# Chasing Lyman $\alpha$ -emitting galaxies at z=8.8

Peter Laursen<sup>1, 2</sup>, Jesper Sommer-Larsen<sup>2, 3, 4</sup>, Bo Milvang-Jensen<sup>2, 5</sup>, Johan P. U. Fynbo<sup>2, 5</sup>, and Alexei O. Razoumov<sup>6</sup>

- <sup>1</sup> Institute of Theoretical Astrophysics, University of Oslo, P.O. Box 1029 Blindern, N-0315 Oslo, Norway. e-mail: pela@astro.uio.no
- <sup>2</sup> Dark Cosmology Centre, Niels Bohr Institute, University of Copenhagen, Juliane Maries Vej 30, 2100, Copenhagen Ø, Denmark.
- Marie Kruses Skole, Stavnsholtvej 29-31, DK-3520 Farum, Denmark.
- <sup>4</sup> Excellence Cluster Universe, Technische Universität München, Boltzmannstraße 2, 85748 Garching, Germany.
- Osmic Dawn Center, Niels Bohr Institute, University of Copenhagen, Juliane Maries Vej 30, 2100 Copenhagen Ø, Denmark.
- <sup>6</sup> WestGrid, Vancouver, BC, Canada.

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#### **ABSTRACT**

With a total integration time of 168 hours and a narrowband filter tuned to  $Ly\alpha$  emission from z=8.8, the UltraVISTA survey has set out to find some of the most distant galaxies, on the verge of the Epoch of Reionization. Previous calculations of the expected number of detected  $Ly\alpha$ -emitting galaxies (LAEs) at this redshift based e.g. on extrapolation of lower-redshift luminosity functions did not explicitly take into account the radiative transfer of  $Ly\alpha$ . In this work we combine a theoretical model for the halo mass function, i.e. the expected number of haloes per volume, with numerical results from high-resolution cosmological hydrosimulations post-processed with radiative transfer of ionizing UV and  $Ly\alpha$  radiation, assessing the visibility of LAEs residing in these haloes. Uncertainties such as cosmic variance and the anisotropic escape of  $Ly\alpha$  are taken into account, and it is predicted that once the survey has finished, the probabilities of detecting none, one, or more than one are roughly 90%, 10%, and 1%, respectively. This is a significantly smaller success rate compared to earlier predictions, due to the combined effect of a highly neutral intergalactic medium (IGM) scattering  $Ly\alpha$  to such large distances from the galaxy that they fall outside the observational aperture, and to the actual depth of the survey being less than predicted.

Because the IGM affects narrowband (NB) and broadband (BB) magnitudes differently, we argue for a relaxed colour selection criterion of NB – BB  $\simeq +0.85$  in the AB system. Since the flux is dominated by the continuum, however, even if a galaxy is detectable in the NB, its probability of being selected as a narrowband excess object is  $\lesssim 35\%$ .

Various additional properties of galaxies at this redshift are predicted, e.g. the Ly $\alpha$  and UV luminosity functions, the stellar mass–halo mass relation, the spectral shape, the optimal aperture, as well as the anisotropic escape of Ly $\alpha$  through both the dusty, interstellar medium and through the partly neutral IGM.

Finally, we describe and make public a fast numerical code for adding numbers with asymmetric uncertainties (" $x_{-\sigma_{-}}^{+\sigma_{+}}$ ") which proves to be significantly better than the standard, but wrong, way of adding upper and lower uncertainties in quadrature separately.

**Key words.** radiative transfer — galaxies: high-redshift — cosmology: reionization

# 1. Introduction

Unveiling the evolution and the constituents of the early Universe is as exciting and important as it is arduous. While the formation of structure from primordial fluctuations to massive haloes can be accounted for purely by gravitational collapse of matter, the mechanisms that lead to the emission of light — the primary way of gaining information from the high-redshift Universe — are less clear. The first generation of stars seem to have emerged some 200 Myr after the Big Bang (Barkana & Loeb 2001; Visbal et al. 2012; Bowman et al. 2018). In a virtually neutral Universe, the escape of ionizing radiation was inhibited, but eventually the Universe was reionized and galaxies became more easily detectable.

Hard UV radiation is emitted from the most massive and hence hot stars of a starburst, attempts to escape the surrounding neutral gas, and carves out bubbles of ionized hydrogen in the interstellar medium (ISM). Because of the high densities involved during the Epoch of Reionization (EoR), recombination happens on very short timescales, eventually reprocessing 1/3 of the radiation bluewards of 912 Å into a single emission line — the Ly $\alpha$  line at 1216 Å. Consequently, up to 10% of the to-

tal, bolometric luminosity can be emitted in Ly $\alpha$ , as first predicted by Partridge & Peebles (1967). At high redshifts, where the metallicity may be expected to be substantially lower and the initial mass function (IMF) may be more top-heavy than the Salpeter (1955)-one assumed by Partridge & Peebles (1967), the fraction may be even higher, up to 20–40% (Raiter et al. 2010). This fortunate fact facilitates observations of galaxies that would otherwise be impossible to detect. In addition to the Ly $\alpha$  precipitated by stars, a notable amount is surmised to be emitted from cooling radiation following the cold accretion of gas onto the galaxies (see discussion in Sec. 3.3.2).

When the UltraVISTA survey (discussed in detail in Sec. 1.1) set out, the most distant known galaxy was the Iye et al. (2006) Ly $\alpha$  emitter (LAE) at z=6.96, which held its record for five years. Eventually, a few LAEs at redshifts beyond 7 were reported (e.g. Vanzella et al. 2011; Shibuya et al. 2012; Finkelstein et al. 2013), and more recently, galaxies at z=8.68 (Zitrin et al. 2015), z=11.09 (Oesch et al. 2016), and z=9.1 (Hashimoto et al. 2018) were detected, showing that the survey should at least have a chance of detecting LAEs at z=8.8. The galaxy detected by Oesch et al. (2016) was detected due to the Ly $\alpha$  break rather than the line, while the one found by

Hashimoto et al. (2018) was detected in O III albeit with tentative evidence for a Ly $\alpha$  line; thus, an UltraVISTA-detection at z = 8.8 could be the highest-redshift LAE to date.

Detecting the most distant astronomical object has long been a goal in itself, but pushing such observations to the limit is not just a question of increasing the volume of the explored part of the Universe, or breaking a record. Although the difference in lookback time between, say, z = 8 and 9 is merely a hundred Myr, this is a significant fraction of the age of the Universe at this time, which was only half a Gyr. Thus, these extreme observations offers crucial insight into the time scales of the formation, evolution and general properties of galaxies and the intergalactic medium (IGM). Moreover, the number density and clustering of LAEs at z > 6 can put constraints on reionization (Furlanetto et al. 2006; McQuinn et al. 2007; Iliev et al. 2008; Jensen et al. 2013). As yet, quantifying the clustering of LAEs has been rather inadequate due to limited sample sizes, but at these redshifts even the detection of a single galaxy provides important constraints.

#### 1.1. The UltraVISTA survey

The comissioning of the 4.1 m survey telescope VISTA, located close to the VLT on a neighbouring peak, and its wide-field infrared camera VIRCAM (Sutherland et al. 2014) was completed in 2009. VISTA is used mainly for large, multi-year, public surveys (Arnaboldi et al. 2017). One of these is UltraVISTA (McCracken et al. 2012), which utilizes the VISTA telescope to obtain deep imaging of  $1.2 \times 1.5 \text{ deg}^2$  of the COSMOS field (Scoville et al. 2007) in the four near-IR filters Y, J, H and  $K_s$ . Half of this field, the four so-called ultra-deep stripes covering about 1 deg<sup>2</sup>, are also observed in a narrowband filter NB118 centered at 1.19 µm (Milvang-Jensen et al. 2013), corresponding to Ly $\alpha$  redshifted from z = 8.8, or less than 600 Myr after the Big Bang. This wavelength was chosen to be relatively free of airglow emission. Unfortunately the filter turned out to be subject to a small shift in wavelength of approximately 3.5 nm when mounted in VIRCAM, which, while still effectively probing the same redshift, is large enough that airglow lines are partly entered, resulting in a somewhat lower sensitivity (Milvang-Jensen et al. 2013).

The narrowband survey, which constitutes  $\sim 10\%$  of the full UltraVISTA survey, set out in December 2009 to construct an ultradeep image from 168 hours of integration. An original  $5\sigma$  detection limit of  $F=3.7\times 10^{-18}\,\mathrm{erg}\,\mathrm{s}^{-1}\,\mathrm{cm}^{-2}$  (corresponding to an AB magnitude of 26.0) was expected (Nilsson et al. 2007); however, due to the above-mentioned shift, as well as a too optimistic sky background assumed by the ESO Exposure Time Calculator used at the time, it turned out to be somewhat shallower: Based on the GTO data (Milvang-Jensen et al. 2013), the detection limit for the final UltraVISTA is predicted to be  $F=1.5-1.7\times 10^{-17}\,\mathrm{erg}\,\mathrm{s}^{-1}\,\mathrm{cm}^{-2}$  (see e.g. Matthee et al. 2014). The depth and the large area still results in a volume much larger than previous surveys.

