Parameterization of the Lyα forest power spectrum

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This is an internal document aimed at clarifying the work-flow related to extracting cosmological information from the Lyα power spectrum, using emulators and hydrodynamical simulations. It could be used for an eventual publication, but for now the main goal is to make sure we are all on the same page, and help build the science case for the 11th DiRAC Call. Some of this discussion started by me (Andreu) trying to understand the details of the SDSS-I analysis, and how one would do an equivalent 3D analysis. Some of it is from chats with Pat and Simeon in 2016, trying to understand why H_0 should not be a parameter in Lyα analyses. Some of it is from discussions with Pat and Anze over email, and some of it is from Anze and I in a whiteboard at the Cosmoparticle hub.

I. INTRODUCTION

Discuss here the unique window opened by Lyman-α (Lyα) forest clustering, to study the linear power spectrum on small scales and redshifts higher than those available from galaxy surveys. Discuss the role of hydrodynamic simulations in these studies, and the need for an emulator. Discuss the importance of chosing the right parameterization in the emulator, since some cosmological parameters are not well measured by the Lyα forest. In particular, mention neutrino-mass degeneracy and the reasons to not use σ_8 defined at redshift zero.

Mention that even though this was studied already in [1], recent papers have ignored this issue [2, 3]. This will be relevant for future analyses, specially from DESI.

Even though past analyses have focused on the 1D power spectrum, the 3D power spectrum can also be measured [4], and it contains most of the information available from future surveys like DESI [5].

In this paper we take another look at this topic, using modern hydrodynamic simulations and explicitely showing the accuracy of some of the approximations. We start in section II with an overview of the different steps involved in a cosmological inference from the Lyα power spectrum, and we continue in III with a description of the likelihood code, its user interface, and its internal parameterization. We describe the link between the likelihood and the *emulator* in section IV. In section V we discuss the simulations used in the emulator, and the post-processing of the snapshots.

II. COSMOLOGICAL ANALYSES WITH THE LYα FOREST POWER SPECTRUM

In this section we present an overview of the different aspects involved in a cosmological analysis of the small scale clustering from the Lyα forest power spectrum.

- Measurement of the flux power spectrum: calibrate the quasar spectra, fit the quasar continua, measure 2-point functions, covariance matrices and possible contaminants.
- *Emulate* the flux power spectrum: using hydrodynamical simulations, build an emulator to translate the measured flux power to constraints on the linear power spectrum of density at the redshift of the measurement ($z \sim 3$).
- Cosmological constraints: combine the inferred linear power spectrum with external datasets (primarily CMB studies) to constrain the parameters of a particular cosmological model.

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A. Measuring the Lyα correlations

Skip over continuuming fitting, instrumental details, and so on. This will not be the main focus of this paper.

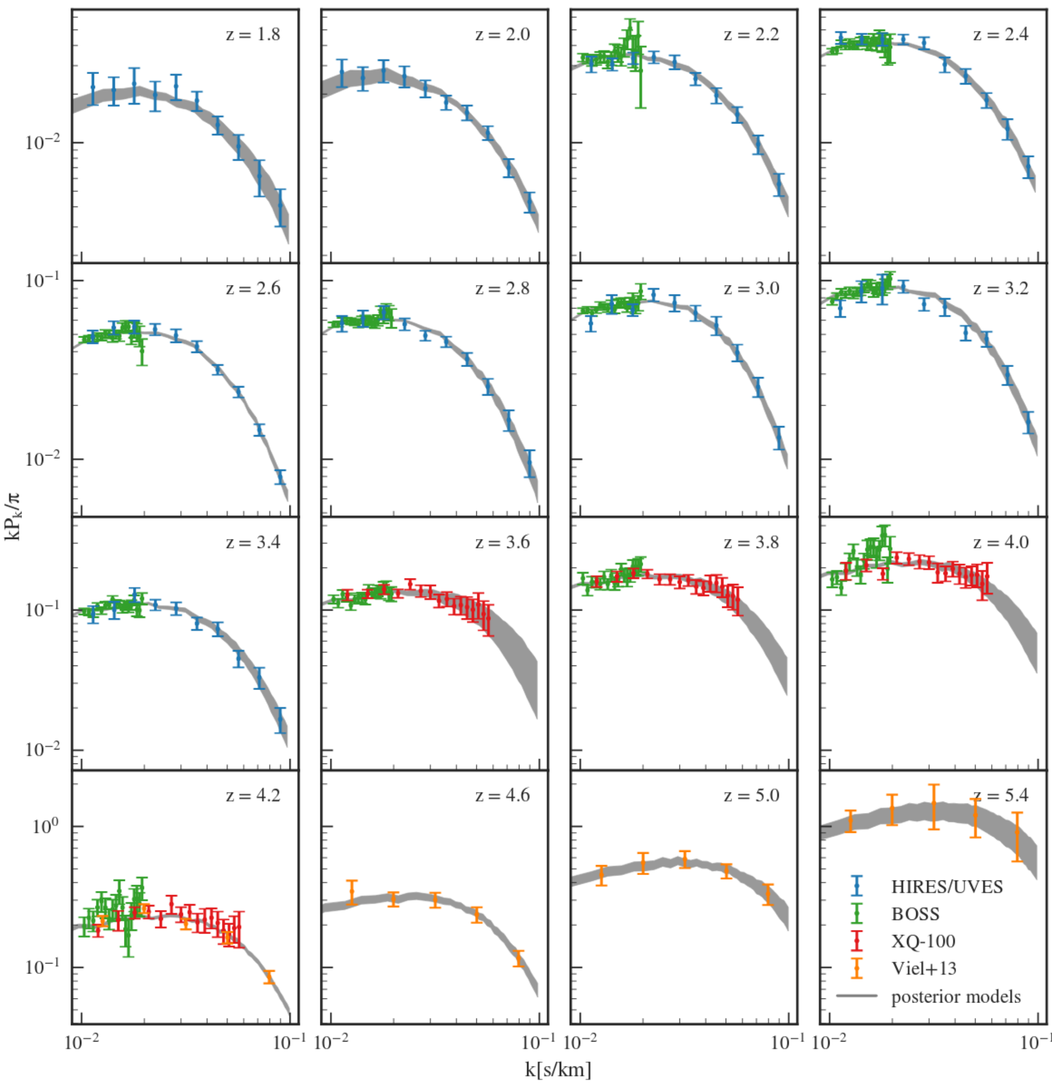

FIG. 1. Compilation of $P_{1D}(z, k_\parallel)$ measurements, including those from [6] (orange), [7] (red), [8] (green) and [9] (blue). AFR: This figure was stolen from [10], it would be better to add one that goes to lower values of $k_\parallel$ covered by SDSS/BOSS.

