approximately the same level of the angular power spectra from both pure isocurvature correlation and cross-correlation at the intermediate scale $l \sim 200$, i.e., $C_l^{\text{pure iso}} \sim C_l^{\text{cross cor}}$, the fractional cross-correlation should satisfy $|\beta| \geq 4 \times 10^{-2}$. Another utility of the β variable comes from the fact that when there are nontrivial transfer functions governing $\Delta_{\zeta\delta_S}^2$ and $\Delta_{\delta_S}^2$ after the end of inflation, the transfer function factors can cancel in the expression for β . We will use this feature later to compute β based on just the (quasi-)dS mode function behavior.

⁸Our sign conventions are such that *negative* values for β correspond to a positive contribution of the cross-correlation term to the Sachs-Wolfe (SW) component of the total temperature spectrum. See, e.g., [3,6].

⁹We will use the exact dS approximation for the massive σ and use the quasi-dS approximation for only the massless scenario. The corrections coming from the deviations away from the exact dS background in principle can be absorbed into the transfer function multiplying the superhorizon mode functions which cancel out in β due to a common appearance in the numerator and the denominator.

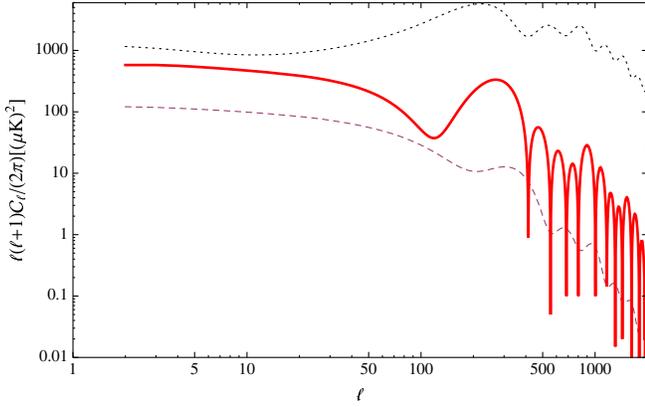


FIG. 1 (color online). Angular power spectra C_l from pure adiabatic (dotted), pure isocurvature (dashed) contributions. The solid red line corresponds to be qualitatively the contribution of the absolute magnitude of the third term in Eq. (24). The plotted pure adiabatic perturbation has the spectral index $n_s = 0.96$. For isocurvature perturbations, the spectral index n_{iso} is 1 and the isocurvature fraction $\alpha = 0.067$ defined at $k_0 = 0.002 \text{ Mpc}^{-1}$, and the fractional cross-correlation $|\beta|$ is 1.

As far as the experimental numbers are concerned, the isocurvature contribution to the CMB temperature perturbation is expected to be roughly less than 10% compared to the curvature contribution. More precisely, the Planck + WP limits [6–8] are

$$\begin{aligned} \alpha|_{\beta=0} &< 0.016(95\% \text{ C.L.}) \quad \text{and} \\ \alpha|_{\beta=-1} &< 0.0011(95\% \text{ C.L.}), \end{aligned} \quad (30)$$

where the isocurvature power spectrum is assumed to be scale invariant, i.e., $n_{iso} = 1$. The significant difference in the upper bound of α between uncorrelated and totally (anti)correlated cases can be explained by the ratio $\beta/\sqrt{\alpha}$ already discussed above. The difficulty in improving the current isocurvature bound with data on short wavelengths can be seen in Fig. 1, where one sees a falloff of the isocurvature spectrum on short scales ($l \gtrsim 100$). This falloff is generic and can be attributed to the transfer function effect encoded by $c_1(k)/c_2(k)$ in Eq. (24) for $k \gtrsim k_{eq}$ (where $k_{eq}/a_0 \sim 10^{-2} \text{ Mpc}^{-1}$ is the wave vector associated

with matter radiation equality). To understand why $c_1(k)/c_2(k)$ generically becomes large for $k \gtrsim k_{eq}$, note that isocurvature modes with $k \gtrsim k_{eq}$ enter the horizon during radiation domination. Because the isocurvature effect on the temperature spectrum is gravitational, the value of $c_1(k)/c_2(k)$ is proportional to the ratio $\rho_R(t(k))/\rho_\sigma(t(k))$ of the radiation energy density to the energy density in the isocurvature degree of freedom at the time $t(k)$ when mode $k \gtrsim k_{eq}$ enters the horizon. Since shorter wavelengths enter the horizon earlier, $\rho_R(t(k))/\rho_\sigma(t(k))$ is larger for shorter wavelengths, making $c_1(k)/c_2(k)$ larger. For those readers not familiar with this physics, some of the details of the transfer function are reviewed in Appendix A.

Because of the large differences in the constraints between $\beta = 0$ and $\beta = -1$, estimating the cross-correlation is crucial to restrict parameters and give observable predictions of isocurvature models. In particular, the axion scenario with a negligible homogeneous vacuum misalignment angle (and similarly the wimpzilla scenario with a negligible homogeneous background field value) predicts detectable non-Gaussianity [24,30,85]

$$f_{\text{NL}} \sim 30 \left(\frac{\alpha}{0.067} \right)^{3/2} \quad (31)$$

provided the assumption that the cross-correlation is zero, i.e., $\beta = 0$. However, as we will explain, this assumption is not obvious for massive field quadratic isocurvature scenarios, and the reexamination of this assumption is one of the goals of this paper.

III. COMPUTATION OF CORRELATORS

In order to provide the initial condition of the classical fluid equations, it is standard to compute the quantum equal time correlators with the inflationary background approximated as a Bunch-Davies vacuum. In this section, we compute the correlators using the “in-in” formalism (e.g., see Weinberg [86]). More specifically, in the context of canonical quantization, we perturbatively compute the expectation value of an operator $\hat{Q}(t)$

$$\langle \hat{Q}(t) \rangle = \sum_n (-i)^n \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n \langle [[\hat{Q}^I(t), \hat{H}^I(t_n)], \hat{H}^I(t_{n-1})], \cdots \hat{H}^I(t_1)] \rangle, \quad (32)$$

where the superscript I stands for the interaction picture and $\hat{Q}(t)$ represents a product of canonically quantized operators.

In the scenario explained in Sec. II, we consider the gravitational coupling whose interaction Hamiltonian is derived from the ADM formalism with a given choice of gauge. For the computation of the cross-correlation to leading order in gravitational coupling, we need at least

up to the cubic coupling $H_{\zeta\sigma\sigma}^I$, where σ is a spectator field during inflation. The interaction Hamiltonian is diffeomorphism gauge dependent. For two commonly used gauges, the comoving gauge ($\delta\phi = 0$) and the uniform curvature gauge ($A = 0$), we have

$$H_{\zeta\sigma\sigma}^I(t) = -\frac{1}{2} \int d^3x a^3(t) T_{\sigma}^{\mu\nu}(t, \vec{x}) \delta g_{\mu\nu}(t, \vec{x}), \quad (33)$$

$$\delta g_{\mu\nu}^{(C)} = \begin{pmatrix} -2\frac{\dot{\zeta}}{H} & \left(-\frac{\zeta}{H} + \epsilon\frac{a^2}{\nabla^2}\dot{\zeta}\right)_{,i} \\ \left(-\frac{\zeta}{H} + \epsilon\frac{a^2}{\nabla^2}\dot{\zeta}\right)_{,i} & a^2\delta_{ij}2\dot{\zeta} \end{pmatrix}, \quad (34)$$

$$\delta g_{\mu\nu}^{(U)} = \begin{pmatrix} 2\epsilon\dot{\zeta} & \epsilon\frac{a^2}{\nabla^2}\dot{\zeta}_{,i} \\ \epsilon\frac{a^2}{\nabla^2}\dot{\zeta}_{,i} & 0 \end{pmatrix}, \quad (35)$$

where $T_{\sigma}^{\mu\nu}$ is the stress energy tensor of the field σ , and $\delta g_{\mu\nu}$ is the metric perturbation and the superscripts (C) and (U) denote the comoving gauge and uniform curvature gauge, respectively. A detailed derivation of the interaction Hamiltonian using the ADM formalism is presented in Appendix C.

The isocurvature perturbation δ_S should be also written in terms of quantum operators associated with the energy density ρ_{σ} of the particle σ . Since the energy density ρ_{σ} is written in bilinear form of σ and since the energy density of CDM are often those of nonrelativistic particles at the time of matching to classical equations, we may approximate the energy density $\rho_{\sigma} \approx m_{\sigma}^2\sigma^2$. We then promote the field σ to a quantum operator:

$$\delta_{\sigma} \equiv \frac{\delta\rho_{\sigma}}{\rho_{\sigma}} \approx \frac{\sigma^2 - \bar{\sigma}^2}{\bar{\sigma}^2} \rightarrow \hat{\delta}_{\sigma} = \frac{\hat{\sigma}^2 - \langle\hat{\sigma}^2\rangle}{\langle\hat{\sigma}^2\rangle}. \quad (36)$$

The field $\hat{\sigma}$ can be decomposed into the classical homogeneous background and the quantized perturbation, i.e., $\hat{\sigma} = \bar{\sigma} + \delta\hat{\sigma}$. Unlike the inflaton ϕ whose classical background is nonzero, because we consider the field $\hat{\sigma}$ without classical background, the leading density perturbation starts with the quadratic in the operator $\delta\hat{\sigma}^2$. As with any quantum composite operator, we renormalize it with counterterms invariant under the underlying gauge symmetry (here, it is diffeomorphism):

$$(\hat{\sigma}^2)_r = \left(\delta\hat{\sigma} + \sum_i \hat{\chi}_i\right)^2 + \delta Z_0 + \delta Z_1 R, \quad (37)$$

where the subscript r denotes that the operator is a renormalized composite operator, R is the Ricci scalar, and $\hat{\chi}_i$ are Pauli-Villars fields, which are described in Appendix D. We apply this to gauge invariant isocurvature variable δ_S defined in Sec. II A. Then we have

$$\hat{\delta}_S^{(C)} = -\frac{3H}{\partial_t\langle(\hat{\sigma}^2)_r\rangle} [(\hat{\sigma}^2)_r - \langle(\hat{\sigma}^2)_r\rangle], \quad (38)$$

$$\hat{\delta}_S^{(U)} = -\frac{3H}{\partial_t\langle(\hat{\sigma}^2)_r\rangle} [(\hat{\sigma}^2)_r - \langle(\hat{\sigma}^2)_r\rangle] - 3\hat{\zeta}. \quad (39)$$

We will not write the hat explicitly from now on.

In the next subsection, we present how a non-diffeomorphism-invariant estimation of the cross-correlation leads to an observationally attractive but grossly incorrect result. In subsections after that, we identify the

problems with the wrong estimate and calculate the cross-correlation properly.

A. Plausible but wrong estimation of the cross-correlation

In this subsection, we present a plausible estimation of the cross-correlation that leads to a large value that is observationally interesting. Unfortunately, we will see in later subsections that the estimate presented in this subsection can be many orders of magnitude off due to the explicit breaking of diffeomorphism invariance in the treatment of the UV physics. Nonetheless, what is presented in this subsection is interesting both as a lesson in field theory and as a motivation for the careful correct computation that follows later.

The isocurvature cross-correlation in the comoving gauge is written as

$$\langle\delta_S^{(C)}\zeta\rangle \approx \frac{\langle(\sigma^2)_r\zeta\rangle}{\langle(\sigma^2)_r\rangle}, \quad (40)$$

where we have used $\partial_t\langle(\sigma^2)_r\rangle + 3H\langle(\sigma^2)_r\rangle \approx 0$ for the isocurvature field number density. For an order of magnitude estimation, we consider a nonderivatively coupled part of the gravitational interaction, $2\zeta a^2\delta_{ij}T_{\sigma}^{ij} \in H_{\zeta\sigma\sigma}^I$. Then the two-point function, shown diagrammatically in Fig. 2, is written in the Fourier space as

$$\begin{aligned} \langle(\widetilde{\sigma^2})_r\zeta\rangle_p^C &\sim \int d^3x e^{-i\vec{p}\cdot\vec{x}} \int^t d^4z a^3(t_z) \\ &\times \left\langle \left[\sigma^2(t, \vec{x})\zeta(t, \vec{0}), \frac{i}{2}(2\zeta a^2\delta_{ij}T_{\sigma}^{ij})_z \right] \right\rangle \quad (41) \\ &\sim -4 \int \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\times \int_{-\infty}^t dt_z a_z^3 \text{Im} \left[\zeta_p^*(t)\zeta_p^*(t_z)u_{k_1}(t)u_{k_2}(t) \left[\frac{1\vec{k}_1\cdot\vec{k}_2}{2a^2} \right. \right. \\ &\left. \left. + 3\left(\frac{1}{2}\partial_t^{(1)}\partial_t^{(2)} - \frac{1}{2}m_{\sigma}^2\right) \right] u_{k_1}^*(t_z)u_{k_2}^*(t_z) \right], \quad (42) \end{aligned}$$

where

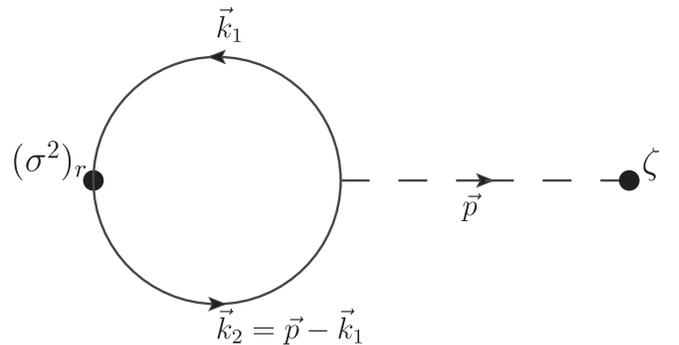


FIG. 2. Two-point function at one-loop order.

$$\langle \widetilde{AB} \rangle_p \equiv \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle A(t, \vec{x}) B(t, 0) \rangle, \quad (43)$$

ζ_p and u_k are mode functions for ζ and σ , respectively, and $\partial_t^{(i)}$ means the time derivative with respect to $u_{k_i}^*(t_z)$.¹⁰ This integral is UV divergent, and thus we introduce the horizon scale UV cutoff

$$\Lambda_{\text{UV}} \sim aH_{\text{inf}}. \quad (44)$$

Moreover, we neglect the contribution from the time range $t < t_p$, where t_p is the time when the scale p exits the horizon since ζ_p is oscillatory before the horizon exit. Using the superhorizon approximation for mode functions during inflation

$$\zeta_k(t) = \frac{1}{\sqrt{4\epsilon}M_p} \frac{H}{k^{\frac{3}{2}}} e^{i\frac{k}{aH}} \left(1 - i\frac{k}{aH}\right), \quad (45)$$

$$u_k(t) \approx a^{-\frac{3}{2}} H^{-\frac{1}{2}} \left\{ \frac{2^{\nu-1} \Gamma(\nu)}{\pi^{\frac{1}{2}}} \left(\frac{k}{aH}\right)^{-\nu} + i \frac{\pi^{\frac{1}{2}}}{2^{\nu+1} \Gamma(1+\nu)} \left(\frac{k}{aH}\right)^{\nu} \right\}, \quad (46)$$

where $\nu \equiv \sqrt{9/4 - m^2/H^2}$, the cross-correlation at the end of inflation time t_e is approximately

$$\langle (\widetilde{\sigma^2})_r \zeta \rangle_p^C \sim \frac{-1}{8\pi^2} |\zeta_p^o|^2 \frac{H^4}{m_\sigma^2} \left[1 - \left(\frac{p}{a_e H}\right)^{\frac{2m_\sigma^2}{3H^2}} \right], \quad (47)$$

where we used the relations $m_\sigma^2 \ll H^2$ and $|\zeta_p^o|^2 p^3 = H^2/4M_p^2 \epsilon$ is the mode function behavior in the long wavelength limit. To understand the magnitude of this expression, note that for physical CMB scale comoving momenta, we have

$$\frac{p}{a_e} = e^{-N(p)} H \quad (48)$$

for $N(p) \sim O(50)$. As long as

$$1 \gg m_\sigma^2/H^2 \gtrsim 1/N(p), \quad (49)$$

we can estimate

$$\langle (\widetilde{\sigma^2})_r \zeta \rangle_p^C \sim \frac{-1}{8\pi^2} |\zeta_p^o|^2 \frac{H^4}{m_\sigma^2}, \quad (50)$$

¹⁰It is also helpful to remember that in terms of Fourier space operators/fields, the tilde notation is equivalent to

$$\langle \widetilde{AB} \rangle_p = \int \frac{d^3p_2}{(2\pi)^3} \langle A(t, \vec{p}) B(t, \vec{p}_2) \rangle,$$

where

$$A(t, \vec{p}) \equiv \int d^3x e^{-i\vec{p}\cdot\vec{x}} A(t, \vec{x})$$

for generic operators/fields A and B .

which is an expression that is valid when the p is far outside of the horizon and a constant H is a good approximation. Note that this does not vanish in the limit $p \rightarrow 0$. We will soon see that this nonvanishing behavior is incorrect and is a signal of explicit breaking diffeomorphism invariance coming from Eq. (44). Note that if Eq. (49) is not satisfied because $m_\sigma = 0$, we have

$$\langle (\widetilde{\sigma^2})_r \zeta \rangle_p^C \sim \frac{H^2}{12\pi^2} |\zeta_p^o|^2 \ln \frac{p}{a_e H} \quad (51)$$

$$\sim -N(p) \frac{H^2}{12\pi^2} |\zeta_p^o|^2, \quad (52)$$

which again does not vanish and is negative.

