Gauge-Invariant Temperature Anisotropies and Primordial Non-Gaussianity

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We provide the gauge-invariant expression for large-scale cosmic microwave background temperature fluctuations at second-order in perturbation theory. It enables to unambiguously define the nonlinearity parameter $f_{NL}$ which is used by experimental collaborations to pin down the level of Non-Gaussianity in the temperature fluctuations. Furthermore, it contains a primordial term encoding all the information about the Non-Gaussianity generated at primordial epochs and about the mechanism which gave rise to cosmological perturbations, thus neatly disentangling the primordial contribution to Non-Gaussianity from the one caused by the post-inflationary evolution.

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Inflation has become the dominant paradigm to understand the initial conditions for the density perturbations in the early Universe which are the seeds for the Large-Scale Structure (LSS) and for the Cosmic Microwave Background (CMB) temperature anisotropies [1]. In the inflationary picture, primordial density and gravity-wave fluctuations are created from quantum fluctuations “redshifted” out of the horizon during an early period of superluminal Universe expansion. Despite the simplicity of the inflationary paradigm, the mechanism by which cosmological curvature (adiabatic) perturbations are generated is not yet established. In the standard slow-roll inflationary scenario associated to one-single field, the inflaton itself when it slowly rolls down along its potential. In the curvaton mechanism [2] the final curvature perturbation $\zeta$ is produced from an initial isocurvature mode associated with the quantum fluctuations of a light scalar (other than the inflaton), the curvaton, whose energy density is negligible during inflation. Recently, other mechanisms for the generation of cosmological perturbations have been proposed, the inhomogeneous reheating scenario [3], ghost-inflation [4] and the D-cceleration scenario [5], to mention a few. A precise measurement of the spectral index $n_\zeta$ of comoving curvature perturbations will provide a powerful constraint to slow-roll inflation models and the standard scenario for the generation of cosmological perturbations which predicts $|n_\zeta - 1|$ significantly below unity. However, alternative mechanisms generically also predict a value of $n_\zeta$ very close to unity. Thus, even a precise measurement of the spectral index will not allow us to efficiently discriminate among them. On the other hand, the lack gravity-wave signals in CMB anisotropies will not give us any information about the perturbation generation mechanism, since alternative mechanisms predict an amplitude of gravity waves far too small to be detectable by future experiments aimed at observing the $B$-mode of the CMB polarization.

There is, however, a third observable which will prove fundamental in providing information about the mechanism chosen by Nature to produce the structures we see today. It is the deviation from a Gaussian statistics, i.e., the presence of higher-order connected correlation functions of CMB anisotropies. Since for every scenario there exists a well defined prediction for the strength of Non-Gaussianity (NG) and its shape as a function of the parameters, testing the NG level of primordial fluctuations is one of the most powerful probes of inflation [6] and is crucial to discriminate among different – but otherwise indistinguishable - mechanisms. For instance, the single-field slow-roll inflation model itself produces negligible NG, and the dominant contribution comes from the evolution of the ubiquitous second-order perturbations after inflation, which is potentially detectable with future observations of CMB temperature and polarization anisotropies. This effect must exist regardless of the inflationary models, setting the minimum NG level of cosmological perturbations. Therefore, if we do not find any evidence for this ubiquitous NG, then it will challenge our understanding of the evolution of cosmological perturbations at a deeper level.

Motivated by the extreme relevance of pursuing NG in the CMB anisotropies, in this Letter we provide the exact expression for large-scale CMB temperature fluctuations at second order in perturbation theory. This expression has various virtues. First, it is gauge-invariant. Second, from it one can unambiguously extract the exact definition of the nonlinearity parameter $f_{NL}$ which is used by the experimental collaborations to pin down the level of NG in the temperature fluctuations. Third, it contains a “primordial” term encoding all the information about the NG generated in primordial epochs, namely during or immediately after inflation, and depends upon the various fluctuation generation mechanisms. As such, the expression neatly disentangles the primordial contribution to the NG from that arising after inflation. Finally, the expression applies to all scenarios for the generation of cosmological perturbations.
In order to obtain our gauge-independent formula for the temperature anisotropies we first perturb a spatially flat Robertson-Walker background. Here we follow the formalism of Ref. [8] expanding metric perturbations in a first and a second-order part as