Beyond BAO analyses [11, 12], the only public results on the clustering of the Lyα forest are measurements of the 1D power spectrum [13–15] or more recently [6–9]. These are usually presented as band powers measured in different redshift bins, spanning the redshift $1.8 < z < 5.4$, and covering a broad range of scales $0.001\text{s km}^{-1} < k_\parallel < 0.1\text{s km}^{-1}$. A compilation of recent measurements is shown in Figure 1.

In most cases, the line of sight wavenumbers are expressed in units of inverse velocity, s km^{-1}, but other mappings from observed wavelength could be used. When measuring the 3D power, we will also need to define transverse wavenumbers, and in this case the natural choice is to use units of inverse angles [4].

B. *Emulating* the flux power spectrum

In order to interpret the measurements, we need to be able to make theoretical predictions for the measured correlations, and setup a statistical method to compare models and compute constraints on their parameters.

Due to its non-linear nature, to simulate the Lyα forest (or flux) power spectrum we need to rely on expensive hydrodynamical simulations. Each model evaluation requires thousands of CPU hours, what makes a *brute-force* approach unfeasible.

Moreover, the flux power spectrum does not only depend on the density clustering, but it also depends on the thermal history of the Inter-Galactic Medium (IGM) (see [10] for a recent review). In order to compute robust cosmological constraints, we need to make sure that we explore all possible thermal histories, and that we fully marginalize over these nuisance parameters.

This large parameter space, and the cost of a single run, makes it impossible to run a simulation for each model we want to compare. A small number of simulations is usually available, and in the past different analysis have used different techniques to circumvent this problem: a smooth dependence was assumed and fit in [1]; a Taylor expansion was used in [8]; a Gaussian Process-based *emulator* was used in [9, 10], although in this analysis the cosmological model was kept fixed and only the thermal history was explored.

Emulators based on Gaussian Processes are an active area of research AFR: cite density emulators, and it is possible that they will have an important role in future Lyα forest analyses. However, in this publication we will use the term *emulator* in a broad sense, to describe any setup to use a finite suite of hydrodynamical simulations to make predictions for the flux power spectrum.

The main topic of this paper is to study the parameter degeneracies in this type of analyses, and discuss how this might affect the parameterization of an emulator for the flux power spectrum.

C. Cosmological constraints

As we will discuss in the next sections, once we have marginalized over the thermal history of the IGM, the flux power spectrum is mostly sensitive to the amplitude and slope of the linear power spectrum around $k \sim 1$ Mpc^{-1} [1] and around $z \sim 3$. For instance, [1] measured these quantities with 15% and 5% precision respectively.

Changes in other (traditional) cosmological parameters are very degenerate with changes in the linear power or in the thermal history. For instance, as discussed in [16] and more recently in [17], at fixed linear power spectrum the effect of massive neutrinos is almost indistinguishable from that of Ω_m. Another example: at fixed linear power spectrum, and fixed Ω_m, the effect of Ω_b is degenerate with the level of UV background assumed.

One of the peculiarities of Lyα forest analyses that we will discuss is that it covers a redshift range $2 < z < 5$ where the universe was close to Einsteint-de Sitter (EdS), i.e., $\Omega_m(z) \sim 1$. This means that the growth of structure in this redshift range is almost independent of cosmology, and so is the expansion history $H(z)/H_0$.

It is only in combination with external datasets, mainly from CMB experiments, that we are able to provide constraints on the traditional cosmological parameters. For instance, by combining our measurement at $k \sim 1$ Mpc^{-1} with the CMB constraints on the amplitude and slope of the linear power spectrum at $k \sim 0.05$ Mpc^{-1} we get tight constraints on the running of the spectral index (α_s) and on the sum of the neutrino masses ($\sum m_\nu$).

This approach of emulating only the linear power was used in [1], but recent analyses [2, 3] have attempted instead to directly emulate the 6+ traditional parameters of a Λ-CDM universe. We will argue that this might not be the best approach, because of the following reasons:

- As discussed above, the traditional parameters have strong degeneracies and this makes the emulator (or Taylor expansion) more challenging.
- In order to break the degeneracies, one needs to adopt priors from CMB experiments, making it more dificult to combine with CMB experiments later without double counting information.

[1] As it will be discussed in the next sections, the pivot point should be specified in velocity units, $k \sim 0.01$s km^{-1}.

- The results are model-dependent, and it is impossible to use them in extended models (curved universe, non-Λ, different $N_{\rm eff}$...) if these were not in the original emulator.

III. PUBLIC LIKELIHOOD CODE

In order to properly discuss our choice of parameterization and simulation setup, it is important to describe how we intend the end product, the *likelihood code*, to be used in a cosmological analysis.

Note that during this discussion we have ignored the differences between baryons and CDM, and always work with their weighted-averaged power.

A. User interface

AS: I don't like the expression "user interface" here. Wouldn't likelihood parameterization be more appropriate? AFR: Anže, this is an internal document, to make sure we are all (including Chris, Hiranya, Andrew, Tom...) in the same page. The second part of this section is about the parameterization, this first part is really just about the interface... As Pat mentiones below, we can give an easy interface to the users, and under the hood we compress that into any set of parameters we want.

The aim of the project is to provide a public likelihood package that others can use to include Lyα results in their cosmological parameter constraints. The end-user does not need to know about the internal details, about the suite of simulations, the nuisance parameters or the interpolation scheme used in the emulator. They do not need to know either whether internally we are describing the power in units of km s^{-1}, Mpc or h^{-1}Mpc.

There are different possible interfaces that we could setup, and probably we will want to provide more than one with different levels of complexity. But we will start discussing a particular interface, where we will ask the user to provide for each cosmological model:

- Linear matter power (baryons+CDM), as a function of redshift and wavenumber, in units of Mpc^{-1}. The redshift range should cover at least $2 < z < 5$, and the wavenumber range should cover at least $0.01\ \mathrm{Mpc}^{-1} < k < 10\ \mathrm{Mpc}^{-1}$. For simplicity, we will restrict ourselves to models with a linear power spectra that can be factorized ,in the range of redshift and scales described above, in a power spectrum at a central redshift, $P_L(z_\star = 3, k)$, and a scale independent growth factor, $D(z)$. AS: If you are to compress flux measurement over X redshift bins into one linear power constrain, just ask for the linear power at that $z_{\rm pivot}$ and f at that redshift. If you are going to compress into two zs, ask for those two zs and two fs. AFR: Yes, this is an option. But as Pat mentions below, this might not be the easier option for some users. But when I mentioned above that we could have more than one interface, this is what I had in mind.

- Logarithmic growth rate, $f(z)$, that could be computed directly from the evolution of $D(z)$.

