Constraining Density Fluctuations with Big Bang Nucleosynthesis in the Era of Precision Cosmology

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We reexamine big bang nucleosynthesis with large-scale baryon density inhomogeneities when the length scale of the density fluctuations exceeds the neutron diffusion length ($\sim 10^7 - 10^8$ cm at BBN), and the amplitude of the fluctuations is sufficiently small to prevent gravitational collapse. In this limit, the final light element abundances can be determined by simply mixing the abundances from regions with different baryon/photon ratios without interactions. We examine Gaussian, lognormal, and gamma distributions for the baryon/photon ratio, $\eta$. We find that the deuterium and lithium-7 abundances increase with the RMS fluctuation in $\eta$, while the effect on helium-4 is much smaller. We show that these increases in the deuterium and lithium-7 abundances are a consequence of Jensen’s inequality, and we derive analytic approximations for these abundances in the limit of small RMS fluctuations. Observational upper limits on the primordial deuterium abundance constrain the RMS fluctuation in $\eta$ to be less than 17% of the mean value of $\eta$. This provides us with a new limit on the graininess of the early universe.

I. INTRODUCTION

The successful theory of big bang nucleosynthesis (BBN) remains one of the major pillars of modern cosmology. While BBN once treated the baryon/photon ratio, $\eta$, as the main quantity to be determined by comparing BBN predictions with astronomical observations, the independent measurement of $\eta$ by deduction from cosmic microwave background (CMB) observations has led to a minimal BBN theory with no free parameters. Using the CMB values for $\eta$, the predicted BBN abundances of deuterium (D) and $^4$He are in excellent agreement with the observations, while the predicted $^7$Li abundance remains a factor of three larger than the observationally-inferred abundance; for recent reviews of BBN, see refs. [1–3].

Given the excellent agreement between the predicted and observed D and $^4$He abundances, any modification that alters the BBN predictions will probably be sharply constrained. Many such modifications have been proposed, but here we focus on one of the earliest to be investigated: inhomogeneities in the density. Such inhomogeneities are irrelevant if (as in the case of adiabatic fluctuations or temperature fluctuations [4]) they leave $\eta$ unchanged [2]. Here, we will be interested in the different case of isocurvature fluctuations, for which $\eta$ varies from one region of the Universe to another. There is a long history of investigations of these kind of models [5–12] and their baryon inhomogeneity may reflect environmental non-uniformities or symmetry breakings at phase transitions in the very early universe, long before BBN occurred [13]. These investigators showed that it was possible to reconcile the observed D abundance with a closure density of baryons if the baryons were inhomogeneously distributed. During the 1970s there was interest in baryon symmetric cosmologies which had led to the consideration of proton and neutron diffusion effects during BBN [14, 15], and the need to avoid matter-antimatter annihilation effects by requiring that baryon inhomogeneities were larger than the neutron diffusion length at BBN. The subsequent realisation that baryon number would not be conserved in a Grand Unified Theory (GUT) led to a rapid loss of interest in baryon symmetric cosmologies, but there remained an interest in diffusion effects. An important effect arises when the length scale of the fluctuations is longer than the proton diffusion length but shorter than the neutron diffusion length; in this case neutron diffusion from high-density to low-density regions will strongly modify the neutron-proton ratio [16, 17]. This class of models has been explored in great detail (see, e.g., Refs. [18, 19] and references therein for more recent discussions). When neutron diffusion is important and the fluctuation amplitude is large, it is possible to produce heavier elements than those normally considered in standard homogeneous BBN [19, 21], a result which provides additional observational signatures and constraints on such models. Furthermore, fluctuations of sufficiently large amplitude can lead to gravitational collapse, further modifying the standard BBN scenario [22, 24] and creating primordial black holes.

