Parameterization of the Lyα forest power spectrum

Andreu Font-Ribera[1,*]

[1] *Department of Physics and Astronomy, University College London, Gower Street, London, United Kingdom*

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This is an internal document aimed at clarifying the work-flow related to extracting cosmological information from the Lyα forest 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 years ago when I was trying to understand the details of the SDSS-I analyses by Pat and Uroš, 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. The current version is mostly influenced by discussions with Anže in a whiteboard of the Cosmoparticle hub, and by feedback from Pat on an earlier version of this document.

I. INTRODUCTION

We will discuss all the steps involved in extracting cosmological information from the small scale Lyα forest power spectrum, from measuring the Lyα (or flux) power spectrum to presenting a module that can be used by others to include our results in their cosmological constraints.

The goal is to start an internal discussion within the different Co-Is of the DiRAC proposal, and make sure that we are on the same page before starting to write the science case. The idea is not to define the ultimate setting, but rather to present a first possible setting, that we can use as a baseline when discussing possible improvements.

Most of the discussion presented here is in the context of the 1D flux power spectrum, but it should be relatively easy to extend the formalism to 3D. This will be particularly important in the context of DESI, since the information content will be dominated by 3D correlations [1, 2].

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. We finish in section VI with a discussion on how the same simulations could be used to compute Fisher forecasts for different Lyα statistics.

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, estimate covariance matrices and assess possible contaminants.

- Measurement of the linear 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.

* a.font@ucl.ac.uk

A. Measurement of the flux power spectrum

[TO DO: *Add here some text on continuum fitting, instrumental noise, spectrograph resolution, metal contamination...*]