- Hubble parameter as a function of redshift, $H(z)$, over the same redshift range.

- If we want the likelihood code to be able to fit 3D clustering as well, we would need as an input the angular diameter distance, $D_A(z)$, over the full redshift range. AS: I would add r_d and also r_d fiducial for generality. AFR: Yes, I forgot about r_d here. Although we could fit it from the linear power ourselves under the hood, to prevent some users to use EH98 and others using CAMB to compute it.

PVM: I don't think you should skimp on what you want from the outside. E.g., in neutrino mass era it is starting to feel a little quaint to talk about $D(z)$, $f(z)$ – both generally depend on k. At the same time, producing density and velocity power spectra as a function of k and z is just getting easier and easier as people get more comfortable with things like CLASS. (I mean, no I don't actually think k dependence of D and f will ever matter, but it seems just easier to ask for the linear $P(z, k)$ than worry about defining and justifying these things (e.g., I remember kind of laughing at Alexey Makarov for producing $D(z)$ by running CMBfast, which seemed like overkill when I had a little numerical integrator code, but to him this was actually easier than setting up that code...)) I wouldn't worry too much about what you're going to ask for though. Focus on making a good emulator and then ask for what you need for that... AFR: Great, that's all I wanted to hear. For now, let's assume this is a possible option, and we'll come back to it later on. AS: I like Pat's idea of just asking for a bunch of power spectra, including matter, velocity and perhaps baryon as well. For example, you could easily also check if the power spectra are not so pathological that approximations employed are not valid. For example Pat's code wasn't the right thing to use for WDM models and here you can guard against that.

The user will also specify:

- Data products to use: SDSS-I from [15], BOSS from [8], HIRES/UVES from [6], XQSO-100 from [7], HIRES/UVES from [9]. We should also allow the user to specify what redshifts to use from each dataset, since they are independent, and probably also allow the user to specify the scales to be used in the fit for each dataset.
- Extra analysis settings, like whether to allow for running in the linear power, differences in the linear growth, or differences in the BAO wiggles.

AFR: It is not clear to me whether at this point the user would also be able to set other settings of the likelihood or not, like the way we treat contamination by DLAs or metals, resolution or noise corrections, or the parameterization of the temperature-density relation in the simulations. AS: This is implementational detail, no need to worry about this now.

AFR: I believe the answer is that each of these analysis choices would be a different likelihood object, and then the user can decided whether to use the likelihood object where the DLA marginalization used the formula from [18] or whether to use the one that used the formula from [19]. Similarly, every time we want to use a different prior for the nuisance parameters (say we want to include measurements of mean flux or temperature) we would need to recompute the marginalization, and provide a new likelihood look-up table.

The output from the *likelihood code* will be:

- A value of (log-)likelihood for each dataset, possibly a value for each redshift bin. Most users will only care about this.
- For the experts, we would also output the best-fit theoretical prediction for each dataset, for that particular cosmological model. We would also provide the values of the nuisance parameters that correspond to the best fit model (mean flux, temperature-density relation, metal or DLA contamination...).
- We could also provide a random sample of theory lines that are above a likelihood threshold for that particular model, exploring different thermal histories and other nuisance parameters.

AFR: Actually, I don't think at this point you can get any of the above. The user of the final likelihood code will only get a total value for the likelihood for the total dataset. Even though one would compute the un-marginalized likelihood for each redshift and each dataset separately, at the step of marginalizing over nuisance parameters (see section IV) you would need to include them all at the same time. AS: No, no. You don't marginalise over nuissance parameters inside your likelihood code. Some nuissance parameters will have particular degeneracies with the big picture cosmological parameters, and in addition you never know how clever the user's sampler is. It is ok to ask for linear power, f, $H(z)$, $D_A(z)$ and a set of nuissance parameters, which users doesn't need to understand except for valid ranges. You can add a small wrapper that does this marginalisation internally for those who don't care. PVM: In principle I more or less agree with Anže about the nuisance parameters, the core level of the code should be written treating all parameters symmetrically and this should be kept accessible... although, if you were, e.g., importance sampling a Planck chain you would effectively return to needing the code to marginalize over nuisance parameters. On the other hand, I remember long ago in Alexey Makarov days we ended up retreating from this idea because the generic MCMC was painfully slowed by marginalization over these nuisances when we knew how to make it fast internally... Ugh - I'm going to try not to read anything but emulator section since I think this discussion of final public likelihood code is getting way ahead of yourself... ☺ I'd focus on "what do I need to do to get an emulator capable of any kind of fit to a LyaF data set?" ...

AFR: Nooooooo! I need to understand how the final package will be used, before I can think of emulators and simulations!

AFR: Pat, in your 2005 paper, you had χ^2 look-up tables, that were only a function of amplitude and slope (and may be running). I always thougth that this type of look-up table would be the end product of the analysis, with a nice wrapper around it with a public interface to translate cosmology to our cryptic parameters in the lookup table. Isn't it the case? You made the look-up table public, and that table had already marginalized over all nuisance parameters, right? PVM: Yes. This is getting at what I rambled about in comment later. While Anže's desired option to control all parameters simultaneously in a cosmoMC run should certainly *exist,* I don't think you should present this as, e.g., what anyone would run in their first use of your results. I do think you still want to produce some form of "de-forested" linear power main result, that will contain everything most people would want. You need it for "opening the black box" purposes, but also, it will be faster, and why force people to mess with a bunch of forest nuisance parameters they don't care about when you know they can get the same results without it? The option to run global chain with LyaF nuisances should exist for comparison, and so you can see correlations, but not be the lead option... (this is sort of what I was trying to indicate here saying "core level of code", but I didn't really think through how necessary I think the marginalized version really is...). ... I don't think this has to be very "cryptic" even under the hood though... I wouldn't call a χ^2 table in $\Delta_L^2, n_{\rm eff}(z=3, k=0.009s/km)$ cryptic...

AFR: Perfect. Just for the record, in my original text (two days ago) I never meant to talk about the CosmoMC option, I always had in mind to compress it all to a look-up table with $\Delta_L^2, n_{\rm eff}(z=3, k=0.009s/km)$ or equivalent (may be extending to $f_\star$ or running.

PVM: Ok, since it isn't actually perfectly trivial to define $\Delta_L^2, n_{\rm eff}(z=3, k=0.009s/km)$ in practice, e.g., do you really want to do an infinitesimal derivative at exactly this point or some kind of broader thing, I think you will always want to control how that is done by asking for full P(k), and they should be happy to let you take care of it, so maybe it could get a little cryptic, but this is not much related to the more physical stuff related to emulator. AFR: Agreed. AS: I agree as well.

