Cosmological perturbations: Noncold relics without the Boltzmann hierarchy

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We present a formulation of cosmological-perturbation theory where the Boltzmann hierarchies that evolve the neutrino phase-space distributions are replaced by integrals that can be evaluated easily with fast Fourier transforms. The simultaneous evaluation of these integrals combined with the differential equations for the rest of the system (dark matter, photons, baryons) are then solved with an iterative scheme that converges quickly. The formulation is particularly powerful for massive neutrinos, where the effective phase space is three dimensional rather than two dimensional, and even more so for three different neutrino mass eigenstates. Therefore, it has the potential to significantly speed up the computation times of cosmological-perturbation calculations. This approach should also be applicable to models with other noncold collisionless relics.

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I. INTRODUCTION

The publicly available cosmological-perturbation codes CAMB [1] and CLASS [2] lie at the heart of almost all analyses in cosmology. These codes solve the differential equations for the evolution of the gravitational potentials, the baryon and dark-matter fluid equations, the neutrino and photon distribution functions, and possibly more species, depending on the cosmological model considered. The codes, which build upon nearly half a century of technical innovations [3], are now remarkably efficient. However, modern Markov chain Monte Carlo (MCMC) analyses require these codes to be called tens of thousands of times to obtain the posterior in a multidimensional cosmological-parameter space, requiring perhaps days of CPU time. There is thus incentive to accelerate these codes.

The most time-consuming parts in these calculations are the "Boltzmann hierarchies," which evolve the higher moments of the photon and neutrino distribution functions. The real bottleneck, though, is massive neutrinos: Since their momentum distribution occupies a three-dimensional, rather than two-dimensional, space, they require, strictly speaking, an infinitude of hierarchies. Nonzero neutrino masses are, moreover, becoming increasingly important given that they will be probed with forthcoming cosmological measurements [4]. Clever numerical methods are able to reduce the system of ordinary differential equations (ODEs) to a manageable size [2]. But the algorithms are still ultimately limited by the requirement to solve—depending on the target accuracy—$O(500)$ ODEs (for each Fourier wave number k) for the Boltzmann hierarchies of photons and three generations of massive neutrinos. The computational problem is exacerbated further with the increased focus on new-physics models with other noncold relics or neutrino models with nonthermal phase-space distributions; we list in Refs. [5–10] papers from just the past year on such relics.

It has long been known that each Boltzmann hierarchy is formally equivalent to a small set of integral equations [11], but only recently [12] has this formalism been implemented for scalar perturbations numerically. Numerical experiments in which the photon hierarchies were replaced with the integral equations showed that the new "hierarchyless" formalism may have the potential to accelerate cosmological-perturbation codes. We emphasize that this formalism provides a numerical solution to the perturbation equations; it is not an analytical approximation.

Here, we apply this integral-equation approach to neutrinos (and other collisionless noncold relics) and show that it is potentially extremely powerful. First of all, the integral equations for collisionless particles are simply integrals. Moreover, each integral can be written as a convolution of gravitational potentials and a radial eigenfunction, and the convolution can be done trivially with a fast Fourier transform (FFT). The only catch is that the collisionless-sector equations must be solved with the equations for the rest of the system iteratively. Still, as we show, this iteration converges quickly. If the collisionless sector dominates the computational effort, this iterative scheme may provide a more computationally efficient route to a precise numerical solution.

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Below, we first derive the integral equations for the moments of the massive-neutrino distribution functions and show how they can be written as convolutions. We then discuss aspects of the iterative scheme [12] to solve the collisionless-sector perturbations in tandem with the equations for photons, dark matter, baryons, and gravitational potentials. We present numerical results from a proof-of-concept code and end with some concluding remarks.