The observational part of the narrowband survey was completed in January this year. Since the data reduction is extremely time-consuming, the latest data release ("DR3") only contains 60% of the final narrowband exposure; so far there is no sign of the detection of z=8.8 LAEs. Can we hope to detect any at all? This question boils down to estimating the luminosity function (LF) of LAEs at a hitherto unexplored epoch of the history of the Universe. In essence, two complementary approaches exist to this problem: Either one can look at LFs of galaxies probed at lower redshift, and then extrapolate to z=8.8, assuming a model

for the evolution of both galaxies and the IGM. Alternatively, one may resort to numerical simulations, relying on the faith in our understanding of the physics governing the formation of structure.

#### 1.2. Previous predictions and observations at z = 8.8

Prior to the launch of UltraVISTA, Nilsson et al. (2007) made predictions for the expected number of detected LAEs at z=8.8. At this time, realistic Ly $\alpha$  radiative transfer (RT) was at its infancy and unavailable to most astronomers. Instead these authors followed three different approaches: Model 1 used the semi-analytical galaxy formation model GALFORM (Cole et al. 2000) with a common Ly $\alpha$  escape fraction of  $f_{\rm esc}=0.02$  or 0.2 for galaxies of all masses, to match LF observations at lower redshifts (Le Delliou et al. 2006). Model 2 uses the phenomenological model of Thommes & Meisenheimer (2005), normalized to match the observed mass function of galaxy spheroids at z=0. Model 3 uses a Schechter LF with parameters extrapolated linearly from fits at  $3.1 \le z \le 6.5$ . The three models predict between 3 and 20 detections.

With similar extrapolations of lower-redshift LFs, Faisst et al. (2014) predicted a less optimistic  $0.6 \pm 0.3$ , while Matthee et al. (2014, see below) predicted, with their most optimistic LF, a number of  $\lesssim 23$ . However, using the Nilsson et al. (2007) LF extrapolation but with the realistically estimated depth yields only 0.19.

Observations of LAEs at z=8.8 have been attempted before. Willis & Courbin (2005) used the VLT/ISAAC narrowband to sample a volume of 340  $h^{-3}\,\mathrm{cMpc^3}$  to a limiting flux of  $3.28\times10^{-18}\,\mathrm{erg}\,\mathrm{s^{-1}}\,\mathrm{cm^{-2}}$ , while Cuby et al. (2007), using the same instrument, went for a larger area of 31 arcmin² albeit to a shallower threshold of  $\sim 1.3\times10^{-17}\,\mathrm{erg}\,\mathrm{s^{-1}}\,\mathrm{cm^{-2}}$ . Taking advantage of the lensing effect of three clusters, Willis et al. (2008) reached  $3.7\times10^{-18}$  in an area of 12 arcmin². Sobral et al. (2009) surveyed  $1.4\,\mathrm{deg^2}$  down to  $\sim 7.6\times10^{-17}\,\mathrm{erg}\,\mathrm{s^{-1}}\,\mathrm{cm^{-2}}$  with UKIRT/WFCam in the HizELS survey at  $z\simeq9$ , and Matthee et al. (2014) searched the hitherto largest area of  $10\,\mathrm{deg^2}$  with CFHT/WIRCam and VLT/SINFONI followup down to  $7\times10^{-17}\,\mathrm{erg}\,\mathrm{s^{-1}}\,\mathrm{cm^{-2}}$ . However, all surveys returned null-results.

# 1.3. Overview of our approach

Predicting numerically the expected the number of observed galaxies is a challenging task, but can essentially be divided into two subprojects: Calculating the number of galaxies in the cosmic volume surveyed by UltraVISTA, and calculating the observability of those galaxies. In principle, everything could be computed in a single numerical simulation calculating the galaxy formation and emission of light from the galaxies. In practise, however, the simultaneous need for a large volume and high resolution obliges us to split up the project in several parts. In the following, the various constituents of the project are outlined.

Galaxies reside in dark matter haloes, the number density of which is given by the *halo mass function* (HMF) which can be estimated analytically or determined via large cosmological simulations, or using a combination hereof. Whether or not a given halo hosts a galaxy is given by a halo occupation distribution, which is defined once the concept of a galaxy is defined. The easiest approach is to simply define a galaxy as *any* conglomerate of baryons, or even any dark matter (DM) halo, whether or not these particles have made themselves visible by producing

any kind of luminous matter. Subsequently we can then ask the question "Is a given galaxy observable?"

Simulating galaxy formation realistically requires not only inclusion of hydrodynamics, but also higher resolution than what is offered by large-scale simulations. Moreover, for the RT *much* higher resolution is needed, making it impossible to simulate a statistically robust sample of galaxies with sufficient resolution. These difficulties are dealt with by carrying out a fully cosmological, hydrodynamical, but medium-sized, simulation which is large enough that the interaction between individual galaxies is accounted for. Subsequently, a number of galaxies are extracted from the simulation and resimulated at higher resolution. Several different models for star formation and feedback are investigated.

Finally, two RT schemes are employed: While the cosmological simulation uses an on-the-fly approximation of the ionizing UV background (UVB), a full UV RT is performed on the extracted galaxies and their environments, after which the Ly $\alpha$  RT is conducted, monitoring the spatial and spectral distribution of the photons that reach the observer, i.e. those which are not absorbed by dust, or scattered out of the line of sight (LOS) by the IGM.

The two subprojects — calculating the number density and the observability — are described in Secs. 2 and 3, respectively. The results are presented in Sec. 4, discussed in Sec. 5, and summarised in Sec. 6.

#### 2. Galaxy number density

#### 2.1. Halo mass function

The problem of calculating the distribution of the masses  $M_h$  of collapsed haloes was addressed first by Press & Schechter (PS; 1974), who considered the spherical collapse of gravitationally interacting matter from an initial, smoothed density field. The resulting HMF expressed as number density per logarithmic mass bin can be written as

$$\frac{dN}{d\ln M_{\rm h}} = \frac{\rho_{\rm M,0}}{M_{\rm h}} \left| \frac{d\ln \sigma}{dM_{\rm h}} \right| f(\sigma),\tag{1}$$

where  $\rho_{\rm M,0}$  is the present-day average mass density of the Universe,  $\sigma(M_{\rm h},z)$  is the rms fluctuations of the density field smoothed with a top-hat filter W(R) of radius  $R=(3M_{\rm h}/4\pi\rho_{\rm M}(z))^{1/3}$ , and  $f(\sigma)$  is discussed below.

For a linearly extrapolated density field characterised by a power spectrum P(k), the rms fluctuation is given by

$$\sigma^2(M) = \frac{\delta^2(z)}{2\pi^2} \int_0^\infty dk \, k^2 P(k) \widehat{W}(k, M),\tag{2}$$

where  $W(k, M) = 3(\sin kR - kR\cos kR)/(kR)^3$  is the Fourier transform of the real-space filter W(R), and  $\delta(z) = D(z)/D(0)$  is the linear growth rate normalized to unity today. The growth rate function, in turn, involves an integral over the expansion history, but is very well approximated (Lahav et al. 1991; Carroll et al. 1992) by

$$D(z) = \frac{5}{2} \frac{1}{1+z} \frac{\Omega_{\text{M},z}}{\Omega_{\text{M},z}^{4/7} - \Omega_{\Lambda,z} + (1+\Omega_{\text{M},z}/2)(1+\Omega_{\Lambda,z}/70)}$$
(3)

The last term in Eq. 1,  $f(\sigma)$ , is the *multiplicity function* giving the mass fraction associated with halos in a unit range of  $\ln \nu$ , with  $\nu \equiv \delta_{\rm cr}/\sigma$  and  $\delta_{\rm cr} \simeq 1.686$  the critical density contrast needed for gravitational collapse. Only in the PS formalism is an analytical form of  $f(\sigma)$  obtainable; in general it must be empirically derived by fitting to halo abundances in cosmological simulations. The PS HMF gave good fits to simulations at that time, but as computing resources improved, it was found numerically that it over(under)predicts the collapsed fraction at the low-(high-)mass end (e.g. Governato et al. 1999).

By introducing two extra parameters, Sheth & Tormen (ST; 1999) gave an improved formalism (further detailed in Sheth et al. (2001) and Sheth & Tormen (2002)), allowing for ellipsoidal structures to form. In the ST formalism the multiplicity function is given by

$$f(\sigma) = A\sqrt{\frac{2\tilde{\nu}}{\pi}} \left[1 + \tilde{\nu}^{-p}\right] e^{-\tilde{\nu}/2},\tag{4}$$

where  $A \approx 0.322$  is a normalization constant,  $\tilde{v} \equiv av^2$  with a = 0.707 describing a high-mass cutoff in an *N*-body simulation, and p = 0.3 is given by the shape of the HMF at low masses in the simulation. The PS HMF is recovered using  $\{A, a, p\} = \{\frac{1}{2}, 1, 0\}$ ).

While the ST HMF is much more accurate, especially at low redshifts, it still tends to overpredict the abundance of haloes at higher redshifts, when comparing to large, cosmological simulations. On the basis of the so-called Bolshoi simulation — an 8.5 billion particle simulation of comoving volume  $(250 \, h^{-1} {\rm Mpc})^3$  — Klypin et al. (2011) provide a simple z-dependent correction factor which brings the analytical predictions much closer to the results of the simulation:

$$F(z) = \frac{[5.501\delta(z)]^4}{1 + [5.500\delta(z)]^4},\tag{5}$$

The Bolshoi simulation uses a (near-)*WMAP* seven-year data cosmology (Jarosik et al. 2011). For our analysis we adopt the ST HMF with the correction factor in Eq. 5; in Sec. 5.2 we discuss the implications of using other HMFs and the more recent Planck cosmology (Planck Collaboration: et al. 2016).