B. From cosmological model to likelihood parameters

Under the hood, we will use more effective (and cryptic) parameters in our likelihood, to reduce the internal degeneracies between parameters. There are many, many possibilities here, but we will start by discussing a possible setting.

1. *Fiducial cosmological model*

We will choose a fiducial cosmological model, based on a recent Planck+BAO analysis, and use it to compute a fiducial linear power spectrum, $P_L^0(z,k)$, a fiducial Hubble expansion, $H^0(z)$, a fiducial growth rate $f^0(z)$... All quantities with a superscript ^{0} will refer to the fiducial model.

2. *Linear power shape*

Since we have decided to use only models where the linear power spectrum can be factorized, we will describe its shape at the central redshift only, $z_\star = 3$. In general we will use the subscript $_\star$ to refer to quantities that have been evaluated at $z_\star$, but in this sub-section we will ignore the redshift and assume that all power spectra are evaluated at $z_\star$.

We will compress the difference between the input power spectrum, $P_L(k)$, and the fiducial power spectrum, $P_L^0(k)$, into a handful of parameters. We start by fitting the fiducial power with a smooth function, $P_{nw}^0(k)$, using the *no-wiggle* model from [20]. We define the oscillatory (or *wiggle*) component of the fiducial power, $W^0(k)$, as the ratio of these two powers:

$$W^0(k) = \frac{P_L^0(k)}{P_{nw}^0(k)} \ . \tag{1}$$

PVM: Are your boxes actually going to be big enough to worry about BAO? If so, I think you should *definitely* model that part by linear bias/more general PT... you can use that to pull out the feature essentially analytically. Never mind what I said about "units of BAO"... this is surely the way to go since you don't want to be trying to interpolate between raw sim power at that scale anyway... AFR: No, in the main analysis I would not vary r_d as a free parameter. But talking about this option might help others understand what we are doing, even though we then say: "we do not expect our results to be sensitive to BAO, and therefore we fix r_d to Planck value".

We will assume that the oscillatory component of the input model can be described with the oscillations in the fiducial model, shifted by the ratio of their sound horizons at the drag epoch (r_d):

$$W(k) \sim W^0(\beta k) \qquad \beta = \frac{r_d}{r_d^0} \ . \tag{2}$$

We have decided to use β and not α, more common in BAO analyses, because the latter includes a ratio of transformations from observable to commoving coordinates, and we do not need this at this point.

Finally, we will model the differences in the smooth component with a smooth, parameterized function:

$$B(k) = \frac{P_{nw}(k)}{P_{nw}^0(k)} \ . \tag{3}$$

There are different parameterizations possible, but for the rest of this discussion we will assume that we use three parameters: an amplitude, a slope, and a running of the slope, evaluated around $k_p = 1$ Mpc^{-1}.

To summarize, we will describe the input linear power at $z_\star$ as:

$$P_L(k) = B(k)\ P_{nw}^0(k)\ W^0(\beta k) \ . \tag{4}$$

3. *Linear growth*

We will compute the difference of the input logarithmic growth rate with that in the fiducial cosmology, $\Delta f_\star = f(z_\star) - f^0(z_\star)$, evaluated at $z_\star = 3$. We will approximate that the different growth rate at $z_\star$ is enough to compute the difference in linear growth at any redshift (within the range):

$$\frac{D(z)}{D^0(z)} = 1 + \Delta f_\star \ \frac{\Delta z}{1 + z_\star} \ . \tag{5}$$

Note that in LCDM models, and at $2 < z < 5$, the differences in growth rate are typically less than 1%, as shown in Figure 2.

4. *Hubble expansion*

If we could observe the Lyα power spectrum in comoving coordinates, that would be enough. However, we observe the power spectrum in observing coordinates, wavelengths and angles, and a more natural choice is to use velocity units (km s^{-1}) for the clustering measurements. Indeed, all recent measurements of the 1D Lyα power reported their results in units of km s^{-1}, and we will assume the same in this discussion.

In general, we would need to use $H(z)$ from each model to compare measurements in km s^{-1} with model preditions in Mpc:

$$q = \frac{1 + z}{H(z)}\ k = a_v k \ , \tag{6}$$

where we use q to refer to wavenumbers in velocity units, and we have defined a_v as the transformation from km s^{-1} to Mpc. This would force us to add in the emulator some sort of Hubble parameter, either at $z = 0$ (h) or at $z_\star = 3$. However, as suggested by [1], it is possible to avoid this burden if we describe our model (the linear power spectrum) already in units of km s^{-1}. AS: This confused the shit out of me until very recently. I vote for having power spectra in Mpc and also require $H(z_\star)$ and do this conversion internally – it is trivial. AFR: Yes, Anže, that was the entire point of the user interface. We ask the users to provide power in Mpc, and we ask for $H(z)$, and we do the convertions under the hood.

We claim that two models with different expansion histories $H(z)$, but the same linear power in units of km s^{-1}, will have very similar Lyα power spectra, with small remaining differences being caused by astrophysical effects (different reionization history, different thermal history, different mean flux...). And since we plan to marginalize over these to get the final cosmological constraints, we do not need to worry about these differences. For the rest of this discussion, we will assume that this is true.

PVM: I agree with Anže that you should move to just using Mpc and asking for $H(z)$, where, a clincher is in 3D you can't get away from asking for at least $(HD_A)(z)$. The argument about km/s was always that you should quote results as a linear power measurement in km/s at $z \sim 3$, *if you are going to quote results from LyaF ∼alone* – the goal there was to produce "model independent" constraints that could be propagated forward. AFR: My plan was to translate the flux power into linear power, in km s^{-1}, and make that public as a look-up table, with a user interface in Mpc to make it easier for others to use. This is what I was trying to explain all along, mostly in section II, but I guess I didn't do a good job ☺. PVM: But if you're going to be using flux power directly in global chains fitting cosmological parameters, which seems to be what you're talking about here, that argument doesn't apply – you have the only relevant cosmological model on hand point-by-point. AFR: I never talked about doing this! Only Anže talked about it. I only talked about cosmological models as a wrapper, but the likelihood and the emulator would only hear about our compressed parameterization. PVM: This does raise the question though, how much you want to commit to that approach, i.e., to primarily present a likelihood code that does direct fits to flux power measurements on the fly, vs. boiling things down to linear power measurement (which you would again obviously present in observable coordinates). Certainly internally you want to be able to do both, and the code to do linear boil-down should probably wrap the other one, but there is a question where to spend more time cleaning and advertising. Arguments in favor of boil-down to linear could be speed (in old days, like I said, we could do both, but fit to flux power really slowed down global fits, while my χ^2 table gave identical results), and just... it is nice to be able to show the more-or-less LyaF-model-independent cosmological thing you claim to have measured, not just present a big black likelihood box. It helps, e.g., estimate how these constraints will affect new cosmological models. In any case, you can figure out what to advertise later. It seems like first goal should be to produce χ^2 contours for, e.g., $\Delta^2, n_{\rm eff}(z = 3, k = 0.009s/km)$, defined as deviations from a central model (i.e., effectively variations of A_s and n_s with other parameters fixed), to compare to past... this is clearly going to be *most of* what matters. AFR: Yes, I agree with the above.