II. INTEGRAL SOLUTION

We start with the linearized collisionless Boltzmann equation in Fourier space and in synchronous gauge [13,14],[1]

$$\frac{\partial\Psi}{\partial\tau}+ik\mu\frac{q}{\epsilon}\Psi+\frac{d\ln f_0}{d\ln q}\left[\eta'-\frac{h'+6\eta'}{2}\mu^2\right]=0, \quad (1)$$

and follow the notation in Ref. [13] unless stated otherwise. Here the fractional phase-space-density perturbation Ψ is related to the phase-space density via $f(\vec{q},\vec{k},\tau)=f_0(q)[1+\Psi(\vec{q},\vec{k},\tau)]$ with $\vec{q}$ being the neutrino momentum in units of the current neutrino temperature T_0 ($q\equiv|\vec{q}|$) and f_0 being the Fermi-Dirac distribution. Because of symmetry considerations [13], Ψ depends only on the momentum magnitude q, the Fourier wave number $k\equiv|\vec{k}|$, and the angle $\mu\equiv(\vec{q}/q)\cdot(\vec{k}/k)$. We have also introduced the synchronous-gauge metric perturbations $h(k,\tau)$ and $\eta(k,\tau)$, and use a prime to denote derivative with respect to conformal time τ. We follow Ref. [2], thus a small deviation from Ref. [13], in defining the neutrino energy $\epsilon(q,\tau)\equiv[q^2+a^2(\tau)m^2/T_0^2]^{1/2}$ in units of T_0, with $a(\tau)$ the scale factor, and m the neutrino mass. We omit the arguments of all quantities if no confusion is caused.

We recognize Eq. (1) as a first-order ODE of Ψ in τ, labeled by μ, q, and k. Integrating this equation from some initial time τ_i to some final time τ_f, we obtain the formal solution,

$$\Psi(\tau_f)=e^{-i\mu k\chi(\tau_i,\tau_f)}\Psi(\tau_i)+\int_{\tau_i}^{\tau_f}e^{-i\mu k\chi(\tau,\tau_f)}\times\left[-\eta'+\frac{h'+6\eta'}{2}\mu^2\right]\frac{d\ln f_0}{d\ln q}d\tau. \quad (2)$$

Here we define the neutrino comoving horizon $\chi(\tau_1,\tau_2;q)=\int_{\tau_1}^{\tau_2}(q/\epsilon)d\tau$, and omit the q dependence for simpler notation. We now define the multipole moments $\Psi_l\equiv(i^l/2)\int_{-1}^{+1}\Psi(\mu)P_l(\mu)d\mu$ with $P_l(\mu)$ the Legendre polynomials, and use the integral representation

$$\frac{d^n}{dx^n}j_l(x)=\frac{i^l}{2}\int_{-1}^{+1}e^{-i\mu x}(-i\mu)^nP_l(\mu)d\mu \quad (3)$$

of the spherical Bessel functions $j_l(x)$ (and its derivatives) to arrive at the central result,

$$\Psi_l(\tau_f)=\sum_{l'=0}^{\infty}(-1)^{l'}(2l'+1)W_{ll'}[k\chi(\tau_i,\tau_f)]\Psi_{l'}(\tau_i)+\int_{\tau_i}^{\tau_f}\frac{d\ln f_0}{d\ln q}d\tau\left\{-j_l[k\chi(\tau,\tau_f)]\eta'-j_l''[k\chi(\tau,\tau_f)]\frac{h'+6\eta'}{2}\right\}. \quad (4)$$

Here, we have defined the auxiliary function,

$$W_{ll'}(x)\equiv\frac{i^{l+l'}}{2}\int_{-1}^{+1}e^{-i\mu x}P_l(\mu)P_{l'}(\mu)d\mu=i^{l'}P_{l'}\left(i\frac{d}{dx}\right)j_l(x). \quad (5)$$

Now, we discuss the evaluation of the integral solution Eq. (4). We choose the initial time τ_i sufficiently early, ideally close to neutrino decoupling, when the higher multipoles $\Psi_l(\tau_i)$ for $l>2$ are effectively zero. This reduces the infinite sum in Eq. (4) to only three terms (i.e., $l'=0,1,2$). Then, $\Psi_l(\tau_f)$ for arbitrary $\tau_f>\tau_i$ can be computed by performing the integral in Eq. (4). Although this can be done for arbitrary l too, we only need the monopole and dipole (i.e., $l=0,1$), as those are all that appear in the Einstein equations.[2] A schematic comparison between the Boltzmann-hierarchy solver and the new hierarchyless solver presented in this work is shown in Fig. 1.