\[
y_{0a} = -a^2 \left( 1 + 2 \phi^{(1)} + \phi^{(2)} \right),
\]
\[
y_{0i} = a^2 \left( \frac{1}{2} \omega^{(2)} + \frac{1}{2} \omega_i^{(2)} \right),
\]
\[
g_{ij} = a^2 \left( 1 - 2 \psi^{(1)} - \psi^{(2)} \right) \delta_{ij} + \left( \chi^{(1)}_{ij} + \frac{1}{2} \chi^{(2)}_{ij} \right), \tag{1}
\]

where the scale factor \(a(\eta)\) is a function of the conformal time \(\eta\). The functions \(\phi^{(r)}, \omega^{(r)}_i, \psi^{(r)}_i\) and \(\chi^{(r)}_{ij}\), where \((r) = (1, 2)\), stand for the \(r\)-th order perturbations of the metric. It is standard use to split the perturbations into the so-called scalar, vector and tensor parts, according to their transformation properties with respect to the 3-dimensional space with metric \(\delta_{ij}\), where scalar parts are related to a scalar potential, vector parts to transverse (divergence-free) vectors and tensor parts to transverse trace-free tensors. Thus \(\phi \) and \(\psi\) are scalar perturbations, and for instance, \(\hat{\omega}^{(r)}_i = \partial_i \omega^{(r)} + \omega^{(r)}_i\), where \(\omega^{(r)}\) is the scalar part and \(\omega^{(r)}_i\) a transverse vector, i.e. \(\partial^i \omega^{(r)}_i = 0\). The metric perturbations will transform according to an infinitesimal change of coordinates. From now on we limit ourselves to a second-order time shift \(\eta \rightarrow \eta - \alpha(1) + \frac{1}{2} (\alpha'(1) \alpha(1) - \alpha(2))\), where \(\alpha(1)\) denotes differentiation w.r.t. conformal time.

In general a gauge corresponds to a choice of coordinates defining a slicing of spacetime into hypersurfaces (at fixed time \(\eta\)) and a threading into lines (corresponding to fixed spatial coordinates \(x\)), but in this Letter only the former is relevant so that gauge-invariant can be taken to mean independent of the slicing [8]. For example, under the time shift, the first-order spatial curvature perturbation \(\psi^{(1)}\) transforms as \(\psi^{(1)} \rightarrow \psi^{(1)} - \mathcal{H} \alpha(1)\) (here \(\mathcal{H} = a'/a\)), while \(\phi^{(1)} \rightarrow \phi^{(1)} + \alpha'(1) + \mathcal{H} \alpha(1)\), \(\omega^{(1)}_i \rightarrow \omega^{(1)}_i + \partial_i \alpha(1)\), and the traceless part of the spatial metric \(\chi^{(1)}_{ij}\) turns out to be gauge-invariant. At second order in the perturbations we just give some useful examples like the transformation of the energy density and the curvature perturbation \(\delta^{(2)} \rho \rightarrow \delta^{(2)} \rho + \rho' \alpha(2) + \alpha(1) \left( \rho'' \alpha(1) + \rho' \alpha'(1) + 2 \delta^{(1)} \rho \right)\) and \(\psi^{(1)} \rightarrow \psi^{(1)} + 2 \mathcal{H} \psi^{(1)} + (\mathcal{H}' + 2 \mathcal{H}^2) a^2 \alpha(1) - \mathcal{H} \alpha(1) \alpha'(1) - \frac{1}{3} \left( 2 \omega^{(1)}_{ij} - \alpha''(1) \alpha_{ij} - \alpha'(1) \mathcal{H} \alpha(2) \right).\) In particular, there exists an extension at second order of the well-known gauge-invariant variable \(\zeta^{(1)} = -\psi^{(1)} - \mathcal{H} \delta^{(1)} \rho / \rho\) (the curvature perturbation on uniform density hypersurfaces). It is given by \(\zeta = \zeta^{(1)} + (1/2) \zeta^{(2)}\), where

\[
- \zeta^{(2)} = \psi^{(2)} + \mathcal{H} \delta^{(1)} \rho / \rho' - 2 \mathcal{H} \delta^{(1)} \rho / \rho' \psi^{(1)} - 2 \delta^{(1)} \rho / \rho' \psi^{(1)} - 4 \mathcal{H} \delta^{(1)} \rho / \rho' \psi^{(1)} + \left( \delta^{(1)} \rho / \rho' \right)^2 \left( \mathcal{H} \rho'' / \rho' - \mathcal{H}' - 2 \mathcal{H}^2 \right). \tag{2}
\]

