Efficient Computation of Hyperspherical Bessel Functions

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Fast and accurate computations of the power spectrum of cosmic microwave background fluctuations are essential for comparing current and upcoming data sets with the large parameter space of viable cosmological models. The most efficient numerical algorithm for power spectrum calculation, recently implemented by Seljak and Zaldarriaga, involves integrating sources against spherical Bessel functions or, in the cases of a non-flat universe, analogous hyperspherical Bessel functions. Evaluation of these special functions usually dominates the computation time in non-flat spatial geometries. This paper presents a highly accurate and very fast WKB approximation for computing hyperspherical Bessel functions which will greatly increase the speed of microwave background power spectrum computations in open and closed universes.

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I. INTRODUCTION

The power spectra of temperature and polarization fluctuations of the cosmic microwave background contain a rich harvest of cosmological information. From upcoming high-resolution maps of the microwave background, we can hope to determine the basic cosmological parameters to high precision, as well as test the nature of the primordial perturbations and the mechanism for structure formation in the Universe [1]. Extracting this information will require computationally intensive analysis of the parameter space of cosmological models; a basic, general family of inflation-like models requires around ten parameters. Monte Carlo explorations of such a large parameter space will require power spectra evaluations for millions of models, so it is imperative that the fastest possible code be available for calculating power spectra.

Traditionally, microwave background power spectra were computed by expanding the angular dependence of the radiation field in multipole moments and then evolving the resulting set of coupled differential equations. For power spectra at sub-degree scales, typically several thousand coupled equations need to be evolved; the CPU time for such codes on current workstations is generally measured in hours. Even scaling up to supercomputer speeds, large Monte Carlo calculations are not possible with such codes.

A major advance was the realization by Seljak and Zaldarriaga that a formal integral solution to the photon evolution equation allows the solution (in flat space) to be expressed as a source term integrated against spherical Bessel functions [2]. The source term still needs to be calculated via coupled evolution equations, but since only the lowest moments contribute to the source term, far fewer equations must be evolved. In essence, the full set of coupled equations integrates the Bessel equation, whose solution is already known. The spherical Bessel functions depend on radius \( r \) and on two parameters, the wavenumber \( k \) and the index \( l \); however, in flat space, the wavenumber can be scaled with the radial variable so \( j_l(\kappa r) \) is actually a one-parameter family of functions. Microwave background computations generally require values of \( l \) up to a few thousand, and it is computationally feasible to precompute and cache the required Bessel functions. Thus the flat-space power spectrum can be evaluated with a greatly increased speed using the Seljak-Zaldarriaga algorithm.

For open or closed universes, the analogous “hyperspherical” Bessel functions depend on the radial coordinate and the wavenumber separately, so an inordinate number of functions would need to be precomputed and stored. Seljak and Zaldarriaga resort to a numerical integration of the differential equation defining the hyperspherical Bessel functions, which is far slower than calling the precomputed functions in the flat case. This paper calculates the WKB approximation to the hyperspherical Bessel functions, which, while not as fast as precomputation, offers a dramatic increase in computational speed over other methods. Furthermore, the WKB approximation is highly accurate for all but the lowest few values of \( l \).

The following Section gives a brief review of WKB theory. Section III then gives an overview of the relevant properties of the hyperspherical Bessel functions; Section IV derives the WKB approximation for all cases, including

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the usual spherical Bessel functions in the flat space limit. Comparisons with exact functions demonstrate the remarkable accuracy of the approximation. The paper concludes with brief remarks discussing implementation and application of the approximations.

II. REVIEW OF WKB THEORY

The WKB approximation applies to equations of the Schrodinger form
\[ \epsilon^2 y'' = Q(x)y. \]  
(1)

Such equations have exponential behavior in regions where \( Q(x) > 0 \) (dissipative regions) and oscillatory behavior when \( Q(x) < 0 \) (dispersive regions). Points with \( Q(x) = 0 \) are called turning points, marking the transition between the two behaviors. The WKB approximation (away from the turning points) consists of an exponentiated power series in \( \epsilon \):
\[ y(x) = \exp \left[ \frac{1}{\epsilon} \sum_{n=0}^{\infty} S_n(x) \epsilon^n \right]. \]  
(2)

This paper considers the usual first-order WKB approximation, which retains only the \( n = 0 \) and \( n = 1 \) terms of the expansion. This approximation is often surprisingly accurate for \( \epsilon \) as large as 1. For a more detailed exposition of WKB theory, see Ref. [3].