How does this affect the discussion above?

Let us use $\tilde{P}(q)$ to refer to power spectra in units of velocity:

$$\tilde{P}(q) = a_v^3 \; P(k = q/a_v) \; . \tag{7}$$

We can then redo the whole discussion above, but using power spectra in velocity units:

$$\begin{aligned} \tilde{P}^0_L(q) &= (a_v^0)^3 \; P^0_L(q/a_v^0) \\ &= (a_v^0)^3 \; P^0_{nw}(q/a_v^0) \; W^0(q/a_v^0) \\ &= \tilde{P}^0_{nw}(q) \; \tilde{W}^0(q) \; , \end{aligned} \tag{8}$$

where we have also defined $\tilde{W}^0(q) = W^0(q/a_v^0 0$.

We can now define a term for the ratio of the smooth power, in velocity units:

$$\begin{aligned} \tilde{B}(q) &= \frac{\tilde{P}_{nw}(q)}{\tilde{P}^0_{nw}(q)} \\ &= \left(\frac{a_v}{a_v^0}\right)^3 \frac{P_{nw}(q/a_v)}{P^0_{nw}(q/a_v^0)} \; , \end{aligned} \tag{9}$$

and we can finally write

$$\begin{aligned} \tilde{P}_L(q) &= \tilde{P}_{nw}(q) \; W(q/a_v) \\ &= \tilde{B}(q) \; \tilde{P}^0_{nw}(q) \; \tilde{W}^0(\alpha q) \; , \end{aligned} \tag{10}$$

where we have defined α as the ratio of sound horizons in units of velocity:

$$\alpha = \beta \frac{a_v^0}{a_v} = \frac{r_d \; H_\star}{r_d^0 \; H_\star^0} \; . \tag{11}$$

The cosmological model in the likelihood will then be described by a set of parameters θ describing the linear power spectrum, including:

- Ratio of sound horizons in units of km s^{-1}, α, where the conversion from Mpc to km s^{-1} is computed at $z_\star = 3$. This is the inverse of the usual definition of BAO $\alpha_\parallel$.
- Approximately 3 parameters describing the ratio of the smooth linear power at $z_\star = 3$, in units of km s^{-1}.
- Difference of growth rates at $z_\star = 3$, $\Delta f_\star$.

We will ask the likelihood code: for these set of parameters θ, what is the likelihood of getting the measured power, after marginalizing over all nuisance parameters (including mean flux and thermal history)? Or in math, what we want is:

$$L(\mathbf{d}|\theta) = \int d\phi \; \Pi(\phi) \; L(\mathbf{d}|\theta,\phi) \; , \tag{12}$$

where $\mathbf{d}$ is the measured flux power spectrum, ϕ are the nuisance parameters, and $\Pi(\phi)$ are the priors on the nuisance parameters. AS: Again, marginalisation is for the user to do. The code should output total χ^2 at this point and optionally data-points and theory predictions at this point include full gory of nuissance parameters. If you look at eg `cosmomc` it internally marginalises already over some 15 Planck parameters, it can do 15 more for us. AFR: Ok, this is the type of discussion I wanted to have. Is this really how it was done in SDSS-I? What was the look-up table for, then? To make plots? PVM: I guess I should further to un-agree with Anže... If you wanted to assume everyone will be using cosmoMC so you could just make a module for that and broadcast it, I guess it would be ok (but I think still a lot of people would consider your LyaF parameters to be too literally a nuisance... and be less tolerant of it than of Planck nuisance), but I don't think you want to think this way. I don't think one MCMC code will dominate, so you need to assume people are going to be grafting your likelihood code into various things themselves, so you want to make sure to have a very easy option. AFR: Agreed. We should have an easy version for all to use, and a difficult one for testing and for the experts to use.

This likelihood will have been evaluated at a grid of points in θ, and it will be stored as a look up table. Evaluating the likelihood, once the lookup table has been computed, should then be trivial and extremely fast.

IV. THE EMULATOR

For a given combination of linear power parameters θ, i.e., for each point in the lookup table, we want to compute the integral in equation 12. To do this, we need to specify priors $\Pi(\phi)$, but more importantly we need to compute the likelihood $L(\mathbf{d}|\theta,\phi)$.

We need, therefore, to make predictions for the 1D flux power spectrum at a certain set of points, $P_{1D}(z,q)$, in velocity units, given a model defined by (θ,ϕ). We discuss the (nuisance) astrophysical parameters ϕ in more detail later on, but for now we will assume that there are only two parameters: an overall normalization of the logarithm of the mean flux $\ln \bar{F}_0$, multiplying some fiducial redshift evolution, and an overall normalization of the filtering length k_{F0} (associated to the smoothing of the gas), also multiplying a fiducial redshift evolution.

A. Emulating a particular redshift

For each redshift z_i, we compute the corresponding value of the mean flux ($\bar{F}_i$) and filtering length (k_{Fi}).

Using the linear power parameters (θ), and the fiducial power spectrum (in velocity units), we are able to compute the expected linear power for this particular model, in velocity units, at this redshift, $\tilde{P}_i(q)$.