As explained around Eq. (24), the importance of the cross-correlation in the isocurvature bound depends on whether β is of order 10^{-2} or larger and not by whether the cross-correlation by itself is of the order of curvature perturbations. To compute β defined in Eq. (29), we need an estimate of $(\sigma^2)_r$ correlator which we can take from [30]:

$$\langle (\widetilde{\sigma^2})_r (\widetilde{\sigma^2})_r \rangle_p^C \sim \frac{1}{2\pi^2} \frac{H^4}{p^3} f(m_\sigma/H, p/a_e H), \quad (53)$$

where f is a function which can have an exponentially small value owing to the functional behavior

$$f \sim \frac{H^2}{m_\sigma^2} \left(\frac{p}{a_e H}\right)^{\frac{4m_\sigma^2}{3H^2}}. \quad (54)$$

Combining Eqs. (29), (47), and (53), we find

$$\beta^{\text{wrong}} \sim \sqrt{\Delta_\zeta^2} \frac{H}{4m_\sigma} \left(\frac{p}{a_e H}\right)^{-\frac{2m_\sigma^2}{3H^2}} \quad (55)$$

$$\sim \frac{H}{4m_\sigma} e^{\frac{2m_\sigma^2}{3H^2} N - 12}, \quad (56)$$

which, after recalling Eq. (49) and that $N \sim O(50)$, gives some hope that a proper computation would give a large value for β with m_σ/H satisfying Eq. (49).¹¹ For example, if $|\beta| = O(1)$, then any appreciable isocurvature perturbation would be ruled out with the current data, affecting predictions of [24,30,85].

Recall from Eq. (24) that the role of the cross-correlation can become important if β can become sizable while keeping α also sizable. One may worry that the enhancement factor in β of Eq. (53) which is approximately proportional to α may make α negligible in the parameter

¹¹It is important to keep in mind that we are making an assumption here about the isocurvature evolution when identifying the primordial computations of Eqs. (47) and (53) with the CMB observables of Eq. (29) where c_i are computed according to the simple transfer treatment of Appendix A. We will discuss this assumption in more detail in Sec. IVA.

regime in which β is enhanced. However, note that α is controlled not just by Eq. (53) but by

$$\langle \widetilde{\delta_S \delta_S} \rangle_p = \frac{\langle (\sigma^2)_r (\widetilde{\sigma^2})_r \rangle_p^C}{[\langle (\sigma^2)_r \rangle]^2}, \quad (57)$$

which has a one-point function squared in the denominator proportional to the energy density squared of σ . One can straightforwardly check from Ref. [30] that the denominator of Eq. (57) can be tuned such that α can remain constant while $\langle (\sigma^2)_r (\widetilde{\sigma^2})_r \rangle_p^C$ is sufficiently small as to enhance β as described in Eq. (56).

Given this generic possibility of ruling out a large class of isocurvature perturbation models, we consider below the leading gravitational interaction contribution to β carefully. We find that unlike the naive estimate given in Eq. (47), there is a suppression in the limit $p/(aH) \rightarrow 0$ for the mass in the range of Eq. (49). The suppression in the numerator of β precisely cancels the denominator suppression factor coming from f in Eq. (54) such that no enhancement is obtained, contrary to the naive expectation of Eq. (56). This suppression of the numerator in the proper computation not seen in the naive estimate can be attributed to a Ward identity associated with the diffeomorphism group element of constant scaling of the spatial coordinates. Furthermore, a careful computation that we give below will show that the sign of the cross-correlation will be opposite to the naive estimate, owing to the fact that the cross-correlation here is tied to particle production instead of volume dilution.

The detailed computation will address also explicitly how the same answer to the gauge invariant correlator results in two different gauges of comoving gauge and uniform curvature gauge (one can verify this is not obvious from the naive estimate presented in this subsection). Another technical care that is taken in the computations below is to explicitly specify how diffeomorphism invariant counterterms are introduced to renormalize the composite operators intrinsic to δ_S . Since the correct answer relies on a gravitational Ward identity, identifying proper diffeomorphism invariant regulator and counterterms is important for a trustworthy computation. On the other hand, note that the finite parts of the counterterms that remain after the divergences are canceled will not affect the results to the leading \hbar expansion that we are concerned with.¹²

B. Plausible and correct estimation using a soft- ζ theorem

Before we describe the actual computation, we give in this subsection a method akin to the soft- ζ theorem used by [44,47–52,54–60] to estimate the correct answer without a detailed computation. We will also point out what *ad hoc*

assumptions are needed to make this estimate using this theorem. A rigorous computation will be given in Sec. III D.

In the soft- ζ theorem application to the correlators in inflation, one factorizes an N -point function including at least one soft external ζ into an $(N-1)$ -point function times the two-point function $\langle \zeta \zeta \rangle$. The well-known example is the three-point function $\langle \zeta \zeta \zeta \rangle$ in the squeezed limit in quasi-dS space:

$$\int \frac{d^3 q}{(2\pi)^3} \langle \zeta_{\vec{q}} \zeta_{\vec{k}} \zeta_{\vec{p}} \rangle \xrightarrow{p \rightarrow 0} -|\zeta_p^o|^2 \frac{1}{k^3} \frac{\partial}{\partial \ln k} [k^3 \langle \widetilde{\zeta \zeta} \rangle_k] \sim -(n_s - 1) |\zeta_p^o|^2 |\zeta_k^o|^2, \quad (58)$$

where the superscript on the ζ mode functions denote long wavelength parts. To use this, note that if we neglect renormalization of the composite operators, we can write

$$\int \frac{d^3 q}{(2\pi)^3} \langle \zeta_{\vec{p}} \sigma^2(\vec{q}) \rangle = \int \frac{d^3 k_2}{(2\pi)^3} \int \frac{d^3 k_1}{(2\pi)^3} \langle \zeta_{\vec{p}} \sigma(\vec{k}_1) \sigma(\vec{k}_2) \rangle. \quad (59)$$

Using Eq. (58) and replacing two ζ fields with σ fields, we can estimate

$$\int \frac{d^3 q}{(2\pi)^3} \langle \zeta_{\vec{p}} \sigma^2(\vec{q}) \rangle \xrightarrow{p \rightarrow 0} -|\zeta_p^o|^2 \int \frac{d^3 k_2}{(2\pi)^3} \frac{1}{k_2^3} \frac{\partial}{\partial \ln k_2} [k_2^3 \langle \widetilde{\sigma \sigma} \rangle_{k_2}], \quad (60)$$

where the comoving IR cutoff p is required to treat ζ_p^o as a constant background field. This effective lower cutoff p cannot be justified without explicit computation, but this is physically plausible because $\langle \sigma \sigma \rangle$ does not have any IR divergence as long as $m_\sigma^2 > 0$. One can rewrite the integral in Eq. (60) as

$$\int \frac{d^3 q}{(2\pi)^3} \langle \zeta_{\vec{p}} \sigma^2(\vec{q}) \rangle \xrightarrow{p \rightarrow 0} |\zeta_p^o|^2 \frac{\partial}{\partial \ln a} \langle \sigma^2(t, \vec{x}) \rangle_p, \quad (61)$$

where the σ^2 on the right-hand side corresponds to space-time field (and not its Fourier transform), the p subscript on the bracket corresponds to the IR cutoff in the mode function integral, and we assume that there is no contribution from the UV cutoff. It is easy to prove that if $p \rightarrow 0$ is well defined and a UV cutoff is not required, then the right-hand side of Eq. (61) vanishes in the limit $p \rightarrow 0$. This is in contrast with Eq. (47).

The vanishing of this function in the $p \rightarrow 0$ limit for $m_\sigma^2 > 0$ is intuitively understood from the fact that in that limit, ζ_p^o acts as a spatial diffeomorphism

$$\vec{x} \rightarrow \vec{x}(1 + \zeta_p^o) \quad (62)$$

(which in turn effectively rescales the scale factor a by a constant factor if we neglect spatial derivatives on long wavelengths) which cannot change $\langle \sigma^2(t, \vec{x}) \rangle = \langle \sigma^2(t, 0) \rangle$. More explicitly, one can show that the explicit computation can be rewritten as

¹²Note that particle production is nonperturbative in \hbar .

$$\int \frac{d^3q}{(2\pi)^3} \langle \zeta_{\vec{p}} \sigma^2(\vec{q}) \rangle \xrightarrow{p \rightarrow 0} |\zeta_{\vec{p}}|^2 \int_p \frac{d^3k}{(2\pi)^3} \times \int d^3x i \langle [\hat{Q}(t), \hat{\sigma}(t, \vec{x}) \hat{\sigma}(t, 0)] \rangle e^{i\vec{k} \cdot \vec{x}}, \quad (63)$$

where

$$\hat{Q}(t) \equiv \int^t d^4z a^3(t_z) \hat{T}_\sigma^{ij}(z) \delta_{ij} a^2(t_z) \quad (64)$$

is the generator of the diffeomorphism associated with Eq. (62). Note that the right-hand side formally vanishes when the IR cutoff is removed (i.e., $p = 0$) because in that limit, we find the commutator

$$\langle [\hat{Q}(t), \hat{\sigma}^2(t, 0)] \rangle = 0. \quad (65)$$

This can be interpreted also as a Ward identity. On the flip side, as long as $p \neq 0$, $\langle \sigma^2(t, \vec{x}) \rangle_p$ is not invariant under the diffeomorphism Eq. (62). The crucial point from this perspective is that diffeomorphism invariance is extremely important to see that the cross-correlation vanishes for $p \rightarrow 0$ for a massive scalar field. It is this that one failed to preserve in Eq. (44).

As we will show in detail, Eq. (61) is consistent with the explicit computation. Note that a couple of assumptions that we already mentioned in deriving Eq. (61) can only be justified by an explicit computation: namely, the effective lower cutoff p in Eq. (60) and UV cutoff details associated with renormalizing the composite operator σ^2 . Such complications do not arise in isocurvature scenarios without composite operators. Hence, one of the main technical merits of this paper is to provide an explicit justification of Eq. (61). Note that because the diffeomorphism gauge invariance plays a crucial role in obtaining the correct p dependence in Eq. (61) as explained around Eq. (65), we choose a UV regulator that preserves diffeomorphism invariance in the computation below.

C. Gauge invariance of correlators

Before we begin our explicit computation, we will check the setup of our computation by demonstrating that the manifestly gauge invariant quantities $\langle \delta_S \zeta \rangle$ and $\langle \delta_S \delta_S \rangle$ yield the same values in comoving and in the uniform curvature gauges. To accomplish this, we use a gravitational Ward identity.

We first note that the ζ dependent metric perturbations $\delta g^{(C)}$ and $\delta g^{(U)}$ differ by a gauge transformation, i.e.,

$$\begin{aligned} \Delta g_{\mu\nu} &= \delta g_{\mu\nu}^{(U)} - \delta g_{\mu\nu}^{(C)} = \begin{pmatrix} 2 \frac{d}{dt} \left(\frac{\zeta}{H} \right) & \left(-\frac{\zeta}{H} \right)_{,i} \\ \left(-\frac{\zeta}{H} \right)_{,i} & -a^2 \delta_{ij} 2\zeta \end{pmatrix} \\ &= -[\mathcal{L}_{X\bar{g}}]_{\mu\nu}, \end{aligned} \quad (66)$$

where

$$X^0 = -\frac{\zeta}{H}, \quad X^i = 0. \quad (67)$$

Their interaction actions differ by

$$\Delta S_{\sigma\sigma\zeta} = S_{\sigma\sigma\zeta}^{(U)} - S_{\sigma\sigma\zeta}^{(C)} = - \int^{t_f} dt d^3x a^3 T^{\mu\nu}(\bar{g}, \sigma) \nabla_\mu X_\nu. \quad (68)$$

Their interaction Hamiltonians differ by

$$\begin{aligned} \Delta H_{\zeta\sigma\sigma}(t) &= H_{\zeta\sigma\sigma}^{(U)}(t) - H_{\zeta\sigma\sigma}^{(C)}(t) \\ &= \int d^3x a^3(t) T^{\mu\nu}(\bar{g}, \sigma; t, \vec{x}) \nabla_\mu X_\nu(t, \vec{x}). \end{aligned} \quad (69)$$

Then we compare $\langle \sigma_x^2 \zeta_y \rangle$ in the two gauges:

$$\begin{aligned} &\langle \sigma^2(t_f, \vec{x}) \zeta(t_f, \vec{y}) \rangle^U - \langle \sigma^2(t_f, \vec{x}) \zeta(t_f, \vec{y}) \rangle^C \\ &= -i \int^{t_f} dt \langle [\sigma_x^2 \zeta_y, \Delta H_{\zeta\sigma\sigma}(t)] \rangle \\ &= -i \int^{t_f} dt d^3z \langle [\sigma_x^2 \zeta_y, \nabla_\mu (a^3(t) T^{\mu\nu} \\ &\quad \times (\bar{g}, \sigma; t, \vec{x}) X_\nu(t, \vec{x}))] \rangle, \end{aligned} \quad (70)$$

where we have integrated by parts and used the quantum version of $\nabla_\mu T_\sigma^{\mu\nu} = 0$, i.e., in-in formalism gravitational Ward identities

$$\begin{aligned} &i \nabla_\mu \langle in | T_z^{\mu\nu+} \sigma_x^+ \sigma_y^+ | in \rangle_g \\ &= \frac{1}{\sqrt{g_x}} \delta^4(x-z) g_x^{\alpha\nu} \frac{\partial}{\partial x^\alpha} \langle in | \sigma_x^+ \sigma_y^+ | in \rangle_g \\ &\quad + \frac{1}{\sqrt{g_y}} \delta^4(y-z) g_y^{\alpha\nu} \frac{\partial}{\partial y^\alpha} \langle in | \sigma_x^+ \sigma_y^+ | in \rangle_g \end{aligned} \quad (72)$$

$$i \nabla_\mu \langle in | T_z^{\mu\nu-} \sigma_x^+ \sigma_y^+ | in \rangle_g = 0, \quad (73)$$

whose notation is explained in Appendix B. Note that the remaining term in Eq. (71) is a total derivative. Hence, we are left with the boundary contribution

$$\begin{aligned} &\langle \sigma^2(t_f, \vec{x}) \zeta(t_f, \vec{y}) \rangle^U - \langle \sigma^2(t_f, \vec{x}) \zeta(t_f, \vec{y}) \rangle^C \\ &= -i \int d^3z a^3(t_f) \frac{1}{H} \langle [\sigma_x^2, T_{\sigma,z}^{00}] \rangle \langle \zeta_x \zeta_y \rangle \\ &= -\frac{\partial_t \langle \sigma_x^2 \rangle}{H} \langle \zeta_x \zeta_y \rangle. \end{aligned} \quad (74)$$

To make these composite operator correlators well defined while maintaining diffeomorphism invariance [see the discussion surrounding Eq. (65)], we need a proper covariant regulator, such as the Pauli-Villars (PV) regulator. It is straightforward to use the PV regulator here because the above identity holds for PV fields as well. See Appendix D for a more detailed discussion of the prescription of the PV regulator.

Using Eq. (75), it is now trivial to show that $\langle \delta_S \zeta \rangle^U = \langle \delta_S \zeta \rangle^C$ and $\langle \delta_S \delta_S \rangle^U = \langle \delta_S \delta_S \rangle^C$. Because $\delta_S \ni \sigma_x^2 / \langle \sigma_x^2 \rangle$, the denominator of this expression also transforms:

$$\Delta\delta_S \ni -\frac{\Delta\langle\sigma_x^2\rangle}{\langle\sigma_x^2\rangle}\frac{\sigma_x^2}{\langle\sigma_x^2\rangle} = \frac{\zeta_x}{H}\frac{\partial_t\langle\sigma_x^2\rangle}{\langle\sigma_x^2\rangle}\frac{\sigma_x^2}{\langle\sigma_x^2\rangle}, \quad (76)$$

which leads to a cancellation of Eq. (75) consistently to leading $\hbar \rightarrow 0$ approximation. Hence, we have a non-trivial consistency check of the computation that we are setting up.