Equations possessing a single turning point are the most straightforward application of WKB theory. Without loss of generality, translate the dependent variable so that the turning point is at the origin and \( Q(x) > 0 \) for \( x > 0 \). In the dissipative region \( x > 0 \), which will be called region I, a simple asymptotic expansion gives the familiar “WKB formula” for the exponentially decaying solution
\[ y_I(x) \approx C \left[ Q(x) \right]^{-1/4} \exp \left[ -\frac{1}{\epsilon} \int_0^x \sqrt{Q(t)} \, dt \right], \]  
(3)

where \( C \) is an undetermined normalization constant. In region II in the neighborhood of \( x = 0 \), \( Q(x) \) can be replaced by its asymptotic expansion \( Q \sim ax, x \to 0 \) which converts Eq. (1) to an Airy equation with solution
\[ y_{II}(x) \sim 2C \sqrt{\pi(a\epsilon)^{-1/6}} \text{Ai} \left( a^{1/3} \epsilon^{-2/3} x \right), \quad x \to 0 \]  
(4)

where \( \text{Ai}(x) \) is the first type of Airy function and the prefactor has been determined by an asymptotic match with Eq. (3). Finally, in region III with \( x < 0 \), an analytic continuation of Eq. (3) and an asymptotic match to \( y_{II} \) gives
\[ y_{III}(x) \approx 2C \left[ Q(x) \right]^{-1/4} \sin \left[ \frac{1}{\epsilon} \int_x^0 \sqrt{-Q(t)} \, dt + \frac{\pi}{4} \right]. \]  
(5)

Remarkably, there exists a single function which uniformly approximates \( y(x) \) and reduces to the above asymptotic forms in the various limits:
\[ y(x) \approx 2\sqrt{\pi}C \left( \frac{3S_0(x)}{2\epsilon} \right)^{1/6} \left[ Q(x) \right]^{-1/4} \text{Ai} \left[ \left( \frac{3S_0(x)}{2\epsilon} \right)^{2/3} \right], \]  
(6)

\[ S_0(x) = \int_0^x \sqrt{Q(t)} \, dt. \]

This formula is the basis for all approximations presented in this paper.

For the case of a function with two turning points at \( x = A \) and \( x = B \), two single-turning-point solutions can be asymptotically matched to form the general solution, which leads to the eigenvalue condition
\[ \frac{1}{\epsilon} \int_A^B \sqrt{-Q(t)} \, dt = \left( n + \frac{1}{2} \right) \pi \]  
(7)

with \( n \) a non-negative integer. This condition typically is used to approximate the energy eigenvalues of a particle in an arbitrary potential well in quantum mechanics.
III. PROPERTIES OF HYPERSPHERICAL BESSEL FUNCTIONS

It is straightforward to apply these expressions to the case of hyperspherical Bessel functions. A review of their relevant properties is presented here; a more detailed exposition of these functions on which the following discussion is based is given in Ref. [3]. The hyperspherical Bessel functions \( \Phi^\beta_l(r) \) are radial eigenfunctions of the covariant Laplace operator in spherical coordinates, for spaces of constant curvature:

\[
(\nabla^2 + k^2)\Phi^\beta_l(r)Y_{lm}(\theta, \phi) = 0
\]

where the index \( \beta = \sqrt{K^2 + l} \) with \( K = H^2_0(\Omega_0 - 1) \) the spatial curvature, and \( \nabla \) is the covariant 3-derivative associated with the spatial part of the Robertson-Walker metric:

\[
ds^2 = dt^2 - R^2(t)\left[\frac{dr^2}{1 - Kr^2} + r^2d\Omega^2\right].
\]

In this paper, all physical distances will be expressed in units of the curvature scale, giving \( K = 1 \) for a closed universe, \( K = 0 \) for a critical (flat) universe, and \( K = -1 \) for an open universe. The eigenfunctions \( \Phi^\beta_l \), termed “hyperspherical” or “ultraspherical” Bessel functions because they reduce to the usual spherical Bessel functions in the case of a flat universe, are very useful because they serve as the analog of Fourier modes for cosmological models with non-zero curvature. For a critical density universe with no spatial curvature, \( \nabla \) is just the usual gradient operator and \( \Phi^\beta_l(r) = j_l(\beta r) = j_l(kr) \).

