New calculation of the mass fraction of primordial black holes

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We revisit the calculation of the abundance of primordial black holes (PBHs) formed from primordial density perturbations, using a formation criterion derived by Shibata and Sasaki which refers to a metric perturbation variable rather than the usual density contrast. We implement a derivation of the PBH abundance which uses peaks theory, and compare it to the standard calculation based on a Press-Schechter-like approach. We find that the two are in reasonable agreement if the Press-Schechter threshold is in the range \( \Delta_n = 0.3 \) to 0.5, but advocate use of the peaks theory expression which is based on a sounder theoretical footing.

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I. INTRODUCTION

Primordial black holes (PBHs) may have formed during the early Universe, and if so can have observational implications at the present epoch, either from effects of their Hawking evaporation or from a contribution to the present dark matter density [1,2]. That there is no unambiguous observational evidence of PBHs is a significant constraint on some possible types of early Universe physics. In particular, they are the only known way of constraining the density perturbation spectrum on extremely short scales, and indeed until fairly recently provided the most powerful upper limit on the spectral index of perturbations with an exactly power-law power spectrum.

However, the abundance of PBHs formed from a given initial power spectrum remains uncertain. The traditional calculation takes the same form as the Press-Schechter calculation much used in large-scale structure studies [3], where the density field is smoothed on a mass scale \( M \) (in this application taken to be at the time of horizon crossing), and those regions where the density contrast exceeds a threshold value \( \Delta_{\text{th}} \) are assumed to form PBHs with mass greater than \( M \). However the correct value for the threshold is quite uncertain. The “standard” value of 1/3 for a radiation-dominated Universe was derived by Carr [1] (see also Ref. [4]), but was probably only ever intended as an order-of-magnitude estimate. Subsequently, Niemeyer and Jedamzik [5] carried out numerical simulations of the collapse of isolated regions and found the threshold for PBH formation, in terms of the relative excess mass within the horizon, to be \( \Delta M / M_\odot = 0.7 \). However, Shibata and Sasaki [6] have pointed out that they formulate their initial data after horizon crossing, and hence their criterion cannot be related to the initial perturbations produced by, for instance, a period of inflation.

More recently, Shibata and Sasaki [6] devised a new approach to the formation of individual PBHs, seeking to find criteria on the metric perturbation rather than the density field, and in a form which can be applied to superhorizon initial perturbations. They were able to specify a criterion in terms of whether the initial central value of a particular metric perturbation variable \( \psi \) exceeds a threshold value. In this paper, we investigate the implications of this result for the abundance of PBHs formed.

II. THE PBH FORMATION CRITERION

We briefly describe the PBH formation criterion of Shibata and Sasaki, whose paper can be consulted for the full details [6]. They define a metric variable \( \psi \) from the spatial part of the metric on uniform-expansion hypersurfaces [their Eq. (2.2)] as

\[
\gamma_{ij} = a^2 \psi^4 \gamma_{ij},
\]

where \( \gamma_{ij} \) is the metric of the spatial 3-sections (throughout we assume a flat background and only consider scalar perturbations). Shibata and Sasaki numerically explored a range of initial configurations, all spherically symmetric, for the metric variable \( \psi \) in a radiation-dominated Universe, and were able to show that the central value of \( \psi \), denoted \( \psi_0 \), was a good indicator of PBH formation. They found that PBH formation took place provided \( \psi_0 \) exceeded a threshold value \( \psi_{0,\text{th}} \). The precise value of this threshold depended on the environment of the initial configuration, and lay in the range from 1.4 for a density peak surrounded by a low-density region, to 1.8 for a peak surrounded by a flat Friedmann-Robertson-Walker (FRW) region.

We wish to relate the Shibata–Sasaki threshold criterion to quantities given in standard linear perturbation theory, where the spatial part of the metric tensor is given by [7]

\[
g_{ij} = a^2 \left[ (1 + 2 R) \delta_{ij} + 2 \partial_i \partial_j H_T \right],
\]

where \( R \) is the curvature perturbation and \( H_T \) represents the anisotropic part. The gauge-invariant curvature perturbation on uniform-density hypersurfaces \( \zeta \) is defined as [8]

\[
\zeta = R - H_T \frac{\delta \rho}{\rho},
\]

with \( H \), \( \rho \), and \( \delta \rho \) denoting the Hubble parameter, background density, and perturbed density, respectively, which then gives
on superhorizon scales, where the anisotropic part $H_T$ is negligible. Note that on large scales uniform-density hypersurfaces coincide with uniform-expansion hypersurfaces (also known as uniform-Hubble hypersurfaces) [7].