Although similar to the analogous integral equation for photons in Ref. [12], Eq. (4) is different in a very important way. The phase-space perturbation $\Psi_l(\tau)$ does not appear inside the integral in Eq. (4), so Eq. (4) is merely an integral, not a bona fide integral equation, a consequence of the fact that neutrinos are collisionless. As we will see shortly, this allows for considerable simplification and acceleration.

III. ITERATIVE METHOD

The integrals in Eq. (4) require the metric perturbations $h(\tau)$ and $\eta(\tau)$, but the Einstein equations that determine these quantities take as input the neutrino perturbations (as well as those of any other species). To solve this chicken-and-egg problem, we solve the coupled system of equations iteratively, as follows.

We first choose an ansatz for the neutrino sector and solve the non-neutrino sector using a traditional ODE solver; then the metric perturbations are used to evaluate

[1]The hierarchyless approach is equally applicable to the conformal Newtonian gauge.

[2]Here, we use the synchronous gauge, where the (0,0) and $(0,i)$ components of the Einstein equations are sufficient to evolve the metric perturbations h and η. So we only need the $l=0$, 1 moments of the neutrino distribution function.

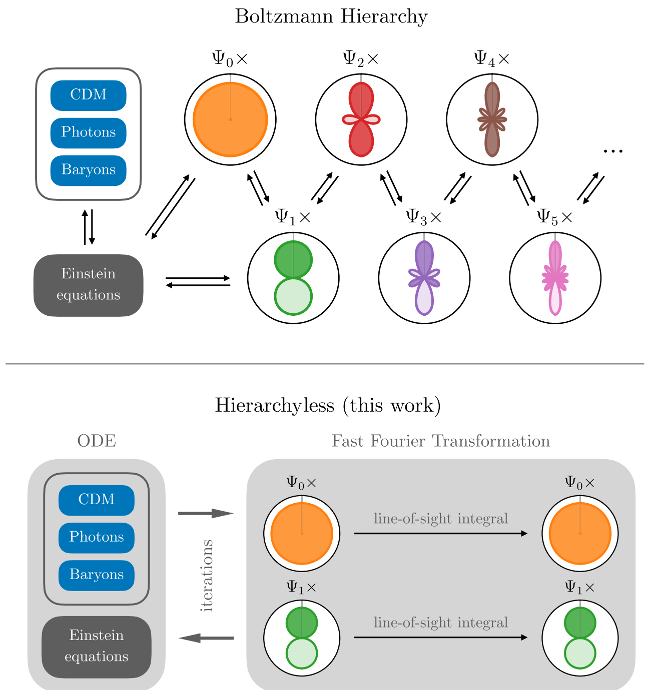

FIG. 1. Comparison between the traditional solver using a truncated Boltzmann hierarchy and the new solver proposed in this paper. In the new approach, the infinite hierarchy is being replaced by two line-of-sight integrals—for the monopole and dipole of the distribution function—that are evolved simultaneously with the differential equations for the rest of the system via an iterative scheme. The line-of-sight integrals are computed very efficiently via fast Fourier transforms.

and update the neutrino sector via Eq. (4). This process is continued until some target precision is achieved. Better choice of the ansatz enables faster convergence of the iterations. Here, we discuss several possibilities.

One simple possibility is to start with a solution to the ODEs truncating the neutrino hierarchies at a low multipole. These trial solutions typically take far shorter to compute compared to the full hierarchy, but nonetheless provide enough crude features in the solution for the iterative process to refine on. The numerical results shown below are obtained with this ansatz.