AFR: This is one of the pieces that is still not crystal clear in my head. Would we just take $\tilde{P}_L(z_\star, q)$, the linear power in velocity units at the central redshift, and rescale it using the discussion around equation 5? If we did that, we would be missing the fact that the transformation between comoving and velocity separations a_v changes with redshift. I guess one could use the fiducial model to compute this difference? The alternative would be to have a 6th cosmological parameter describing the difference in the change in the Hubble expansion around $z_\star$? AS: If DE is truly negligible for sensible models, then just don't worry about it and assumed EdS. If it makes small corrections, then the best course of action would be to also specify $dH^2/da = -3\Omega_m/a^4$ at $z = z_\star$. PVM: I think there is a key thing you (Andreu) should add to your thinking about these things: don't focus on the parameters you put in when running the simulation, focus on the effective parameters you *achieve* for each redshift output, i.e., the numbers you can associate most directly with the flux power spectrum produced from that redshift output. E.g., there is a linear power spectrum associated with each redshift output, which you can easily compute using CLASS – you don't really care where it came from in terms or evolution from higher z, or, if you do, it is only as a very subdominant correction. AFR: Yes, I got that. That's what I was trying to say here... PVM: Even if you decided you needed to track differences in evolution for fixed output-time linear power, you would probably want to do that by extracting $dP_{lin}/dz(z_{output})$ from CLASS, i.e., keep everything you associate with an output local in z. Going on, there is an $F(z_{out})$, there is a $T(z_{out})$, there is a $k_F(z_{out})$ – there is no need to talk about a "fiducial z" at all at this level. You only need to think about that at a higher level of fitting, when, e.g., you want to produce χ^2 contours in $\Delta_L^2(z=3), n_{\rm eff}(z=3)$ plane (fixing linear power at other z assuming some model), or you want to enforce physically reasonable temperature evolution connecting $T(z)$, $k_F(z)$. This isn't an entirely non-trivial attitude. E.g., if you didn't think you could summarize pressure by a $k_F(z)$ you could calculate for each output, maybe you'd want to associate a full temperature history with each output instead of only writing down local-in-z quantities, and then you might want to parameterize that thermal history somehow, but I would worry about that only when pushed to it (and probably it would always be better to invent some local-in-z quantity you could compute to capture the physical effect you were missing). To put it another way: you want to separate your picture into things you can calculate about the conditions in the Universe at a given z without sims (including if necessary derivatives) – you want to take advantage of these kinds of things as much as possible – and then a simulation mapping of those things into non-linear power (in more or less arbitrary units, followed by observation, applying the necessary units – this part I think is easy for everyone to agree on). AFR: Yes, that was my plan. PVM: This is an opportunity to say something I've been thinking about all this including neutrino, etc., sim testing: by *far* the most efficient way to test whether an idea you have for simplifying the emulator parameterization is good enough is to just do the simple version and then see if it works in the case you think it might not. Probably it will work, and if not you haven't lost anything since you should just need to expand parameter space a little and add some sims to probe the new effect, still using what you have done (assuming it was sensible and the addition is more or less perturbative).

AFR: Pat, that is what I was trying to write... See discussion below, about computing some quantities at the particular redshift, and then completely dropping the redshift altogether.

AFR: But I don't think I've got an answer to my question. We define a model, by choosing θ (linear power at $z_\star = 3$, in km s^{-1}, and may be $f_\star$) and by choosing ϕ ($\bar{F}$, k_F...); We then ask the emulator to give us the prediction for flux power spectrum at $z = 4$, and the emulator needs to figure out how to translate this model (θ,ϕ) to the parameters describing the simulations outputs, to figure out which one to use (imagine we have infinit simulations); For the IGM parameters it is easy, we have a way to use ϕ parameters and the fiducial evolution, and turn that into a prediction for $\bar{F}_i$ and $k_{F\ i}$; However, we also need a way to translate the θ parameters, and the fiducial cosmological model, to a linear power at $z_i = 4$, in km s^{-1}. How do we do this? If we had still access to the full $P(z,k)$ and $H(z)$ that entered the user interface, that would be trivial. But we threw that information away because we claimed that the only thing that matters (the only parameters in our final likelihood) were there θ parameters. So we need to be able to reconstruct any linear power from these, so that then we can look at the simulations and try to look for a "snapshot" (more precisely, one of the multiple reproccessed snapshots) that had this particular power spectrum. I'm not sure this is any clearer...

PVM: *For the emulator*, who says you need to "define a model" by choosing power at $z_\star = 3$? Where by "emulator" I mean this thing that takes some kind of relatively easy to compute quantities and produces what it thinks would be simulation results given them. Maybe it is easiest to think of it by sort of back-propagation: you have a 1D flux power spectrum measurement at $z = 4$, you need a prediction for it, what does your emulator need to know to predict it? I'd say at first approximation it needs to know $P(k, z = 4)$, in km/s. So the input to the emulator is $P(k, z = 4)$ in km/s, period, end of story for emulator – it has a hard enough job doing this well, it doesn't need to worry about where this $P(kinkm/s, z = 4)$ came from. AFR: Yes, I agree. I realize now that I was using the word *emulator* in the wrong way, including what you call bellow "code to make a χ^2 table". PVM: If you're asking like "how would I use this emulator to make a χ^2 table of final results for $\Delta^2, n_{\rm eff}(z = 3, k = 0.009s/km)$", worrying about broader z (and k) dependence, I think you just pick the current best cosmological model as fiducial, and define $\Delta^2, n_{\rm eff}(z = 3, k = 0.009s/km)$ effectively as variations of A_s and n_s – this gives you your $P(kinkm/s, z = 4)$ to feed the emulator, but it is really a completely separate thing from the emulator. AFR: Just to be sure. θ parameters describe the different shape of the linear power, in km s^{-1}, at $z_\star = 3$. I can try to use these, and $H^0(z_\star)$ from the fiducial model, to compute the equivalent linear power in comoving coordinates. Then I can translate that to a different redshift using the linear growth of the fiducial model (may be corrected by difference in $f_\star$), and then use the Hubble parameter of the fiducial model at the redshift, $H^0(z_i = 4)$ to compute the final power we needed to talk to the simulations. Correct? The only thing this could break is if the redshift evolution of $H(z)$ and $H^0(z)$ were very different, but that should not be the case for most models, and if it was we could add an extra parameter to take care of this. Did I understand it? PVM: Of course, maybe you want to fit for growth deviations, and this gives you a different way of getting $P(kinkm/s, z = 4)$, or maybe you are doing a big global MCMC chain... the emulator who's job is to predict 1D flux power at z=4 doesn't want to know what you are doing globally, it just wants to know $P(kinkm/s, z = 4)$... (I've been writing $P(kinkm/s, z = 4)$ because I carefully wrote 1D power and it is shorter than writing "$P(kinMpc, z = 4)$ and $H(z = 4)$", which I think we agree is probably how things should really go for pedagogical reasons, and add $D_A(z = 4)$ for 3D.) AFR: Ok, I think we are getting closer. I think part of the confusion was my poor use of the word *emulator*, and the other part of the confusion is that I always wanted to focus on the "look-up table" version, and not on the cosmomc version.

At this point, we can completely forget about the redshift z_i.

Instead, we will go to our simulation database, and ask: is there any simulated flux power spectra that was computed from a snapshot with similar linear power (in velocity units) $\tilde{P}_i(q)$, similar mean flux $\bar{F}_i$ and similar filtering length k_{Fi}? AS: And similar f for velocity effects? Again, only matters if non-EdS matters. PVM: Remember that much of non-EdS effects can still be accounted for by just linear theory. AS: But it changes growth, which in turn changes velocity smoothing. So yes, linear power spectrum but also most likely its time derivative (or equivalently velocity power spectrum) PVM: Thinking of neutrinos, I think it is really best to get away from talking about $f(z)$, which is not well-defined when it is really $f(z, k)$. Remember that you can easily compute from CLASS the velocity power spectrum as well as density, which gives you your leading order handle on changes in evolution... (arguably if you had to choose you'd probably want this instead of density power for LyaF, but you don't have to choose...) AFR: Yes, we could add linear velocity power instead of $f(z)$, and compute from there any parameter we want to use internally.