A reasonable prescription for relating $\zeta$ and $\psi$ in the quasi-linear regime is

$$\exp(2\zeta) = \psi^4,$$  \hspace{1cm} (5)

since by definition $\psi^4 = \exp(2\Delta N)$ where $\Delta N$ is the difference in $e$-foldings between uniform-expansion hypersurfaces, and we can argue that the uniform-expansion and uniform-density slices are almost equivalent even in the non-linear regime, so that $\zeta = \Delta N$ [8,9]. Using Eq. (5), we find that the threshold values of $\psi_0$ ($\psi_{0,th} = 1.4$ and 1.8) correspond to thresholds on $\zeta$ of $\zeta_{th} = 0.7$ and 1.2 respectively.

### III. THE PBH ABUNDANCE

The observational constraints on the fraction of the energy density of the Universe in PBHs at the time they form, $\Omega_{\text{PBH}}(M)$, can be very roughly summarized as

$$\Omega_{\text{PBH}}(M) = \frac{\rho_{\text{PBH}}}{\rho_{\text{tot}}} \leq 10^{-20},$$  \hspace{1cm} (6)

on any interesting mass scale. Detailed examination of particular constraints can give more accurate values for the limits at particular masses [1,2], but for our present purpose we need only have an approximate guideline. In any event, PBH formation calculations remain uncertain enough that high-accuracy observational constraints are unnecessary; nevertheless the production rate is normally so sensitive to quantities we might wish to constrain, such as the density perturbation amplitude, that useful constraints can be extracted even from quite approximate calculations and constraints.

#### A. Review of the standard calculation

The traditional PBH abundance calculation (e.g. Refs. [1,10]) refers to a quantity which in modern terminology would be known as the density contrast on the comoving (velocity-orthogonal) slicing, which we denote by $\Delta$. The density contrast is smoothed on a scale $R$, and the calculation simply integrates the probability distribution $P(\Delta(R))$ over the range of perturbation sizes which form PBHs: $\Delta_{\text{th}} < \Delta(R) < \Delta_{\text{cut}}$, where the upper limit arises since very large perturbations would correspond to a separate closed universe in the initial conditions [11]. In practice $P(\Delta(R))$ is such a rapidly decreasing function of $\Delta(R)$ above $\Delta_{\text{th}}$ that the upper cutoff is not important. The threshold density is taken as $\Delta_{\text{th}} \approx w$, where $w = p/\rho$ is the equation of state [1]. This cannot of course be valid in the limit $w \to 0$, but is thought to be acceptable for the radiation-dominated case $w = 1/3$ which is the main one of interest.

The smoothed density contrast $\Delta(R,x)$ is found by convolving the density contrast $\Delta(x)$ according to

$$\Delta(R,x) = V^{-1} \int W(|x - y|/R) \Delta(x') \, d^3x',$$  \hspace{1cm} (7)

where $R$ is the smoothing scale, $W(y)$ is the window function used for the smoothing and $V$ is the volume of the window function. If the initial perturbations are gaussian, this property will be inherited by the smoothed density perturbation so that

$$P(\Delta(R)) = \frac{1}{\sqrt{2\pi} \sigma_\Delta(R)} \exp \left( -\frac{\Delta^2(R)}{2\sigma_\Delta^2(R)} \right),$$  \hspace{1cm} (8)

where $\sigma_\Delta(R)$ is the variance of $\Delta(R,x)$.

Here $P_\Delta(k) = (k^3/2\pi^2)(|\Delta(k)|^2)$ is the power spectrum of $\Delta$ and $W(kR)$ is the volume-normalized Fourier transform of the window function used to smooth $\Delta$. It is not obvious what the correct smoothing function to use is; a top-hat smoothing function has often been used in the past [10] although it is sensitive to scales well within the horizon, which requires careful treatment [12]. We prefer to use a gaussian window function:

$$W(kR) = \exp \left( -\frac{k^2R^2}{2} \right).$$  \hspace{1cm} (10)

On comoving hypersurfaces there is a simple relation between the density perturbation and the curvature perturbation (e.g., Ref. [13])

$$\Delta(t,k) = \frac{2(1+w)}{5+3w} \left( \frac{k}{aH} \right)^2 R_\zeta(k),$$  \hspace{1cm} (11)

where $R_\zeta$ is the curvature perturbation on comoving hypersurfaces, which coincides with the curvature perturbation on uniform-density hypersurfaces, Eq. (3), on large scales. The power spectra are related by

$$P_\Delta(k) = \frac{4(1+w)^2}{(5+3w)^2} \left( \frac{k}{aH} \right)^4 P_{\zeta}(k).$$  \hspace{1cm} (12)

Then at horizon crossing we have

$$P_\Delta(k) = \frac{4(1+w)^2}{(5+3w)^2} P_{\zeta}(k).$$  \hspace{1cm} (13)