# 2.2. UltraVISTA area and depth

To get the total number of galaxies, the number density must be multiplied by the volume surveyed by UltraVISTA. However, not all parts of the area are exposed equally. VIRCAM comprises 16 detectors (each with its own NB118 filter) which cannot be placed adjacently but instead are separated by a large fraction of a detector size. To acquire a contiguous image, the camera is shifted in the declination direction between exposures (or "paw prints"), resulting in most of the area being exposed twice, while the top and bottom 5.5' are exposed once, in units of a single paw print exposure time. With a final, total exposure time of 168 hours, split equally in the three paw prints, most of the area will reach an exposure time of 112 hours. Moreover, detector #16 and, to a lesser extend, #4 have sizable unreliable regions that are excluded from the analysis. The result is that various parts of the area is sensitive to different depths. For details on exposures, see www.vista.ac.uk. The total (non-dead) area exposed at least once is 1.07 deg<sup>2</sup>, which at z = 8.8 corresponds to  $150 h^{-2}$  Mpc<sup>2</sup>, or  $14.5 \times 10^3 h^{-2}$  cMpc<sup>2</sup>.

The depth of the volume is also not unequivocal; since the transmission curves of the filters are not tophats, different distances are probed to different depths. Moreover, the 16 filters are

<sup>&</sup>lt;sup>1</sup> Note that other functional forms of the filter are possible, e.g. a Gaussian filter for which  $\widehat{W}(k,M)=e^{-(kR)^2/2}$ , where the relation between mass and radius is  $M_{\rm h}=(2\pi)^{3/2}R^3\rho_{\rm M}$ .

slightly different, and have slightly different central wavelengths. In general, they all have roughly "full" transmission (i.e. around 60%) in a window of  $\sim 70$  Å. Outside of this region the transmission tapers off in such a way that the average FWHM is  $123\pm3$  Å. If the emission lines were delta functions, at z=8.8 this would translate into galaxies within a slab  $19\ h^{-1}$  cMpc thick being detected. Since in fact resonant scattering broadens the emission lines by several Ångström (in the rest frame), galaxies on the edges of this slab are less conspicuous than more centrally located ones. For an extensive description of the filters and transmission curves, see Milvang-Jensen et al. (2013).

The consequence is that the exact volume becomes a function of the flux limit of the observation; whereas a faint galaxy may only be detected if it lies at the centre of a filter, a bright galaxy may be detected even if it lies in the wing. Thus, any survey probes bright galaxies in a larger volume than fainter. An approximate volume can be computed from the average filter FWHM and the area exposed at least once; this estimate yields  $290 \ h^{-3} \ \mathrm{Mpc^3}$ , or  $2.7 \times 10^5 \ h^{-3} \ \mathrm{cMpc^3}$ .

Likewise, line broadening from RT effects may make galaxies both more and less visible: A Ly $\alpha$  line that would be detectable if it were a delta-like line can be smeared out over tens of Ångströms (in the observer's frame), lowering the flux density below the sensitivity threshold. On the other hand, a (bright) line lying so far out in the wing of the filter that it would be undetectable as a delta-line, could be broadened into the sensitive part of the filter.

To address these complications, in the following calculations we integrate the simulated spectra over the exact filter shapes for each of the 16 filters, and split the detector up in 52 regions with individual limiting magnitudes.

# 3. Galaxy observability

Whether a galaxy is observable depends on many factors, from its history of formation, to its ability to create luminous objects, to the emitted light making its way out through the galaxy and down to us. To simulate this numerically requires detailed modelling; in particular high resolution and a realistic HI field is needed for the  $\text{Ly}\alpha$  RT. In the following, the simulations of the galaxies and the RT is described.

#### 3.1. Cosmological hydrosimulations

# 3.1.1. The code

The TreeSPH type code used to simulate the formation and evolution of galaxies to z = 8.8 is in most aspects identical to the code described by Sommer-Larsen & Fynbo (2017). In particular, the superwind prescription for starburst-driven energy feedback is implemented, and a Chabrier (2003) IMF is employed. This enables the continuing formation of starburstdriven (metal-enriched) outflows (discussed further in Sec. 5.5), in line with indications of recent observations of Ovi and Ovii absorption in the Galactic CGM. Such outflows are also of great significance to the Ly $\alpha$  RT (see Sec. 5.5), especially during the EoR (Dijkstra & Wyithe 2010; Dijkstra et al. 2011). The code used for the present work differs from the one described in Sommer-Larsen & Fynbo (2017) in a few aspects: i) a "stretched" version of the Haardt & Madau (1996) UVB is used, rather than the Haardt & Madau (2012) UVB — the stretched UVB turns on at z = 12, whereas the original Haardt & Madau (1996) UVB turns on at z = 6 (see Laursen et al. 2011 for more detail), ii) early stellar feedback (ESF) was not implemented in the simulations described in this work, and *iii*) the effects of self-shielding of the UVB by gas is not described using the mean field approximation of Rahmati et al. (2013). Instead it is assumed that the UVB is fully shielded off in regions where the mean free path of Lyman limit photons is less than 0.1 kpc.

#### 3.1.2. The simulations

One expects the brightest and most Ly $\alpha$ -luminous galaxies observable at z=8.8 to be located in higher-density, proto-cluster regions of the Universe. Hence, emphasis is placed on simulating such regions at high resolution. To this end, the well-known "zoom-in" technique (e.g. Navarro & White 1994; Oñorbe et al. 2013, and references therein) is applied in two steps, as will be detailed in the following.

First, a low resolution, DM-only simulation is run to z=0, using  $128^3$  particles in a  $(150\,h^{-1}\,\mathrm{cMpc})^3$  box with periodic boundary conditions, and starting at  $z_i=39$ . The cosmological parameters of the simulation (and the subsequent simulations described below) are  $\{\Omega_{\mathrm{M}}, \Omega_{\Lambda}, h, n, \sigma_8\} = \{0.3, 0.7, 0.7, 0.95, 0.9\}$ . This is somewhat different from the cosmology of the HMF, but we will only use these simulations to assess the link between DM and baryons, and will moreover, unless otherwise stated, factor out the h-dependence from cosmological quantities.

Two of the most massive DM haloes, at z = 0, are selected for re-simulation using the zoom-in technique; they correspond in several aspects to the Virgo and (sub)Coma clusters, with virial masses at z = 0 of about  $3 \times 10^{14}$  and  $1.2 \times 10^{15}$  $M_{\odot}$  and "temperatures" of  $kT \sim 3$  and 6 keV, respectively (see Sommer-Larsen et al. 2005; Romeo et al. 2006 for more detail). For each cluster, all DM particles within the virial radius at z = 0have been traced back to the initial conditions at  $z_i$ . The particles are contained within "virial volumes" having a linear extent of  $20-30 \,h^{-1}$  cMpc, and within these volumes the numerical resolution is increased by 512 times in mass, and eight times in linear resolution. In addition, each higher resolution DM particle is split into an SPH particle and a DM particle — a baryonic fraction  $f_b = m_{SPH}/(m_{DM} + m_{SPH}) = 0.15$  is assumed, in quite good agreement with recent values reported by the WMAP and Planck collaborations.

The mass resolution reached inside the resampled Lagrangian sub-volumes is  $m_{\rm DM} = 2.2 \times 10^8 h^{-1} M_{\odot}$  and  $m_{\rm SPH} = m_{\star} = 3.9 \times 10^7 h^{-1} M_{\odot}$ . Using the code described in Sec. 3.1.1, the evolution of the two virial volumes and the lower-resolution regions around these is then simulated from  $z_i = 39$  to z = 8.8. The gravity softening lengths  $\epsilon$  are kept fixed in comoving coordinates until a redshift of 15, and at later times they are constant in physical coordinates. In the higher-resolution regions, at z < 15,  $\epsilon_{\rm SPH} = \epsilon_{\star} = 0.75 h^{-1} \rm kpc$  and  $\epsilon_{\rm DM} = 1.3 h^{-1} \rm kpc$ .

At z=8.8, 20 galaxies of stellar mass  $M_{\star} \gtrsim 3 \times 10^8 M_{\odot}$ , corresponding to an absolute UV magnitude at 1600 Å of  $M_{\rm UV} \lesssim -20$  (see Fig. 3), are selected from the two simulations. The galaxies are identified in the higher-resolution regions of the two proto-cluster simulations using the algorithm described, e.g., in Sommer-Larsen et al. (2005). For each of the 20 galaxies, the DM particles inside of the virial radius (at z=8.8) are traced back to the initial conditions at  $z_i$  of the two resolution-increased proto-cluster simulations described above. It is found that, in each case, this virial volume is contained within a sphere of radius  $3 h^{-1}$  cMpc. For each galaxy, the numerical resolution in this sphere (which is located within the higher-resolution region of the corresponding proto-cluster initial conditions) is increased (additionally) by 64 times in mass, and four times in

linear resolution. Consequently, the mass resolution reached inside these resampled spheres is  $m_{\rm DM}=3.4\times10^6h^{-1}M_{\odot}$  and  $m_{\rm SPH}=m_{\star}=6.1\times10^5h^{-1}M_{\odot}$ .