D. Two-point functions

In this subsection, we present a rigorous computation of β defined in (29). To this end, we need to calculate the two-point functions $\langle(\sigma^2)_r\zeta\rangle$ and $\langle(\sigma^2)_r(\sigma^2)_r\rangle$ where the renormalized composite operator [67,87–98] is

$$(\sigma^2)_r \equiv \left(\sigma + \sum_n \chi_n\right)^2 + \delta Z_0(\Lambda, m_\sigma) + \delta Z_1(\Lambda, m_\sigma)R, \quad (77)$$

which is discussed in greater detail in Appendix D 2. Here we are going to use the comoving gauge for the computation because of its advantages that we state below.¹³ As shown in Eqs. (33) and (34), the gravitational interactions in the comoving gauge are derivatively (i.e., p^2/a^2) suppressed except the (ij) -components. In other words, the contributions from $T_\sigma^{00}\delta g_{00}^{(C)}$ and $T_\sigma^{0i}\delta g_{0i}^{(C)}$ interactions are $O(p^2/a^2)$, where \vec{p} is an external 3-momentum. Furthermore, all counterterm contributions are also derivatively suppressed in the comoving gauge: $\delta Z_0\langle\zeta\rangle = 0$ and $\delta Z_1\langle R\zeta\rangle_p^C = O(p^2/a^2)$. Therefore, we do not need the counterterms to compute the nonderivatively suppressed contributions, but we still need a regulator for UV divergences in the computation. The regulator dependences and the UV divergences will automatically disappear together in our final result.

Now we compute the two-point function shown in Fig. 2, which is written in the Fourier space as

$$\begin{aligned} \langle(\widetilde{\sigma^2})_r\zeta\rangle_p^C &= \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle(\sigma^2(t, \vec{x}))_r \zeta(t, \vec{0})\rangle^C \\ &= \int d^3x e^{-i\vec{p}\cdot\vec{x}} \int^t d^4z a^3(t_z) \\ &\quad \times \sum_{N=0}^s \left\langle \left[\sigma_N^2(t, \vec{x}) \zeta(t, \vec{0}), \frac{i}{2} (2\zeta a^2 \delta_{ij} T_\sigma^{ij})_z \right] \right\rangle + O\left(\frac{p^2}{a^2}\right), \end{aligned} \quad (78)$$

where we have introduced the PV regulator (see Appendix D for more details) and

¹³This computation has been done also in the uniform curvature gauge, which is presented in Appendix E. Particularly, in the massless limit, we explicitly calculate up to the next leading term including all gravitational couplings. This shows that the next leading terms are indeed suppressed by the factor p^2/a^2 .

$$a^2 \delta_{ij} T_\sigma^{ij} = -3\mathcal{L}_\sigma + \sum_{N=0}^s C_N \left(\frac{\nabla}{a} \sigma_N\right)^2, \quad (80)$$

where σ_0 and σ_n are the physical field σ and the PV field χ_n (here, $n \in \{1, 2, \dots, s\}$), respectively, and s is the number of introduced PV fields.

Interestingly, this integral can be computed in any Friedmann-Robertson-Walker space-time. We first compute the second term contribution in Eq. (80) defined as

$$\begin{aligned} I_N^{(2)}(p) &\equiv \int d^3x e^{-i\vec{p}\cdot\vec{x}} \int^t d^4z \sqrt{-g_z} \\ &\quad \times \left\langle \left[\sigma_N^2(t, \vec{x}) \zeta(t, \vec{0}), i\zeta_z C_N \left(\frac{\nabla}{a} \sigma_N\right)_z^2 \right] \right\rangle. \end{aligned} \quad (81)$$

Expanding in mode functions, this becomes

$$\begin{aligned} I_N^{(2)}(p) &= -4C_N^{-1} \int \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\quad \times \int_{-\infty}^t dt_z a_z^3 \left(-\frac{\vec{k}_1 \cdot \vec{k}_2}{a_z^2} \right) \\ &\quad \times \text{Im}[\zeta_p(t) \zeta_p^*(t_z) u_{N,k_1}(t) u_{N,k_1}^*(t_z) u_{N,k_2}(t) u_{N,k_2}^*(t_z)], \end{aligned} \quad (82)$$

where u_N are the mode functions for fields σ_N . Because ζ oscillates before and freezes after the horizon exit, we neglect the contribution before the horizon exit. Furthermore, we can neglect the $O(p^2/a^2)$ term and factor ζ_p out of the time integral. We thus find

$$\begin{aligned} I^{(2)}(p) &\approx 4|\zeta_p^o(t)|^2 \int \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\quad \times \int_{t_p}^t dt_z a_z^3 \left(\frac{\vec{k}_1 \cdot \vec{k}_2}{a_z^2} \right) \text{Im}[u_{k_1}(t) u_{k_1}^*(t_z) u_{k_2}(t) u_{k_2}^*(t_z)] \\ &\quad + O\left(\frac{p^2}{a^2}\right), \end{aligned} \quad (83)$$

where t_p is the time at which scale p exits the horizon. Note that we drop subscript N and field normalization C_N for convenience, but we will put it back later in the final result. Moreover, we neglect the low momentum phase space, i.e., $\min\{k_1, k_2\} < p$, because of $|u_k|^2 \lesssim O(k^{-3})$ and the spatial gradient factor $\vec{k}_1 \cdot \vec{k}_2/a^2$:

$$\begin{aligned} &\int_{k_1 < p} \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\quad \times \int_{t_p}^t dt_z a_z^3 \left(\frac{\vec{k}_1 \cdot \vec{k}_2}{a_z^2} \right) \text{Im}[u_{k_1}(t) u_{k_1}^*(t_z) u_{k_2}(t) u_{k_2}^*(t_z)] \\ &\lesssim O\left(\frac{p^2}{a^2}\right). \end{aligned} \quad (84)$$

Then the main contribution of the integral comes from the phase space $k_1, k_2 > p$, and thus p behaves as an IR cutoff

[see the importance of this IR cutoff in the discussion surrounding Eq. (61)].

Since $k_1, k_2 > p$, we Taylor-expand the integrand with respect to p and take the leading term. Then we have

$$I^{(2)}(p) \approx 4|\zeta_p^o(t)|^2 \int_p \frac{d^3 k_1}{(2\pi)^3} \times \int_{t_p}^t dt_z a_z^3 \left(-\frac{k_1^2}{a_z^2} \right) \text{Im}[u_{k_1}^2(t) u_{k_1}^{*2}(t_z)] + O\left(\frac{p^2}{a^2}\right). \quad (85)$$

Now we are going to compute the time integral. Recall that the differential equation for mode function u_k is

$$\ddot{u}_k + 3H u_k + \left(\frac{k^2}{a^2} + m^2 \right) u_k = 0. \quad (86)$$

Applying $\frac{\partial}{\partial \ln k}$ to the equation, we obtain

$$\ddot{y}_k + 3H y_k + \left(\frac{k^2}{a^2} + m^2 \right) y_k = -2 \frac{k^2}{a^2} u_k, \quad (87)$$

where $y_k \equiv \frac{\partial}{\partial \ln k} u_k$. Note that the homogeneous solutions for y_k are u_k and u_k^* . Thus, we use the Green's function method to find a solution

$$y_k(t) = \int^t dt' \frac{a^3(t')}{i} (u_k^*(t) u_k(t') - u_k(t) u_k^*(t')) \times \left(-2 \frac{k^2}{a^2} \right) u_k(t'). \quad (88)$$

From this, we find

$$\frac{d}{d \ln k} |u_k(t)|^2 = 2 \text{Re}[u_k^*(t) y_k(t)] \quad (89)$$

$$= 4 \int_{-\infty}^t dt_z a_z^3 \frac{k^2}{a_z^2} \text{Im}[u_k^2(t) u_k^{*2}(t_z)] \quad (90)$$

$$= \left[\int_{t_p}^t dt_z + \int_{-\infty}^{t_p} dt_z \right] 4 a_z^3 \frac{k^2}{a_z^2} \times \text{Im}[u_k^2(t) u_k^{*2}(t_z)]. \quad (91)$$

The second term is oscillatory with respect to k so that we can safely neglect it after the momentum integral. Inserting this back into the integral (85), we obtain

$$I_N^{(2)}(p) \approx -C_N^{-1} |\zeta_p^o(t)|^2 \int_p \frac{d^3 k}{(2\pi)^3} \frac{d}{d \ln k} |u_{N,k}(t)|^2 + O\left(\frac{p^2}{a^2}\right) \quad (92)$$

$$= -C_N^{-1} |\zeta_p^o(t)|^2 \left[-\frac{k^3}{2\pi^2} |u_{N,k}(t)|^2 \Lambda_{UV} + 3 \langle (\sigma_N^2)_p \rangle \right] + O\left(\frac{p^2}{a^2}\right), \quad (93)$$

where we have put the subscript N and the field normalization C_N back, and

$$\langle (\sigma_N^2)_p \rangle \equiv \int_p \frac{d^3 k}{(2\pi)^3} |u_{N,k}(t)|^2, \quad (94)$$

where the subscript p stands for the comoving IR cutoff of momentum. One can then compute the contribution of the first term in Eq. (80) in a similar manner:

$$I_N^{(1)} \equiv \int d^3 x e^{-i\vec{p}\cdot\vec{x}} \times \int^t d^4 z \sqrt{-g_z} \langle [\sigma_N^2(t, \vec{x}) \zeta(t, \vec{0}), i(-3) \mathcal{L}_\sigma(z) \zeta(z)] \rangle \quad (95)$$

$$= 3C_N^{-1} |\zeta_p^o|^2 \langle (\sigma_N^2)_p \rangle + O\left(\frac{p^2}{a^2}\right). \quad (96)$$

Hence, we obtain

$$\langle (\sigma^2)_{r,\zeta} \rangle_p^C = \sum_{N=0}^s I_N^{(1)} + I_N^{(2)} + O\left(\frac{p^2}{a^2}\right) \quad (97)$$

$$= |\zeta_p^o|^2 \frac{p^3}{2\pi^2} |u_p(t)|^2 + O\left(\frac{p^2}{a^2}\right), \quad (98)$$

where u_p is the mode function for physical field σ .

Comparing the computation of Eq. (98) with the estimate in Sec. III A, we see two crucial differences:

- (1) There is a cancellation of the $3C_N^{-1} |\zeta_p^o|^2 \langle (\sigma_N^2)_p \rangle$ term that is sensitive to mode summation that extends to subhorizon modes.
- (2) The Λ_{UV} dependent term in Eq. (93) in the present computation disappears after accounting for the PV regulator fields. In contrast, the estimate in Sec. III A leaves behind a $\Lambda_{UV} = aH_{\text{inf}}$ dependent contribution due to the *ad hoc* nature of the UV cutoff which does not preserve diffeomorphism.

Finally, putting the results (93) and (96) together, the two-point function becomes

$$\langle (\sigma^2)_{r,\zeta} \rangle_p^C |_{t_e} = |\zeta_p^o|^2 \times \begin{cases} \frac{\Gamma^2(\nu) H^2}{\pi^3} \left(\frac{p}{2a(t_e)H} \right)^{3-2\nu} & \text{massive scalar in dS} \\ \frac{H_p^2}{4\pi^2} & \text{massless during quasi-dS} \end{cases} + O\left(\frac{p^2}{a^2}\right), \quad (99)$$

where H_p denotes the Hubble scale at which scale p exits the horizon, $\nu = \sqrt{9/4 - m^2/H^2}$, and t_e reminds us that we are evaluating this at the end of inflation. We have applied the (quasi-)dS mode function in evaluating (99).¹⁴ One can easily check that Eq. (47) is consistent with Eq. (60).

As explained near Eq. (65), the vanishing of the cross-correlation in the limit $p \rightarrow 0$ is expected from the diffeomorphism Ward identity. For a nonvanishing p , one might expect the cross-correlation should be $O(p^2/a^2)$ by Taylor-expanding the cross-correlation at $p = 0$. However, Eq. (99) interestingly shows that the leading term of the cross-correlation is not analytic at $p = 0$ and thus not p^2/a^2 -suppressed. Indeed, for any small $p/a(t_e)$, we can diminish the suppression by making $3 - 2\nu \rightarrow 0^+$ through the limit $m/H \rightarrow 0$.

To finish the computation of β , we also consider the two-point correlator $\langle(\sigma^2)_r(\sigma^2)_r\rangle$ showing up in the denominator. Again, the comoving gauge is convenient for this computation. Although the correlator is UV divergent, because the counterterms associated with the divergence are derivatively suppressed, we do not need to include the counterterms in computing the IR contributions and the nonderivative contribution of the correlator is insensitive to renormalization. Furthermore, the IR contribution using the superhorizon approximation is not UV divergent. That means the UV contribution and the IR contribution are cleanly separated. Thus, we can estimate $\langle(\sigma^2)_r(\sigma^2)_r\rangle$ using only the superhorizon approximation unlike in the computation of $\langle(\sigma^2)_r\zeta\rangle$. We find

$$\begin{aligned} \langle(\sigma^2)_r(\sigma^2)_r\rangle_p^C &= 2 \int_{\Lambda_{\text{IR}}} \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\times |u_{k_1}(t)|^2 |u_{k_2}(t)|^2 + O\left(\frac{p^2}{a^2}\right), \end{aligned} \quad (100)$$

where Λ_{IR} is a comoving IR cutoff. Evaluating this with dS superhorizon modes and assuming $m < 3H/2$, we find the value at the end of inflation to be

¹⁴After inflation ends at time t_e , the cross-correlation is expressed as

$$\langle(\sigma^2)_r\zeta\rangle_p^C = f_T \langle(\sigma^2)_r\zeta\rangle_p^C|_{t_e},$$

where f_T accounts for the change in the mode-function behavior after the end of inflation. As alluded to in the discussion near Eq. (24), the factor f_T cancels out of the expression in β due to its appearance in the denominator $\sqrt{\Delta_\zeta^2 \Delta_\delta^2}$. The factor f_T can also account for the corrections in the superhorizon mode function behavior during inflation due to deviations away from the exact dS background.

$$\begin{aligned} \langle(\sigma^2)_r(\sigma^2)_r\rangle_p^C|_{t_e} &\approx 2 \int_{\Lambda_{\text{IR}}} \frac{d^3k_1}{(2\pi)^3} d^3k_2 \delta^3(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\times \frac{2^{-4+4\nu} |\Gamma(\nu)|^4}{\pi^2} \frac{1}{a^6(t_e) H^2} \\ &\times \left(\frac{k_1}{a(t_e)H}\right)^{-2\nu} \left(\frac{k_2}{a(t_e)H}\right)^{-2\nu} \end{aligned} \quad (101)$$

$$\begin{aligned} &\approx \frac{1}{2\pi^2} \frac{H^4}{p^3} \frac{1}{3 - 2\nu} \left(\frac{p}{a(t_e)H}\right)^{6-4\nu} \\ &\times \left[1 - \left(\frac{\Lambda_{\text{IR}}}{p}\right)^{3-2\nu}\right]. \end{aligned} \quad (102)$$

In Eq. (100), we have introduced a comoving IR cutoff Λ_{IR} which corresponds to the statement that the inflationary era had a beginning in the finite past. Explicitly, we cannot use the Bunch-Davies vacuum boundary condition for modes that left the horizon before the beginning of inflation. This means that

$$\frac{\Lambda_{\text{IR}}}{p} \sim e^{-(N_{\text{tot}} - N(p))}, \quad (103)$$

where N_{tot} is the total number of e-folds of inflation, $N(p)$ is the number of e-folds before the end of inflation at which the mode p left the horizon, i.e., $p/a(N) = H$. This cutoff is related to the box cutoff introduced in [85,99,100]. Numerically, $\Lambda_{\text{IR}} \ll p$ is irrelevant when

$$\frac{m_\sigma^2}{H^2} \gg \frac{1}{N_{\text{tot}} - N(p)}. \quad (104)$$

For situations in which this condition is violated, IR effects are important, and our computation is only qualitatively suggestive since Λ_{IR} has to be resolved using more detailed description of the beginning of inflation. In particular, since we do not physically expect $N_{\text{tot}} = \infty$, the $m_\sigma = 0$ situation is not accurately captured by our computation. Of course, the IR sensitivity here is not important as far as the importance of the cross-correlation is concerned since the qualitative behavior of having $p/\Lambda_{\text{IR}} \rightarrow \infty$ is to make the correlation even larger making the β parameter even smaller. Finally, note that Eq. (104) can easily be more stringent than Eq. (49).