The fraction of the Universe which exceeds the threshold for PBH formation $\Delta(M) > \Delta_{\text{th}}$ when smoothed on scale $M$, and hence will form a PBH with mass $> M$, is given as in Press-Schechter theory by

\footnote{Throughout we assume for simplicity that the PBH mass is equal to the horizon mass $M_H$ corresponding to the smoothing scale. This is not strictly true (and in fact the PBH mass appears to depend on the size and shape of the perturbations [5,6]); however, this uncertainty is not important when applying PBH abundance constraints, due to their relatively weak mass dependence.}
\[ \Omega_{\text{PBH,PS}}(\Delta, > M) = 2 \int_{\Delta}^{\infty} \frac{\Delta d\Delta}{d\Delta} \]

In this expression we have followed the usual Press-Schechter practice of multiplying by a factor 2, which can be thought of as allowing for the fact that the PBH formation happens in regions which are overdense with respect to the mean cosmological density.

For the purpose of specific calculations in this paper, we assume a power-law primordial power spectrum \( P_A(k) = A_{R_e}(k/k_0)^{n-1} \), so that

\[ \sigma_A^2(M) = \frac{2(1 + w)^2 A_{R_e} \Gamma[(n - 1)/2]}{(5 + 3 w)^2 (k_0 R)^{n-1}}. \]  

(Sp)ergel et al. [14,15] found, from the WMAP2x+2dFGRS dataset as described in their paper, that \( A_{R_e} = (0.8 \pm 0.1) \times 2.95 \times 10^{-9} \) for \( k_0 = 0.05 \text{ Mpc}^{-1} \).

**B. A new calculation using peaks theory**

The Shibata and Sasaki PBH formation criterion is expressed in terms of the peak value of the fluctuation, \( \psi_0 \), at \( t = 0 \) (equivalently, at some early time when the perturbation is on superhorizon scales, since \( \psi \) is constant on superhorizon scales). Rather than the Press-Schechter form, it is therefore best suited to a calculation of the mass function using the theory of peaks, as extensively described by Bardeen et al. [16]. We will apply peaks theory to the initial value of the variable \( \zeta \).

After smoothing the density field on a scale \( M \), the number density of peaks with height greater than \( \nu \), where \( \nu = \zeta_0 / \sigma_\zeta(M) \), is given (for high peaks) by [16,17]

\[ n_{\text{peaks}}(\nu, M) = \frac{1}{(2 \pi)^2} \left( \frac{\langle k^2 \rangle(M)}{3} \right)^{3/2} (\nu^2 - 1) e^{-\nu^2/2}, \]  

(16)

where \( \langle k^2 \rangle(M) \) is the second moment, with respect to \( k \), of the power spectrum

\[ \langle k^2 \rangle(M) = \frac{1}{\sigma_\zeta^2(M)} \int_0^{\infty} k^2 W^2(kR) P_\zeta(k) \frac{dk}{k}. \]  

(17)

For a power-law power spectrum \( P_\zeta(k) = A_\zeta(k/k_0)^{n-1} \) (with \( A_\zeta = A_{R_e} \) since on superhorizon scales \( \zeta = R_e \)) and a Gaussian window function, we have

\[ \langle k^2 \rangle(M) = \frac{n-1}{2 R^2}. \]  

(18)

The number density of peaks with height greater than \( \nu \), when smoothed with a Gaussian filter on scale \( M \), is then given by

\[ n_{\text{peaks}}(\nu, M) = \frac{1}{(2 \pi)^2} \left( \frac{\langle k^2 \rangle(M)}{3} \right)^{3/2} (\nu^2 - 1) e^{-\nu^2/2}, \]  

(19)

where

\[ \nu = \left( \frac{2(k_0 R)^{n-1}}{A_\zeta \Gamma((n - 1)/2)} \right)^{1/2} \xi_\text{th}. \]  

(20)

The number density of peaks is related to the fraction of the Universe in peaks above the threshold by \( \Omega_{\text{PBH,peaks}}(\nu, \nu > M) = n_{\text{peaks}}(\nu, M) / \rho \). Here \( M \) is the mass associated with the filter (which for a Gaussian window function is given by \( M = \rho(2 \pi)^{3/2} R^3 \)) so that

\[ \Omega_{\text{PBH,peaks}}(\nu, \nu > M) = \frac{(n-1)^{3/2}}{(2 \pi)^{1/2} 6^{3/2} \sigma_\zeta^2(M)} \left( \frac{\xi_\text{th}}{2 \sigma_\zeta^2(M)} \right)^2 \]  

\times \exp \left( -\frac{\xi_\text{th}^2}{2 \sigma_\zeta^2(M)} \right), \]  

(21)

where

\[ \sigma_\zeta(M) = \frac{5 + 3 w}{2(1 + w)} \sigma_A(M) = \left( \frac{A_\zeta \Gamma((n - 1)/2)}{2(k_0 R)^{n-1}} \right)^{1/2}. \]  