If we had an extremely large number of simulations, we could just setup a metric to find the closest snapshot, and directly read the flux power from the snapshot. Since we will have a sparse sampling of the parameter space, we will need to do some interpolation between them. AS: This is a good way to think about this, yes. This interpolation is precisely the role of the *emulator*.

Note that the internal metric used for the interpolation does not need to use the same parameters θ describing the linear power.

V. SIMULATIONS

Describe here the simulations, include the initial conditions code (GenIC), the code to evolve the fields (MP-Gadget), the different boxes used, and the code to extract skewers (fake_spectra).

Discuss also here the optical depth rescaling, different transfer functions (if any), and thermal history effects (that will be mostly ignored in this paper).

A. Rescaling of the optical depth

From each simulation we will get a set of snapshots, outputs at different redshifts.

From each snapshot, we will extract Lyα skewers, and use these to compute their power spectra. We will repeat this exercise for different rescalings of the optical depth, i.e., we will multiply the optical depth in all cells by a constant factor in the range $0.8 < A_\tau < 1.2$ (approximately), and for each value of A_τ we will compute the transmitted flux fraction F, its mean value (mean flux), and the power spectra of their fluctuations δ_F.

Therefore, from each snapshot we will get a set of power spectra for different values of A_τ. We can label the different power spectra by their associated value of A_τ, or we can label them by their resulting value of the mean flux $\bar{F}$.

[21] showed that the rescaling might introduce biases in the 1D power spectrum for values of A_τ very different than one. However, their test compared two simulations with different thermal history and different pressure, so it is difficult to tell whether the bias came from the rescaling or from the different IGM physics. AFR: It would be great to repeat this exercise in two simulations that have very similar thermal history but different mean flux, I will ask Jose Onorbe for help (he is visiting UCL soon). It is also possible that the test is clearer if we look at the 3D power, where pressure only affects the high-k limit, and the scale independent linera bias.

B. Rescaling of the temperature

The Temperature-Density Relation (TDR) in the Lyα forest can be reasonably well described by a power law,

$$T(\rho) = T_0 \left(\frac{\rho}{\rho_0}\right)^{\gamma-1} , \tag{13}$$

with a typical values for γ between 1 and 1.6. If we use $\rho_0 = \bar{\rho}$, T_0 varies between 10,000 and 20,000K [21].

We can change the thermal history of the simulations by running the same box with different *TREECOOL* files, that contain the redshift evolution of different heating and ionizing rates.

For each snapshot, we can fit their values of T_0 and γ, and use these to label the snapshot, instead of using the name of the TREECOOL, or the parameters that we have used to modify a given file (MP-Gadget can implement the recipes in [22] to modify TRECOOL files by setting the parameters *HeatAmplitude* and *HealSlope*).

Just like we did with the optical depth, we can rescale the temperatures in post-processing. We could do this at two different levels:

- Thermal broadening: when extracting the skewers from the boxes, the last step is to compute the redshift-space-distorted optical depth. To do that, the temperature at each cell is used to decide the local smoothing that we need to apply, what is known as the thermal broadening. It is trivial to take the same optical depth skewer, and convolve it for different temperature rescalings.
- Recombination rates: the temperature also sets the recombination rate, $\alpha(T) \sim T^{-0.7}$. It would also be possible to change the recombination rate at each cell, propagate this into a change in the neutral fraction (proportional to the recombination rate), and finally to the optical depth (proportional to the neutral fraction). PVM: Note that these two are both essentially instantaneous, i.e., I don't think there is any physical possibility of them not using the same temperatures... (so I wouldn't mess with it, except maybe in some pedagogical example) AFR: Great, thanks.

Note that, even though this would capture most of the effects of having a different temperature, we would miss the effect that different temperature have in the pressure smoothing. PVM: Which is of course not really the same temperature (unlike above), i.e., the functional derivative of $P(z)$ with respect to $T(z')$ through the effect of pressure is zero at $z = z'$, while it is a delta function through thermal broadening and recombination rate... I know you know this, this is just a different way to say it... if all pressure came from temperature in observable range I'd say this is a little bit of a nitpicky distinction, but the contribution from pressure at early times sort of fundamentally decouples the two uses of temperature... AFR: Agreed. However, we will include a parameter to study the dependence on the pressure smoothing, the filtering length k_F, and this should be able to capture the differences.

C. Adding pressure smoothing

The small scale structure is suppressed on very small scales because of the pressure in the gas. As described in [23, 24], the smoothing can be described by a characteristic scale, $k_F(z)$, the *filtering scale*, that is an integral version of the Jeans length that depends also on the temperature in the past.

It would be interesting to see if we can add smoothing in postprocessing, effectively lowering the value of k_F in the simulation by hand. Of course, it would not be possible to reduce the smoothing, and to do that one would need to run a simulation with an earlier redshift of reionization.

AFR: We could also ask Jose Onorbe for help to setup this type of test. We would also need to discuss the best way to measure k_F in the snapshots: fit a Gaussian kernel in the power spectrum of $F_{\rm real}$, where no redshift-space distortions have been included? I believe that is what is used in all papers by Hennawi / Lukic / Onorbe. AS: I remember having massive trouble with this when Nishi was still around. I naively imagined that I would just plot the 3D baryon power spectrum, see supression by eye and call k at the midpoint of supression the smoothing. No cigar – the baryon power spectrum is dominated by shot-noise of baryons in halos, you really need to be a bit clever about this. Perhaps this has been solved.

D. Labelling the snapshots

In the linear regime, and for a single specie, the growth of structure is scale independent, and it can be described by the growth factor $D(z)$.

If the Lyα power spectra depended only on the linear power spectrum, this would suggest that there would be a complete degeneracy between changing the overall amplitude of the linear power spectrum and changing the redshift at which we ouput the snapshot. Therefore, we could use the amplitude of the linear power at a given snapshot to label it, and we could potentially use different snapshots of the same simulation to study models with different amplitudes of the linear power.