In this paper, we ignore these latter possibilities (and also the possibility of inhomogeneities in fundamental “constants” like $G$ [25] or the neutron half-life) and concentrate on the simplest case: low-amplitude, large-scale fluctuations. In this case, BBN proceeds in the standard way in independent regions with different values of $\eta$, and the elements in these regions mix after BBN to give the observed abundances today. There are two reasons why this is an opportune time to revisit this scenario. First, observational limits on the primordial element abundances have improved significantly since the earlier investigations cited above. In particular, high-redshift quasar absorption sys-
tems allow high-precision measurements of the primordial value of D/H (the number ratio of deuterium to hydrogen) \[26, 27\]. Second, \( \eta \) is no longer a free parameter to be determined from the results of BBN calculations. Instead, it is fixed by measurements of CMB fluctuations and then becomes a well determined input parameter for BBN. This is particularly salient for the case of BBN with density fluctuations, as much of the motivation for these models was the possibility that they might allow a wider range of values for \( \eta \) than in the standard model, and previous work concentrated on determining the allowed range for \( \eta \) in these models. Here, instead, we will be able to use a combination of a fixed value for \( \eta \), along with improved estimates of the primordial element abundances, to place limits on the magnitude and type of allowed density fluctuations in the early universe.

In the next section, we will briefly review the standard model for BBN and discuss the observational limits on the element abundances that we incorporate in this paper. In Sec. III, we will examine a variety of statistical distributions for \( \eta \) and calculate the corresponding predicted element abundances using a version of the Kawano nucleosynthesis code \[28\] with updated reaction rates \[29\]. We will then use the observational limits to bound the fractional RMS fluctuation, \( \sigma \), in each case. We discuss our results in Sec. IV.

\section{II. STANDARD BBN}

Consider the standard model for BBN \[1\–3\]. For \( T \gtrsim 1 \text{ MeV} \), the weak interactions inter-convert protons and neutrons, maintaining a thermal equilibrium ratio:

\[ n + \nu_e \leftrightarrow p + e^-, \]
\[ n + e^+ \leftrightarrow p + \bar{\nu}_e, \]
\[ n \leftrightarrow p + e^- + \bar{\nu}_e, \]

while a thermal abundance of deuterium is maintained by

\[ n + p \leftrightarrow D + \gamma. \]

After the weak reactions drop out of thermal equilibrium at \( T \sim 0.8 \text{ MeV} \), free-neutron decay continues until \( T \sim 0.1 \text{ MeV} \), when rapid fusion into heavier elements occurs. Almost all of the remaining neutrons end up bound into 4\text{He}, with a small fraction remaining behind in the form of deuterium, tritium, and 3\text{He}, and some production of 7\text{Li} and 7\text{Be}, with the latter decaying into the former via electron capture at the beginning of the recombination era \[30\]. The element abundances produced in BBN depend on the baryon/photon ratio \( \eta \), which can be independently determined from the CMB. We adopt a value of \( \eta = 6.1 \times 10^{-10} \), consistent with recent results from Planck \[31\]. This value of \( \eta \) yields predicted abundances of \( D \) and 4\text{He} consistent with observations.

Recent observational estimates of D/H include those of the Particle Data Group (PDG) \[32\]: D/H = (2.569±0.027) \times 10^{-5}, Cooke et al. \[26\]: D/H = (2.527 ± 0.030) \times 10^{-5}, and Zavarygin et al. \[27\]: D/H = (2.545 ± 0.025) \times 10^{-5}. Here we will adopt the PDG estimate:

\[ \text{D/H} = (2.569 \pm 0.027) \times 10^{-5}. \]

The primordial 4\text{He} abundance, designated \( Y_p \), is not so well established. Izotov et al. \[33\] give \( Y_p = 0.2551 \pm 0.0022 \), while Aver et al. \[34\] give \( Y_p = 0.2449 \pm 0.0040 \). The PDG limit is \[32\]: \( Y_p = 0.245 \pm 0.003 \). However, as we will see, the primary limit on the models we will examine here comes from deuterium, rather than 4\text{He}, so the observational limit on 4\text{He} will have little effect on our results.