Hence, we conclude

$$\beta \approx \begin{cases} -\frac{m_\sigma}{H} \sqrt{\frac{\Delta_\zeta^2}{6}} & \text{massive scalar in dS} \\ -\frac{\sqrt{\Delta_\zeta^2}}{2} \left(\ln \frac{p}{\Lambda_{\text{IR}}}\right)^{-1/2} & \text{massless during quasi-dS} \end{cases}, \quad (105)$$

which for the massive scalar case is assumed to satisfy Eq. (49). Although this in principle is a generic prediction of an isocurvature scenario, the magnitude of around 10^{-5} is difficult to probe experimentally since the current sensitivity is at the level of 10^{-2} .

IV. APPLICATION

The β computation presented in Eq. (105) is not sensitive to $\dot{\rho}_\sigma$ that is involved in the definition of the isocurvature perturbation δ_S . Instead, it is a property of quadratic nature of the scalar composite operator during inflation. Since Eq. (105) does depend on the masses, in this section, we motivate a couple of the mass parameters from well-motivated nonthermal dark matter models: wimpzillas [101–120] and axions [121–123]. Although these two particles have different physical origins, they share some common properties as a cosmological component. Firstly, since they are massive (at the CMB time at least) and weakly interacting, they both are good CDM candidates. Also, they can be gravitationally produced during or after inflation, and this gives rise to isocurvature from their density perturbations. Furthermore, when their background field values are negligibly small, the isocurvature perturbation from these particles is approximated by quadratic form σ^2 . In that case, they would present detectable non-Gaussianities [24,30,85] and their cross-correlation is characterized by Eq. (105).

A. Weakness of σ interactions with ψ

To connect our computation of β to observables, a postinflationary isocurvature scenario is necessary. For the illustrative situations of axions and wimpzillas, it is sufficient to assume that σ has an extremely weak interaction with the reheating degrees of freedom ψ and the inflaton ϕ such that the transfer function of σ is trivial after inflation: with sufficiently small interactions, α and β of Eqs. (28) and (29) computed during inflation can be directly matched without any further transfer function computations to the isocurvature initial condition for CMB codes such as CMBFAST. In this section, we quantify the requisite weakness of the interactions and qualitatively discuss the situation when the weakness assumption is invalid. For example, we will show below that ordinary WIMPs are too strongly interacting with the reheating degrees of freedom for this assumption to be valid while axions and wimpzillas are sufficiently weakly interacting. We also qualitatively describe what extra work needs to be done to apply this paper for observations in situations in which the dark matter particles are not extremely weakly interacting.¹⁵

At the linearized classical equation of motion level, we have the gauge invariant perturbations $\{\zeta_j\}$ being governed by a linear time evolution operator

¹⁵Because the cross-correlation result in this paper is small, the discussion here is a bit academic if this discussion applied only to the cross-correlation result. However, the discussion here applies to the isocurvature two-point function found in the literature [9,30,41–43,99,124,125] which has a realistic chance of being observable in near future experiments.

$$O[\{\zeta_j\}] = 0, \quad (106)$$

where the initial condition for the isocurvature species $j = \sigma^{16}$ is given by

$$\zeta_\sigma(t_i) = f(t_i) \quad (107)$$

which in turn is set by the inflationary physics. For example, the initial time t_i can be set to be the time of the end of inflation. The final $\zeta_\sigma(t_f)$ will contain a contribution which does not vanish in the limit $f \rightarrow 0$. Hence, one can write

$$\zeta_\sigma(t_f) = G_{t_f}^\sigma[f(t_i), 0] + G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)], \quad (108)$$

where $G_{t_f}^\sigma[D]$ is the σ component of the Green's function derived from the linear operator O which takes the initial data D and maps it to the final value of $\zeta_\sigma(t_f)$. Note that we have implicitly assumed the boundary condition such that $G_{t_f}^\sigma[0, 0] = 0$ which means that $G_{t_f}^\sigma[f(t_i), 0]$ vanishes as $f(t_i) \rightarrow 0$.

Now, we will consider two situations which bound the picture of super-weakly-interacting scenarios. In the first scenario, the thermal plasma generated by the inflaton decay will interact with σ sufficiently strongly to make δ_S mix strongly with ζ . In the second scenario, the inflaton decay to σ directly will realign σ fluctuations during radiation domination to those of ζ , even though σ and reheating products are not interacting appreciably.

First, consider the effects of radiation dominated thermal plasma on σ . The mixing rate governing $G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)]$ is the production rate of σ particles from the thermal plasma. Typically a single channel involving particle y dominates the production of the σ particle from the plasma. (If there are more channels, the discussion below can easily be generalized.) We thus expect a qualitative behavior of

$$G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)] \sim \left(1 + \tanh \left[\frac{\Gamma(yy \rightarrow \sigma\sigma, t_{\max})}{H(t_{\max})} \right]\right) \zeta_y, \quad (109)$$

where $\Gamma(yy \rightarrow \sigma\sigma, t_{\max})$ is the reaction rate for this process at the time that the production rate is maximum (in $\Gamma(yy \rightarrow \sigma\sigma, t)$ is maximum at $t = t_{\max}$ where $t_{\max} \in [t_i, t_f]$), H is the expansion rate, and $\zeta_y = O(\zeta_{\text{tot}})$.

Hence, one sees that the information about the isocurvature perturbations depends not only on

$$\Gamma(yy \rightarrow \sigma\sigma, t_{\max})/H(t_{\max})$$

but on t_f since t_{\max} is restricted to be in the range $t_{\max} \in [t_i, t_f]$. For example, the usual CMB code is run starting with an initial condition at $T \ll T_{\text{BBN}}$. This means that $t_f \gg t_{\text{BBN}}$ is required to use the inflationary correlator computations in the CMB code. A general computation

¹⁶In our scenario, the isocurvature species stand for the degrees of freedom in contrast with the radiation degrees of freedom.

of $G_{t_f}^\sigma$ needed for the prediction of the isocurvature perturbation effect on CMB temperature is beyond the scope of current work. To be able to trust the trivial transfer function of

$$G_{t_f}^\sigma[f(t_i), 0] \approx f(t_i) \gg G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)], \quad (110)$$

for superhorizon modes (where t_i is, say, at the end of inflation¹⁷), we can require

$$\frac{\Gamma(yy \rightarrow \sigma\sigma, t_{\max})}{H(t_{\max})} \ll \frac{\zeta_\sigma(t_i)}{\zeta_{\text{tot}}}, \quad (111)$$

where t_{\max} can be at any time between inflation and the time at which boundary conditions are set for the CMB code. This sets a bound on the cross section $\langle \sigma\nu \rangle$ for $yy \rightarrow \sigma\sigma$ to be

$$\langle \sigma\nu \rangle \ll \frac{\zeta_\sigma(t_i)}{\zeta_{\text{tot}}(t_i)} \frac{g_*^{3/4}}{g_y} \left(\frac{T_{\text{RH}}}{10^6 \text{ GeV}} \right)^{-1} 4.2 \times 10^{-25} \text{ GeV}^{-2}, \quad (112)$$

where the bound becomes more stringent for higher reheating temperatures.

This number should be compared to the typical thermal WIMP DM candidate annihilation cross section of 10^{-9} GeV^{-2} and a high energy s -channel scattering at T_{RH} mediated through a vector boson with a dimensionless coupling $g = \sqrt{4\pi\alpha_g}$:

$$\langle \sigma\nu_{yy \rightarrow A^\mu \rightarrow \text{light states}} \rangle \sim \frac{\alpha_g^2}{T_{\text{RH}}^2} \quad (113)$$

$$= \left(\frac{\alpha}{10^{-1}} \right)^2 \left(\frac{T_{\text{RH}}}{10^6 \text{ GeV}} \right)^{-2} 10^{-14} \text{ GeV}^{-2}. \quad (114)$$

Hence, one sees that WIMP dark matter cannot play the role of the isocurvature perturbations. That is why if we are to identify our computation of α and β directly to physical observables, we have to choose the isocurvature degree of freedom to be nonthermal.¹⁸

Even though the current work applies most immediately without changes to nonthermal dark matter scenarios having extremely weak interactions, Eq. (112) is still much bigger than gravity mediated s -channel interactions

$$\langle \sigma\nu_{yy \rightarrow g_{\mu\nu} \rightarrow \sigma\sigma} \rangle \sim \frac{1}{16\pi^2} \frac{T_{\text{RH}}^2}{M_p^4} \quad (115)$$

$$\sim \left(\frac{T_{\text{RH}}}{10^6 \text{ GeV}} \right)^2 10^{-64} \text{ GeV}^{-2}. \quad (116)$$

¹⁷Note that as discussed in footnote 14, α can also receive corrections from the departures from the ideal dS mode function evolution as well as from the time when m/H becomes larger than unity. As discussed there, the quantity β is not as sensitive to these corrections.

¹⁸Similar arguments can also be made from unitarity [126].

For example, axion cross sections for gluon coannihilation behave as [127]

$$\langle \sigma\nu_{ag \rightarrow X} \rangle \sim \frac{\alpha_s^2}{8\pi^2} \frac{1}{f_a^2} \quad (117)$$

$$\sim \left(\frac{f_a}{10^{12} \text{ GeV}} \right)^{-2} 10^{-28} \text{ GeV}^{-2}, \quad (118)$$

where f_a is the Peccei-Quinn (PQ) breaking VEV. Hence, there is a large class of weakly interacting models for which this work directly applies without modification. For models for which Eq. (112) is not satisfied, one needs to compute the transfer function associated with the mixing. Nonetheless, this work will still be useful in setting the initial conditions for such computations.

Let us see qualitatively what happens when Eq. (112) is not satisfied. In that case, we expect mixing between isocurvature and curvature perturbations

$$\zeta_\sigma(t_f) = G_{t_f}^\sigma[f(t_i), 0] + G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)] \sim O(\zeta_\sigma) + O(\zeta_{\text{tot}}). \quad (119)$$

Since the curvature perturbations will analogously be

$$\zeta(t_f) = G_{t_f}^R[f(t_i), 0] + G_{t_f}^R[0, \zeta_{j \neq \sigma}(t_i)], \quad (120)$$

we would then have

$$\delta_S = 3(\{G_{t_f}^\sigma[f(t_i), 0] - G_{t_f}^R[f(t_i), 0]\} + \{G_{t_f}^\sigma[0, \zeta_{j \neq \sigma}(t_i)] - G_{t_f}^R[0, \zeta_{j \neq \sigma}(t_i)]\}). \quad (121)$$

Up to the accuracy that all species are equipartitioned, this quantity may vanish since there is cancellation in each of the terms in the bracket. Since it is beyond the scope of the current work to compute more precisely this cancellation, we are focusing on scenarios which satisfy Eq. (112).

Suppose there is a direct decay of the inflaton to σ , and suppose there is no other appreciable interaction between σ and other decay products of the inflaton. In that case, it is better to set the initial time t_i to be at the time of inflaton decay completion such that $G_{t_f}^\sigma[f(t_i), 0]$ is still trivial.

In that case, we have

$$\zeta_\sigma \equiv -\frac{A}{2} + \frac{\delta\rho_\sigma^{(\text{grav})} + \delta\rho_\sigma^{(\text{decay})}}{3(\bar{\rho}_\sigma^{(\text{grav})} + \bar{\rho}_\sigma^{(\text{decay})} + \bar{P}_\sigma^{(\text{grav})} + \bar{P}_\sigma^{(\text{decay})})} \quad (122)$$

$$= r_\sigma^{(\text{grav})} \zeta_\sigma^{(\text{grav})} + r_\sigma^{(\text{decay})} \zeta_\sigma^{(\text{decay})}, \quad (123)$$

where r_i has been defined in Eq. (11). Hence, we have

$$\delta_S = 3(\zeta_\sigma - \zeta_R) \quad (124)$$

$$= 3(r_\sigma^{(\text{grav})} \zeta_\sigma^{(\text{grav})} + r_\sigma^{(\text{decay})} \zeta_\sigma^{(\text{decay})} - \zeta_R). \quad (125)$$

If $\zeta_\sigma^{(\text{decay})} = \zeta_R$ is assumed, then

$$\delta_s = 3[1 - r_\sigma^{(\text{decay})}](\zeta_\sigma^{(\text{grav})} - \zeta_R). \quad (126)$$

This equation says that if most of the inflaton energy density goes to σ , then the isocurvature is negligible.

In the next two subsections, we now consider a couple of mass motivations for nonthermal dark matter isocurvature candidates.

B. WIMPZILLA

The wimpzilla was originally proposed to avoid the restriction from the assumption that the dark matter is a thermal relic. Thus, the wimpzilla is supposed to be either very heavy and/or very weakly interacting. In particular, we consider the possibility that the wimpzilla is gravitationally produced during the phase transition out of the quasi—de Sitter phase of inflation. In that case, the model is controlled by two parameters: the ratio of mass to the Hubble scale of inflation m_X/H_{inf} , and the reheating temperature T_{RH} , where X denotes a massive scalar field. Since the energy density is approximated as $\rho_X \sim m_X^2 X^2$ the relic density of X is estimated as

$$\Omega_X h^2 \sim 10^{-1} \left(\frac{H_e}{10^{12} \text{ GeV}} \right)^2 \left(\frac{T_{\text{RH}}}{10^6 \text{ GeV}} \right), \quad (127)$$

where we have assumed that $m_X \sim H_e$, because *a priori* we know that we can find proper isocurvature and relic density in this mass range. (For a more detailed discussion of the relic abundance, see for example [30].) The isocurvature power spectrum depends on the details of the evolution of the background during inflation because the mode function of massive particle decays as $a^{-3+2\nu}$ (see a related discussion in footnote 17). However, we can generally obtain $\alpha \sim 0.067$ if $m_X \lesssim H_{\text{inf}}$, where H_{inf} is the Hubble expansion rate when the CMB scale crosses the horizon [30]. The wimpzilla isocurvature has also the quadratic form like the axion. It thus generates the observable non-Gaussianities estimated as Eq. (31). Equation (105) translates to the fractional cross-correlation of

$$\beta_{\text{WIMPZILLA}} \approx -0.4 \frac{m_X}{H_{\text{inf}}} \sqrt{\Delta_\zeta^2}, \quad (128)$$

which justifies the constraint used in [30]. Since the naive estimate of Eq. (56) gives a gross overestimate β , one of

the merits of this paper is to put such worries to rest through the proper computation.

C. Axion

In this subsection we assess the relevance of Eq. (105) to the axion scenario. Firstly, we review the axion scenario. In 1997, Peccei and Quinn proposed the global $U(1)_{\text{PQ}}$ symmetry in order to solve to the strong CP problem in QCD. The axion is the Nambu-Goldstone boson associated with the symmetry after it is broken spontaneously. Many mechanisms have been proposed to produce axions in the early Universe. We focus only on the “vacuum misalignment” mechanism here following Refs. [43,125,128–134]. In the early Universe, the axions are effectively massless and gain their mass when the QCD anomaly term (which explicitly breaks PQ symmetry) becomes physical after the chiral symmetry breaking QCD phase transition. After the Universe cools down and the Hubble friction drops below the axion mass, the axions begin to coherently oscillate and they contribute to the CDM component of the Universe because of their long lifetime.

Let us denote the PQ symmetry breaking scale by f_a . Because $n_a \propto \theta^2$ where θ is the axion angle, the relic axion density is estimated as

$$\Omega_a h^2 \sim \begin{cases} 2 \times 10^4 \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^{7/6} \langle \theta^2 \rangle & \text{for } T_{\text{osc}} \geq \Lambda_{\text{QCD}} \\ 5 \times 10^3 \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^{3/2} \langle \theta^2 \rangle & \text{for } T_{\text{osc}} \leq \Lambda_{\text{QCD}}, \end{cases} \quad (129)$$

where we have neglected $O(1)$ factors due to diffusion, anharmonic correction, and temperature dependent mass correction, and T_{osc} is the temperature at which the axion starts to oscillate. The axion isocurvature in comoving gauge is written as

$$\delta_s^{(C)} = \omega_a \frac{\theta^2 - \langle \theta^2 \rangle}{\langle \theta^2 \rangle} = \omega_a \frac{2\theta_i \delta\theta + \delta\theta^2 - \langle \delta\theta^2 \rangle}{\langle \theta^2 \rangle}, \quad (130)$$

where $\omega_a \equiv \Omega_a/\Omega_{\text{CDM}}$, θ_i is the average of initial QCD vacuum angle θ over the observable Universe, and $\delta\theta$ is the inhomogeneity of θ , i.e., $\theta(t, \vec{x}) = \theta_i(t) + \delta\theta(t, \vec{x})$. Then the isocurvature power spectrum becomes

$$\langle \widetilde{\delta_s \delta_s} \rangle \sim \omega_a^2 \begin{cases} 3.5 \times 10^{10} \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^{7/3} \widetilde{F} & \text{for } f_a/N \geq 6 \times 10^{17} \text{ GeV} \\ 2 \times 10^9 \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^3 \widetilde{F} & \text{for } f_a/N \leq 6 \times 10^{17} \text{ GeV}, \end{cases} \quad (131)$$

where

$$\widetilde{F} = 4\theta_i^2 \langle \widetilde{\delta\theta \delta\theta} \rangle + \langle \delta\theta^2 \delta\theta^2 \rangle + \theta_i [\langle \delta\theta \delta\theta^2 \rangle + \langle \delta\theta^2 \delta\theta \rangle]. \quad (132)$$

Since our primary interest is in the cross-correlation with $\theta_i \approx 0$, we set it to zero.