The 20 sets of nested, twice resolution-increased initial conditions form the base of the "production" simulations presented in this work. For each of the 20 sets, the code described in Sec. 3.1.1 is used to simulate the evolution of the formation region of a fairly massive galaxy, from  $z_i = 39$  to z = 8.8. For computational reasons, the 20 high-resolution (HR) regions are not evolved at the same time as one simulation, but are rather simulated one-by-one, resulting in a total of 20 production simulations. At z < 15,  $\epsilon_{\rm SPH} = \epsilon_{\star} = 188 h^{-1} \rm pc$  and  $\epsilon_{\rm DM} = 335 h^{-1} \rm pc$ in the HR regions. At z = 8.8, the HR regions reach out to distances of about 150 kpc (physical) from the central galaxies. The virial radii of the central galaxies range from 12–25 kpc, so the HR regions around the galaxies stretch 6–12 times as far as the virial radius. Consequently, other (typically smaller) galaxies are also present in these 20 simulations. Using the galaxy detection algorithm referred to above, a total of about 500 galaxies are identified — most of the analysis presented in this work builds on this sample of simulated galaxies.

In addition to the 20 simulations discussed above, for convergence study purposes, seven of the 20 galaxies were also simulated at eight times higher mass resolution and twice better linear resolution. The initial conditions for these seven simulations were constructed in the same way as described above, except that (for computational purposes) each galaxy was represented by a radius  $1 h^{-1}$  cMpc sphere in the initial conditions (rather than the radius  $3h^{-1}$  cMpc spheres described above), in which the mass resolution is increased by 512 times (rather than the 64× above), and the linear resolution was increased by a factor of eight (rather than the  $4\times$  above). The seven simulations were then run with the code described above, from  $z_i = 39$ to z = 8.8. The mass resolution reached inside these resampled spheres is, consequently,  $m_{\rm DM} = 4.3 \times 10^5 h^{-1} M_{\odot}$  and  $m_{\rm SPH} =$  $m_{\star} = 7.6 \times 10^4 h^{-1} M_{\odot}$ . Moreover, at z < 15,  $\epsilon_{\rm SPH} = \epsilon_{\star} = 94$  and  $\epsilon_{\rm DM} = 167 h^{-1} {\rm pc}$  in the (ultra-)HR regions. At z = 8.8, the HR regions only reach out to a couple of virial radii from the central galaxies, but the simulations can nevertheless be used for some aspects of convergence studies, detailed in App. A.

# 3.2. Ionizing UV radiative transfer

As described above, the hydrosimulations employ an approximate scheme for the RT of ionizing UV radiation. Beginning at  $z_{\rm re}=12$ , a UVB field similar in shape to Haardt & Madau (1996) is assumed to build up, exposing all regions characterised by a Lyman-limit photon mean free path greater than 0.1 kpc fully to the field, while the remaining regions are assumed to be self-shielded. This results in roughly half of the hydrogen in the simulation being ionized at  $z\sim10-11$ , consistent with what is inferred from WMAP polarization maps (Bennett et al. 2013,  $z_{\rm re}=10.6\pm1.0$ ), but  $\sim100$  Myr earlier than the more recent result by Planck Collaboration: et al. (2016,  $z_{\rm re}=8.8^{+1.7}_{-1.4}$ ).

To model the local UV coming from stars in the galaxy, we post-process the snapshots at z=8.8 with a detailed UV RT scheme. The physical properties of the SPH particles are first interpolated onto an adaptively refined grid of base resolution  $128^3$ , with up to 15 additional levels of refinement, such that no cell contains more than one particle. The smallest cells thus have a linear extent  $20 h^{-1} \text{Mpc}/(1 + 8.8)/128/2^{15} = 0.7 \text{ pc}$ . The same adaptive mesh refinement (AMR) is used in the subsequent Ly $\alpha$  RT. At each stellar source in the simulation we start twelve rays covering all  $4\pi$  directions isotropically which are

then split recursively into four rays each to maintain adequate resolution (at least several ray segments per every cell in the volume) as we move further away from the source or enter refined cells. Along these rays, the equlibrium photoionization state of each cell is calculated iteratively taking into account both transfer of stellar UV photons and the above-mentioned UVB. The stellar UV RT is computed separately in the frequency bands [13.6, 24.6] eV, [24.6, 54.4] eV, and [54.4,  $\infty$ ] eV. For details, see Razoumov & Sommer-Larsen (2006, 2007).

#### 3.3. Ly $\alpha$ radiative transfer

#### 3.3.1. Galactic radiative transfer

To conduct the Ly $\alpha$  RT we use the code MoCaLaTA (Laursen et al. 2009a,b). MoCaLaTA is a ray-tracing Monte Carlo code that operates on an AMR grid, so we use the same grid that was constructed for the UV RT. In the following, the characteristics of the code are briefly outlined:

Each cell contains the physical variables important for the RT, which are Ly $\alpha$  and continuum emissivity  $L_{\rm Ly}\alpha$  and  $L_{\rm FUV}$ , gas temperature T, velocity field  ${\bf v}_{\rm bulk}$ , as well as densities  $n_{\rm HI}$  and  $n_{\rm d}$  of neutral hydrogen and dust. Ly $\alpha$  emissivity is calculated as the sum of Ly $\alpha$  photons produced from recombinations following ionization (mainly from hot stars, but also from the UVB field) and cooling radiation, discussed in more detail in the next section.

Individual photons are emitted from a given cell with a probability proportional to the emissivity in that cell, in a random direction, and is followed as it scatters stochastically on the neutral hydrogen out through the ISM, until it either escapes the galaxy or is absorbed by dust. The position and wavelength of the photons are recorded in an IFU-like array along the Cartesian axes, i.e. the galaxy is observed simultaneously from six different directions. This provides a measure of the anisotropic escape of Ly $\alpha$  from the galaxies.

#### 3.3.2. Cooling radiation from cold accretion

As mentioned in the previous section, accretion of gas onto galaxies is expected to give rise to some emission of Ly $\alpha$  photons in addition to the photons resulting from star formation. Exactly how much is a matter of debate, since numerical predictions (e.g. Goerdt et al. 2010; Faucher-Giguere et al. 2010) require accurate knowledge of the thermal state of the gas, which is difficult, and since observations are lacking or indirect (see discussions in Dijkstra 2014 and Prescott et al. 2015). As a (semi-)analytical estimate showing that at least it should not be readily neglected, we can take cooling radiation  $L_{\rm Ly\alpha,cool}$  to be proportional to the gas mass accretion rate  $\dot{M}_{\rm gas}$  and the potential difference  $|\Delta\Phi|$  from the gas begins to accrete till it settles at the core.

Free-falling gas will deposit its released energy in bulk kinetic form. In contrast, gas falling at constant velocity will heat and subsequently cool. Taking the ambient temperature of the halo gas to be equal to the virial temperature and the velocity of gas in the cold streams to be equal to the sound speed implies that the gas falls at a constant velocity roughly equal to the virial velocity. In this case, all the energy released will go into heat, and one proportionality factor will be  $f_{\gamma} \simeq 1$ . This approximation tends to be accurate especially at high redshifts (Goerdt & Ceverino 2015). A more conservative choice might be  $f_{\gamma} = 0.3$  (Dijkstra & Loeb 2009). The amount of radiation emitted as Ly $\alpha$  depends on the temperature of the gas, but as discussed in Fardal et al. (2001), the vast majority of the cool-

ing radiation comes from gas with  $T \sim 10^4$  K, implying that a fraction  $f_{\alpha} \sim 0.5$  is emitted as Ly $\alpha$ .

The gravitational potential will have the form  $f_{\phi}GM_{\rm vir}/r_{\rm vir}$ , where  $f_{\phi}$  is a factor that depends on the exact density profile, e.g.  $\sim 5$  for an NFW profile with a halo concentration of 5 (Binney & Tremaine 2008). For a virial overdensity  $\Delta_c \simeq 200$  and absolute density  $\rho_{\rm crit}(z) \simeq \rho_{\rm M,0}(1+z)^3$  (valid at high z), the virial mass and radius are related as  $r_{\rm vir} = (3/[4\pi\Delta_c\rho_{\rm M,0}])^{1/3}(1+z)^{-1}M_{\rm vir}^{1/3}$ .

The accreted gas sparks star formation, and the star formation rate will thus be SFR =  $\epsilon \dot{M}_{\rm gas}/(1-R+\eta)$ , where the proportionality accounts for the accretion efficiency  $\epsilon=0.5$ –1 (Bouché et al. 2010), gas which is quickly recycled from shortlived stars with a return fraction  $R\sim0.3$ –0.5 (Vincenzo et al. 2016), and gas ejected due to galactic outflows with typical mass loading factors  $\eta=\dot{M}_{\rm out}/{\rm SFR}\sim0.5$ –3 (Schroetter et al. 2015; Heckman et al. 2015). Expressing the accretion rate in this way allows us to compare to the Ly $\alpha$  caused by star formation.