In the context of parameter inference, where a thorough exploration of the parameter space is needed, another possibility is to use the neutrino-sector solution from the previous MCMC step as the ansatz. A converging MCMC typically only samples fairly concentrated points around the best-fit model in the parameter space. Thus, presumably, a solution from the previous step is a very good approximation to the true solution of the current step. Along this line of reasoning, one can even maintain a small cache of certain previous MCMC steps that more or less uniformly cover the parameter space of interest, then, in the current step, only retrieve the closest candidate as the ansatz (although the required interpolation may be costly). A related possibility is to do something similar using the solutions for Ψ_l from a previous k value in the calculation, rescaling the conformal time so that $k\tau$ is fixed.

IV. FFT ACCELERATION

The line-of-sight integral can be written as a convolution between a cosmology-independent kernel and the metric perturbations. The integral in Eq. (4) can be written schematically as

$$I(\tau_f) = \int_{\tau_i}^{\tau_f} F(\tau)K[x(\tau_f) - x(\tau)]d\tau. \tag{6}$$

For the first term in the integral in Eq. (4),

$$F(\tau) \equiv -\eta' \frac{d\ln f_0}{d\ln q} \quad \text{and} \quad K(x) = j_l(x), \tag{7}$$

and for the second term in the integral in Eq. (4),

$$F(\tau) \equiv -\frac{h' + 6\eta'}{2}\frac{d\ln f_0}{d\ln q} \quad \text{and} \quad K(x) = j_l''(x), \tag{8}$$

but the following derivation applies to both cases. We define $x(\tau) \equiv k\chi(\tau_i, \tau)$, and we have used the fact that these distances are additive, i.e., $\chi(\tau_i, \tau) + \chi(\tau, \tau_f) = \chi(\tau_i, \tau_f)$. Now, we change the integration variable using the inverse function $\tau = \tau(x)$ and $d\tau/dx = \epsilon(x)/(qk)$, giving

$$I[\tau(x_f)] = \int_0^{x_f} \frac{\epsilon(x)}{qk} F[\tau(x)]K(x_f - x)dx, \tag{9}$$

where $x_f \equiv k\chi(\tau_i, \tau_f)$. Defining the function $G(x) \equiv \epsilon(x) F[\tau(x)]/(qk)$, we have

$$I[\tau(x_f)] = \int_0^{x_f} G(x)K(x_f - x)dx = (G\star K)(x_f). \tag{10}$$

Here, $G\star K$ denotes the Laplace convolution between G and K. The discrete samples of $I[\tau(x_f)]$ can be computed from the discrete samples of $G(x)$ and $K(x)$ very efficiently via FFT. Note that the x-samples (or τ-samples) do not need to be uniform, in which case the nonuniform FFT can be used without impacting the $O(N\log N)$ complexity.

V. NUMERICAL DEMONSTRATIONS

Our calculation proceeds as follows. (1) We first solve the complete set of ODEs for the baryons, dark matter, photon moments, gravitational potentials, and neutrinos. However, we truncate all the neutrino Boltzmann hierarchies at $l = 3$. This then provides an initial solution for the potentials $h(\tau)$