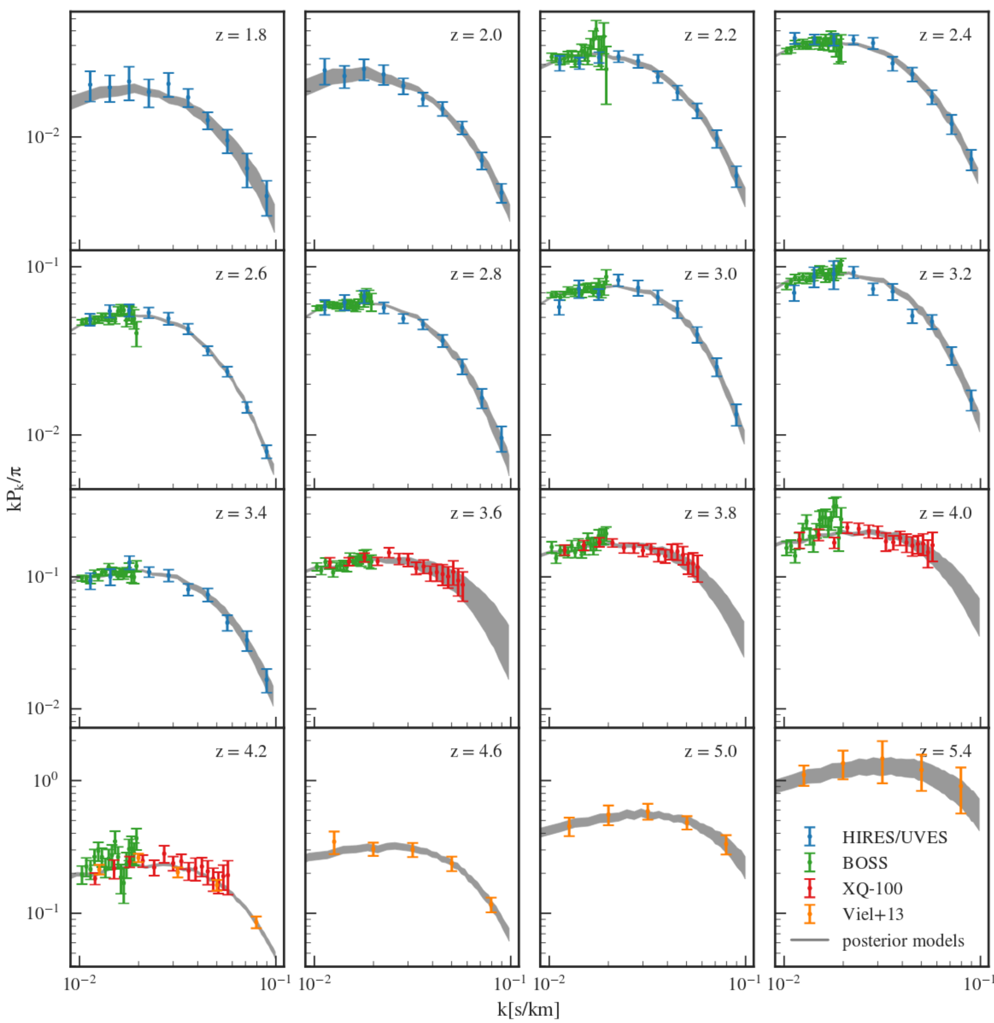

FIG. 1. Compilation of $P_{1D}(z, k_\parallel)$ measurements, including those from [3] (orange), [4] (red), [5] (green) and [6] (blue). [TO DO: *This figure was stolen from [7], it would be better to add one that goes to lower values of $k_\parallel$ covered by SDSS/BOSS.*]

Beyond BAO analyses [8, 9], the only public results on the clustering of the Lyα forest are measurements of the 1D power spectrum [10–12] or more recently [3–6]. 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 will be units of inverse angles [2].

In the rest of this paper we will assume that the flux power spectrum has already been measured, and we will focus on its interpretation. We will mostly discuss the 1D power spectrum, but we will comment on the differences that one would need to add to apply similar techniques to the 3D power.

B. Measurement of the linear power spectrum

In order to interpret the measurement of the Lyα (or flux) power spectrum, we need to be able to make theoretical predictions, and set up a statistical method to compare models and compute constraints on their parameters. Due to its non-linear nature, to model the 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 [7] for a recent study). 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 [13]; a Taylor expansion was used in [5]; a Gaussian Process-based *emulator* was used in [6, 7], 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 [14–16], and its application in Lyα studies is now being studied [6, 17, 18]. 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. 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 $k \sim 0.01\mathrm{s\ km}^{-1}$ (roughly $k \sim 1\ \mathrm{Mpc}^{-1}$) around $z \sim 3$ [1]. For instance, [13] 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 [19] and more recently in [20], 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.

Another peculiarity of Lyα forest analyses is that the measurement 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 $H(z)/H_0$.

This approach of emulating only the linear power was used in [13], but recent analyses [21, 22] have attempted instead to directly emulate the 6+ traditional parameters of a Λ-CDM universe. We 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.
- The results are model-dependent, and it is impossible to use them in extended models (curved universe, non-Λ, different N_{eff}...) if these were not in the original emulator.

C. Cosmological constraints

It is only in combination with external datasets, mainly from CMB experiments, that we are able to provide constraints on the traditional cosmological parameters.

[1] As it will be discussed in the next sections, it is convenient to specify the pivot point in velocity units, since these are the typical units of the measured flux power.

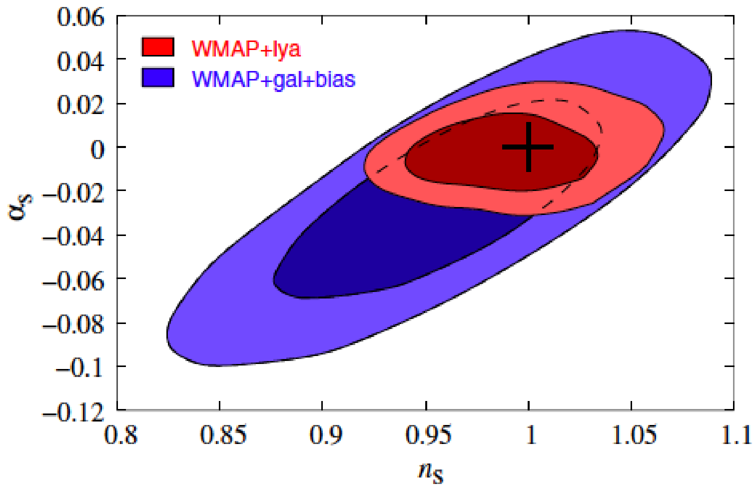

FIG. 2. Constraints on the shape of the primordial power spectrum of perturbations, slope n_s and running α_s, from [23]. The blue contours show the constraints from a joint analysis of WMAP CMB data and SDSS galaxy clustering, while the red contours use the same WMAP data and the linear power spectrum inferred from the Lyα analysis of [13].