Thus we may write

$$L_{\text{Ly}\alpha,\text{cool}} \sim f_{\gamma} f_{\alpha} |\Delta \Phi| \dot{M}_{\text{gas}}$$

$$\sim f_{\gamma} f_{\alpha} f_{\phi} \frac{G M_{\text{vir}}}{r_{\text{vir}}} \frac{1 - R + \eta}{\epsilon} \text{SFR}$$

$$\sim 0.5 - 2 \times 10^{41} \text{erg s}^{-1} \frac{1 + z}{1 + 8.8} \frac{\text{SFR}}{M_{\odot} \text{yr}^{-1}} \left(\frac{M_{\text{vir}}}{10^{11} M_{\odot}}\right)^{2/3} (6)$$

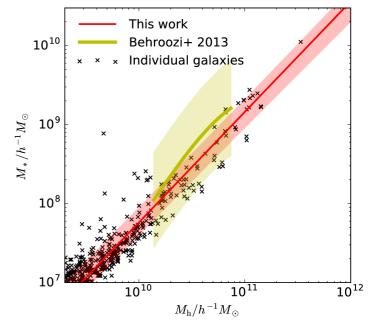
Having expressed the accretion rate in terms of SFR, we can then compare to the Ly $\alpha$  originating from star formation (Kennicutt 1998):

$$L_{\rm Ly\alpha,SF} \sim 10^{42} \frac{\rm SFR}{M_{\odot} \, \rm yr^{-1}} \, {\rm erg \, s^{-1}},$$
 (7)

and see that cooling radiation will account for roughly 10% of the total emitted Ly $\alpha$ , also bearing in mind that in dusty galaxies,  $L_{\rm Ly}\alpha,\rm SF$  will be more susceptible to absorption than  $L_{\rm Ly}\alpha,\rm cool}$ , since the former is produced by stars which tend to inhabit the same regions as the dust, while the latter predominantly is produced farther out in the galaxy. In reality, the mass loading factor decreases somewhat with mass (e.g. Dutton & Van Den Bosch 2009; Hayward et al. 2016; Muratov et al. 2015) such that the dependency on  $M_{\rm vir}$  in Eq. 6 will be shallower for larger masses than the exponent 2/3 suggests. This result is consistent with Faucher-Giguere et al. (2010) who find a fraction of  $\sim 0.18$  at z=8.8 and  $M_{\rm vir}=10^{11}M_{\odot}$  through similar considerations.

# 3.3.3. Intergalactic radiative transfer

Because of the high neutral fraction of the Universe at z=8.8, in general the blue peak of the Ly $\alpha$  emission line is completely suppressed; as light leaves a galaxy, the CGM and the IGM starts "erasing" the spectrum from around the line centre, or even somewhat into the red wing, gradually working its way out through the line towards bluer and bluer wavelengths. As the lines are broadened substantially due to the scattering in the ISM, the necessary distance travelled before the full line is out of resonance with the CGM is longer than our computational box. The often-used approximation of simply removing the blue half of the spectrum is rather imprecise and will underestimate the impact of the IGM at these high redshifts where the density of neutral gas is so high. Even if IGM absorption were not an issue, a neighbouring galaxy at a modest distance can still induce a sizable reduction of both peaks.



**Fig. 1.** Stellar mass  $M_{\star}$  as a function of halo mass  $M_{\rm h}$  for individual galaxies in the hydro-simulation (*black crosses*), and a power law fit (*red*) to this distribution. For comparison, a model of the stellar masshalo mass relation by Behroozi et al. (2013) at z=8.8 is shown in *yellow*. Shaded areas show the 68% CIs.

To achieve a less stochastic description of the observed profiles we use another approach: "Inside" the galaxies, where photons are all the time scattered both into and out of the LOS, we use the accurate RT described in Sec. 3.3.1, but after a certain distance  $r_0$  from the centre, when the probability of being scattered into the LOS can be neglected, we instead multiply the spectrum at that point with the average transmission curve  $F(\lambda) = \langle e^{-\tau(\lambda)} \rangle$ . Here, the average is taken over  $10^3$  sightlines per galaxy in a cosmological volume, and a confidence interval (CI) is defined by the range of F enclosing 68% of the individually calculated transmission functions. To calculate  $F(\lambda)$ , we use the publically available RT code IGMTRANSFER. IGMTRANSFER has previously been used to model the impact of the CGM on Ly $\alpha$  line profiles at lower redshift; Laursen et al. (2011) found that setting  $r_0 \sim 1.5 r_{\rm vir}$  was a reasonable value of the threshold between the full and the approximative RT scheme. At z = 8.8, however, where the large neutral fraction of the IGM gives rise to significant scattering out to large distances from the galaxies, this value will underestimate the transmitted flux considerably. Hence, in this work we calculate the full RT out to  $10r_{\rm vir}$ , which convergence tests reveal to be sufficient.

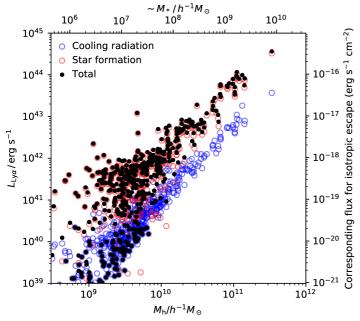
#### 4. Results

#### 4.1. Stellar masses

Figure 1 shows, as a function of halo mass, the stellar mass of the simulated galaxies. Fitting a power law to the distribution for masses above  $10^9 M_{\star}$ , we find that the stellar mass is related to the virial mass roughly as

$$M_{\star} \sim 1.5 \times 10^9 \left(\frac{M_{\rm h}}{10^{11}}\right)^{1.4},$$
 (8)

where masses are measured in  $h^{-1}M_{\odot}$ . Behroozi et al. (2013) present a model of the relation between stellar masses and halo masses which is consistent with observed stellar mass functions,



**Fig. 2.** Total, "intrinsically" emitted Ly $\alpha$   $L_{\text{Ly}\alpha,\text{tot}}$  (black dots), and the contributions from star formation ( $L_{\text{Ly}\alpha,\text{SF}}$ ; blue circles) and cooling radiation ( $L_{\text{Ly}\alpha,\text{cool}}$ ; red circles). The secondary y axis on the right shows the corresponding flux that would be measured at Earth, if the Ly $\alpha$  photons escaped isotropically, and were not absorbed by dust or scattered out of the LOS by neutral hydrogen. As seen in Fig. 8, the actual measured values are quite a lot smaller.

specific SFRs, and cosmic SFRs from z=0–8. Extrapolating the model to z=8.8 (in the  $M_{\rm h}$  range that Behroozi et al. (2013) use for z=8), Fig. 1 shows that our stellar masses are in rough agreement with their model. In the following figures, most quantities are shown as functions of halo mass, because this is what is predicted from the HMF, but a secondary y axis in the top of the plots display an approximate scale for the corresponding stellar mass, based on the relation in Eq. 8.

As discussed in Sec. 3.3, a fraction of the stars emit enough ionizing radiation to give rise to Ly $\alpha$  emission; from the H II regions, assuming a Salpeter (1955) IMF,  $1.1 \times 10^{42} \, \mathrm{erg \ s^{-1}}$  is produced per SFR of  $1 \, M_{\odot} \, \mathrm{yr^{-1}}$  (Kennicutt 1998), while for a Chabrier (2003) IMF the Ly $\alpha$  luminosity is a factor  $\sim 1.8$  times higher, with a modest dependency on stellar mass. In addition to this, accreting gas gets shock-heated, subsequently cooling and emitting Ly $\alpha$ . Figure 2 show the "intrinsically" emitted Ly $\alpha$  — i.e. before any RT effects — for the two processes. For masses up to  $M_{\rm h} \sim 10^{10} h^{-1} M_{\odot}$ , star formation is sufficiently stochastic that cooling radiation can dominate the total (albeit small) luminosity, but at the high-mass end, the contribution is of the order of ten per cent, in accord with our estimate in Sec. 3.3.2.

#### 4.2. UV luminosity function

As discussed in the introduction, the Ly $\alpha$  luminosity is primarily linked to star formation, specifically the massive O and B stars. Since these stars are responsible not only for Ly $\alpha$  but for the bulk of the entire UV spectrum, the Ly $\alpha$  LF and the UV LF are interlinked (see, e.g. Gronke et al. 2015), so comparing the predicted UV LF to observations will support our confidence in the simulations. Because of the small size of our cosmological volume, it cannot be used for determination of the HMF. Instead we use the ST HMF (Eq. 1, calibrated to the Bolshoi simulation) to give us the number density of halo masses, and then translate this to

a LF by using the relation between halo mass and brightness for our simulated galaxies. That is, with halo number density and masses measured in  $h^3 {\rm Mpc}^{-3}$  and  $h^{-1} M_{\odot}$ , respectively, the LF can be written as

$$\frac{\Phi}{\text{Mpc}^{-3} \,\text{mag}^{-1}} = h^3 \ln 10 \, \frac{dN}{d \ln M_h} \left( \frac{dM_{\text{UV}}}{d \log M_h} \right)^{-1}. \tag{9}$$

In the following section, we describe how to obtain the last term in Eq. 9.

# 4.2.1. Relation between halo mass and UV luminosity

Trac et al. (2015) argue for a triple power law relation between the UV luminosity and the halo masses. In terms of magnitudes this may be written

$$M_{\text{UV}} = -2.5 \left[ \log L_0 + a \log \left( \frac{M_{\text{h}}}{M_{\text{h},a}} \right) + (b-a) \log \left( 1 + \frac{M_{\text{h}}}{M_{\text{h},b}} \right) + (c-b) \log \left( 1 + \frac{M_{\text{h}}}{M_{\text{h},c}} \right) \right] + 51.6$$
(10)

where  $L_0$  is an overall amplitude,  $M_{h,a}$ ,  $M_{h,b}$ , and  $M_{h,c}$  are three characteristic mass scales, and a, b, and c are three power law slopes.