The key point here is that the gauge-invariant comoving curvature perturbation \(\zeta^{(2)}\) remains constant on super-horizon scales after it has been generated and possible isocurvature perturbations are no longer present. Therefore, \(\zeta^{(2)}\) provides all the necessary information about the “primordial" level of NG generated either during inflation, as in the standard scenario, or immediately after it, as in the curvaton scenario. Different scenarios are characterized by different values of \(\zeta^{(2)}\), while the post-inflationary nonlinear evolution due to gravity is common to all of them [8, 10, 11, 12]. For example, in standard single-field inflation \(\zeta^{(2)}\) is generated during inflation and its value is \(\zeta^{(2)} = 2 (\zeta^{(1)})^2 + \mathcal{O}(\alpha - 1)\) [10, 13].

We now construct in a gauge-invariant way temperature anisotropies at second order. Temperature anisotropies beyond the linear regime have been calculated in Refs. [14], following the photons path from last-scattering to the observer in terms of perturbed geodesics. The linear temperature anisotropies read [14]

\[
\frac{\Delta T^{(1)}}{T} = \phi^{(1)} - \psi^{(1)} e_i + \tau^{(1)} e_i - \int_{s_{\odot}} d\lambda A^{(1)}(\lambda), \tag{3}
\]

where \(A^{(1)} \equiv \psi^{(1)} + \phi^{(1)} + \hat{\omega}^{(1)}_i e_i - \frac{1}{2} \chi^{(1)}_{ij} e^i e^j\), the subscript \(\odot\) indicates that quantities are evaluated at last-scattering, \(e^i\) is a spatial unit vector specifying the direction of observation and the integral is evaluated along the line-of-sight parametrized by the affine parameter \(\lambda\). Eq. (3) includes the intrinsic fractional temperature fluctuation at emission \(\tau^{(1)}\), the Doppler effect due to emitter’s velocity \(v^{(1)}\) and the gravitational redshift of photons, including the integrated Sachs-Wolfe (ISW) effect. We omitted monopoles due to the observer \(O\) (e.g. the gravitational potential \(\psi^{(1)}\) evaluated at the event of observation), which, being independent of the angular coordinate, can be always recast into the definition of temperature anisotropies [15]. Notice however that the physical meaning of each contribution in Eq. (3) is not gauge-invariant, as the different terms are gauge-dependent. However, it is easy to show that the whole expression [14] is gauge-invariant. Since the temperature \(T\) is a scalar, the intrinsic temperature fluctuation transforms as \(\tau^{(1)} \rightarrow \tau^{(1)}_{\odot} + (T'/T) \alpha(1) = \tau^{(1)}_{\odot} - \mathcal{H} \alpha(1)\), having used the fact that the temperature scales as \(T \propto a^{-3}\). Notice, instead, that the velocity \(v^{(1)}\) does not change. Therefore, using the transformations of metric perturbations we find

\[
\frac{\Delta T^{(1)}}{T} \rightarrow \frac{\Delta T^{(1)}}{T} + \alpha'(1) - \int_{s_{\odot}} d\eta \frac{d\alpha'(1)}{d\eta} = \frac{\Delta T^{(1)}}{T} + \mathcal{O}, \tag{4}
\]