For instance, by combining our measurement around $k \sim 1$ 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 can be seen in Figure 2, copied from [23], where WMAP data was used in combination with the linear power spectrum inferred from the Lyα power spectrum [13].

III. PUBLIC LIKELIHOOD CODE

In order to properly discuss our choice of parameterization and simulation setup, it will be helpful to start by describing how we intend the end product, the *likelihood code*, to be used in a cosmological analysis.

A. User interface

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, etc.

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 by discussing a particular interface, where we will ask the user to provide for each cosmological model:

- $P(z, k)$, the linear density power spectrum [2], 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 Mpc^{-1} $< k <$ 10 Mpc^{-1}.

- $P_\theta(z, k)$, the linear power spectrum of velocity divergence, or *velocity power*, over the same range of redshift and scales. Equivalently we could ask for $f(z, k)$, since one could compute one from the other.

[2] During the rest of this paper we will use linear power spectrum to refer to the baryons+CDM power.

- Hubble parameter as a function of redshift, $H(z)$, over the same redshift range.
- If we wanted the likelihood to be able to describe 3D clustering as well, we would need as an input the angular diameter distance $D_A(z)$ (or the Alcock-Paczyński coefficient, $\propto D_A(z)H(z)$, [24]) over the full redshift range.

In exchange, the user will get a value of the (log-) likelihood for this model, that can be then combined with other cosmological probes.

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B. Full likelihood vs look-up table

We will consider two type of users: the experts, who will like to access the full likelihood, and the non-experts that will like to have a quick and easy access to the marginalized likelihood, i.e., where simulation details have been hidden away and astrophysical / nuisance parameters have already been marginalized over.

As an example, in the SDSS-I analysis of [13] the authors made public a look-up table with the tabulated value of the marginalized likelihood as a function of three parameters: the amplitude, the slope, and the running of the linear power spectrum at $z = 3$ and $k = 0.009$s km^{-1}.

In the next sections we will discuss slightly different parameterizations, but we will still have the goal of publishing a simple and fast look-up table that can be easily pluged in *CosmoMC*, *MontePhyton*, etc. We will refer to this object as the *compressed likelihood*, the *look-up table*, or the *marginalized likelihood*, and we will use θ to refer to the parameters in this final product.

However, in order to compute this compressed likelihood, we will first need to marginalize the *full likelihood* over the nuisance astrophysical parameters, that we will refer as ϕ, and that include mean flux, thermal history, contaminants in the data, etc. Both likelihoods are related by:

$$L(\mathbf{d}|\theta) = \int d\phi \; \Pi(\phi) \; L(\mathbf{d}|\theta, \phi) \; , \tag{1}$$

where $\mathbf{d}$ is the measured flux power spectrum, and $\Pi(\phi)$ are the priors on the nuisance parameters.

We will do this marginalization ourselves, and published the already marginalized likelihood for everyone else to use.

The emulator discussed later in this paper is only used to compute the full likelihood, but once we have the marginalized likelihood we do not need to use it any more. In other words, most users will not even need to install the emulator code, they will directly use the pre-computed look-up table.

We could make available different look-up tables for different combinations of Lyα measurements: SDSS-I from [12], BOSS from [5], HIRES/UVES from [3], XQSO-100 from [4] and HIRES/UVES from [6]. Since these measurements share many nuisance parameters (mean flux, thermal history...) it will be important to do the marginalization at the same time.

Of course, we will still make public the code that can compute the full likelihood $L(\mathbf{d}|\theta, \phi)$. This will be important to allow external experts to cross-check our results, and to test whether the results depend on the compression step. It will also be important to allow others to generate new look-up tables by using different priors on the nuisance parameters $\Pi(\phi)$, or by adding new datasets $\mathbf{d}$.