It is convenient to change variables to the radial coordinate \( \chi \) defined by \( d\chi = dr/\sqrt{1 - Kr^2} \); explicitly,

\[
r(\chi) = \begin{cases} 
\sin\chi, & K = 1; \\
\chi, & K = 0; \\
\sinh\chi, & K = -1.
\end{cases}
\]

Then it is straightforward to demonstrate from Eq. (8) that the hyperspherical Bessel functions satisfy the Schrodinger equation

\[
d^2u^\beta_l(d\chi) = \left[\frac{l(l + 1)}{r(\chi)^2} - \beta^2\right]u^\beta_l
\]

where \( u^\beta_l(\chi) = r(\chi)\Phi^\beta_l(\chi) \). The hyperspherical Bessel functions are normalized so as to match the normalization of \( j_l(kr) \) in the flat-space limit. For the cases \( K = 0 \) and \( K = -1 \), the momentum variable \( \beta \) can have any positive value, Eq. (11) has a single turning point for \( \chi > 0 \), and the WKB approximation can be applied directly.

The \( K = 1 \) case is more complicated: the spatial sections of the spacetime are compact, resulting in a discrete eigenvalue spectrum for the eigenfunctions. It is possible to express the closed-universe functions in terms of associated Legendre polynomials as

\[
\Phi^\beta_l \propto (\sin\chi)^{-l/2}P^l_{-\frac{1}{2}}(\cos\chi);
\]

this form shows that \( \Phi^\beta_l \) is periodic in \( \chi \) with period \( 2\pi \). As with spherical Bessel functions, \( \Phi^\beta_l \) is symmetric (antisymmetric) around \( \chi = 0 \) for \( l \) even (odd); thus the function is determined by its values on the interval \([0, \pi]\). Requiring \( \Phi^\beta_l \) to be single-valued gives the condition

\[
\Phi^\beta_l(-\cos\chi) = \cos((\beta - l - 1)\pi)\Phi^\beta_l(\cos\chi).
\]

Two conclusions follow immediately: \( \beta \) must be a positive integer, and the functions are symmetric (antisymmetric) around \( \chi = \pi/2 \) if \( \beta - l - 1 \) is even (odd). Thus the value of \( \Phi^\beta_l(\chi) \) must be computed only on the interval \([0, \pi/2]\) and can be determined for all other values of \( \chi \) by symmetry. It can be demonstrated that \( \beta = 1 \) and \( \beta = 2 \) represent gauge modes, not physical perturbations [3], so \( \beta \) takes integer values of 3 or larger, and \( \beta > l \) follows from Eq. (12).

The hyperspherical Bessel functions also satisfy several useful recursion relations which are given in Ref. [3]. A closed-form expression for \( \Phi^\beta_l \) can be obtained as \( l + 1 \) derivatives of an elementary function; it is practicable to use these exact expressions for evaluating the hyperspherical Bessel functions up to \( l = 4 \) or 5. For precise calculation of the functions for larger values of \( l \), recursion techniques can be used for the open case, in analogy with the Miller’s method evaluation of Bessel functions in Ref. [4]. However, for the closed case, downwards recursion is not always available due to the restriction \( l < \beta \), so direct integration of Eq. (11) is better [7].
IV. WKB APPROXIMATIONS

To apply the WKB formalism most effectively, first divide both sides of Eq. (11) by \( l(l + 1) \) to obtain Eq. (1) with

\[
Q(\chi) = \frac{1}{r^2(\chi)} - \alpha^2
\]

with \( \alpha \equiv \beta \epsilon \) and \( \epsilon = 1/\sqrt{l(l + 1)} \). Turning points \( \chi_0 \) are located where

\[
r(\chi_0) = 1/\alpha;
\]

note that the \( K = 0 \) and \( K = 1 \) cases each have a single turning point, while the \( K = 1 \) case has a single turning point within the range \( [0, \pi/2] \). Thus Eq. (1) can be applied directly to each case. The WKB approximation is an asymptotic series in powers of \( \epsilon \), which in this case is the inverse of \( l \). For larger \( l \) values, the approximation becomes progressively better; it is also better away from the region of the turning point where the various asymptotic solutions are matched. As demonstrated below, the approximation is remarkably good even for \( l = 2 \) and 3.