Therefore, the adiabaticity parameter α defined in Eq. (28) is estimated as

$$\alpha \sim \omega_a^2 \begin{cases} 1.3 \times 10^{19} \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^{7/3} \Delta_\theta^2 & \text{for } f_a/N \gtrsim 6 \times 10^{17} \text{ GeV} \\ 8.1 \times 10^{17} \left(\frac{f_a/N}{10^{16} \text{ GeV}} \right)^3 \Delta_\theta^2 & \text{for } f_a/N \lesssim 6 \times 10^{17} \text{ GeV,} \end{cases} \quad (133)$$

$$\Delta_\theta^2(p) = \frac{p^3}{2\pi^2} \langle \delta\theta^2 \widetilde{\delta\theta^2} \rangle = \left(\frac{f_a}{N} \right)^{-4} \left(\frac{H_p^2}{2\pi^2} \right)^2 \ln \frac{p}{\Lambda_{\text{IR}}}, \quad (134)$$

where H_p is the Hubble scale at the horizon exit of mode p , and Λ_{IR} is an IR cutoff. Here we have used Eq. (102) with the assumption that the axion is effectively massless during inflation. In the case that $\theta_i \ll \delta\theta$, the isocurvature has the quadratic form of Gaussian variable $\delta\theta$, and it naturally becomes non-Gaussian perturbation. The isocurvature non-Gaussianity is estimated as Eq. (31).

These parameter constraints and predictions (129), (133), and (31) already have been investigated in the literature [24,43,85,125] with the assumption that the axion isocurvature and the curvature is uncorrelated. Our result from Eq. (105) is

$$\beta_{\text{axion}} = -\frac{\sqrt{\Delta_\zeta^2}}{2} \left(\ln \frac{p}{\Lambda_{\text{IR}}} \right)^{-1/2} \lesssim 2.5 \times 10^{-5} \quad (135)$$

which is consistent with the assumptions made in the literature.

V. SUMMARY

In this paper, we have presented the first explicit computation of the gravitational interaction contribution to the cross-correlation between the curvature and quadratic isocurvature perturbations (which include dark matter isocurvature candidates such as axions and wimpzillas). Since the necessary and sufficient condition for the cross-correlation to dominate over the isocurvature perturbations in the temperature two-point function is $|\beta| \gtrsim 4 \times 10^{-2}$, we have explicitly computed β , which incidentally is not sensitive to the background number density of the isocurvature degrees of freedom and postinflationary mode function changes on superhorizon scales. Although a naive estimate of β based on a diffeomorphism violating UV cutoff leads to the possibility of $\beta \sim O(1)$ due to a large ratio that can appear between the numerator and the denominator of the expression for β , our explicitly diffeomorphism invariant computation leads to $|\beta| \lesssim \Delta_\zeta/2 \approx 2.5 \times 10^{-5}$ because the numerator has a suppression as a consequence of a diffeomorphism Ward identity. Unfortunately, this is far below the current observational sensitivity of $|\beta| \gtrsim 10^{-2}$.

The smallness of the cross-correlation is explained by the fact that the superhorizon mode of the curvature perturbation ζ can be smoothly connected to the gauge mode, which is the spatial dilatation, in the zero external momentum limit. Hence, Eq. (98) vanishes when $p = 0$

and $m \neq 0$. In other words, this can be seen as a suppression due to a diffeomorphism Ward identity (i.e., uniform spatial rescaling invariance). A nontrivial structure revealed through our explicit computation is the suppression's nonanalytic structure with respect to p : the cross-correlation cannot be Taylor-expanded at $p = 0$, and this contribution is not p^2/a^2 -suppressed.

Our rigorous result which incorporates UV renormalization of the composite operator in the curved background is also shown to be consistent with an estimate based on a soft- ζ theorem, which allows one to factorize $\langle \zeta \zeta \rangle$ from $\langle \sigma^2 \zeta \rangle$ as explained in Eq. (61). However, Eq. (61) requires two assumptions that can only be justified by an honest computation such as what is presented in Sec. III D:

- (1) There is an effective IR cutoff of p in evaluating $\langle \sigma^2 \rangle$ due to the external momentum p inserted into the composite operator.
- (2) The only UV renormalization property of $\langle \sigma^2 \rangle$ that is relevant to leading \hbar approximation is the preservation of diffeomorphism invariance.

Note that the proper diffeomorphism invariant UV treatment also allowed us to demonstrate that the cross-correlation is indeed gauge invariant with one-loop correction through the gravitational coupling. This gauge invariance is checked explicitly by computing our cross-correlation in both the comoving gauge and the uniform curvature gauge.

Physically, the curvature perturbation ζ can affect the particle density ρ_σ and generate correlations only at its horizon crossing, because ζ freezes out after its horizon exit, after which it can be effectively treated as a gauge mode. Positive cross-correlation corresponds to the situation in which the $1 + \zeta$ enhancement in the expansion enhances the particle production (assuming that this enhances inhomogeneity) while the negative cross-correlation corresponds to the situation in which the $1 + \zeta$ enhancement in the expansion dilutes the particle inhomogeneity. The latter dilution effect leads to $\beta > 0$, while the particle production enhancement effect corresponds to the quadratic scenario that we explored in this paper. This explains the sign $\beta < 0$ of our result.

Given the robustness of the smallness of β , the gravitational interaction contribution to the cross-correlation should be negligible in most nonthermal dark matter isocurvature scenarios. In addition to giving a concrete computation that supports this statement, our work serves as an interesting lesson in computing correlators of composite operators in curved spacetime in the context of inflationary cosmology.

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APPENDIX A: BEHAVIORS OF TRANSFER FUNCTIONS FOR ADIABATIC AND ISOCURVATURE INITIAL CONDITION

The CMB temperature fluctuation with the leading order approximation (the integrated Sachs-Wolfe term is neglected) in the Newtonian gauge ($B = F = 0$, $E = 2\Phi$, $A = -2\Psi$) is

$$\frac{\Delta T}{T} \approx \frac{1}{4} \delta_\gamma|_r + \Phi|_r, \quad (\text{A1})$$

where the perturbations on the rhs are evaluated at the recombination. We can obtain these perturbations by solving the Einstein and Boltzmann equations with given initial conditions. A projection from a given initial condition to the final CMB temperature fluctuation is called transfer function. In the following subsections, we calculate that the k -dependence of the transfer functions for the adiabatic and the isocurvature initial conditions. In particular, we show that the isocurvature transfer function has the additional suppression factor k_{eq}/k compared to the adiabatic one for small scale $k \gg k_{\text{eq}}$. Here we basically follow the calculation by Refs. [135,136].

1. Perturbation equations

For explicit computation, we choose the Newtonian gauge for the scalar metric perturbation (2). For simplicity, we consider only photon and CDM fluids, which are denoted in the following equations by subscripts γ and m , respectively. This assumption is valid for the sake of identifying the difference between transfer functions for adiabatic and isocurvature initial conditions, although baryon and neutrino should be taken into account for accurate description for transfer functions.

The conservation equations for dark matter and photon fluids in Fourier space are

$$\delta'_m = k^2 V_m + 3\Psi, \quad (\text{A2})$$

$$V'_m = -\mathcal{H} V_m - \Phi, \quad (\text{A3})$$

$$\delta'_\gamma = \frac{4}{3} k^2 V_\gamma + 4\Psi', \quad (\text{A4})$$

$$V'_\gamma = -\frac{1}{4} \delta_\gamma - \Phi, \quad (\text{A5})$$

where $'$ denotes the time derivative with respect to conformal time η , $\mathcal{H} \equiv a'/a$, $\delta_a \equiv \delta\rho_a/\rho_a$. Note that $\Phi = \Psi$

since they are perfect fluids. V_X is the peculiar velocity for fluid X . These four equations are combined by eliminating V_X , and we have

$$(a(\delta'_m - 3\Phi'))' = ak^2\Phi, \quad (\text{A6})$$

$$\delta''_\gamma = 4\Phi'' - \frac{k^2}{3}(\delta_\gamma + 4\Phi). \quad (\text{A7})$$

The evolution of the metric perturbation is encoded in the Einstein equations. (00) and (ii) components are

$$k^2\Phi + 3\mathcal{H}(\Phi' + \mathcal{H}\Phi) = -\frac{1}{2M_p^2} a^2(\rho_m \delta_m + \rho_\gamma \delta_\gamma), \quad (\text{A8})$$

$$\Phi'' + 3\mathcal{H}\Phi' + \left(2\frac{a''}{a} - \mathcal{H}^2\right)\Phi = \frac{1}{6M_p^2} a^2 \rho_\gamma \delta_\gamma. \quad (\text{A9})$$

Combining with other components, we also find the Poisson equation

$$-k^2\Phi = \frac{3}{2} \mathcal{H}^2 \left[\Omega_m \delta_m + \Omega_\gamma \delta_\gamma - 3\mathcal{H} \left(\Omega_m V_m + \frac{4}{3} \Omega_\gamma V_\gamma \right) \right]. \quad (\text{A10})$$

With the definition of isocurvature (20) in Sec. II

$$\delta_S = \delta_m - \frac{3}{4} \delta_\gamma, \quad (\text{A11})$$

where we have used $p_\gamma = \rho_\gamma/3$ and $p_m = 0$, we rewrite the differential equations of fluid and metric perturbations in terms of Φ and δ_S

$$\begin{aligned} \Phi'' + 3\mathcal{H}(1 + c_s^2)\Phi' + [2\mathcal{H}' + \mathcal{H}^2(1 + 3c_s^2)]\Phi + k^2 c_s^2 \Phi \\ = -\frac{2}{3} \frac{c_s^2}{M_p^2} a^2 \rho_m \delta_S, \end{aligned} \quad (\text{A12})$$

$$\frac{1}{3c_s^2} \delta_S'' + \frac{a'}{a} \delta_S' + \frac{k^2 y}{4} \delta_S = -\frac{1}{6} y^2 k^4 \tau_{\text{eq}}^2 \Phi, \quad (\text{A13})$$

where

$$\begin{aligned} y \equiv \frac{a}{a_{\text{eq}}} = \frac{\rho_m}{\rho_\gamma}, \quad \tau_{\text{eq}} = \frac{\sqrt{2}}{a_{\text{eq}} H_{\text{eq}}}, \\ c_s^{-2} \equiv 3 \left(1 + \frac{3}{4} y \right). \end{aligned} \quad (\text{A14})$$

In the $\eta \rightarrow 0$ limit, Eqs. (A12) and (A13) admit two linearly independent solutions $\Phi(k, \eta \rightarrow 0) = \Phi^i(k)$, $\delta_S(k, \eta \rightarrow 0) = 0$, and $\Phi(k, \eta \rightarrow 0) = 0$, $\delta_S(k, \eta \rightarrow 0) = \delta_S^i(k)$, which corresponds to adiabatic initial condition and isocurvature initial condition, respectively.

2. Adiabatic initial condition

For large scale perturbations, which enter the horizon later than the recombination, δ_S remains zero according to Eq. (A13), and thus Eq. (A12) is rewritten as

$$\frac{d^2\Phi}{dy^2} + \frac{21y^2 + 54y + 32}{2y(y+1)(3y+4)} \frac{d\Phi}{dy} + \frac{\Phi}{y(y+1)(3y+4)} = 0, \quad (\text{A15})$$

which is called the Kodama-Sasaki equation. This differential equation can be exactly solved, and we find

$$\Phi(k_l, y \gg 1) = \frac{9}{10} \Phi^i(k_l), \quad (\text{A16})$$

where the subscript l stands for ‘‘superhorizon.’’ For photon energy density δ_γ , Eq. (A4) in the long wavelength limit yields

$$\frac{1}{4} \delta_\gamma - \Phi = \text{const} \quad (\text{A17})$$

and also Eq. (A8) gives

$$\delta_\gamma(k_l, \eta \rightarrow 0) = -2\Phi(k_l, \eta) = -2\Phi^i(k_l). \quad (\text{A18})$$

For small scale perturbation, which enters the horizon during the radiation dominated (RD) era, in the early RD limit $\eta \ll \eta_{\text{eq}}$, Eq. (A12) becomes

$$\Phi'' + \frac{4}{\eta} \Phi' + \frac{k^2}{3} \Phi = 0, \quad (\text{A19})$$

and its solution with the adiabatic initial condition

$$\Phi(k_s, \eta < \eta_{\text{eq}}) = \frac{3}{(w\eta)^3} (\sin w\eta - w\eta \cos w\eta) \Phi^i(k_s), \quad (\text{A20})$$

where $w = k/\sqrt{3}$. After the perturbation enters the horizon,

$$\Phi(k_s, \eta < \eta_{\text{eq}}) \approx -\frac{3 \cos w\eta}{(w\eta)^2} \Phi^i(k_s), \quad (\text{A21})$$

$$\delta_\gamma(k_s, \eta < \eta_{\text{eq}}) \approx -\frac{2M_p^2}{\rho_\gamma a^2} \Phi(k_s, \eta) = 6\Phi^i(k_s) \cos w\eta, \quad (\text{A22})$$

where the subscript s means ‘‘subhorizon,’’ and the second equation is obtained by the Poisson equation (A10). Plugging this solution into Eq. (A6), we find that

$$\delta_m(k_s, \eta < \eta_{\text{eq}}) \approx -9\Phi^i(k_s) \left(\ln w\eta + \gamma - \frac{1}{2} \right), \quad (\text{A23})$$

where γ is the Euler gamma constant. This shows that the dark matter density perturbation grows logarithmically during the RD era.

Now we should match this with the solutions in the matter dominated (MD) era. Because the time derivatives

of Φ are negligible compared to the spatial derivatives, Eq. (A6) is approximated as

$$\delta_m'' + \mathcal{H} \delta_m' \approx -k^2 \Phi \approx \frac{3}{2} \mathcal{H}^2 \Omega_m \delta_m, \quad (\text{A24})$$

where we have used the Poisson equation (A10). Then, it is rewritten as

$$y(1+y) \frac{d^2\delta_m}{dy^2} + \left(1 + \frac{3}{2}y\right) \frac{d\delta_m}{dy} - \frac{3}{2}\delta_m = 0, \quad (\text{A25})$$

and its general solution is

$$\delta_m = c_1 \left(1 + \frac{3}{2}y\right) + c_2 \left[\left(1 + \frac{3}{2}y\right) \ln \frac{\sqrt{1+y} + 1}{\sqrt{1+y} - 1} - 3\sqrt{1+y} \right]. \quad (\text{A26})$$

Matching this solution with Eq. (A23) at $y \ll 1$, we find

$$\begin{aligned} \delta_m(k_s, \eta > \eta_{\text{eq}}) &= -9\Phi^i(k) \left(\ln 2w\eta_* + \gamma - \frac{7}{2} \right) \left(1 + \frac{3}{2}y\right) \\ &\quad + 9\Phi^i(k) \left[\left(1 + \frac{3}{2}y\right) \ln \frac{\sqrt{1+y} + 1}{\sqrt{1+y} - 1} - 3\sqrt{1+y} \right], \\ &\rightarrow -\frac{27}{2} y \Phi^i(k) \left(\ln 2w\eta_* + \gamma - \frac{7}{2} \right) \quad \text{when } y \gg 1, \end{aligned} \quad (\text{A27})$$

where $\eta_* \equiv \eta_{\text{eq}}/(\sqrt{2} - 1) = 2\tau_{\text{eq}}$. Note that we have used the results from the Friedmann equation

$$\mathcal{H}^2 = \frac{a_{\text{eq}}^2 H_{\text{eq}}^2}{2} \left(\frac{1}{y} + \frac{1}{y^2} \right), \quad (\text{A28})$$

$$y = \frac{\eta^2}{(2\tau_{\text{eq}})^2} + \frac{\eta}{\tau_{\text{eq}}}, \quad (\text{A29})$$

and Eq. (A27) corresponds to Eq. (150) in Ref. [136].