Those accessing the full likelihood will be able to ask also for the value of the (log-) likelihood for a particular data point, or a particular redshift. They will be able to run their own MCMC chain and compute the best fit values for the nuisance parameters, and their confidence intervals.

C. From cosmological model to likelihood parameters

We asked the user for the full linear density and velocity power, in comoving coordinates and over a wide range of redshift and scales, as well as the expansion history. In this section we will describe how we compress all this information into a handful of parameters that will be used to describe our likelihood. We claim that this is an almost lost-less compression.

Note that this discussion is only relevant because we want to be able to generate and publish the compressed likelihood, the look-up table that has already marginalized over nuisance parameters. If we only wanted to use the full likelihood, there would be no need to do this compression. For each model we could compute the required linear power at each redshift, in velocity units, and ask the emulator for the flux power.

1. *Fiducial cosmological model*

We will choose a fiducial cosmological model, based on a recent Planck+BAO analysis [25], and use it to compute a fiducial linear power spectrum, for density $P^0(z,k)$ and velocity $P^0_\theta(z,k)$, and a fiducial Hubble expansion, $H^0(z)$. All quantities with a superscript ^{0} will refer to the fiducial model.

2. *Linear power shape*

We will assume that we can factorize the linear power spectrum in a constant shape (in comoving coordinates) and scale-independent growth around the central redshift, $z_\star = 3$. In general we will use the subscript $_\star$ to refer to quantities that have been evaluated at $z_\star$.

The goal is then to compress the difference between the input power spectrum at $z_\star$, $P_\star(k)$, and the fiducial power spectrum, $P^0_\star(k)$, into a handful of parameters. It would be trivial to extend this analysis to include BAO information, but for simplicity we will ignore the (small) BAO information in the simulations and focus on the differences in the overall shape of the power spectra.

$$B(k) = \frac{P_\star(k)}{P^0_\star(k)} \ . \tag{2}$$

We could use different parameterizations for $B(k)$, but we probably only need 2-3 parameters.

3. *Linear growth*

The velocity power spectrum $P_\theta(z,k)$ is related to the linear density power $P(z,k)$ by the logarithmic growth rate $f(z,k)$.

In the redshift and scales of interest, this growth rate is very close to scale-independent, and we will only use the input velocity power spectrum to compute an effective growth rate as a function of redshift, $f(z)$ [3].

This scale-independent growth rate $f(z)$ has two main effects: it sets the redshift evolution of the linear power around $z_\star$, and it sets the amount of velocity power in the model, that will contribute to the flux power spectrum via redshift space distortions.

As we discuss in Appendix A, in relevant LCDM models, and at $2 < z < 5$, the differences in growth rate are typically less than 1% (see Figure 3). To absorb this difference, we will add as a likelihood parameter the difference between the growth rate with that in the fiducial cosmology, $\Delta f_\star = f(z_\star) - f^0(z_\star)$, evaluated at $z_\star = 3$. This compression is equivalent to assuming that the different growth rate at $z_\star$ is enough to compute the difference in linear growth at any redshift (within the range):

$$\frac{D(z)}{D^0(z)} = 1 + \Delta f_\star \ \frac{\Delta z}{1+z_\star} \ . \tag{3}$$

We discuss this approximation further in Appendix A.

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

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[3] Note that this would be true even in cosmologies with relatively massive neutrinos, as shown in [19, 20]. [TO DO: *Quantify*]

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:

$$q = \frac{1+z}{H(z)}\, k = a_v k \ , \tag{4}$$

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 [13], it is possible to avoid this burden if we parameterize our likelihood (the linear power spectrum) already in units of km s^{-1}.

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.

Therefore, we will use the expansion rate $H(z_\star)$ provided by the user to compute a_v and the linear power in velocity units at $z_\star = 3$:

$$\tilde{P}(q) = a_v^3 \ P(z_\star, k = q/a_v) \ . \tag{5}$$

where we use $\tilde{P}$ to refer to power spectra in units of velocity. We can now redefine a term for the ratio of the power spectra, in velocity units:

$$\tilde{B}(q) = \frac{\tilde{P}(q)}{\tilde{P}^0(q)} = \left(\frac{a_v}{a_v^0}\right)^3 \frac{P(z_\star, q/a_v)}{P^0(z_\star, q/a_v^0)} \ . \tag{6}$$

We will use β to refer to the (2 or 3) parameters describing the shape of the linear power.