AFR: How do we measure the linear power in the snapshot? I could see three options (in order of my preference): predict it using the power measured in the initial conditions, and the relative growth as computed from CAMB/CLASS; measure the density power in the snapshot, and fit the growth factor from the low-k part; run a very cheap simulation without hydro and a very low value of A_s, to compute the actual linear power in the simulation (that might sadly differ from the predicted by CAMB/CLASS because of issues in the linear growht). AS: By far preferrable, in fact the only way that wouldn't look dodgy would be not to measure it at all. :) It is a known quantity give linear codes. :) AFR: Pat always claims that measured power is better than predicted power, given cosmic variance in the box. We shouldn't care about the mean power over infinite number of realizations, it is more useful to talk about the actual power than went into the simulation, and that is why we could measure linear power in the initial conditions. AS: Ok, but then you have the IC power spectrum that you can multiply by the correct transfer function.

To sum up, each snapshot will be used to generate multiple simulated fields, and we can label each of them by their values of: mean flux (1 parameter) $\bar{F}$, linear power (3 parameters) P_L, TDR (2 parameters) T_0 and γ, filtering scale k_F. AS: Perhaps you need f again. AFR: Yes, good point.

Redshift will NOT be a label describing the simulated field, and neither will be the TREECOOL file or the redshift of reionization. Since we will define the linear power in units of km s^{-1}, we will not need to include the Hubble parameter at the box as a label. We will not care about any other cosmological parameter in the box either.

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Appendix A: Derivation of equations in the main text

1. Different growth rate

I write below the equations deriving equation 5.

For the input cosmology, we define:

$$P(z,k) = P_\star(k) \left[\frac{D(z)}{D_\star} \right]^2 \ , \tag{A1}$$

where $D(z)$ is the growth factor and $_\star$ means that the quantity is evaluated at $z_\star = 3$.

The evolution of the growth factor is quite similar to Einstein-de Sitter (EdS), i.e., $D(z) \propto a(z)$, and we define the deviation from that growth as follows:

$$\frac{D(z)}{D_\star} = \frac{a(z)}{a_\star} \ \eta(z) \ , \tag{A2}$$

with $\eta_\star = 1$ by definition and $\eta(z) = 1$ in an EdS universe.

We can then do a Taylor expansion of $\eta(z)$ around $z_\star$:

$$\begin{aligned} \eta(z_\star + \Delta z) &= 1 + \frac{\partial \eta}{\partial z}\Big|_{z_\star} \Delta z \\ &= 1 - a_\star^2 \ \frac{\partial \eta}{\partial a}\Big|_{z_\star} \Delta z \\ &= 1 + (1 - f_\star) \, \frac{\Delta z}{1 + z_\star} \ , \end{aligned} \tag{A3}$$

where we have used

$$\frac{\partial \eta}{\partial a}\Big|_{z_\star} = \frac{a_\star}{D_\star} \frac{\partial D}{\partial a}\Big|_{z_\star} = \frac{1}{a_\star} \left(f_\star - 1 \right) \ . \tag{A4}$$

In Figure 2 we show the difference in growth between different cosmologies, with the dashed lines showing the residual differences after matching at $z_\star = 3$.

2. Different expansion rate

The expansion history at $z > 2$ is not quite Einstein-de Sitter (EdS), so we might need to worry about the different expansion history of each model with respect to the fiducial model. These differences are shown in Figure 3.

We could do something similar to what we did for the growth factor, and define a single parameter (derivative of $H(z)$ at z=3) to parameterize that, and add this as an extra likelihood parameter.

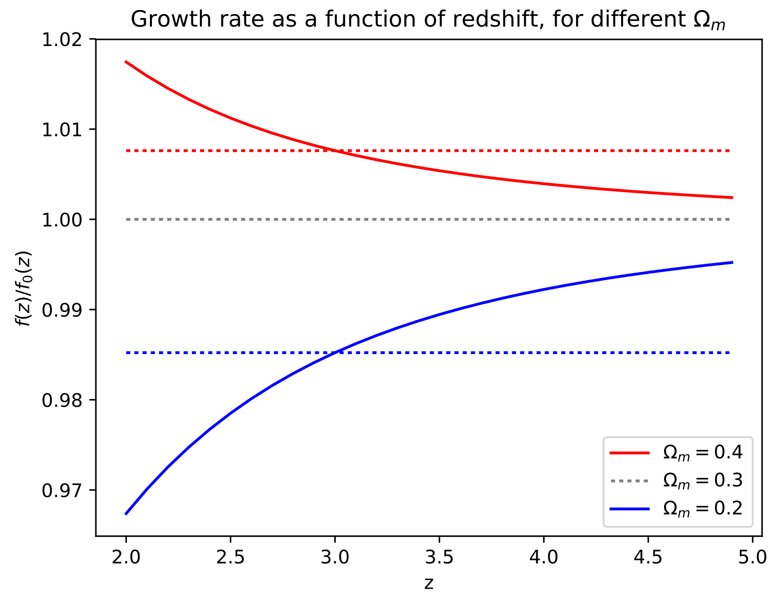

FIG. 2. Logarithmic growth rate, $f(z)$, for different cosmologies. Solid lines show the ratio with respect to fiducial ($\Omega_m = 0.3$), and dashed lines the value at $z_\star = 3$, assumed to be constant in this paper.

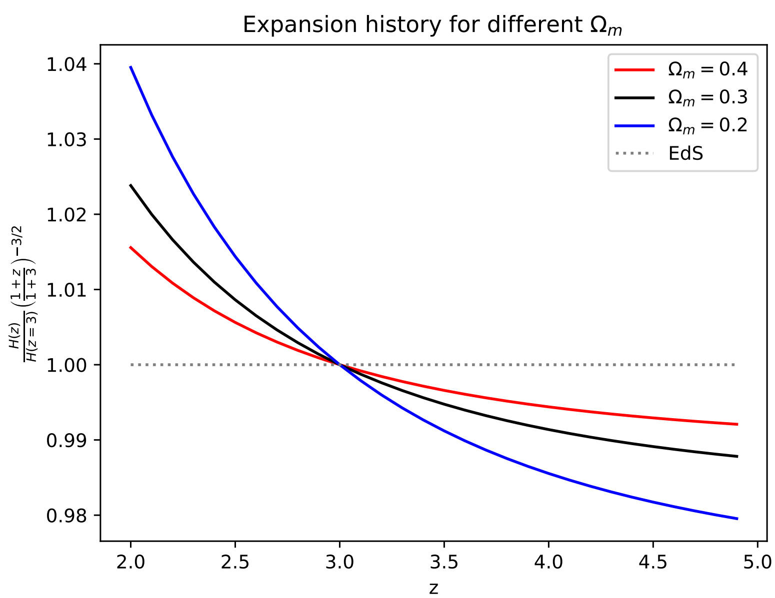

FIG. 3. Differences in the expansion rate, $H(z)$, with respect of EdS, for different cosmologies