To determine the UV magnitudes of the simulated galaxies, each galaxy's UV spectrum is calculated using the stellar population synthesis code STARBURST99 (Leitherer et al. 1999). Subsequently, for each galaxy 10<sup>4</sup> sightlines are followed from the locations of star formation in random directions, with the probability of starting a sightline from a given location proportional to the UV luminosity of stars in that region. Integrating dust extinction along the lines of sight, a distribution of observed UV magnitudes at 1600 Å in different directions is obtained.

Figure 3 shows the halo mass–magnitude relation thus obtained, with the reddened values (red points with error bars) showing the median and the 68% CI enclosed by the 16th and 84th percentiles. Comparing to the *un*reddened values (blue points), effects of reddening are seen to only affect the most massive galaxies, with  $M_{\star} \gtrsim 10^9 h^{-1} M_{\odot}$ .

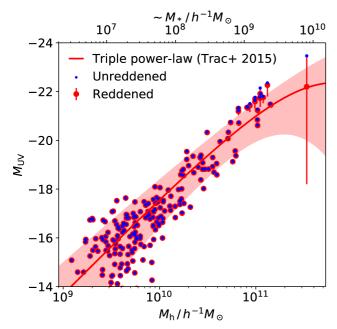
In addition to the simulated  $M_{\rm UV}$  magnitudes, the best fit of the functional form in Eq. 10 with 68% CI is shown in red. At low masses, this CI primarily reflects a scatter in the galaxies' intrinsic luminosities, while at high masses the anisotropic escape of the UV radiation due to dust, as well as the fact that we have so few galaxies more massive than  $\sim 10^{11} M_{\odot}$  comes into play.

#### 4.2.2. Comparing to observations

The derivative of Eq. 10, needed to evaluate Eq. 9, is

$$\frac{dM_{\rm UV}}{d\log M_{\rm h}} = -2.5 \left( a + \frac{(b-a)}{1 + M_{\rm h,b}/M_{\rm h}} + \frac{(c-b)}{1 + M_{\rm h,c}/M_{\rm h}} \right) \eqno(11)$$

The parameters of the fit to  $M_{\rm UV}(M_{\rm h})$  (Eq. 10) can now be plugged into Eq. 11, which in turn enables us to evaluate the UV LF Eq. 9. Due to the small number of galaxies detected at such high redshift, no concensus of a  $z\sim 9$  LF exists, but Bouwens et al. (2015) report a rather well-constrained UV LF at  $z\sim 8$ , as well as a less well-constrained one around  $z\sim 10$  which is improved in Oesch et al. (2017). Figure 4 shows our calculated UV LF, together with the those observations. It is reassuring to see that the z=8.8 LF lies between those of  $z\sim 8$  and  $z\sim 10$ .



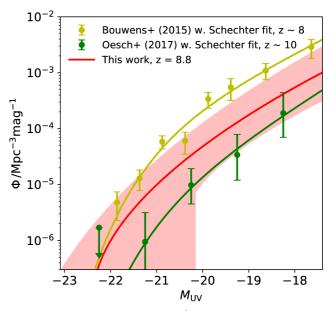
**Fig. 3.** UV magnitude  $M_{\rm UV}$  at 1600 Å as a function of their halo masses  $M_{\rm h}$ . For each galaxy the "intrinsic" UV magnitude calculated with STARBURST99 (*blue dots*) and the reddened magnitudes calculated using the median and 68% CI of the luminosity-weighted extinction along isotropically distributed sightlines from the star (*red dots with errorbars*) are shown. The *red line* shows the best estimate of the analytical relation in Eq. 10, with the *red shaded* region showing the region within which 68% measurements would fall.

# 4.3. Typical line shapes

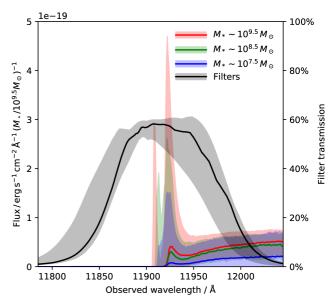
The most prominent feature of a LAE is arguably the emission line profile; much valuable knowledge can be extracted herefrom. Scattering on neutral hydrogen slowly pushes the photons farther from the line centre, so larger column densities are associated with broader emission lines. The same is true for larger temperatures, as the thermal motion of hotter atoms will engender larger Doppler shifts (e.g. Harrington 1973; Neufeld 1990). The relative height of the red and the blue peaks provides a measure of the global kinematics of the galaxy, since blue (red) photons are suppressed by outflowing (infalling) gas, by being Doppler-shifted into the frame of reference of the gas elements (e.g. Dijkstra et al. 2006). At higher redshifts the blue peak is also influenced by the CGM (e.g. Laursen et al. 2011). The longer the photons travel, the more prone they are to dust absorption, so photons emitted in the dense and dusty star-forming regions, which would have to scatter to the wings of the spectrum, escape less easily than photons emitted in the outskirts of the galaxy (e.g. from cooling radiation); hence, dust is expected to narrow the spectrum (Laursen et al. 2009b).

The intertwinement of these effects, however, also makes the interpretation of  $Ly\alpha$  observations notoriously difficult, motivating the need for a more profound theoretical understanding.

Figure 5 shows the average spectra for galaxies in different mass ranges. In the figure, the spectra have been normalized to the same stellar mass, namely  $M_{\star}=10^{9.5}h^{-1}M_{\odot}$ , which is the mass of the most massive mass range. In each mass range a few tens of galaxies have been used, and for each galaxy, the median and the dispersion of six directions, each with 100 different realizations of the impact of the IGM, has been used. While the average spectrum of even the most massive galaxies is virtually erased by the IGM, within  $1\sigma$  many lines do rise above the continuum. Despite the normalization, the lines decrease in

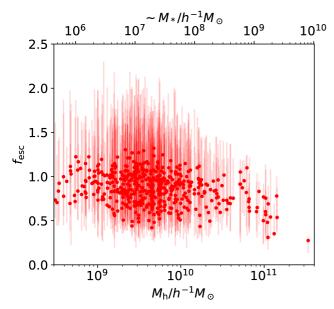


**Fig. 4.** Luminosity function  $\Phi$  at 1600 Å of the simulated galaxies (*red solid*). The *red shaded* region shows the 68% spread in  $\Phi$ , which at the faint end reflects a scatter in the intrinsic UV luminosity, and at the bright end is due mostly to the anisotropic escape of UV radiation due to dust, as well as small-number statistics. *Purple* and *dark yellow* dots with errorbars show the observed LFs at  $z \sim 8$  (Bouwens et al. 2015) and  $z \sim 10$  (Oesch et al. 2017), respectively, with the associated *solid lines* showing the best-fit Schechter (1976)-functions.



**Fig. 5.** Median spectra of galaxies in various halo mass ranges, normalized to the same stellar mass  $(10^{9.5} M_{\odot})$ , and including the impact of the IGM on the line. The shaded areas shows the region in which 68% per cent of the lines fall. Also shown, in *black*, is the median transmission (right *y* axis) of the 16 filters, with the grey region showing the 68% CI. Although the average flux in the line hardly rises above the continuum, prominent lines are seen for a significant fraction of the galaxies.

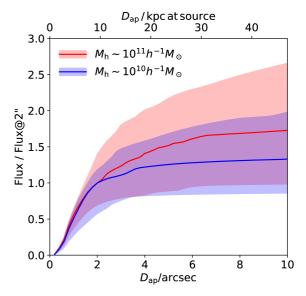
intensity with decreasing stellar mass. While this may in part be attributed to less cooling radiation, the main reason is that more massive galaxies are more likely to ionize larger bubbles around themselves, facilitating the transfer of  $Ly\alpha$ .



**Fig. 6.** Escape fraction  $f_{\rm esc}$  of  ${\rm Ly}\alpha$  as a function of halo mass  $M_{\rm h}$ , defined as the ratio of the number of  ${\rm Ly}\alpha$  photons that make it out through the galaxy to the total number emitted. The points and the error bars denote the median and the 68% CI of the six directions along the Cartesian axes. If there were no dust and galaxies were isotropic,  $f_{\rm esc}$  would be 1. The extent of the error bars is chiefly dictated by the anisotropy of the ISM. Only for galaxies above  $M_{\rm h} \sim 10^{10} h^{-1} M_{\odot}$  does dust play a significant role for the escape fraction. After escaping the galaxy, photons may still be scattered out of the LOS, so the observed  $f_{\rm esc}$  would be (much) smaller than these values.

#### 4.4. Escape fractions

As soon as the first generation of stars end their lives, the ISM is polluted with metals. A fraction of these metals deplete to form dust grains. As galaxies must probably have gone through at least some star formation episodes to make themselves visible, it therefore comes as no surprise that most visible galaxies must also contain some amount of dust. Because of the long path length of Ly $\alpha$  (compared to continuum photons) due to scattering, Ly $\alpha$  is particularly prone to dust absorption<sup>2</sup>. Observationally, it is difficult to distinguish between photons lost to dust and photons scattered out of the LOS by the IGM, but in the simulations this is possible. However, only the most massive galaxies have been able to generate enough dust to give to a measurable colour excess; thus, averaged over all directions the Ly $\alpha$  escape fraction  $f_{\rm esc}$  is close to unity. Nevertheless, the complex density field entails a quite anisotropic escape, where some sightlines are blocked by dense clouds, instead beaming the radiation in other directions. Defining the escape fraction as the ratio of observed Ly $\alpha$  flux to what would be observed if all photons escaped isotropically,  $f_{\rm esc}$  will thus exceed unity in some directions. This is seen in Fig. 6, where also the large spread between different sightlines is noticed.