To sum up, all cosmological information will be compreseed to the following parameters:

- 2 or 3 β parameters describing $\tilde{B}(q)$, the ratio of the linear power at $z_\star = 3$ with respect to the fiducial, in velocity units.
- $\Delta f_\star$, the difference of growth rates at $z_\star = 3$.

AFR: As discussed below, we *might* also add a parameter describing the (des-)acceleration of the Universe at $z_\star$, to describe the differences in expansion history between the cosmologies below and above $z_\star$, similarly to what we have done with growth in equation 3.

Note that in [13] the main result was a look-up table with only two β parameters (amplitude and slope around $q = 0.009$s km^{-1}), but they also discussed extensions with extra parameters: a third β parameter (running) and a parameter describing the linear growth around $z_\star = 3$, similar to the $\Delta f_\star$ presented here, for which they found they did not have much constraining power.

D. Constructing the compressed likelihood

We want to compute a look-up table with the likelihood as a function of the cosmologically relevant parameters θ, describing the shape of the linear power at $z_\star = 3$ in velocity units (β) and the linear growth ($\Delta f_\star$). There are many possible implementations, but in this section we will focus on a simple one.

We start by specifying a grid of values of the θ parameters [4], and for each of these we will compute the marginalized likelihood by integrating equation 1:

$$L(\mathbf{d}|\theta) = \int d\phi \ \Pi(\phi) \ L(\mathbf{d}|\theta, \phi) \ , \tag{7}$$

[4] We could probably get away with an irregular grid. It would make interpolation a tiny bit more complicated, but it would help us in setting up the simulations.

where ϕ are the nuisance parameters (mean flux, temperature...), and $\Pi(\phi)$ are the priors on the nuisance parameters. We will compute this integral using MCMC or similar.

In order to compute the full likelihood $L(\mathbf{d}|\theta, \phi)$ we will need an *emulator* that will use whatever simulations are available to make a prediction for the flux power in a particular model. However, we will not pass the parameters (θ, ϕ) to the emulator and ask for a prediction for all data points $P_{1\mathrm{D}}(z, k_\parallel)$. Instead, we will do the following:

- For each redshift z_i, we use the nuisance parameters ϕ to make a prediction for the mean flux at the redshift $(\bar{F}_i)$, the values of the temperature-density relation at the redshift (T_{0i},γ_i) and the filtering scale at the redshift (k_{Fi}). T_0 sets a thermal broadening length σ_0, in velocity units, that can be used as a parameter instead. The filtering length, k_F, is discussed in more detail in the next section, but it is also naturally described in velocity units.

- At the same time, we use the parameters describing the linear power θ and the fiducial cosmology to make a prediction for the linear power in velocity units at the redshift $(\tilde{P}_i(q))$ and for the logarithmic growth rate at the redshift (f_i). How exactly this is done is described in Appendix B.

- We then ask the emulator to give us a prediction for the flux power spectrum corresponding to $\left(\bar{F}_i,\ T_{0i},\ \gamma_i,\ k_{Fi},\ \tilde{P}_i(q),\ f_i\right)$. Note that we do not tell the emulator what redshift this corresponds to, and we do not tell it either anything about the θ or ϕ parameters.

IV. THE EMULATOR

As we discussed in the previous section, in order to evaluate the likelihood of a given dataset we ask the emulator to provide the predicted flux power spectrum $P_{1\mathrm{D}}(z_i, k_\parallel)$ for a given model, specified by $\left(\bar{F}_i,\ T_{0i},\ \gamma_i,\ k_{Fi},\ \tilde{P}_i(q),\ f_i\right)$. Note, again, that the emulator does not need to know about the concept of redshift. Yes, snapshots from simulations have associated output redshifts, but this information does not need to be passed to the emulator.