The WKB approximation offers a great increase in numerical speed because the required integrals can be performed exactly in terms of elementary functions. For the \( K = 0 \) case,

\[
\int_{\chi_0}^{\chi} \left( \alpha^2 - \frac{1}{\epsilon^2} \right)^{1/2} dt = \sqrt{\alpha^2\chi^2 - 1} - \sec^{-1}(\alpha\chi),
\]

\[
\int_{\chi}^{\chi_0} \left( \frac{1}{\epsilon^2} - \alpha^2 \right)^{1/2} dt = \log(1 + \sqrt{1 - \alpha^2\chi^2}) - \sqrt{1 - \alpha^2\chi^2}.
\]

For the \( K = -1 \) case, defining \( w \equiv \alpha \sinh \chi \),

\[
\int_{\chi_0}^{\chi} \left( \alpha^2 - \frac{1}{\sinh^2 t} \right)^{1/2} dt = \alpha \log\left( \frac{\sqrt{w^2 - 1} + \sqrt{w^2 + \alpha^2}}{\sqrt{1 + \alpha^2}} \right) + \tan^{-1}\left[ \frac{1}{\alpha} \left( \frac{w^2 + \alpha^2}{w^2 - 1} \right)^{1/2} \right] - \frac{\pi}{2},
\]

\[
\int_{\chi}^{\chi_0} \frac{1}{\sinh^2 t} - \alpha^2 \right)^{1/2} dt = \frac{\alpha}{2} \tan^{-1}\left( \frac{2\sqrt{(1 - w^2)(w^2 + \alpha^2)}}{2w^2 + \alpha^2 - 1} \right) + \log\left( \frac{\alpha \sqrt{1 - w^2} + \sqrt{\alpha^2 + w^2}}{w^2 \sqrt{1 + \alpha^2}} \right).
\]

And similarly, for the \( K = 1 \) case, defining \( v \equiv \alpha \sin \chi \),

\[
\int_{\chi_0}^{\chi} \left( \alpha^2 - \frac{1}{\sin^2 t} \right)^{1/2} dt = \tan^{-1}\left[ \frac{1}{\alpha} \left( \frac{\alpha^2 - v^2}{v^2 - 1} \right)^{1/2} \right] - \frac{\alpha}{2} \tan^{-1}\left( \frac{2\sqrt{(v^2 - 1)(\alpha^2 - v^2)}}{2v^2 - \alpha^2 - 1} \right) - \frac{\pi}{2},
\]

\[
\int_{\chi}^{\chi_0} \frac{1}{\sin^2 t} - \alpha^2 \right)^{1/2} dt = \tanh^{-1}\left[ \alpha \left( \frac{1 - v^2}{\alpha^2 - v^2} \right)^{1/2} \right] - \log\left( \frac{\sqrt{1 - v^2} + \sqrt{\alpha^2 - v^2}}{\sqrt{\alpha^2 - 1}} \right).
\]

Care must be taken to use the correct branch of the inverse tangent functions.

In the closed case, the eigenvalue condition Eq. (6) becomes

\[
\beta = n + \frac{1}{2} + \frac{1}{\epsilon}
\]

with \( n \) an integer, so for a given exact integer value of \( \beta \), the corrected WKB eigenvalue can be obtained by the replacement

\[
\beta \to \beta - \frac{1}{8l} + \frac{1}{16l^2},
\]

which is sufficiently accurate for a first-order WKB approximation. If the eigenvalue \( \beta \) is not corrected when evaluating the approximate function, the function or its first derivative will be discontinuous at \( \chi = \pi/2 \).

The other necessary numerical ingredient is the evaluation of the Airy function in Eq. (7). If a fast routine is not available, a reasonable approximation is to use the leading asymptotic behavior at large arguments and a Taylor series around the origin. With a crossover at \( |x| = 1.6 \) and a series including \( x^{13} \) terms, the residual error in \( \text{Ai}(x) \) is at the 1% level. Fast routines based on Chebyshev polynomial fits or Pade expansions are readily obtainable in both
FIG. 1. The WKB approximation for the usual spherical Bessel functions $j_l(\chi)$, for $l = 2$ and $l = 5$. The exact functions are solid lines, the approximate functions dashed lines. For $l > 5$ the exact and approximate functions are indistinguishable on the scale of the plot.
Fortran and C. Note that since the Airy function is evaluated for every hyperspherical Bessel function, errors in Airy function evaluation translate into systematic errors in $\Phi^\beta_l$. Using the simple asymptotic approximation to $\text{Ai}(x)$, for example, leads to a systematic 1% error when integrating smooth functions against $\Phi^\beta_l$ independent of $l$; this error is reduced to 0.01% or less when an accurate Airy function evaluation is employed \cite{8}.