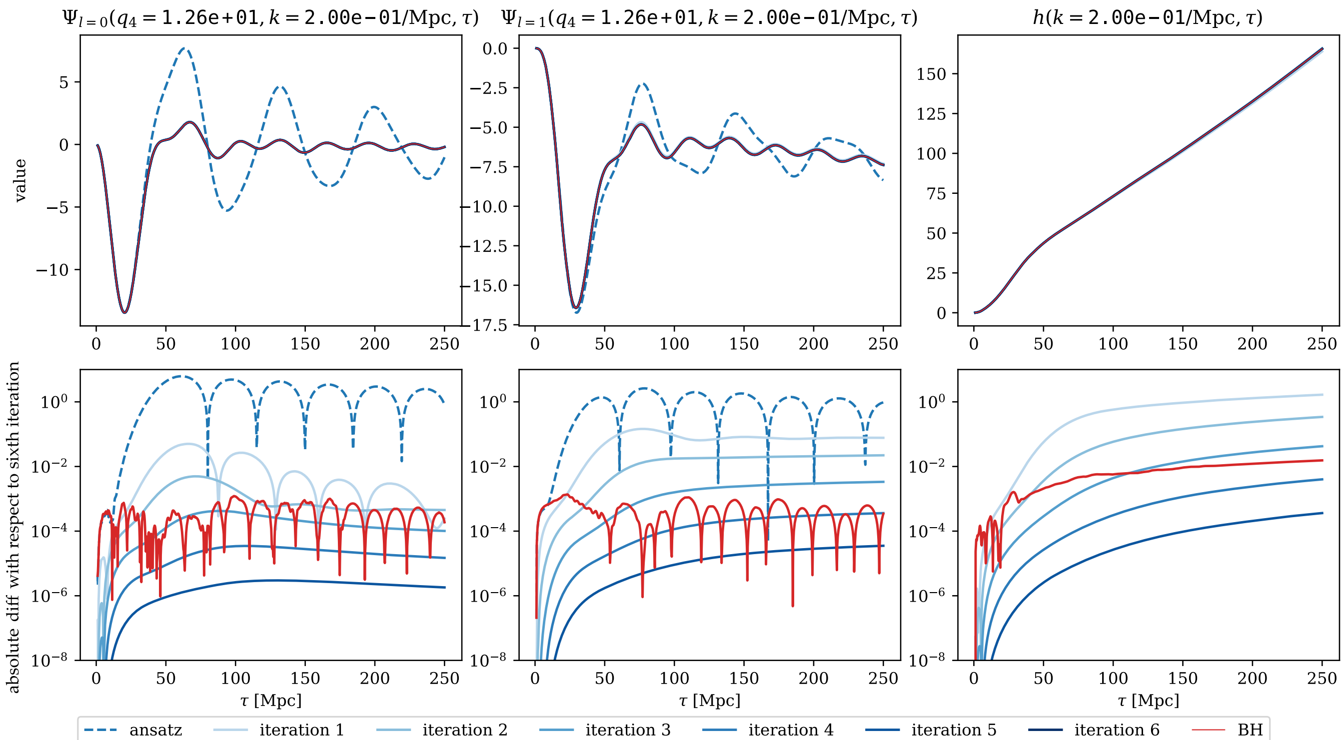

FIG. 2. Numerical results of the hierarchyless solver. We show (from left to right) the evolution of the neutrino distribution-function monopole Ψ_0, dipole Ψ_1, and the synchronous-gauge metric perturbation h. The top panels show the initial ansatz (blue dashed, obtained by solving a very short hierarchy cut at $l = 3$), the results of six iterations (light blue to dark blue, solid), and the solution obtained from a Boltzmann hierarchy truncated at $l = 30$ (red solid). Note that the iterations are overlapping due to the rapid convergence. Each bottom panel shows the absolute differences between the lines in the corresponding top panel comparing to the results of the sixth iteration.

and $\eta(\tau)$. (2) We then evaluate the neutrino monopoles $\Psi_0(\tau)$ and dipoles $\Psi_1(\tau)$ for all momenta q from Eq. (4) using the FFT method described above. (3) We then go back and solve the ODEs for the baryons, dark matter, photon moments, and gravitational potentials. However, this time we use the results of step (2) for the neutrino source terms in the Einstein equations. (4) We then iterate steps (2) and (3) until the desired precision in the neutrino moments or the gravitational potentials are achieved.

For step (2), one could alternatively simply evaluate the integral equation for either the monopole or the dipole (rather than both) and then obtain the other from the continuity equation. We have found, though, that the solutions converge more rapidly if they are both evaluated with the integral equation, with little additional computational effort.