where we have used the fact that the integral is evaluated along the line-of-sight which can be parametrized by the background geodesics \(x^{(0)} = (\lambda, (\lambda_{\odot} - \lambda_{\odot}) e^i\) (with
\[d\lambda/d\eta = 1\), and the decomposition for the total derivative along the path for a generic function \(f(\lambda, x^i(\lambda))\), \(f' = \frac{\partial f}{\partial \lambda} + \partial_i f e^i\). Eq. 4 shows that the expression for first-order temperature anisotropies is indeed gauge-invariant (up to monopole terms related to the observer \(O\)). Temperature anisotropies can be easily written in terms of particular combinations of perturbations which are manifestly gauge-invariant. For the gravitational potentials we consider the gauge-invariant definitions \(\psi^{(1)}_I = \psi^{(1)} - \Delta \omega^{(1)}\) and \(\phi^{(1)}_I = \phi^{(1)} + \Delta \omega^{(1)} + \omega^{(1)}\). For the \((0 - i)\) component of the metric and the trace-less part of the spatial metric we define \(\omega^{(1)}_{iI} = \omega^{(1)}_{iI}\) and \(\lambda^{(1)}_{iI} = \lambda^{(1)}_{iI}\). For the matter variables we use a gauge-invariant intrinsic temperature fluctuation \(\tau^{(1)}_I = \tau^{(1)} - \Delta \omega^{(1)}\), where the velocity itself is gauge-invariant \(v^{(1)}_i = v^{(1)}_i\) under time shifts. Following the same steps leading to Eq. 1 one gets the linear temperature anisotropies in Eq. 3 in terms of these gauge-invariant quantities

\[
\frac{\Delta T^{(1)}_{GI}}{T} = \phi^{(1)}_{GI} - v^{(1)}_i e_i + \tau^{(1)}_I - \int_{\lambda^0}^{\lambda^e} d\lambda A^{(1)}_{I GI}, \tag{5}
\]

where \(A^{(1)}_{I GI} = \phi^{(1)}_{GI} + \psi^{(1)}_{GI} + \omega^{(1)}_{I GI} - \frac{1}{2} \nabla^i \nabla_j \phi^{(1)}_{GI} e^i e^j\) and we omitted the subscript \(E\). For the primordial fluctuations we are interested in the large-scale modes set by the curvature perturbation \(\zeta^{(1)}\). Defining a gauge-invariant density perturbation \(\delta^{(1)}_{p GI} = \delta^{(1)} p + \rho \omega^{(1)}\), we write the curvature perturbation as \(\zeta^{(1)}_I = -\psi^{(1)}_{GI} - \tilde{H} \delta^{(1)} \rho GI / \rho')\). Since for adiabatic perturbations in the radiation \((\gamma)\) and matter \((m)\) eras (1/4)\(\delta^{(1)} \rho / \rho_m\) = (1/3)\(\delta^{(1)} \rho_m / \rho_m\), one can write the intrinsic temperature fluctuation as \(\tau^{(1)} = (1/4)\(\delta^{(1)} \rho / \rho_m\) = -\(H\delta^{(1)} \rho / \rho')\) and a gauge-invariant definition is \(\tau^{(1)}_I = -\tilde{H} \delta^{(1)} \rho GI / \rho')\). In the large-scale limit, from Einstein equations, in the matter era \(\phi^{(1)}_{GI} = \psi^{(1)}_{GI} = -\frac{3}{2} \phi^{(1)}\). Thus we obtain the large-scale limit of temperature anisotropies \[
\frac{\Delta T^{(1)}_{GI}}{T} = 2 \psi^{(1)}_{GI} - \phi^{(1)}_{GI} = \omega^{(1)}_{I GI} / 3, \tag{6}
\]

At second order, the procedure is similar to the one described so long, though more lengthy and cumbersome. We only provide the reader with the main steps to get the final expression. The second-order temperature fluctuations in terms of metric perturbations read \[14\]

\[
\frac{\Delta T^{(2)}_{GI}}{T} = \frac{1}{2} \left( \frac{\phi^{(2)} - \phi^{(2)}_{GI} - \phi^{(1)}_{GI}^2}{2} - \frac{\phi^{(2)}_{GI}}{2} e^i + \frac{1}{2} \phi^{(2)}_I - I_2(\lambda e) \right) \\
+ \left( I_1(\lambda e) + \phi^{(1)}_{GI} e_i \right) \left( -\phi^{(1)}_{GI} - \phi^{(2)}_{GI} - \phi^{(1)}_{GI} e_i + I_1(\lambda e) \right) \\
+ x^{(1)}_{i j} \phi^{(1)}_{GI} + \phi^{(1)}_{GI} e^i \phi^{(1)}_{GI} + H_1(\lambda e) \\
+ \frac{\phi^{(1)}_{GI}}{2} e_i \phi^{(1)}_{GI} + \phi^{(1)}_{GI} e_i + \frac{\phi^{(1)}_{GI} e_i}{2} e^i - \phi^{(1)}_{GI} e_i \phi^{(1)}_{GI} \\
+ v^{(1)}_i \left( -\phi^{(1)}_{GI} - I_1(\lambda e) \right), \tag{7}
\]