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. This interpolation is precisely the role of the *emulator*. There are different options for the emulator itself, for instance one could use Gaussian Processes [6, 14–18], but the exact interpolation scheme will not be discussed futher in this paper.

In order to reduce the cosmic variance noise in the simulated flux power, we could decide to emulate instead the ratio of the flux power with respect to the flux power in the fiducial model, and use the same random seed in all simulations. However, in different cosmologies we will have the same fluctuations in the initial conditions (defined in comoving coordinates) mapped into different noise spikes in the band powers (defined in velocity units). We could avoid this by using different box sizes for different cosmologies, so that they all have the same box size in velocity units at $z_\star = 3$. Even then, we would only match the noise spikes at one redshift, and there could be (very minor) differences at other redshifts that could confuse the emulator.

AFR: Actually, we could avoid this nuisance by letting the emulator work in comoving coordinates, in Mpc. We could use the expansion history from the fiducial model $H^0(z)$ to convert all quantities back and forth when needed. The only important thing is that if we use Mpc for the linear power spectrum and for the flux power spectrum, we have to use Mpc for the thermal broadening at T_0, σ_0, and for the filtering scale k_F. In any case, it would not affect the setting of the simulations, only the internal interpolation of the emulator, and we could try and compare both approaches.

In order to reduce the effect of cosmic variance and noise spikes, we could also decide to run *paired-fixed* simulations [26–29].

Finally, we could decide to fit the simulated flux power with a handful of coefficients (polynomials or PCA components), and interpolate these instead of the noisy band powers.

AFR: Written this way, it is clear that we are talking about emulating the theory, and not emulating the likelihood. This has not been clear to me in the past... One of the key features of GP emulators is that they can provide an estimate on the uncertainty in the theoretical prediction. In [18] we have been looking at how to implement a *refinement* step, where we combine the posterior probability for (a very different) set of parameters with the predicted theoretical uncertainty to decide where to run the next batch of simulations to more efficiently improve the description of the posterior. I wonder how could one implement something similar in the setting described here.

AFR: I guess there are two things that should be addressed: How do we propagate the theoretical uncertainty reported by the emulator to uncertainties in the likelihood? And once we identify the points in parameter space that we would like to refine, specified by (θ,ϕ), how do we translate this into a configuration for the simulation to run, specified by a linear power spectrum at $z_{\rm ini} = 99$, a cosmology to evolve the density fields, and a TRECOOL file specifying the heating and ionization rates? I am sure there are approximated ways to do this, but we'd need to think about it.

V. SIMULATIONS

Even though we could always move to Gadget-3, we would like to start the project with MP-Gadget as our main code to evolve the initial conditions. We should do a comparison of the linear growth in both codes, and that should help us make a final decision.

Our baseline plan is to run simulations with $N = 1024^3$ particle per especies (baryons and CDM) in boxes of roughly 100 Mpc. This would give us a mean particle separation of roughly 100 kpc, or 70 h^{-1}kpc, that should be enough to have a first decent emulator working. AFR: This might not be enough to properly study the higher redhift bins in HIRES/UVES, $z > 5$, where the gas is less smooth and it is harder to resolve all the structure. But I think it is better to err on this side than to have boxes that are too small, since poor resolution is somewhat degenerated with different reionization / filtering length that we want to marginalize over anyway.

We discuss here the different post-processing of the snapshots, and how we store the simulated power spectrum that the emulator will later use to make predictions.

A. Rescaling of the optical depth

From each simulation we will get a serie 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 $0.5 < A_\tau < 2.0$ (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 could label the different power spectra by their associated value of A_τ, but we will label instead by their resulting value of the mean flux $\bar{F}$. [30] argued 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. It is true that collisional ionization could break the rescaling, but this type of ionization should only be relevant on very high-density regions, where we know that our simulations are not correct anyway [5].

B. Rescaling of the temperature

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

$$T(\rho) = T_0 \left(\frac{\rho}{\rho_0} \right)^{\gamma - 1} , \tag{8}$$

[5] So if we found that collisional ionizations mattered we would have to consider using more realistic (and expensive!) simulations.

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 [30].

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 [31] to modify TRECOOL files by setting the parameters *HeatAmplitude* and *HeatSlope*).