As noted above, both the D and 4\text{He} abundances are consistent with the predictions of standard BBN with the CMB value for \( \eta \), but this is not the case for the 7\text{Li} abundance. The primordial lithium abundance is estimated to be:\[32\]

\[ ^7\text{Li}/\text{H} = (1.6 \pm 0.3) \times 10^{-10}. \]

However, standard BBN with \( \eta \sim 6 \times 10^{-10} \) predicts a primordial value for 7\text{Li}/H that is roughly three times higher than this observationally-inferred value. (For this value of \( \eta \), most of the primordial 7\text{Li} is produced in the form of 7\text{Be}, which decays into 7\text{Li} much later, as noted above). This discrepancy between the predicted and observationally-inferred primordial 7\text{Li} abundances is called the “lithium problem,” and it remains unresolved at present (for a further discussion, see Ref. \[35\]). Clearly, we cannot use the 7\text{Li} abundance to constrain inhomogeneous BBN, since it is already inconsistent with standard BBN. However, it will be interesting to see whether the inhomogeneous models examined here can help to solve the lithium problem.
III. INHOMOGENEOUS BBN

Our modeling of inhomogeneous BBN will closely parallel that of Refs. [11] and [12]. We will assume isocurvature fluctuations, with $\eta$ varying across different regions of the universe. We will take the length scales of these fluctuations to be larger than the neutron diffusion length, so that diffusion of neutrons relative to protons is not a significant effect. Note that the Planck CMB measurements strongly constrain isocurvature modes [36], but there are many orders of magnitude between the comoving neutron diffusion length at BBN ($\sim 10^7 - 10^8$ cm at BBN [37]) and the smallest length scales probed by Planck, so our model has a nontrivial range of application. We assume further that the inhomogeneous element abundances are smoothed out by post-BBN diffusion of all of the nuclei, so that the observable universe ends up with a single, uniform abundance of each element. Treatments of post-BBN element diffusion in the standard (homogeneous) case can be found in Refs. [38, 39].

Our model can be entirely characterized by the distribution of $\eta$, given by the distribution function $f(\eta)$ which specifies the fraction of the universe with $\eta$ in the interval $(\eta, \eta + \delta\eta)$ at the time of nucleosynthesis. We will consider a variety of choices for $f(\eta)$. Since $f(\eta)$ is a probability distribution for $\eta$, it must integrate to unity:

$$\int_0^\infty f(\eta) \, d\eta = 1. \quad (5)$$

We assume that the inhomogeneities present at BBN are erased by diffusion before recombination, so that the mean value of $\eta$ today (and at recombination) is given by

$$\overline{\eta} = \int_0^\infty f(\eta) \, \eta \, d\eta. \quad (6)$$

The final average element abundances, i.e., the abundances inferred from present-day measurements, are mass-weighted averages of the element abundances produced in the different regions. These are most easily expressed in terms of the mass fraction $X_A$ of a given nuclide $A$, for which we have

$$\overline{X}_A = \int_0^\infty X_A(\eta) \, f(\eta) \, \eta \, d\eta / \overline{\eta}. \quad (7)$$

The factor of $\eta$ in the integral comes from the fact that the abundances must be weighted by the baryon density in each region before they mix. The only complication is that the deuterium and $^7$Li abundances are expressed as number ratios relative to hydrogen, $\text{D}/\text{H}$ and $\text{^7Li}/\text{H}$, rather than as mass fractions, where the relationship between $A/\text{H}$ and $X_A$ is given by

$$A/\text{H} = X_A / AX_H, \quad (8)$$

and the hydrogen mass fraction, $X_H$, is, to a good approximation, given by $X_H = 1 - Y_p$, where $Y_p$ denotes the primordial mass fraction of $^4$He. Then the mean value of $A/\text{H}$ averaged over different values of $\eta$ is

$$\overline{A/\text{H}} = \frac{1}{A(1 - \overline{Y}_p)} \int_0^\infty X_A(\eta) \, f(\eta) \, \eta \, d\eta / \overline{\eta}. \quad (9)$$

where $\overline{Y}_p$ is the mean primordial value of the $^4$He mass fraction in a given inhomogeneous model. In practice, $\overline{Y}_p$ never varies a great deal from the homogeneous value, $Y_p$, for the models considered here, so the correction given by including the factor of $1/(1 - \overline{Y}_p)$ instead of $1/(1 - Y_p)$ in Eq. (9) is negligible.