Here \(I_2(\lambda e) = \int_{\lambda^0}^{\lambda^e} \frac{d\lambda}{2} \left( A^{(1)}_{I GI} + (\tilde{\omega}^{(1)}_I - \phi^{(1)}_{GI}) e_i \phi^{(1)}_{GI} + e^i \phi^{(1)}_{GI} e_i \phi^{(1)}_{GI} \right) \), where \(A^{(1)}_I = \phi^{(1)}_I + \phi^{(1)}_I e_i + \phi^{(1)}_I e_i e_j + \phi^{(1)}_I e_i + \phi^{(1)}_I e_i e_j + \phi^{(1)}_I e_i e_j + \phi^{(1)}_I e_i e_j + \phi^{(1)}_I e_i e_j + \phi^{(1)}_I e_i e_j \) is the photon wave vectors, with \(I_1(\lambda e) = \frac{1}{2} \left( \frac{\phi^{(1)}_{GI} - \phi^{(1)}_{GI}}{2} \right) \), is the direction of the photon emission. As usual we have omitted the monopole terms due to the observer. Using the transformation rules of Ref. 11, it is possible to check that the expression \[12\] is gauge-invariant. We can express the second-order anisotropies in terms of explicitly gauge-invariant quantities, whose definition proceeds as for the linear case, by choosing the shifts \(\alpha^{(1)}\) such that \(\omega^{(1)} = 0\). For example, the second-order gravitational potential \[12\]

\[
\phi^{(2)}_{GI} = \phi^{(2)} + \omega^{(1)} \left[ 2 \left( \frac{\psi^{(1)}_{CI}}{2} + \frac{\phi^{(1)}_I}{\alpha^{(1)}} \right) + \omega^{(1)} + \frac{\alpha^{(1)}}{\alpha^{(1)}} \right] \\
+ \left( H + 2H^2 \right) \alpha^{(1)} + 2 \left( \phi^{(1)}_{CI} + \phi^{(1)}_I \right) \left[ \frac{1}{2} \left( \frac{\phi^{(1)}_{GI}}{2} \right) - \phi^{(1)}_I \right) \right], \tag{8}
\]

where \(\alpha^{(1)} = \omega^{(1)} + \omega^{(1)} + \nabla^{-2} \partial^i \partial_j \left( 4 \psi^{(1)} \partial_i \omega^{(1)}j - 2 \omega^{(1)} \partial_i \omega^{(1)}j \right)\). Expressing the second-order temperature anisotropies \[15\] in terms of our gauge-invariant quantities and taking the large-scale limit we find \(\Delta T^{(2)}_{GI}/T = (1/2)\phi^{(2)}_{CI} - (1/2) \left( \frac{\phi^{(1)}_{GI}}{2} + \omega^{(1)} \right) + \phi^{(1)}_I \) (having dropped the subscript \(E\)), and the gauge-invariant intrinsic temperature fluctuation at emission is \(\tau^{(2)}_I = (1/4)\phi^{(2)}_{CI} / \rho / \rho_m - 3 \phi^{(1)}_{CI} \). We have dropped those terms which represent integrated contributions and other second-order small-scale effects that can be distinguished from the large-scale part through their peculiar scale dependence. At this point we make use of Einstein’s equations. We take the expression for \(\zeta^{(2)}\) in Eq. 24, and we use the \((0 - 0)\) component and the traceless part of the \((i - j)\) Einstein’s equation at second order (see Eqs. (153) and (155) of Ref. 11). Thus, on large scales we find that

\[
\frac{\Delta T^{(2)}_{GI}}{T} = \frac{1}{18} \left( \frac{\phi^{(1)}_{GI}}{2} \right) - \frac{K}{10} - \frac{\zeta^{(2)}_{GI} - 2 \phi^{(1)}_{CI} \phi^{(1)}_I}{10}, \tag{9}
\]