**Fig. 7.** Measured flux as a function of aperture diameter  $D_{\rm ap}$ , normalized to the flux measured at  $D_{\rm ap}=2''$ , for  $M_{\rm h}\sim 10^{11}M_{\odot}$  (red) and  $M_{\rm h}\sim 10^{10}M_{\odot}$  (blue) galaxies, with the shaded regions giving the 68% confidence interval. For the  $M_{\rm h}\sim 10^{11}M_{\odot}$  galaxies, the observed flux for  $D_{\rm ap}=2''$  is  $\sim 50\%$  compared to  $D_{\rm ap}\to\infty$ , but since a smaller  $D_{\rm ap}$  means less noise, slightly better results are achieved for  $D_{\rm ap}=1''4$ .

#### 4.5. Observed flux

# 4.5.1. Optimal aperture

As discussed in Sec. 3.3.3, scattering in the IGM persists out to many virial radii. Photons travelling in the direction towards the observer are lost from the LOS, but do not vanish; instead they become part of the background. Similarly, photons that leave the galaxy initially in another direction, have a small chance of being scattered towards the observer. This mechanism creates a halo of Ly $\alpha$  light around the galaxy, which has indeed been observed at all redshifts down to  $z \sim 0$  (Hayes et al. 2013; Leclercq et al. 2017).

The half-light radii of our simulated galaxies increase from a few kpc, to roughly 5 kpc, to  $\sim 10$  or even tens of kpc for small, intermediate, and massive halos, respectively. When measuring the total flux received from a galaxy, a larger aperture will always result in more flux, but of course also in more background noise. The standard aperture for measuring flux has a diameter of 2", corresponding at z=8.8 to just under 10 kpc. For the most massive galaxies, which as yet are the only ones we have a chance of detecting, we will hence miss of the order half of flux (see Fig. 7). In fact, due to the increased noise for large apertures, the "optimal" aperture turns out to be a slightly smaller 1"4, although the difference in the total number of observed galaxies is on the < 10% level when comparing to using a 2" aperture.

Sadoun et al. (2016) similarly discuss the fraction of photons that fall outside an aperture of diameter 2" for a strong and a weak ionizing background. For the weak UVB, corresponding to early in the EoR, they predict that the flux should be suppressed by a larger factor of  $\sim 10$ . However, their LAE model is modeled as a smooth gas distribution, which forces photons to scatter to larger distances than in a clumpy medium before being able to escape.

 $<sup>^2</sup>$  Note that, theoretically, it is possible to have the reverse effect, i.e. to have a dusty, multiphase ISM that preferentially lets Ly $\alpha$  escape (Neufeld 1991; Hansen & Peng Oh 2006). However, as was shown by Laursen et al. (2013) and Duval et al. (2014) this requires physically unrealistic scenarios; in particular an almost vanishing velocity field together with (super-)Solar metallicities and very high density contrasts between the phases.

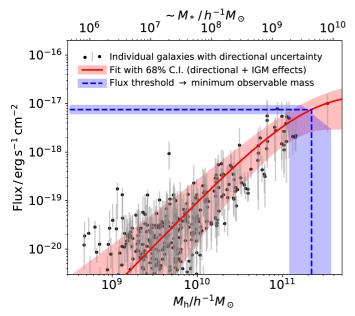


Fig. 8. Flux F measured inside a 1".4 circular aperture (black dots) with errors given by the 68% CI of the six directions of observation, as a function of halo mass  $M_h$ . Additional to this "intrinsic" variation, the inhomogeneous IGM, as well as the fact that galaxies of similar masses exhibit a variety in physical properties, introduces a scatter in possible values of observed flux; the 68% CI of this scatter is represented by the red, shaded region, while the solid, red line is the double power law given in Eq. 12. The dashed, blue line shows how the flux threshold of the detectors results in a minimum, observable halo mass  $M_{h,min}$ , and the shaded, blue region shows how the spread in detector thresholds, combined with the spread in fluxes, results in a spread in  $M_{h,min}$ .

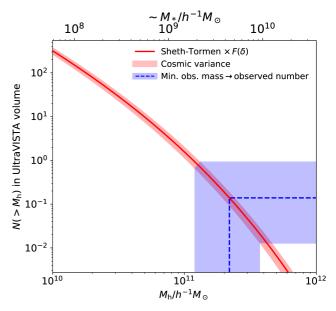
#### 4.6. Translating flux threshold to minimum observable mass

Figure 8 shows the expected observed flux F measured within a 1"4 circular aperture centered on the brightest pixel for the simulated galaxies as a function of their halo mass. Viewing the galaxies from different directions introduce a large scatter in the observed flux, both due to the anisotropy of the galaxies, and due to the inhomogeneous IGM. The scattered points show the median observed flux (i.e. of the radiation that makes it through both ISM and IGM), while the error bars show the 68% CI in the flux introduced by the anisotropic ISM alone. Assuming a power law-like relation between F and  $M_h$  (which ought to be suitable at least over a limited mass range), but with a turnover at high masses where dust and possibly a more compact ISM makes Ly $\alpha$  escape harder (see Laursen et al. 2009b), a double power law given by

$$\frac{F(M_{\rm h})}{\text{erg s}^{-1} \text{ cm}^{-2} \text{ Å}^{-1}} = 10^{-19} \left(\frac{M_{\rm h}}{10^{10}}\right)^{1.8} \left(1 + \frac{M_{\rm h}}{3 \times 10^{11}}\right)^{-2.3}$$
(12)

with masses, again, measured in  $h^{-1}M_{\odot}$  is seen to be a good fit to the data in the relevant range (the negative exponent in the last term probably makes this functional form impractical at higher masses). The red, shaded region captures the 68% CI from both the anisotropic escape, the inhomogeneous IGM, and the spread in flux from galaxies of similar masses; that is, it shows the most probable region that a new measurement would fall.

The 16 detectors of UltraVISTA have a varying threshold for detecting sources at a given significance, and even have variations in different regions of the detectors. For a  $5\sigma$  detection and an aperture of 1".4, they have an average threshold of  $m_{\text{AB,thres}} = 25.25 \pm 0.24$ , corresponding to a flux threshold of



**Fig. 9.** Cumulative halo mass function (*solid red*), normalized to the approximate volume surveyed by UltraVISTA. The *red-shaded* region represent the  $1\sigma$  standard deviation on the number counts resulting from cosmic variance. The *dashed blue* line shows the minimum observable halo mass (Eq. 13) in the UltraVISTA survey and the corresponding number of observed galaxies. The *blue-shaded* region shows the 68% confidence interval for this.

 $F_{\rm thres} = (7.5^{+1.5}_{-1.9}) \times 10^{-18} \, {\rm erg \ s^{-1} \ cm^{-2}}$ , shown in Fig. 8 as the horizontal, blue, dashed line with the shaded region marking the spread. These values are as measured in a 1".4 aperture, and do not include an aperture correction, since we measure the flux in our simulated images using this aperture.

The first thing to notice is that indeed some of the simulated galaxies make it above the flux threshold, at least in certain directions — the question is whether such galaxies are sufficiently common that there is a significant probability that UltraVISTA will detect them. Assuming the relation Eq. 12 to hold true, this flux threshold can be translated into a *minimum observable halo mass* 

$$M_{\rm h,min} = (2.2^{+1.5}_{-1.0}) \times 10^{11} h^{-1} M_{\odot},$$
 (13)

seen in Fig. 8 as the vertical, blue, dashed line. This corresponds roughly to a minimum observable *stellar* mass of  $M_{\star, \text{min}} = (5^{+5}_{-3}) \times 10^9 h^{-1} M_{\odot}$ .

# 4.7. Translating minimum observable halo mass to expected number of observed galaxies

Integrating the HMF from a given mass scale M' to infinity, the total number of haloes at least as massive as M' is found. Figure 9 shows the resulting *cumulative halo mass function* in the volume surveyed by UltraVISTA.

#### 4.7.1. Cosmic variance

Density fluctuations in the large-scale structure lead to uncertainties in the number counts, known as *cosmic variance*. The expected standard deviation due to this effect is shaded red in Fig. 9. This uncertainty is obtained following Trenti & Stiavelli (2008), who estimate the cosmic variance employing a combination of excursion set theory (Bond et al. 1991) and *N*-body

simulations. We have made use of the associated online calculator³ which allows for a Sheth & Tormen (1999) bias instead of a Press & Schechter (1974) bias, as well as changing the value of  $\sigma_8$  to our preferred value of 0.82. All their simulations have  $\{\Omega_{\rm M},\Omega_{\Lambda}\}=\{0.26,0.74\},$  rather close to the  $\{0.27,0.73\}$  of the Bolshoi simulation. Taking into account cosmic variance results in a relative uncertainty on the number of galaxies increasing from 17% at  $M_{\rm h}=10^{10}h^{-1}M_{\odot}$  to 48% at  $M_{\rm h}=10^{12}h^{-1}M_{\odot}$ .