To perform this calculation, all that is needed is a choice for $f(\eta)$ and the values of the element abundances as a function of $\eta$ in the standard (homogeneous) case. A variety of choices for $f(\eta)$ have been investigated: unimodal distributions have included the gamma distribution [8, 10], the lognormal distribution [9], and the gaussian distribution [11]. We will examine the same set of distributions here.

Taking $\overline{\eta}$ to be given by $\overline{\eta} = 6.1 \times 10^{-10}$, consistent with the Planck results [31], we define the comparison ratio, $\phi$, to be given by

$$\phi \equiv \eta / \overline{\eta} = \eta / 6.1 \times 10^{-10}, \quad (10)$$

so that our earlier expressions become

$$\int_0^\infty f(\phi) \, d\phi = 1, \quad (11)$$

$$\int_0^\infty f(\phi) \phi \, d\phi = 1, \quad (12)$$
along with

\[ \mathcal{X}_A = \int_0^\infty X_A(\phi) \ f(\phi) \ \phi \ d\phi, \quad (13) \]

\[ \frac{A}{H} = \frac{1}{A(1 - Y_p)} \int_0^\infty X_A(\phi) \ f(\phi) \ \phi \ d\phi. \quad (14) \]

Since our goal is to use current observations to bound the magnitude of the fluctuations, we will express all of our results in terms of the RMS fluctuation in \( \phi \), with mean value 1, given by

\[ \sigma^2 = \int_0^\infty f(\phi) \ (\phi - 1)^2 \ d\phi, \quad (15) \]

and \( \sigma \) corresponds to the RMS fractional fluctuation in \( \eta \) for a given model (defined by a choice of inhomogeneity distribution \( f \)).

We now express the gaussian, lognormal, and gamma distributions in terms of \( \phi \), parametrizing each one by \( \sigma \).

First, consider the gaussian distribution with unit mean, given by

\[ f(\phi) = \frac{1}{\sqrt{2\pi\sigma}} e^{-(\phi-1)^2/2\sigma^2}. \quad (16) \]

Note that this distribution has the well-known problem that it implicitly allows negative values for \( \phi \) (and therefore for \( \eta \)) which are, of course, unphysical. However, we will confine our attention to sufficiently small values of \( \sigma \) (\( \sigma < 0.25 \)) that the negative values of \( \phi \) correspond to \( 4 - \sigma \) fluctuations and therefore have no significant effect on the final results. (In effect, we are truncating our gaussian at \( \phi = 0 \)).

The second distribution we consider is the lognormal with unit mean, given by

\[ f(\phi) = \frac{1}{\sqrt{2\pi s\phi}} e^{-(\ln(\phi) - \mu)^2/2s^2}, \quad (17) \]

where

\[ s = \sqrt{\ln(1 + \sigma^2)}, \quad (18) \]

and

\[ \mu = -\ln(1 + \sigma^2)/2. \quad (19) \]

Our final test distribution is the gamma distribution with unit mean, given by

\[ f(\phi) = \frac{\alpha^\alpha \phi^{\alpha-1} e^{-\alpha\phi}}{\Gamma(\alpha)}, \quad (20) \]

where \( \Gamma(\alpha) \) is the gamma function, and \( \alpha \) is related to \( \sigma \) by

\[ \alpha \equiv 1/\sigma^2. \quad (21) \]

Since our calculations of the mean element abundances involve an integration over \( X_A(\phi) \), we use a version of the Kawano nucleosynthesis code \[28\] with updated reaction rates \[29\] and a neutron lifetime of \( \tau = 880.2 \text{ sec} \[32\] to calculate the element abundances as a function of \( \phi \). Our predicted element abundances at \( \phi = 1 \) (\( \eta = 6.1 \times 10^{-10} \)) are \( \text{D/H} = 2.592 \times 10^{-5}, \ Y_p = 0.247, \) and \( 7\text{Li/H} = 4.544 \times 10^{-10} \). These abundances are in good agreement with the corresponding values in Ref. \[1\], but somewhat discrepant (for deuterium and lithium) from those in Ref. \[3\]. (The differences in the abundances predicted in Ref. \[1\] and those in Ref. \[3\] are most likely due to differences in the reaction rates used in the corresponding computer codes).