Figure 1 displays the exact and WKB-approximated spherical Bessel functions $j_l(\chi)$ for $l = 2$ and $l = 5$. The accuracy is very good even for $l = 2$, with an error of 1.5% at the first peak in the $l = 2$ case and 0.6% at the first peak in the $l = 5$ case. For higher values of $l$, the actual and approximated functions are indistinguishable on the scale of the plot; by $l = 20$, the first peak is accurate to 0.05%. As mentioned above, the harmonics for the lowest few $l$ values can be evaluated exactly in terms of trigonometric functions.

![Figure 1](image1.png)

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Figures 2 and 3 compare the exact and WKB-approximated hyperspherical Bessel functions for open and closed universes, respectively. The level of accuracy is essentially the same as in the flat case, with approximations for $l > 5$ indistinguishable from the exact values on the scales of the plots. One particular set of closed-universe functions always has a significant error: the lowest eigenvalue corresponding to a given $l$ with the unperturbed value $\beta = l + 1$. As shown in Figure 4, the approximate functions have discontinuous derivatives at $\chi = \pi/2$ for all $l$. The reason is that the turning point $\chi_0$ is so close to $\pi/2$ for the lowest eigenvalue that the solution does not have enough room between $\chi_0$ and $\pi/2$ to attain its asymptotic behavior away from the turning point, so an asymptotic match around

![Figure 2](image2.png)

FIG. 2. The WKB approximation for the open universe hyperspherical Bessel functions $\Phi^2_2$ and $\Phi^5_5$, shown as the dashed lines, compared with the solid exact functions.

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FIG. 3. The WKB approximation for the closed universe hyperspherical Bessel functions $\Phi_7^2$ and $\Phi_5^7$, shown as the dashed lines, compared with the solid exact functions.
\( \chi = \pi/2 \) is unsuccessful. This behavior can be circumvented with an exact form for the lowest eigenfunctions:

\[
\Phi_l^{l+1}(\chi) = \left[ \frac{(2l)!!}{(l+1)(2l+1)!!} \right]^{1/2} \sin^l \chi \quad (K = 1)
\]

\[
\sim \left[ \frac{2\pi}{2l+1} \right]^{1/4} \left[ \frac{l}{(l+1)(2l+1)} \right]^{1/2} \left[ 1 + \frac{9}{48l} - \frac{7}{512l^2} \right] \sin^l \chi, \quad l \to \infty; \quad (21)
\]

the asymptotic expression is good to 0.02% at \( l = 2 \). Fortunately, the second and higher eigenvalues are not greatly affected by this problem (see Fig. 3, for example).

**FIG. 4.** The WKB approximation for the closed universe hyperspherical Bessel functions \( \Phi_3^3 \) and \( \Phi_5^5 \), shown as the dashed lines, compared with the solid exact functions. The discrepancy near \( \chi = \pi/2 \) is because the matching solution does not have enough space between the two turning points to reach its asymptotic value. This artifact persists in the lowest eigenfunction for all values of \( l \).
V. CONCLUDING REMARKS

The above calculations demonstrate that the WKB approximation to hyperspherical Bessel functions is highly accurate, with increasing accuracy as \( l \) becomes larger. Furthermore, the computation of one of the functions at a given value of \( \chi \) requires around ten elementary function calls, plus some arithmetic, so the approximation is much faster than evaluation based on recursion methods or integration of Eq. (11). The computation time is also independent of \( l \), in marked contrast to other methods, and is completely stable for any values of \( l \) and \( \beta \). This approximation will substantially speed the computation of microwave background power spectra in open or closed universes, potentially by an order of magnitude based on rough timings of the CMBFAST code [9].

A further speedup in evaluating these functions can be accomplished by precomputing and caching the integrals in Eqs. (16) to (18); each is a function of the two variables \( \chi \) and \( \alpha \). The integrals are very uneventful functions of these variables, and accurate interpolation is possible based on a small number of computed values. With this scheme, the computational work for a hyperspherical Bessel function is reduced to evaluating a power and a sine or exponential in Eq. (13) or (14), an inverse sine or hyperbolic sine to evaluate \( \chi_0 \), and a small amount of arithmetic.

The uniform WKB approximation presented here is useful for evaluating any functions defined by a second-order differential equation in Schrödinger form, especially when speed of evaluation is more important than accuracy to many significant figures. This is often the case in physics problems, and particularly in the case where a special function is integrated against another function. If it is impracticable to cache all needed values of the special function, WKB offers a fast, simple, and remarkably accurate alternative.

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