Then using Eqs. (A10) and (A27), we get

$$\Phi(k_s, \eta > \eta_{\text{eq}}) \approx \frac{\ln(0.15k_s \eta_{\text{eq}})}{(0.27k_s \eta_{\text{eq}})^2} \Phi^i(k_s). \quad (\text{A30})$$

This shows that the gravitational potential is frozen after the matter-radiation equality. Similarly, we first find the general solution of Eq. (A7) for subhorizon modes

$$\delta_\gamma = c_1 \cos w\eta + c_2 \sin w\eta - 4\Phi, \quad (\text{A31})$$

where we have neglected the time derivatives of Φ . Then matching this with Eq. (A22), we get

$$\delta_\gamma(k_s, \eta > \eta_{\text{eq}}) \approx \left[6 \cos(w\eta) - 4 \frac{\ln(0.15k_s \eta_{\text{eq}})}{(0.27k_s \eta_{\text{eq}})^2} \right] \Phi^i(k_s). \quad (\text{A32})$$

Now we return factors due to the Silk damping and the acoustic sound speed

$$\begin{aligned} \delta_\gamma(k_s, \eta > \eta_{\text{eq}}) &\approx \left[3^{5/4} \sqrt{4c_s} \cos\left(k_s \int^\eta c_s(\eta') d\eta'\right) e^{-(k_s/k_D)^2} \right. \\ &\quad \left. - \frac{4}{3c_s^2} \frac{\ln(0.15k_s \eta_{\text{eq}})}{(0.27k_s \eta_{\text{eq}})^2} \right] \Phi^i(k_s), \end{aligned} \quad (\text{A33})$$

which is Eq. (153) in Ref. [136]. Notice that the the first term is dominant for the scales we are interested in. However, the second term becomes important for very small scales where the diffusion damping is not negligible, $k \gtrsim k_D$.

Finally, the SW term (A1) becomes

$$\frac{\Delta T}{T} \approx \begin{cases} 6\Phi^i(k) \cos w\eta & \text{if } k > k_{\text{eq}} \\ \frac{3}{10}\Phi^i(k) & \text{if } k < \eta_r^{-1}. \end{cases} \quad (\text{A34})$$

Note that

$$\zeta^i \approx \zeta_R^i = -\Phi^i + \frac{1}{4}\delta_\gamma^i = -\frac{3}{2}\Phi^i. \quad (\text{A35})$$

3. Isocurvature initial condition

For large scale perturbations, δ_S remains constant, and Eq. (A12) has the solution

$$\Phi(k_l, \eta) = -\left(\frac{x}{5}\right) \frac{x^2 + 6x + 10}{(x+2)^3} \delta_S^i(k_l), \quad (\text{A36})$$

where $x \equiv \eta/\eta_{\text{eq}}$. In the MD era, Eq. (A36) gives

$$\begin{aligned} \Phi(k_l, \eta \gg \eta_{\text{eq}}) &= -\frac{1}{2} \delta_m(k_l, \eta \gg \eta_{\text{eq}}) \\ &= \frac{1}{4} \delta_\gamma(k_l, \eta \gg \eta_{\text{eq}}) \\ &= -\frac{1}{5} \delta_S^i(k_l), \end{aligned} \quad (\text{A37})$$

where the last two equations are obtained from Eq. (A8).

Now, we will see how the perturbations evolve during the RD era, and how they are connected to small scale perturbations. In the early RD era, the source term and the last term on the left-hand side of Eq. (A13) are negligible because they are higher order in y . Thus, the solution δ_S remains constant even inside the horizon. In that case, Eq. (A12) becomes Eq. (A19) with the source term $\delta_S/2y\eta_{\text{eq}}^2$. Then we find its solution that matches with Eq. (A36)

$$\begin{aligned} \Phi(k, \eta < \eta_{\text{eq}}) &= -\frac{\eta}{\eta_{\text{eq}}} \frac{1}{(w\eta)^4} \left[1 + \frac{(w\eta)^2}{2} - (\cos w\eta + w\eta \sin w\eta) \right] \\ &\quad \times \delta_S^i(k). \end{aligned} \quad (\text{A38})$$

Furthermore, in the $w\eta \rightarrow 0$ limit, we have

$$\Phi(k_l, \eta < \eta_{\text{eq}}) \approx -\frac{1}{8} \delta_S^i(k_l) \left(1 - \frac{(w\eta)^2}{18} \right) y, \quad (\text{A39})$$

and putting this into Eq. (A8), we find that

$$\delta_\gamma(k_l, \eta < \eta_{\text{eq}}) \approx -\frac{1}{2} \delta_S^i(k_l) \left(1 - \frac{7}{18} (w\eta)^2 \right) y, \quad (\text{A40})$$

$$\delta_m(k_l, \eta < \eta_{\text{eq}}) \approx \delta_S^i(k_l) \left(1 - \frac{3}{8} y \right) + \frac{7}{48} \delta_S^i(k_l) y (w\eta)^2. \quad (\text{A41})$$

As explained in Sec. II B, we have that Φ and δ_γ grow like a during the RD era; meanwhile δ_m decreases.

For subhorizon modes, Eq. (A38) becomes

$$\Phi(k_s, \eta < \eta_{\text{eq}}) \approx -\frac{y}{(w\eta)^3} \left(\frac{w\eta}{2} - \sin w\eta \right) \delta_S^i(k_s), \quad (\text{A42})$$

and again plugging this into Eq. (A8) yields

$$\delta_m(k_s, \eta < \eta_{\text{eq}}) \approx -\left(\frac{3}{2} \frac{\sin w\eta}{w\eta} y - 1 \right) \delta_S^i(k_s), \quad (\text{A43})$$

$$\delta_\gamma(k_s, \eta < \eta_{\text{eq}}) \approx -\frac{2 \sin w\eta}{w\eta} y \delta_S^i(k_s). \quad (\text{A44})$$

Matching these with general solutions of perturbations (A26) and (A31), and also using Poisson equation (A10) in the MD era, we get

$$\delta_m(k_s, \eta > \eta_{\text{eq}}) \approx \left(1 + \frac{3}{2} y \right) \delta_S^i(k_s), \quad (\text{A45})$$

$$\begin{aligned} \delta_\gamma(k_s, \eta > \eta_{\text{eq}}) &\approx \left[-\frac{1}{0.35k_s \eta_{\text{eq}}} \sin(w\eta) \right. \\ &\quad \left. + 4 \frac{1}{(0.8k_s \eta_{\text{eq}})^2} \right] \delta_S^i(k_s), \end{aligned} \quad (\text{A46})$$

$$\Phi(k_s, \eta > \eta_{\text{eq}}) \approx -\frac{1}{(0.8k_s \eta_{\text{eq}})^2} \delta_S^i(k_s). \quad (\text{A47})$$

Then the SW term becomes

$$\frac{\Delta T}{T} \approx \begin{cases} -\frac{1}{0.35k\eta_{\text{eq}}} \delta_S^i(k) \sin(w\eta) & \text{if } k > k_{\text{eq}} \\ -\frac{2}{5} \delta_S^i(k) & \text{if } k < \eta_r^{-1}. \end{cases} \quad (\text{A48})$$

Now we see from Eqs. (A34) and (A48) that the isocurvature transfer function has the additional suppression factor k_{eq}/k compared to the adiabatic one for small scale $k > k_{\text{eq}}$.

APPENDIX B: REVIEW OF DIFFEOMORPHISM INVARIANCE

A symmetry in a classical field theory is preserved at the quantum level, if the regulator preserves this symmetry and

if the functional measure is invariant under the symmetry transformation. The quantum symmetry is reflected in the transformation of the correlation functions.

For example, consider a scalar field σ on a fixed manifold (\mathcal{M}, g) . The two-point function is

$$\langle \sigma(x)\sigma(y) \rangle_g = \int D\phi e^{iS(\sigma;g)} \sigma(x)\sigma(y). \quad (\text{B1})$$

The two-point function only depends on the metric field g and points x, y . Intuitively, the symmetry says for any diffeomorphism $\varphi: \mathcal{M} \mapsto \mathcal{M}$, the metric field and the points change as

$$g \mapsto \tilde{g} = (\varphi^{-1})^* g, \quad x \mapsto \tilde{x} = \varphi(x), \quad y \mapsto \tilde{y} = \varphi(y); \quad (\text{B2})$$

then the two-point function should remain invariant, i.e.,

$$\langle \sigma(x)\sigma(y) \rangle_g = \langle \sigma(\tilde{x})\sigma(\tilde{y}) \rangle_{\tilde{g}}. \quad (\text{B3})$$

The Ward identity is the infinitesimal version of this relation.

Let $\varphi = \exp(\epsilon X)$; then

$$\tilde{g} = \exp(-\epsilon X)^* g = g - \epsilon \mathcal{L}_X g + \dots \quad (\text{B4})$$

$$S(\tilde{g}, \sigma) = S(g, \sigma) - \epsilon \int d^4x \sqrt{g} \frac{1}{2} T_{\sigma}^{\mu\nu} \mathcal{L}_X(g)_{\mu\nu} + \dots \quad (\text{B5})$$

$$\sigma(\tilde{x}) = \sigma(x) + \epsilon \mathcal{L}_X \sigma(x) + \dots \quad (\text{B6})$$

Plugging this into Eq. (B3) and Taylor-expanding with respect to ϵ , one gets

$$-i \int d^4z \sqrt{g} \frac{1}{2} \mathcal{L}_X(g)_{\mu\nu}(z) \langle T_z^{\mu\nu} \sigma_x \sigma_y \rangle_g + \langle \mathcal{L}_X(\sigma)_x \sigma_y \rangle_g + \langle \sigma_x \mathcal{L}_X(\sigma)_y \rangle_g = 0. \quad (\text{B7})$$

Or equivalently, using

$$\mathcal{L}_X(g)_{\mu\nu} = \nabla_\mu X_\nu + \nabla_\nu X_\mu \quad (\text{B8})$$

and performing integration by part, we obtain

$$i \nabla_\mu \langle T_z^{\mu\nu} \sigma_x \sigma_y \rangle_g = \frac{1}{\sqrt{g_x}} \delta^4(x-z) g_x^{\alpha\nu} \frac{\partial}{\partial x^\alpha} \langle \sigma_x \sigma_y \rangle_g + \frac{1}{\sqrt{g_y}} \delta^4(y-z) g_y^{\alpha\nu} \frac{\partial}{\partial y^\alpha} \langle \sigma_x \sigma_y \rangle_g \quad (\text{B9})$$

which is the Ward identity for the path ordered vacuum expectation value. We can then write down the in-in expectation value Ward identity as

$$i \nabla_\mu \langle in | T_z^{\mu\nu+} \sigma_x^+ \sigma_y^+ | in \rangle_g = \frac{1}{\sqrt{g_x}} \delta^4(x-z) g_x^{\alpha\nu} \frac{\partial}{\partial x^\alpha} \langle in | \sigma_x^+ \sigma_y^+ | in \rangle_g + \frac{1}{\sqrt{g_y}} \delta^4(y-z) g_y^{\alpha\nu} \frac{\partial}{\partial y^\alpha} \langle in | \sigma_x^+ \sigma_y^+ | in \rangle_g \quad (\text{B10})$$

$$i \nabla_\mu \langle in | T_z^{\mu\nu-} \sigma_x^+ \sigma_y^+ | in \rangle_g = 0, \quad (\text{B11})$$

where we kept the external operator inserted on the forward branch. The fact that Eq. (B11) has no contact term is easy to understand: since $T_z^{\mu\nu-}$ is inserted on the backward time branch of the manifold, it can never *contact* points x and y .

APPENDIX C: ADM FORMALISM AND INTERACTION HAMILTONIAN

We consider an inflationary model with the inflaton ϕ and an extra free massive scalar σ , where σ is only gravitationally coupled with ϕ :

$$S = \int (dx) \frac{1}{2} M_p^2 R + \left[-\frac{1}{2} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - V(\phi) \right] + \left[-\frac{1}{2} g^{\mu\nu} \partial_\mu \sigma \partial_\nu \sigma - U(\sigma) \right], \quad (\text{C1})$$

where $M_p^2 = \frac{1}{8\pi G} = 1$ and $(dx) = d^4x \sqrt{|\det(g_{\mu\nu})|}$. The metric can be parametrized using ADM formalism [137],¹⁹

$$g_{\mu\nu} = \begin{pmatrix} -N^2 + h_{ij} N^i N^j & h_{ij} N^j \\ h_{ij} N^j & h_{ij} \end{pmatrix}, \quad (\text{C2})$$

$$g^{\mu\nu} = \begin{pmatrix} -N^{-2} & N^i N^{-2} \\ N^i N^{-2} & h^{ij} - N^i N^j N^{-2} \end{pmatrix},$$

where h_{ij} is the metric tensor on the constant time hypersurface, and h^{ij} is the inverse metric. We use Latin indices i, j, \dots for objects on the three-dimensional constant time hypersurface, and we use h_{ij} and h^{ij} to raise and lower the indices. Then the action (C1) is rewritten as

$$S = \frac{1}{2} \int (dx) \sqrt{h} [NR^{(3)} - 2NV(\phi) - 2NU(\sigma) + N^{-1}(E_{ij}E^{ij} - E^2) + N^{-1}(\dot{\phi} - N^i \partial_i \phi)^2 - Nh^{ij} \partial_i \phi \partial_j \phi + N^{-1}(\dot{\sigma} - N^i \partial_i \sigma)^2 - Nh^{ij} \partial_i \sigma \partial_j \sigma], \quad (\text{C3})$$

where E_{ij} and E are given by

$$E_{ij} = \frac{1}{2} (\dot{h}_{ij} - \nabla_i^{(3)} N_j - \nabla_j^{(3)} N_i), \quad (\text{C4})$$

¹⁹We use $(-+++)$ sign convention for the metric, and physical time t .

$$E = E_{ij}h^{ij}. \quad (\text{C5})$$

Consider the background solution driven by the inflaton,

$$\phi^{(0)} = \bar{\phi}(t), \quad \sigma^{(0)} = 0, \quad g_{\mu\nu}^{(0)} = \begin{pmatrix} -1 & 0 \\ 0 & a^2(t)\delta_{ij} \end{pmatrix}, \quad (\text{C6})$$

where they satisfy the background equations of motion

$$3H^2 = \frac{1}{2}\dot{\bar{\phi}}^2 + V(\bar{\phi}) \quad (\text{C7})$$

$$\dot{H} = -\frac{1}{2}\dot{\bar{\phi}}^2 \quad (\text{C8})$$

$$\ddot{\bar{\phi}} + 3H\dot{\bar{\phi}} + V'(\bar{\phi}) = 0. \quad (\text{C9})$$

The action for the perturbations can be obtained by Taylor-expanding the full action around the background solution. However, we may reduce the number of variables by imposing the ADM constraints:

$$0 = \frac{1}{N} \left[R^{(3)} - \frac{1}{N^2} (E_{ij}E^{ij} - E^2) \right] - 2NT^{00} \quad (\text{C10})$$

$$0 = \frac{2}{N} \nabla_i^{(3)} \left[\frac{1}{N} (E^{ij} - Eh^{ij}) \right] + 2N^j T^{00} + 2T^{0j}, \quad (\text{C11})$$

where

$$T^{\mu\nu} = T_{\phi}^{\mu\nu} + T_{\sigma}^{\mu\nu}, \quad (\text{C12})$$

$$T_{\phi}^{\mu\nu} = -g^{\mu\nu} \left[\frac{1}{2} (\partial\phi)^2 + V(\phi) \right] + \partial^\mu\phi\partial^\nu\phi, \quad (\text{C13})$$

$$T_{\sigma}^{\mu\nu} = -g^{\mu\nu} \left[\frac{1}{2} (\partial\sigma)^2 + U(\sigma) \right] + \partial^\mu\sigma\partial^\nu\sigma, \quad (\text{C14})$$

and choose a gauge.