Since we can only calculate the element abundances at discrete values of \( \phi \), we divide the range in \( \phi \) into logarithmic bins and change the integrals in Eqs. \[13\] and \[14\] into the corresponding sums:

\[ \mathcal{X}_A = \sum_i X_A(\phi_i) \ f(\phi_i) \ \phi_i \ \Delta\phi_i, \quad (22) \]

\[ \frac{A}{H} = \frac{1}{A(1 - Y_p)} \sum_i X_A(\phi_i) \ f(\phi_i) \ \phi_i \ \Delta\phi_i. \quad (23) \]
We now proceed to calculate the inhomogeneous element abundances. Although our ultimate goal will be a limit on the magnitude of the density fluctuations, this limit will necessarily depend on current observational limits. To derive a result less prone to obsolescence, we will first determine the general effect on the element abundances by calculating the ratio, \( R \), of each element abundance in the inhomogeneous case to the corresponding homogeneous abundance as a function of \( \sigma \). We will denote this ratio by \( R_D \) for deuterium and \( R_{\text{Li}} \) for \(^7\text{Li}\). For each test distribution, we evaluate Eq. (23) using the binned abundances calculated numerically as a function of \( \phi \) to derive \( R_D \) and \( R_{\text{Li}} \) as a function of \( \sigma \). In standard (homogeneous) BBN, \(^4\text{He} \) varies much more slowly with \( \eta \) than do D and \(^7\text{Li} \) [1]. Consequently, the change in \(^4\text{He} \) is negligible for the range of \( \sigma \) values considered here; we find that \( Y_p \) is altered by less than 0.1%.

Our results for D and \(^7\text{Li} \) are displayed in Figs. 1-2. We first make some general observations. The effect of the inhomogeneities is to increase the abundance of deuterium and \(^7\text{Li} \) for all three of our choices for \( f(\phi) \). Further, the specific choice for the distribution function \( f(\phi) \) has only a small effect: the variation of the element abundances with \( \phi \) is very similar for all three of our choices for \( f(\phi) \). In the limit where \( \sigma \to 0 \), all three of our distributions give nearly identical results; this is because both the gamma and lognormal distributions approach a gaussian distribution in this limit.
FIG. 2: The ratio \( R_{Li} \) of the value of \( ^{7}\text{Li}/\text{H} \) for inhomogeneous BBN to the value of \( ^{7}\text{Li}/\text{H} \) in standard homogeneous BBN as a function of \( \sigma \) (the RMS fluctuation in \( \eta/\bar{\eta} \)) for the gaussian distribution (blue, solid), the lognormal distribution (red, dotted), and the gamma distribution (green, dashed).

It is possible to derive accurate analytic estimates for \( R \) in the small-\( \sigma \) limit. Ref. [1] provides approximations for the element abundances as a function of \( \eta \) when \( \eta \) is near the standard model value (\( \eta = 6.1 \times 10^{-10} \)). Reexpressing these abundances in terms of \( \phi \), we have [1]

\[
\begin{align*}
\text{D}/\text{H} &= (\text{D}/\text{H})_{\phi=1} \phi^{-1.60}, \\
^{7}\text{Li}/\text{H} &= (^{7}\text{Li}/\text{H})_{\phi=1} \phi^{2.11},
\end{align*}
\]

where the \( \phi = 1 \) subscript denotes the predicted element abundances at \( \phi = 1 \) (\( \eta = 6.1 \times 10^{-10} \)). Assuming that \( Y_p \) varies very little from its homogeneous value (a good approximation), we can substitute \( X(\phi) = X_{\phi=1} \phi^n \) along with the gaussian expression for \( f(\phi) \) (Eq. 10) into Eq. (14) and expand to second order in \( \sigma \) to obtain