where we have defined a kernel \(K = 10 \nabla^{-4} \partial^i \partial^j \left( \partial_i \psi^{(1)} \partial_j \psi^{(1)} \right) - 2 \nabla^{-2} \left( \frac{10}{3} \partial_i \psi^{(1)} \partial_j \psi^{(1)} \right)\). Eq. 25 is the main result of this Letter. It clearly (6) shows that there are two contributions to the final
nonlinearity in the large-scale temperature anisotropies. The contribution, \( \zeta_{NL}^{(2)} \), comes from the “primordial” conditions set during or after inflation. They are encoded in the curvature perturbation \( \zeta \) which remains constant once it has been generated. The remaining part of Eq. (8) describes the post-inflation processing of the primordial non-Gaussian signal due to the nonlinear gravitational dynamics, including also second-order corrections at last scattering to the Sachs-Wolfe effect \( L \). Thus, the expression in Eq. (8) allows to neatly disentangle the primordial contribution to NG from that coming from that arising after inflation. While the nonlinear evolution after inflation is the same in each scenario, the primordial content will depend on the particular mechanism generating the perturbations. We parametrize the primordial NG in the terms of the conserved curvature perturbation in the radiation or matter dominated epochs \( \zeta^{(2)} = 2a \left( \zeta^{(1)} \right)^2 \), where \( a \) depends on the physics of a given scenario. For example, in the curvature case \( a = (3/4r) - r/2 \), where \( r = \rho_c/\rho_{\phi} \) is the relative curvature contribution to the total energy density at curvature decay \( f \). In the minimal picture for the inhomogeneous reheating scenario, \( a = 1/4 \). For the other scenarios we refer the reader to Ref. [6]. From Eq. (8) we can extract the nonlinearity parameter \( f_{NL} \), which is usually adopted to phenomenologically parametrize the NG level of cosmological perturbations and has become the standard quantity to be observationally constrained by CMB experiments \( \Omega \). The definition of \( f_{NL} \) adopted in the analyses performed in Refs. \( \Omega \), goes through the conventional Sachs-Wolfe formula \( \Delta T/T = -\Phi/3 \), where \( \Phi \) is Bardeen’s potential \( \Phi \), which is conventionally expanded as (up to a constant offset, which only affects the temperature monopole) \( \Phi = \Phi_L + f_{NL} \Phi_L \Phi_L \), with \( \Phi_L = -\phi_{\phi}^{(1)} \). Here the * product reminds the fact that the nonlinearity parameter might have a non-trivial scale dependence \( \zeta \). Therefore, using \( \zeta^{(1)} = -\frac{5}{2} \phi_{\phi}^{(1)} \) during matter domination, from Eq. (8) we read the nonlinearity parameter in momentum space

\[
f_{NL}(k_1, k_2) = -\left[ \frac{5}{3} (1 - a) + \frac{1}{6} - \frac{3}{10} \mathcal{K} \right] + 1
\]

where \( \mathcal{K} = 10 (k_1 \cdot k_3) (k_2 \cdot k_3) / k^4 - \frac{10}{3} k_1 \cdot k_2 / k^2 \) with \( k_3 + k_1 + k_2 = 0 \) and \( k = |k_3| \). In fact the formula \( \Omega \) already accounts for an additional nonlinear effect entering in the CMB angular 3-point function from the angular averaging performed with a perturbed line element \( d\Omega(1-2\phi_{\phi}^{(1)}) \), implying a +1 shift in \( f_{NL} \). In particular within the standard scenario where cosmological perturbations are due to the inflaton the primordial contribution to NG is given by \( a = 1 - \frac{1}{3} (n_{\phi} - 1) \), where the spectral index is expressed in terms of the usual slow-roll parameters as \( n_{\phi} - 1 = -6\epsilon + 2\eta \). The nonlinearity parameter from inflation now reads

\[
f_{NL} = -\frac{5}{12} (n_{\phi} - 1) + \frac{5}{6} + \frac{3}{10} \mathcal{K}.
\]

Therefore the main NG contribution comes from the post-inflation evolution of the second-order perturbations which give rise to order-one coefficients, while the primordial contribution is proportional to \( |n_{\phi} - 1| \ll 1 \). This is true even in the “squeezed” limit first discussed by Maldacena \( \Omega \), where one of the wavenumbers is much smaller than the other two, \( e.g. \ k_1 \ll k_{2,3} \) and \( \mathcal{K} \to 0 \).

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