One commonly used gauge is the comoving gauge, defined by²⁰

$$\delta\phi = 0, \quad \gamma_{ii} = 0, \quad \partial_i\gamma_{ij} = 0, \quad (\text{C15})$$

where

$$h_{ij} = a^2(t)[e^\Gamma]_{ij}, \quad \Gamma_{ij} = 2\zeta\delta_{ij} + \gamma_{ij}. \quad (\text{C16})$$

The solution of N and N^i is

$$N^{(1,C)} = \frac{\dot{\zeta}}{H}, \quad N_i^{(1,C)} = \partial_i \left[-\frac{\zeta}{H} + \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta} \right]. \quad (\text{C17})$$

We find the scalar metric perturbations are

$$\delta g_{\mu\nu}^{(C)} = \begin{pmatrix} -2\frac{\dot{\zeta}}{H} & \left(-\frac{\zeta}{H} + \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta} \right)_i \\ \left(-\frac{\zeta}{H} + \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta} \right)_i & a^2\delta_{ij}2\zeta \end{pmatrix}, \quad (\text{C18})$$

where $\epsilon \equiv \dot{H}/H^2$. Plugging in the linear metric perturbation back to the action (C3), we can get the perturbed action up to cubic order

$$S^{(C)} = S_{\zeta\zeta}^{(C)} + S_{\sigma\sigma}^{(C)} + S_{\gamma\gamma}^{(C)} + S_{\zeta\zeta\zeta}^{(C)} + S_{\zeta\sigma\sigma}^{(C)} + \dots, \quad (\text{C19})$$

where

$$S_{\zeta\zeta}^{(C)} = \int dt d^3x a_x^3 \epsilon \left(\dot{\zeta}^2 - \left(\frac{\nabla}{a} \zeta \right)^2 \right) \quad (\text{C20})$$

$$S_{\zeta\sigma\sigma}^{(C)} = \int d^4x a_x^3 \left[T_{\sigma}^{ij} a^2 \delta_{ij} \zeta + T_{\sigma}^{0i} \left(-\frac{\zeta}{H} + \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta} \right)_i - T_{\sigma}^{00} \frac{\dot{\zeta}}{H} \right]. \quad (\text{C21})$$

The ζ cubic interaction and graviton actions can be found in [44].

Another commonly used gauge is the uniform curvature gauge, in which

$$h_{ij} = a^2(t)[e^\gamma]_{ij}, \quad \gamma_{ii} = 0, \quad \partial_i\gamma_{ij} = 0. \quad (\text{C22})$$

In this gauge, the inflaton degree of freedom is in $\delta\phi$. However, this degree of freedom can be represented using the gauge invariant variable

$$\zeta = -\frac{H}{\dot{\phi}} \delta\phi^{(U)}. \quad (\text{C23})$$

In this gauge, the ADM constraint renders

$$N^{(1,U)} = -\epsilon\zeta, \quad N_i^{(1,U)} = \partial_i \left[\epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta} \right]. \quad (\text{C24})$$

We get the linear metric perturbation as

$$\delta g_{\mu\nu}^{(U)} = \begin{pmatrix} 2\epsilon\zeta & \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta}_{,i} \\ \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta}_{,i} & 0 \end{pmatrix}. \quad (\text{C25})$$

The free action is the same as in Eq. (C20), and the σ - ζ cubic interaction action is

$$S_{\zeta\sigma\sigma}^{(U)} = \int d^4x a_x^3 \left[T_{\sigma}^{00} \epsilon\zeta + T_{\sigma}^{0i} \epsilon \frac{a^2}{\sqrt{2}} \dot{\zeta}_{,i} \right]. \quad (\text{C26})$$

From these perturbed actions, we can obtain the interaction Hamiltonian. Particularly, note that up to the cubic interaction, $\mathcal{L}_{\text{int}} = -\mathcal{H}_{\text{int}}$. Thus $S_{\zeta\sigma\sigma} = -\int dt H_{\zeta\sigma\sigma}(t)$.

APPENDIX D: RENORMALIZATION OF COMPOSITE OPERATORS

In renormalized perturbation theory, one requires a regulator and renormalization condition. In order to preserve the diffeomorphism invariance, we need to adopt a

²⁰In this section, latin indices i, j are raised and lowered by δ_{ij} , and repeated indices are contracted.

covariant regulator. Here we choose the PV regulator, following [138,139]. We will first review PV regularization in Appendix D 1, and renormalize σ^2 in Appendix D 2. For correlators involving time integrals, we describe the adiabatic expansion of time integral in Appendix D 3.

1. Pauli-Villars regularization

We introduce a set of scalar regulator fields χ_n for $n = 1, \dots, s$ with the following free Lagrangian:

$$\mathcal{L}_{\text{PV}} = \sum_{n=1}^s C_n \left(-\frac{1}{2} g^{\mu\nu} \partial_\nu \chi_n \partial_\nu \chi_n - \frac{1}{2} M_n^2 \chi_n^2 \right). \quad (\text{D1})$$

The number of regulator fields s depends on how many independent divergences one needs to remove. In order to eliminate UV divergences up to some even order $2D$, we must take the C_n and regulator masses M_n to satisfy

$$\sum_{N=0}^s C_N^{-1} = 0, \quad \sum_{N=0}^s C_N^{-1} M_N^2 = 0, \dots \quad (\text{D2})$$

$$\sum_n C_n^{-1} M_n^{2D} = -m_\sigma^{2D}, \quad (\text{D3})$$

where we used the notation $M_0^2 = m_\sigma^2$ and $C_0 = 1$, and let $\sigma_0 = \sigma$ and $\sigma_n = \chi_n$. We use Λ to represent the set of M_n , and the regulator dependence should be removed by counterterms when M_1, M_2, \dots, M_s go to ∞ together.

On a homogeneous Friedmann-Robertson-Walker background, the physical and regulator scalar field can be quantized as

$$[\sigma_N, \dot{\sigma}_M] = i a^{-3}(t) \delta^3(\vec{x} - \vec{y}) \delta_{NM} C_N^{-1} \quad (\text{D4})$$

with the following mode decomposition:

$$\sigma_N(\vec{x}, t) = \int \frac{d^3 k}{(2\pi)^3} (a_{N,\vec{k}} u_{N,\vec{k}}(t) + \text{c.c.}) \quad (\text{D5})$$

$$[a_{N,\vec{p}}, a_{M,\vec{k}}^\dagger] = (2\pi)^3 C_N^{-1} \delta_{NM} \delta^3(\vec{k} - \vec{p}), \quad (\text{D6})$$

where $u_{N,\vec{p}}(t)$ satisfies the usual equation of motion

$$\ddot{u}_{N,k} + 3H\dot{u}_{N,k} + \left(\frac{k^2}{a^2} + M_N^2 \right) u_{N,k} = 0 \quad (\text{D7})$$

with the Bunch-Davies initial condition

$$u_{N,k}(t) \rightarrow \frac{1}{\sqrt{2ka(t)}} \exp\left(-i \int^t \frac{k}{a(t')} dt'\right) \quad \text{for } t \rightarrow -\infty \quad (\text{D8})$$

and Wronskian conditions²¹

²¹Our treatment here differs from [138] in that the physical scalar field ϕ here has no background solution, and the regulator field χ_n does not mix with ϕ by the mass term.

$$u_{N,k} \dot{u}_{N,k}^* - \dot{u}_{N,k} u_{N,k}^* = i/a^3. \quad (\text{D9})$$

Because $M_n \gg H$, Eq. (D7) possesses the WKB-type solution

$$u_{n,k}(t) = \frac{1}{\sqrt{2\omega_k(t)a^3(t)}} \exp\left(-i \int^t \omega_k(t') dt'\right) \left[1 + \frac{f_1(t)}{\omega_k(t)} + \frac{f_2(t)}{\omega_k^2(t)} + O(\omega_k^{-3}) \right], \quad (\text{D10})$$

where $\omega_k = \sqrt{k^2/a^2 + M_n^2}$ and f_i are of zeroth order in ω_k . Since we have to regulate up to quadratic divergence in correlator computations, we need to know

$$|u_{n,k}(t)|^2 = \frac{1}{2\omega_k(t)a^3(t)} \left[1 + \frac{2\text{Re}f_1(t)}{\omega_k(t)} + \frac{|f_1(t)|^2 + 2\text{Re}f_2(t)}{\omega_k^2(t)} + O(\omega_k^{-3}) \right] \quad (\text{D11})$$

up to second order. Due to the equation of motion (D7), f_1 should satisfy

$$\frac{d}{dt} \left(\frac{f_1}{\omega_k} \right) = \frac{i}{2\omega_k} \left(\dot{H} + 2H^2 + \frac{1}{2} \frac{(\dot{H} + 3H^2)M_n^2}{\omega_k^2} - \frac{5}{4} \frac{H^2 M_n^4}{\omega_k^4} \right). \quad (\text{D12})$$

Also, the Wronskian condition (D9) yields

$$\text{Re} f_1 = 0, \quad |f_1|^2 + 2\text{Re}f_2 = \omega_k \frac{d}{dt} \left(\frac{\text{Im}f_1}{\omega_k} \right). \quad (\text{D13})$$

Then plugging these two results into Eq. (D11) gives

$$|u_{n,k}|^2 = \frac{1}{2\omega_k a^3} \left[1 + \frac{\dot{H} + 2H^2}{2\omega_k^2} + \frac{(\dot{H} + 3H^2)M_n^2}{4\omega_k^4} - \frac{5H^2 M_n^4}{8\omega_k^6} + O(\omega^{-3}) \right]. \quad (\text{D14})$$

2. Renormalization of composite operator

The renormalization of composite operators in curved space-time is the same as in flat space-time (see, e.g., [87,88,139]), just with new possible counterterms made from the curvature tensor. For an operator of dimension n , one needs to consider all possible counterterms of dimension n or less. In our example model with free massive scalar σ , we renormalize σ^2 as

$$(\sigma^2)_r = \left(\sigma + \sum_n \chi_n \right)^2 + \delta Z_0(\Lambda, m_\sigma) + \delta Z_1(\Lambda, m_\sigma) R, \quad (\text{D15})$$

where R is the Ricci scalar.

Next, we compute δZ_i 's divergent part. For example, let us consider the one-point function

$$\langle\langle\sigma^2\rangle_r\rangle = \sum_{N=0}^s C_N^{-1} \int \frac{d^3k}{(2\pi)^3} |u_{N,k}|^2 + \delta Z_0 + \delta Z_1 R. \quad (\text{D16})$$

In order to determine the counterterms δZ_0 and δZ_1 , we introduce a comoving scale Q such that $H \ll Q/a \ll M_n$ to break the Fourier space into the UV and the IR sector. Then we use the WKB solution (D14) for $k \gg Q$. Furthermore, the contribution from the PV fields for $k \ll Q$ vanishes since it is suppressed by $1/M_n$:

$$\begin{aligned} & \sum_N C_N^{-1} \int \frac{d^3k}{(2\pi)^3} |u_{N,k}|^2 \\ &= \int^Q \frac{d^3k}{(2\pi)^3} |u_{0,k}|^2 + \sum_{N=0}^s C_N^{-1} \int_Q^{\Lambda_{uv}} \frac{d^3k}{(2\pi)^3} |u_{i,k}|^2 \\ &= \int^Q \frac{d^3k}{(2\pi)^3} |u_{0,k}|^2 + \frac{1}{48\pi^2} R \left(\ln \frac{a}{2Q} + \frac{10}{12} \right) \\ &\quad - \frac{1}{96\pi^2} R \sum_{N=0}^s C_N^{-1} \ln M_N^2 \\ &\quad + \frac{1}{16\pi^2} \sum_{N=0}^s C_N^{-1} M_N^2 \ln M_N^2. \end{aligned} \quad (\text{D17})$$

Note that the arbitrary comoving scales Q in the first two terms should cancel each other.

In order to absorb the PV regulator dependence, we need

$$\delta Z_0 = \frac{1}{16\pi^2} \left[-\sum_N C_N^{-1} M_N^2 \ln M_N^2 + \mu_0^2 \right], \quad (\text{D18})$$

$$\delta Z_1 = \frac{1}{96\pi^2} \left[\sum_N C_N^{-1} \ln \frac{M_N^2}{\mu_1^2} \right], \quad (\text{D19})$$

where μ_0 and μ_1 are unknown mass scales determined by renormalization conditions. We set $\mu_0 = 0$ to have $\langle\langle\sigma_r^2\rangle\rangle = 0$ for flat space-time.

3. Adiabatic expansion of time integral

In order to compute some correlators using the in-in formalism (32), such as two-point function $\langle\sigma^2 \zeta\rangle$, we need to integrate PV field contributions over time. In this subsection, we present how to calculate the time integral of PV fields by adiabatically expanding the integral.

For simplicity, consider a diagram with one internal vertex. Using the WKB solution (D14) of a PV field, the general form of the time integral is

$$I(k_1, k_2, \dots, t_f) = \int_{-\infty}^{t_f} dt G(k_1, k_2, \dots; t_f, t) e^{-i \int_t^{t_f} \omega(t') dt'}, \quad (\text{D20})$$

where $\omega(t) = \omega_{k_1}(t) + \omega_{k_2}(t) + \dots$ and $G(k_1, k_2, \dots; t_f, t) = O(\omega^n)$. Because the integrand is a rapidly oscillatory

function, the dominant contribution comes near the final time t_f . Thus, using integration by parts we expand the integral with respect to ω :

$$\begin{aligned} & I(k_1, k_2, \dots, t_f) \\ &= \frac{G(k_1, k_2, \dots; t_f, t_f)}{i\omega(t_f)} \\ &\quad - \int_{-\infty}^{t_f} dt \left(\frac{d}{dt} \frac{G(k_1, k_2, \dots; t_f, t)}{i\omega(t)} \right) e^{-i \int_t^{t_f} \omega(t') dt'} \end{aligned} \quad (\text{D21})$$

$$\begin{aligned} &= \frac{G(k_1, k_2, \dots; t_f, t_f)}{i\omega(t_f)} - \left(\frac{1}{i\omega(t)} \frac{d}{dt} \frac{G(k_1, k_2, \dots; t_f, t)}{i\omega(t)} \right) \Big|_{t=t_f} \\ &\quad + \left[\frac{1}{i\omega(t)} \frac{d}{dt} \left(\frac{1}{i\omega(t)} \frac{d}{dt} \frac{G(k_1, k_2, \dots; t_f, t)}{i\omega(t)} \right) \right] \Big|_{t=t_f} \\ &\quad + O(\omega^{n-4}). \end{aligned} \quad (\text{D22})$$

Note that the mode functions $u_{n,k}$ and $u_{n,k}^*$ appear in pairs because of Wick contraction. Hence, the final result should be written in terms of $|u_{n,k}(t_f)|^2$ and their time derivatives, and we can compute the time integral up to an arbitrary order of ω . It is straightforward to generalize this to the cases with any number of internal vertices.

APPENDIX E: TWO-POINT FUNCTION $\langle\langle\sigma^2\rangle_r \zeta\rangle$ IN THE UNIFORM CURVATURE GAUGE

In this section, we compute $\langle\langle\sigma^2\rangle_r \zeta\rangle$ using the uniform curvature gauge in the quasi-dS background, where the slow-roll factor ϵ is constant. Then we will show that the results in both gauges are consistent with each other. Particularly, for the massless limit, the next leading order term in the uniform curvature gauge indeed decays as p^2/a^2 .

The two-point function is the same as in the comoving gauge except that the counterterm contribution appears in the leading order:

$$\begin{aligned} \langle\langle\sigma^2\rangle_r \zeta\rangle_p^U &= \int d^3x e^{-i\vec{p}\cdot\vec{x}} \int^t d^4z a^3(t_z) \\ &\quad \times \sum_{N=0}^n \left\langle \left[\sigma_N^2(t, \vec{x}) \zeta(t, \vec{0}), \frac{i}{2} (T_{\sigma}^{\mu\nu} \delta g_{\mu\nu}^{(U)})_z \right] \right\rangle \\ &\quad + \delta Z_1 \langle \widetilde{R} \zeta \rangle_p, \end{aligned} \quad (\text{E1})$$

where R is the Ricci scalar. After taking nonderivative interaction term $T_{\sigma}^{00} \delta g_{00}^{(U)}$ only, factoring ϵ and ζ out from the integral, we get

$$\begin{aligned} \langle\langle\sigma^2\rangle_r \zeta\rangle_p^U &= i |\zeta_p^0|^2 \epsilon \int^t d^4z a^3(t_z) \sum_{N=0}^n \langle [\sigma_N^2(t, \vec{x}), (T_{\sigma}^{00})_z] \rangle \\ &\quad + 24\epsilon H^2 |\zeta_p^0|^2 \delta Z_1 + O\left(\dot{\epsilon}, \epsilon^2, \frac{p^2}{a^2}\right), \end{aligned} \quad (\text{E2})$$

where we have used the perturbed curvature in the uniform curvature gauge

$$R = 12H^2 - 6\epsilon H^2 + 24\epsilon H^2 \zeta + 4\epsilon H \dot{\zeta} + \dots, \quad (\text{E3})$$

where \dots denotes $O(\dot{\epsilon}, \epsilon^2)$ terms or terms proportional to the equation of motion of ζ .