Just like we did with the optical depth, we can rescale the temperatures in post-processing. This would capture correctly two different physical effects:

- 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, $\alpha(T) \sim T^{-0.7}$. We could recompute 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).

It does not matter whether we use different TREECOOL files or different *HeatAmplitude* and *HeatSlope* parameters, at the end of the day we will compute the actual values of (T_0,γ) in the snapshots and store that information to described the power measured in the post-processed snapshot.

C. Pressure smoothing

The small scale structure is suppressed on very small scales because of the pressure in the gas. As described in [32, 33], 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 is important to distinguish the effect of pressure from the effect of temperature, since one can have two snapshots with very similar temperature but very different values of k_F because of a different reionization history.

Note that it is not trivial to measure k_F from a snapshot. One could be tempted to measure the gas density power spectrum and fit an effective Gaussian cut-off, but this power spectrum is completely dominanted by the non-linear regime (high densities) that we do not trust in our simulations. In several papers by Onorbe/Lukic/Hennawi [6, 7, 30, 34] they fit k_F from the power spectrum of $e^{-\tau}$ in real space, without adding redshift space distortions. An alternative would be to use the information about the temperature in previous snapshots to compute k_F using equation 8 in [33].

AFR: I wonder whether this would require storing even more snapshots, increasing even further the total amount of disk space required. It is possible that we can compute the temperature on the fly, or write only a sub-sample of particles for "intermediate" snapshots.

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.

To sum up, each snapshot will be used to generate multiple simulated fields in post-process (rescaling optical depth, temperature...), and we will compute the power spectrum for each of the simulated fields. We will also compute (using CAMB/CLASS) the predited linear power for the snapshot (in velocity units) and its logarithmic growth rate, and will measure from the snapshots other IGM properties like the mean flux $\bar{F}$, the TDR parameters (T_0 and γ) and the filtering scale k_F.

The emulator will have a list of all the models for which we have simulated power spectra, and it will specify a metric quantifying the separation between two models. Every time we ask for a the prediction for a given model (specified by $\bar{F},\ T_0,\ \gamma,\ k_F,\ \tilde{P}(q),\ f$), the emulator will use the nearest points and (somehow) interpolate between these.

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.

VI. FISHER FORECASTS

AFR: I will add here some discussion on how one would use the same set of simulations to compute Fisher forecasts for the 1D power, the 3D power and different type of bispectrums.

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Appendix A: Derivation of equations in the main text

1. Different growth rate

I write below the equations deriving equation 3.
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 3 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 4.
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.

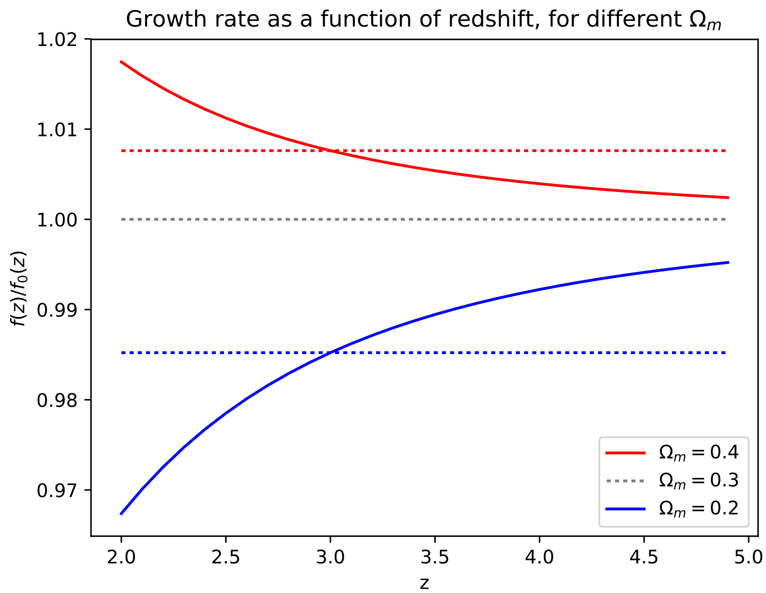

FIG. 3. Logarithmic growth rate, $f(z)$, for different cosmologies. Solid lines show the ratio with respect to fiducial ($\Omega_m = 0.3$), and dashed lines the value at $z_\star = 3$, assumed to be constant in this paper.