\[
R \approx 1 + \frac{1}{2} n (n + 1) \sigma^2,
\]

where \( n = -1.60 \) for deuterium and \( n = 2.11 \) for \( ^{7}\text{Li} \). Eq. (26) provides an excellent approximation to \( R_D \) and \( R_{Li} \) for small values of \( \sigma \). While this analytic argument assumes a gaussian distribution, our other two distributions, as we have noted, approach a gaussian in the limit of small \( \sigma \), so Eq. (26) applies to them as well in the small-\( \sigma \) limit.
Eq. (26) shows that $R - 1$ increases quadratically with $\sigma$ in the small-$\sigma$ limit, but we can derive a more general result that is valid even when Eqs. (24) and (25) are no longer good approximations. The quantity multiplying $f(\phi)$ in Eq. (14) is $X_A(\phi)\phi$. When Eqs. (24)-(25) are valid, this quantity is, respectively, $\phi^{-0.60}$ for deuterium, and $\phi^{3.11}$ for $^7$Li. These are both convex functions (i.e., with positive second derivative). However, $X_A(\phi)\phi$ for both $^7$Li and deuterium remains a convex function beyond the range of validity of Eqs. (24)-(25). Whenever this quantity is convex, Jensen’s inequality applied to Eq. (14) implies that $R > 1$, i.e., the effect of inhomogeneities is to increase the deuterium and $^7$Li abundances relative to their homogeneous abundances. Furthermore, this result is independent of the functional form for $f(\phi)$ as long as $f(\phi)$ is small outside the range where $X_A(\phi)\phi$ is convex. As a corollary, the kinds of inhomogeneities we are considering here cannot solve the lithium problem, since a solution of that problem requires that the $^7$Li abundance predicted by BBN be decreased, not increased.

Not surprisingly, the observed deuterium abundance gives the best upper bound on $\sigma$. Using the $2-\sigma$ upper limit on D/H from the observational estimate in Eq. (3) and taking $D/H = 2.592 \times 10^{-5}$ for the theoretical value in the homogeneous case at $\phi = 1$, we obtain an upper bound on $R_D$:

$$R_D < 1.012.$$  

(27)

This limit is displayed in Fig. 1. While there is some small variation between the results for our three distributions, a conservative bound derived from the observational limit is

$$\sigma < 0.17,$$  

(28)

i.e., the RMS fluctuation in $\eta$ must be smaller than 17% of the mean value of $\eta$.

Lithium-$7$ increases more sharply with $\sigma$ in the inhomogeneous case than does deuterium. However, as we have noted, BBN already predicts a primordial $^7$Li abundance much larger than the observationally-estimated primordial abundance, so our $^7$Li results cannot be used to place useful limits on inhomogeneous BBN. The best we can do is to note that this model cannot ameliorate the primordial lithium problem; indeed, it makes the problem worse.

**IV. DISCUSSION**

It is clear that the combination of sharp upper bounds on the deuterium abundance, along with CMB limits on $\eta$, allows us to place tight constraints on the graininess of cosmological models of the early universe with large-scale baryon inhomogeneities. For all of the models examined here, the RMS fluctuation in $\eta$ is constrained to be less than 17% of the mean value of $\eta$. These constraints are due entirely to the upper bound on deuterium. The $^4$He abundance is much less sensitive to inhomogeneities in $\eta$, while the observationally-inferred primordial $^7$Li abundance is already in conflict with the predictions of standard BBN and so cannot constrain variations to BBN. Note further that the effect of inhomogeneities is to increase the $^7$Li abundance, so inhomogeneous BBN cannot provide a solution to the primordial lithium problem.

The obvious generalization of this work would be a reconsideration of fluctuations on smaller scales, where differential neutron and proton diffusion becomes important. Such models, however, are considerably more complex, since the geometry and magnitude of the fluctuations both have a strong influence on the final results.

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