Since $T_\sigma^{00} = \mathcal{L}_\sigma + \sum_N [(\frac{\nabla}{a} \sigma_N)^2 + M_N^2 \sigma_N^2]$, together with the identities (93) and (96), and

$$i \int^t d^4 z a^3(t_z) \langle [\sigma_N^2(t, \vec{x}), \sigma_N^2(z)] \rangle = -2 \frac{\partial}{\partial M_N^2} \langle (\sigma_N^2)_p \rangle, \quad (\text{E4})$$

with $T_\sigma^{00} = \mathcal{L}_\sigma + \sum_N [(\frac{\nabla}{a} \sigma_N)^2 + M_N^2 \sigma_N^2]$, we have

$$\begin{aligned} & \langle (\sigma^2)_R \zeta \rangle_p^U + \frac{1}{H} \frac{d}{dt} \langle (\sigma^2)_R \rangle \langle \zeta \zeta \rangle_p \\ &= \sum_N F_N(t) + O(\dot{\epsilon}, \epsilon^2, \frac{p^2}{a^2}), \end{aligned} \quad (\text{E5})$$

$$\begin{aligned} F_N(t) &= \epsilon \left(2 \langle (\sigma_N^2)_p \rangle - Z_N^{-1} \frac{k^3}{2\pi^2} |u_{N,k}|^2 \right)^{\Lambda_{UV}} \\ &\quad - 2M_N^2 \frac{\partial}{\partial M_N^2} \langle (\sigma_N^2)_p \rangle + \frac{1}{H} \frac{d}{dt} \langle \sigma_N^2 \rangle. \end{aligned} \quad (\text{E6})$$

Although the rhs of Eq. (E1) is well defined and regulator independent, individual terms are not. Thus, we insert counterterms to have each term regulator independent:

$$\begin{aligned} \sum_N F_N(t) &= \epsilon \left(2 \langle (\sigma^2(t))_{r,p} \rangle + \frac{p^3}{2\pi^2} |u_p(t)|^2 \right. \\ &\quad \left. - 2m_\sigma^2 \frac{\partial}{\partial m_\sigma^2} \langle (\sigma^2(t))_{r,p} \rangle + \frac{1}{H} \frac{d}{dt} \langle (\sigma^2)_r \rangle \right), \end{aligned} \quad (\text{E7})$$

where we have put the counterterms δZ_0 and $\delta Z_1 R$ into each one-point function, and the PV field contribution from the third term cancels with those from the other terms. Then, using the relation (75) one can find that the rhs of Eq. (E7) is consistent with the result (99) in the comoving gauge in the quasi-dS background after explicitly computing renormalized one-point function $\langle (\sigma^2(t))_{r,p} \rangle$. On the other hand, the rhs does not depend on the renormalization as all counterterms cancel. Hence, we can arrive at the same conclusion using the one-point function using super-horizon approximation in the dS space-time,

$$\begin{aligned} \langle (\sigma^2(t))_{r,p} \rangle &\approx \int_p^{caH} \frac{d^3 k}{(2\pi)^3} |u_k(t)|^2 \\ &\approx \int_p^{caH} \frac{d^3 k}{(2\pi)^3} \frac{|\Gamma(\nu)|^2}{4\pi H a^3} \left(\frac{k}{2aH} \right)^{-2\nu}, \end{aligned} \quad (\text{E8})$$

where the arbitrary constant $c \lesssim O(1)$. Note that the UV boundary of the integral should be a comoving scale in order to keep the spatial dilatation symmetry.

1. Massless limit

For the massless limit $m_\sigma^2/H^2 \ll \ln p/aH$, we can compute the two-point function explicitly without neglecting any gravitational couplings. We calculate up to the next leading term here. We decompose Eq. (E1) as

$$\langle (\sigma^2)_r \zeta \rangle_p^U = I_0(p, t) + \sum_{n=1}^s I_n(p, t) + I_{c.t.}(p, t), \quad (\text{E9})$$

where I_0 , I_n , and $I_{c.t.}$ are the contributions from the physical field σ , the PV field χ_i and the counterterms, respectively. Since all the gravitational couplings are $O(\epsilon)$ [see Eq. (C26)], we may use the mode functions ζ_p and u_k in the pure dS for $O(\epsilon)$ correction to the two-point function. Then a long but straightforward calculation gives

$$\begin{aligned} I_0(p, t) &= \int d^3 x e^{-i\vec{p}\cdot\vec{x}} \int^t d^4 z a^3(t_z) \\ &\quad \times \sum_{N=0}^n \left\langle \left[\sigma^2(t, \vec{x}) \zeta(t, \vec{0}), \frac{i}{2} (T_\sigma^{\mu\nu} \delta g_{\mu\nu}^{(U)})_z \right] \right\rangle \\ &= \frac{1}{4\pi^2} \epsilon H^2 |\zeta_p^o|^2 \left[-\frac{1}{3} \frac{p^3}{a^3 H^3} \frac{\Lambda}{aH} + 2 \log \frac{\Lambda}{p} \right. \\ &\quad \left. + \frac{5}{3} \frac{p^2}{a^2 H^2} \log \frac{\Lambda}{p} + 1 - \frac{p^2}{a^2 H^2} + O\left(\frac{p^4}{a^4 H^4}\right) \right] \\ &\quad + O(\epsilon^2, \dot{\epsilon}). \end{aligned} \quad (\text{E10})$$

The PV field contribution I_n requires some more technical explanation. If we write the WKB solution (D11) as

$$u_{n,k}(t) = \alpha_k(t) e^{-i \int^t \omega_k(t') dt'}, \quad (\text{E12})$$

the PV field contribution I_n is written as

$$\begin{aligned} I_n(p, t) &= C_n^{-1} \int_Q \frac{d^3 k_1}{(2\pi)^3} d^3 k_2 \delta^{(3)}(\vec{k}_1 + \vec{k}_2 - \vec{p}) \\ &\quad \times \text{Im} \left[\int^t dt_z e^{i \int_{t_z}^t (\omega_{k_1}(t') + \omega_{k_2}(t')) dt'} G_n(k_1, k_2; t, t_z) \right], \end{aligned} \quad (\text{E13})$$

where

$$\begin{aligned} G_n(k_1, k_2; t, t_z) &= -2a_z^3 \zeta_p(t) \alpha_{k_1}(t) \alpha_{k_2}(t) \\ &\quad \times \left(\sum_i \widehat{O}_i \right) \zeta_p^*(t_z) \alpha_{k_1}^*(t_z) \alpha_{k_2}^*(t_z), \end{aligned} \quad (\text{E14})$$

$$\begin{aligned} (\widehat{O}_1) &= \frac{1}{2} \left[(i\omega_{k_1}(t_z) + \partial_{t_z}^{(1)}) (i\omega_{k_2}(t_z) + \partial_{t_z}^{(2)}) \right. \\ &\quad \left. - \frac{\vec{k}_1 \cdot \vec{k}_2}{a_z^2} + M_n^2 \right] (2\epsilon), \end{aligned} \quad (\text{E15})$$

$$\begin{aligned} (\widehat{O}_2) &= \left[\frac{\vec{k}_2 \cdot \vec{p}}{a_z^2} (i\omega_{k_1}(t_z) + \partial_{t_z}^{(1)}) + \frac{\vec{k}_3 \cdot \vec{p}}{a_z^2} (i\omega_{k_2}(t_z) + \partial_{t_z}^{(2)}) \right] \\ &\quad \times \left(\epsilon \frac{a_z^2}{p^2} \partial_{t_z}^\zeta \right), \end{aligned} \quad (\text{E16})$$

where $\partial_{t_z}^{(i)}$ and $\partial_{t_z}^\zeta$ denote the time derivative with respect to $\alpha_{k_i}^*(t_z)$ and $\zeta_p^*(t_z)$, respectively, and (\widehat{O}_1) and (\widehat{O}_1) correspond to the (00) and the (i0) components of the gravitational couplings, respectively. Notice that $\alpha_k = O(\omega^{-1/2})$ and $G(k_1, k_2; t, t_z) = O(\omega^0)$, and thus I_n has quadratic divergences superficially. However, the quadratic divergences arising from (\widehat{O}_1) vanish in the $M_n \rightarrow \infty$ limit. Effectively, the integral (E13) is linearly divergent. That means we have to adiabatically expand the integral to the second order. Similarly, the integral of the two-point function in the comoving gauge is quadratic divergent, and thus one needs to expand the integral to the third order. This makes the computation easier in the uniform curvature gauge. Using

$$|\alpha_k(t)|^2 = \frac{1}{2\omega_k a^3} [1 + \beta_2(k, t) + O(\omega_k^{-3})], \quad (\text{E17})$$

$$\alpha_k(t) \dot{\alpha}_k^*(t) = \frac{1}{2\omega_k a^3} [\gamma_0(k, t) - i\omega_k \beta_2(k, t) + O(\omega_k^{-2})], \quad (\text{E18})$$

$$\alpha_k(t) \ddot{\alpha}_k^*(t) = \frac{1}{2\omega_k a^3} \left[-3iH - 2i\gamma_0(k, t) + i \frac{k^2/a^2}{\omega_k^2} H + O(\omega_k^{-1}) \right], \quad (\text{E19})$$

where

$$\gamma_0(k, t) = -\frac{3}{2}H + \frac{1}{2} \frac{k^2/a^2}{\omega_k^2} H, \quad (\text{E20})$$

$$\beta_2(k, t) = \frac{\dot{H} + 2H^2}{2\omega_k^2} + \frac{(\dot{H} + 3H^2)M_n^2}{4\omega_k^4} - \frac{5H^2 M_n^4}{8\omega_k^4}, \quad (\text{E21})$$

which are obtained by combining Eq. (D14) with Eq. (E12), the integral (E13) becomes

$$I_n(p, t) = \frac{C_n^{-1}}{4\pi^2} \epsilon H^2 |\zeta_p^o|^2 \left[-\frac{1}{3} \frac{p^3}{a^3 H^3} \frac{\Lambda}{aH} + 2 \log \frac{2\Lambda}{aM_n} + \frac{5}{3} \frac{p^2}{a^2 H^2} \log \frac{2\Lambda}{aM_n} - \frac{5}{3} - \frac{25}{18} \frac{p^2}{a^2 H^2} + O\left(\frac{p^4}{a^4 H^4}\right) \right] + O(\epsilon^2, \dot{\epsilon}). \quad (\text{E22})$$

Note that all Λ dependent terms in $I_0 + \sum_n I_n$ vanishes by the PV field normalization conditions (D3).

Putting Eqs. (E11) and (E22) together into Eq. (E9), we have

$$\langle (\sigma^2)_{R\zeta} \rangle_p^U = \frac{1}{4\pi^2} \epsilon H^2 |\zeta_p^o|^2 \left[2 \log \frac{a\mu_1}{2p} + \frac{5}{3} \frac{p^2}{a^2 H^2} \log \frac{a\mu_1}{2p} + \frac{8}{3} + \frac{7}{18} \frac{p^2}{a^2 H^2} + O\left(\frac{p^4}{a^4 H^4}\right) \right] + O(\epsilon^2, \dot{\epsilon}). \quad (\text{E23})$$

We still need to compute one-point function $\frac{d}{dt} \langle (\sigma^2) \rangle_r$ up to $O(\epsilon)$ in order to compare the results in both gauges. Because mode functions for a massless scalar field are $O(\epsilon^0)$, we need $O(\epsilon)$ correction on it. In a quasi-dS background, we take an ansatz for the mode function

$$u_k(t) = \left(\frac{1}{\sqrt{2ka(t)}} + i \frac{H(t)}{\sqrt{2k^3}} \right) e^{i \frac{k}{a(t)H(t)}} + \frac{\epsilon(t)}{\sqrt{2ka(t)}} f_k(t) e^{i \frac{k}{a(t)H(t)}}, \quad (\text{E24})$$

where $f_k(t) = O(\epsilon^0)$ so that it recovers the dS solution in the $\epsilon \rightarrow 0$ limit. Applying this to the differential equation

$$\ddot{u}_k(t) + 3H\dot{u}_k(t) + \frac{k^2}{a^2} u_k(t) = 0, \quad (\text{E25})$$

we get

$$\begin{aligned} \ddot{f}_k + \left(H(t) - 2i \frac{k}{a(t)} \right) \dot{f}_k - H(t)^2 f_k \\ = 3H(t)^2 - 2i \frac{k}{a(t)} H(t) - 2 \frac{k^2}{a(t)^2} + O(\epsilon), \end{aligned} \quad (\text{E26})$$

whose solution is

$$f_k(t) = -\frac{3}{2} + iq + \frac{i}{2} \frac{1}{q} + \left(1 - \frac{i}{q} \right) e^{-2iq} Ei(2iq) \quad (\text{E27})$$

$$+ c_1 \left(1 + \frac{i}{q} \right) + c_2 \left(1 - \frac{i}{q} \right) e^{-2iq}, \quad (\text{E28})$$

where $q = \frac{k}{a(t)H(t)}$, and Ei is the exponential integral function

$$Ei(z) = - \int_{-z}^{\infty} \frac{e^{-t}}{t} dt \quad (\text{E29})$$

$Ei(\pm ix \rightarrow \infty)$

$$\rightarrow \pm i\pi + e^{\pm ix} \left(\frac{0!}{(\pm ix)} + \frac{1!}{(\pm ix)^2} + \frac{2!}{(\pm ix)^3} + \dots \right). \quad (\text{E30})$$

Matching this solution with the Bunch-Davies initial condition (D8) and the Wronskian condition (D9), respectively, gives

$$c_2 = -i\pi \quad \text{and} \quad c_1 = \frac{1}{2}. \quad (\text{E31})$$

Then the mode function with $O(\epsilon)$ correction in a quasi-dS space-time becomes

$$u_k(t) = \left(\frac{1}{\sqrt{2ka}} + i \frac{H}{\sqrt{2k^3}} \right) e^{i \frac{k}{aH}} \quad (\text{E32})$$

$$\begin{aligned} + \frac{\epsilon}{\sqrt{2ka}} \left[-1 + i \frac{k}{aH} + i \frac{aH}{k} \right. \\ \left. + \left(1 - i \frac{aH}{k} \right) \left(-i\pi + Ei\left(2i \frac{k}{aH} \right) \right) e^{-2i \frac{k}{aH}} \right] e^{i \frac{k}{aH}} \\ + O(\epsilon^2, \dot{\epsilon}). \end{aligned} \quad (\text{E33})$$

Now we calculate the one-point function using this mode function as shown in Appendix D 2, and we get

$$\frac{d}{dt}\langle(\sigma^2)_r\rangle = \frac{H^3}{4\pi^2} + \frac{\epsilon H^3}{2\pi^2}\left(\log\frac{H}{\mu_1} + \frac{1}{6} - \gamma\right) + O(\epsilon^2, \dot{\epsilon}). \quad (\text{E34})$$

Finally, we find

$$\begin{aligned} & \frac{1}{H} \frac{d}{dt} \langle(\sigma^2)_r\rangle \langle\widetilde{\zeta\zeta}\rangle_p + \langle(\sigma^2)_r\rangle \langle\widetilde{\zeta\zeta}\rangle_p^U \\ &= \frac{H^2(t)}{4\pi^2} |\zeta_p(t)|^2 + \frac{\epsilon H^2}{2\pi^2} |\zeta_p^o|^2 \left[\log\frac{aH}{2p} + \frac{3}{2} - \gamma \right] \\ &+ \frac{\epsilon H^2}{4\pi^2} |\zeta_p^o|^2 \frac{p^2}{a^2 H^2} \left[\frac{13}{18} - 2\gamma + \frac{5}{3} \log\frac{a\mu_1}{2p} + 2 \log\frac{H}{\mu_1} \right] \\ &+ O\left(\epsilon^2, \dot{\epsilon}, \frac{p^4}{a^4 H^4}\right). \end{aligned} \quad (\text{E35})$$

The non- p^2/a^2 -suppressed terms are rewritten as

$$\begin{aligned} & \frac{H^2(t)}{4\pi^2} |\zeta_p^o|^2 + \frac{\epsilon H^2}{2\pi^2} |\zeta_p^o|^2 \left[\log\frac{aH}{2p} + \frac{3}{2} - \gamma \right] \\ & \approx \frac{H^2(t)}{4\pi^2} |\zeta_p^o|^2 \times \left(1 + 2\epsilon \log\frac{aH}{p} \right) \end{aligned} \quad (\text{E36})$$

$$\approx \frac{H^2(t)}{4\pi^2} |\zeta_p^o|^2 \left(\frac{p}{aH} \right)^{-2\epsilon} \quad (\text{E37})$$

$$\approx \frac{H_*^2}{4\pi^2} |\zeta_p^o|^2. \quad (\text{E38})$$

As expected, this is the result (99) in the comoving gauge. The other terms are suppressed by the factor p^2/a^2 . This explicitly proves that the next leading terms for the two-point function $\langle(\sigma^2)_r, \zeta\rangle$ are $O(p^2/a^2)$.

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