Appendix B: Reconstructing the linear power from the parameters

In section III we discussed how we compress the cosmological information provided by the user to a handful of θ parameters describing the linear power spectrum over the relevant redshift and scales. This reduced set of parameters θ will be the ones used in the compressed (or marginalized) likelihood.

In order to compute the marginalized likelihood we need to use the default cosmological model ($P^0(z,k)$, $P^0_\theta(z,k)$ and $H(z)$) and the set of θ parameters to compute the corresponding linear power at a particular redshift z_i and in velocity units, $\tilde{P}_i(q)$, as well as the growth rate in that redshift f_i. In this section I will describe in detail how we do this.

- Using the linear power in the fiducial model $P^0_\star(k)$ and the Hubble parameter $H^0_\star$, both evaluated at $z_\star = 3$, we compute the linear power spectrum in velocity units for the fiducial model, $\tilde{P}^0_\star(q)$.
- Using the shape parameters β, we compute the linear power spectrum in velocity units for the input model, $\tilde{P}_\star(q)$.
- Using the Hubble parameter in the fiducial cosmology $H^0_\star$ we convert this to a linear power spectrum in comoving coordinates, $P_\star(k)$.
- Using the linear growth in the fiducial cosmology, $f_0(z)$, we translate that to the desired redshift, $P(z_i,k)$. If we had $\Delta f_\star$ as a free parameter, we would use that to slightly modify this redshift evolution.
- We finally use the Hubble expansion in the fiducial cosmology, $H^0(z_i)$, to convert the linear power in velocity units at the desired redshift, $\tilde{P}(z_i,q)$. If we had an extra parameter describing the different expansion history, we would use it here to slightly modified this last step.

Another way to look at it, is that we will take the linear power at $z_\star = 3$, in velocity units, and try to find a modification of the primordial power in the fiducial model that matches the power. For instance, by trying to find different values of (A_s,n_s and α_S) with which the fiducial model can be modified to match the input power. We would then use call CAMB/CLASS with the fiducial model cosmology, but this modified

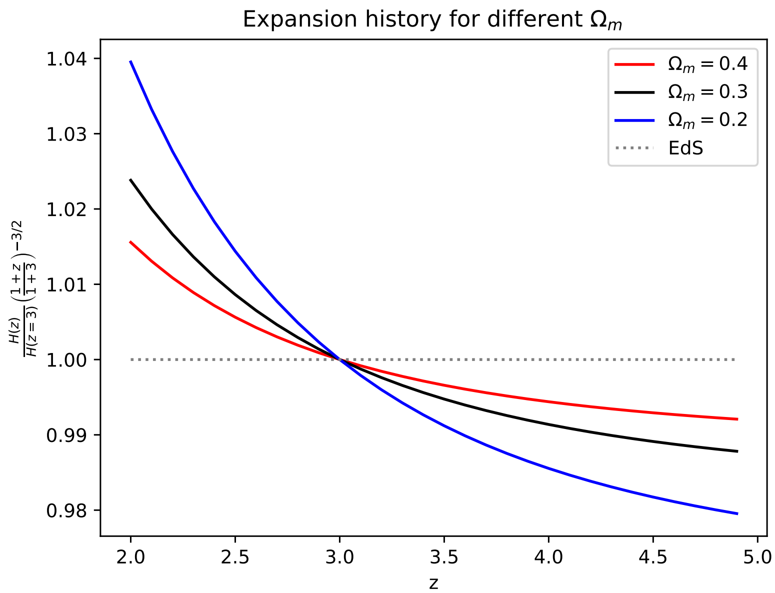

FIG. 4. Differences in the expansion rate, $H(z)$, with respect of EdS, for different cosmologies

primordial power, to make predictions for the linear power at any redshift. This, of course, is for cases where we ignore differences in $f(z)$ or $H(z)$, but these could easily be introduced as well.

AFR: I actually prefer the itemized description, but it is a matter of taste.