We develop a proof-of-concept PYTHON code to demonstrate the potential of the new hierarchyless solver. We adopt a ΛCDM (cold dark matter) cosmology with one species of massive neutrino with $m_\nu = 0.06$ eV. The cosmological parameters are chosen to be the default in CLASSv3.0.1. As an example, we solve the $k = 0.2\ \mathrm{Mpc}^{-1}$ mode in the conformal-time interval $\tau \in [1, 250]$ Mpc, and discretize the q integration with five Gauss-Laguerre nodes. We choose $\tau_{\max} = 250$ Mpc so that $k\tau_{\max} = 50$, which is significantly larger than the standard values to switch on the fluid approximation for the noncold collisionless relics (e.g., the standard value in CLASS is 31).

In Fig. 2, we demonstrate the rapid convergence of the iterative process and the accuracy of the converged solution. Here, we construct the ansatz by solving the system with a short neutrino hierarchy truncated at $l = 3$, and iterate six times from that. We then compare the result from the last iteration with the Boltzmann-hierarchy approach truncated at $l = 30$. (We note that this does not necessarily give a better solution than the final iteration.) In each iteration, we compute the neutrino line-of-sight integral via a FFT of $N = 1024$ points. Whenever there is a need to solve ODEs, we use the RK45 adaptive integrator with $\mathtt{rtol} = 10^{-4}$ and $\mathtt{atol} = 10^{-8}$.

In Fig. 3, we compare the computation time for neutrinos in obtaining Fig. 2 defined to be the total time spent on the neutrino hierarchy (for the Boltzmann-hierarchy case and for obtaining the ansatz) or on the neutrino line-of-sight integral (for the iterations). The time for the ansatz can be eliminated if we obtain the ansatz from the previous MCMC step, or a previous k. The time for each iteration is expected to scale as $O(N \log N)$.

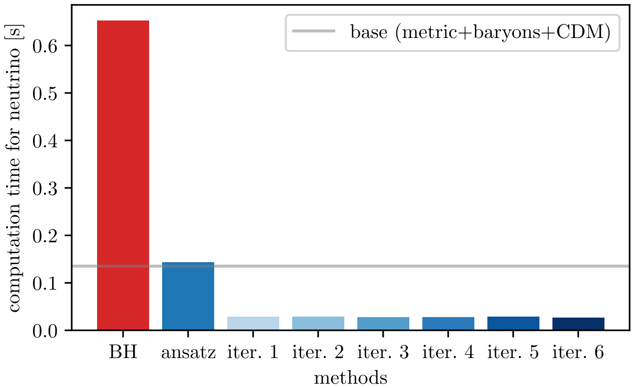

FIG. 3. Comparison of computation time for neutrinos in obtaining Fig. 2. Here, the computation time is defined to be the total time spent on the neutrino hierarchy (for the Boltzmann-hierarchy case and for obtaining the ansatz) or the neutrino line-of-sight integral (for the iterations). As a reference, we plot the computation time for baryons, CDM, and metric as a gray horizontal line.

VI. CONCLUSIONS

We have shown that each of the Boltzmann hierarchies for collisionless species can be replaced by a set of integrals that can be evaluated efficiently with FFT, but at the price of solving the equations for the rest of the system iteratively. Even so, our simple numerical experiments suggest that the iteration can converge quickly with even a simple initial ansatz and thus hold the prospect to accelerate cosmological-perturbation calculations, especially in models with multiple mass eigenstates.

Moreover, we emphasize that the new approach described in this work can be used to accelerate models with other noncold collisionless species [5–9], without much adaptation. It should also apply to scenarios where these (or the neutrino) species have nonthermal homogeneous distribution function f_0 [10]. In general, we expect the acceleration to be more significant with a larger noncold collisionless sector. Still, the optimization of the computational efficiency subject to some precision threshold is a difficult problem, both for the traditional approach and the one we have suggested here. It will require more work to determine more conclusively whether this can be implemented to improve the performance while providing the type of reliability and flexibility available with current codes.

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