(22)

**C. Comparison**

To use our results, we need to relate the comoving smoothing scale \( R \) to the horizon mass. The main case of interest is radiation domination, where \( w = 1/3 \). The horizon mass is given by

\[ M_H = \frac{4 \pi}{3} \rho(H^{-1})^3, \]  

(23)

when the scale enters the horizon, \( R = (aH)^{-1} \). During radiation domination \( aH \propto a^{-1} \), and expansion at constant entropy gives \( \rho \propto g_* a^{-4} \) [18] (where \( g_* \) is the number of relativistic degrees of freedom, and we have approximated the temperature and entropy degrees of freedom as equal). This implies

\[ M_{\text{H,eq}} = M_{\text{H,eq}}(k_{\text{eq}} R)^2 \left( \frac{g_{* \text{eq}}}{g_*} \right)^{1/3}. \]  

(24)

In the early Universe \( g_* \) is expected to be of order 100, while \( g_{* \text{eq}} \approx 3, k_{\text{eq}} = 0.07 \Omega_m h^2 \text{ Mpc}^{-1} \). The horizon mass at matter-radiation equality is given by

\[ M_{\text{H,eq}} = \frac{4 \pi}{3} \rho_{\text{rad,eq}} H_{\text{eq}}^{-3} = \frac{8 \pi}{3} \rho_{\text{rad,eq}} k_{\text{eq}} a_{\text{eq}}^{2/3}, \]  

(25)

where \( a_{\text{eq}}^{-1} = 24000 \Omega_m h^2 \text{ and (assuming three species of massless neutrinos) } \Omega_{\text{rad,eq}} h^2 = 4.17 \times 10^{-3} \text{ so that } M_{\text{H,eq}} = 1.3 \times 10^{40} (\Omega_m h^2)^{-2} \text{ g.} \]  

(26)
If we take $\Omega_{bh} h^2 = 0.14$ [15], then $M_{1h, eq} = 7 \times 10^{50}$ g.

In Fig. 1 we show various calculations of the abundance $\Omega_{bh}(M)$ for power-law primordial power spectra with spectral indices $n = 1.25$ and 1.5. The traditional calculation with $\Delta_{th} = 1/3$ is compared with the peaks theory calculation for the two thresholds $\zeta_{th} = 0.7$ and 1.2. We see that the two peaks theory calculations actually bracket the traditional calculation. The high value of $\zeta_{th}$, corresponding to the lower abundance of PBHs, is the one which corresponds to peaks surrounded by a FRW Universe, and hence is likely to be more appropriate for the cosmological models under discussion.

While we advocate use of the peaks theory expression Eq. (21) to calculate the mass function, we see in the figure that the curves have similar shapes to those of the traditional calculation. In fact, if the peak theory and Press-Schechter expressions were exactly the same, the thresholds would simply be related by Eq. (13), which in radiation domination would give $\Delta_{th} = 4 \zeta_{th}/9$. It turns out that this correspondence does hold quite accurately for our results even at the low abundances $\Omega_{bh} \sim 10^{-20}$ which are close to current observational bounds, breaking down only at much lower abundances where peaks theory is systematically higher than the Press-Schechter formalism. We therefore have quite a good correspondence: $\zeta_{th} = 1.2$ is equivalent to $\Delta_{th} = 0.5$, and $\zeta_{th} = 0.7$ to $\Delta_{th} = 0.3$.

IV. DISCUSSION

We have provided a new calculation of the abundance of PBHs generated by primordial density perturbations. By using a metric perturbation variable rather than the density contrast, a PBH formation criterion can be applied directly to the initial perturbation spectrum. Within this formalism, we have found that the PBH mass spectrum is best computed using the theory of peaks, rather than the standard Press-Schechter-like calculation.

Given the considerable uncertainties involved, our results do not lead to any drastic revision of the PBH formation rate, but do put the calculation on a sounder theoretical footing. Our mass function can be fairly well approximated by that of the standard calculation in the region of interest ($\Omega_{bh} \sim 10^{-20}$), if the threshold density $\Delta_{th}$ is taken in the range 0.3 to 0.5. This range of threshold values is however significantly lower than the value $\Delta_{th} = 0.7$ suggested by the simulations of Niemeyer and Jedamzik [5], and in fact encompasses the value $\Delta_{th} = 1/3$ used in the earliest PBH literature. However, we advocate that anyone using our results adopts the peaks theory expression for the mass function given by Eq. (21).

Note added. Recently, Ref. [19] was brought to our attention. This paper uses the constraints on the metric perturbation variable $\psi$ from Ref. [6] to calculate the PBH abundance, but does not use the peak formalism.

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