The vertical blue dashed line shows the minimum observable halo mass  $M_{\rm h,min}$ , discussed in the previous section, and the horizontal line shows the corresponding number of galaxies that will be observed. When the 68% CI of the  $M_{\rm h,min}$ , shown as the blue-shaded region, is combined with the cosmic variance, the resulting expectation value of the number of observed galaxies is  $N(M_{\rm h} \geq M_{\rm h,min}) = 0.12^{+0.79}_{-0.11}$ .

#### 4.7.2. Poisson noise

In addition to cosmic variance, there will be an uncertainty from usual Poisson noise. For large values of N, the Poisson noise converges towards  $\sqrt{N}$ , but for small values this approximation becomes increasingly inaccurate, as the 68% CI becomes increasingly asymmetric<sup>4</sup>.

Since the number of galaxies is an integer, it makes little sense to quote a number such as the one found in the previous section; instead it is more illuminating to find the probability of detecting a given integer number. From the standard definition of the Poisson distribution, we can then finally state the disheartening probabilities of observing 0, 1, or 2 or more galaxies as

$$P(0) = 88^{+11}_{-45}\%,$$

$$P(1) = 11^{+25}_{-10}\%,$$

$$P(2+) = 1^{+14}_{-1}\%.$$
(14)

#### 4.8. Luminosity function

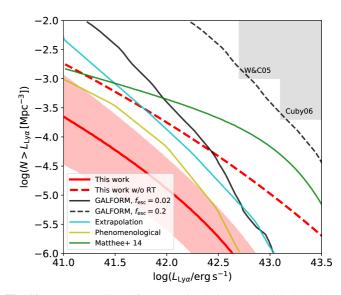
Following the same approach as in Sec. 4.2, a Ly $\alpha$  LF can be constructed. This is seen in Fig. 10, where we also compare to the models presented in Nilsson et al. (2007) and Matthee et al. (2014); the latter is the most optimistic LF allowed by the limits of their survey. Our LF lies well below all models, but is less steep at the bright end, compared to the closest models.

Figure 10 also shows how the predicted Ly $\alpha$  LF would look if we did not take into account Ly $\alpha$  RT. At the bright end, this differs from the correct LF by almost two orders of magnitude, highlighting the crucial role of a proper RT treatment.

# 5. Discussion

#### Colour selection — differing impact of the IGM on narrowband and broadband

In Sec. 4.7 we predicted that the probability of detecting just one, or two or more, galaxies in the UltraVISTA survey is of the order of 10% and 1%, respectively. But even if a galaxy is brighter than the detection threshold, it still needs to be selected as a narrowband excess object, i.e. to have a higher flux density in a narrowband than in a broadband in the same wavelength region, in this case the J band.



**Fig. 10.** Ly $\alpha$  LF predicted from our simulations (red with shaded area showing the 68% CI), compared to the three models of Nilsson et al. (2007, described in Sec. 1.1). Also shown, with the red, dashed line, is the Ly $\alpha$  LF predicted from our simulations if we did not take into account RT effects. Additionally, the "optimistic" LF of Matthee et al. (2014) is shown in green. The grey region marks observational upper limits from Willis & Courbin (2005) and Cuby et al. (2007).

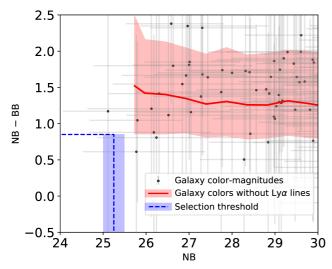
If there were no emission line, a flat spectrum would have NB – BB = 0, where NB is the magnitude in the Ly\$\alpha\$ narrowband filter, and BB is the \$J\$ band magnitude. However, at such high redshifts where the IGM suppresses not only the blue half of the Ly\$\alpha\$ line, but also a significant part of the red half, the NB and the BB are affected differently. The reason is that the NBs are centered on the line, so that (less than) 50% of the flux is transmitted, whereas in the \$J\$ band — which transmits in \$\lambda \sim [11 650–13 500] \text{ Å}\$ the Ly\$\alpha\$ break is located quite far to the blue, so that roughly 85% is transmitted. For 50% transmission in the NB, a flat spectrum with no emission line would have a zeropoint of NB – BB = -2.5 log(50/85) \preceq 0.6. In reality, the NB transmission is closer to 25%, in which case the zeropoint lies at \$\sim 1.3\$. In these calculations, the Ly\$\alpha\$ line centers have been assumed to coincide with the NB center.

Figure 11 shows a colour-magnitude diagram of the simulated galaxies. The error bars correspond to different LOSs. To calculate a more realistic zeropoint, the colours and magnitudes are also calculated in the hypothetical case where the galaxies have no Ly $\alpha$  emission lines. In this case, the scatter is much smaller and is caused mainly by IGM inhomogeneities in the IGM. A running median (with 16th and 84th percentiles) of the galaxies' colours in this case is shown in the figure in red. The median colour is seen to be rather independent of NB magnitude, with a value around NB – BB  $\simeq 1.25$ , except for the brightest galaxies where dust begins to play a role; here the reddening causes a slight upturn in the colour index. The lower limit of the 68% CI lies around NB – BB  $\simeq +0.85$ . Using this value as the colour threshold, together with the magnitude limit of the individual detectors, a "selection square" is defined, shown with blue, dashed lines in Fig. 11 (the blue-shaded region shows the spread in the detector limits).

Considering only the median colours and magnitudes of the galaxies, not even the brightest ones fall inside the selection square. However, taking into account the variability in brightness in different directions, the brightest ones do in fact have a non-zero probability  $P_{\rm sel}$  of being selected as LAEs. The bright-

<sup>3</sup> casa.colorado.edu/~trenti/CosmicVariance.html.

 $<sup>^4</sup>$  For instance, the Poisson uncertainty on the numbers 100 and 10, is not 10 and 3.16 as one might naively expect, but  $^{+11.0}_{-9.98}$  and  $^{+4.27}_{-3.11}$ , respectively (Gehrels 1986).



**Fig. 11.** Colour-magnitude diagram of the simulated galaxies. *Black dots* show individual galaxies, with *grey* error bars showing the 68% CI for different sightlines. The *red* line shows a running median (with shaded 68% CI) of the NB – BB colour as a function of NB magnitude for all galaxies in the hypothetical case where they would have no  $Ly\alpha$  emission lines. The selection criteria are shown with *blue dashed* lines; the magnitude threshold is the same as in 4.6, while the colour threshold is set to NB – BB < +0.85, corresponding roughly to the lower limit of the "no  $Ly\alpha$ ". Although no galaxy on average falls inside the selection square, the directional variance results in a probability of a few tens of % of being selected, albeit only for the brightest galaxies.

est galaxy in the sample, which is also the most massive with  $M_{\rm h}=3.4\times 10^{11}h^{-1}M_{\odot}$ , has a 35% chance of being selected, i.e. to meet the colour selection criterion *and* being brighter than the detection limit of the survey. There is no clear trend of  $P_{\rm sel}$  with halo mass, but for  $M_{\rm h}\gtrsim 10^{11}h^{-1}M_{\odot}$ ,  $P_{\rm sel}$  lies between a few % and 35%, while for  $M_{\rm h}\lesssim 10^{11}h^{-1}M_{\odot}$ ,  $P_{\rm sel}$  is virtually zero.

#### 5.2. Halo mass function and cosmology

The HMF was, and typically is, calculated considering dark matter only. Although baryons make up only  $\sim 1/6$  of the total mass, their ability to cool and condense leads to more concentrated mass profiles, resulting in principle in higher halo masses. Thus, Stanek et al. (2009) and Cui et al. (2012) find an increased number density of cluster scale haloes in simulations including gas cooling and star formation. However, also taking into account the effect of AGN feedback prevents overcooling of the gas, counteracting this concentration. Martizzi et al. (2014) find that, incidentally, the resulting mass function is quite close to the DM-only HMF. We therefore choose to ignore baryonic effects on the HMF.

Of greater concern might be the functional form of the multiplicity function  $f(\sigma)$  (Eq. 4). Both the PS and the ST HMFs are "universal", in the sense that their multiplicity functions are independent of power spectrum and expansion history of the Universe. Several successive authors have noted departures from universality (e.g. Tinker et al. 2008; Crocce et al. 2010; Watson et al. 2013). Tinker et al. (2008) let the parameters of  $f(\sigma)$  be a function of redshift, and in the BolshoiP simulation (an "updated" version of the Bolshoi simulation with Planck Collaboration: et al. (2016) cosmology), Klypin et al. (2016) showed that this HMF fitted their halo abundances well, albeit only in the range 0 < z < 2.5.

Behroozi et al. (2013) extended the Tinker et al. (2008) HMF to z=8, although only for masses up to  $M_{\rm h}\sim 10^{11.5}h^{-1}M_{\odot}$ , which is lower than the upper limit for the minimum detectable mass in UltraVISTA. However, Rodríguez-Puebla et al. (2016) provide a fitting formula for a HMF that gives good fits to the BolshoiP simulation at higher masses. Extending that fit to z=8.8 increases the number density of haloes with masses around the minimum detectable halo mass in by a factor of five from the  $0.12^{+0.79}_{-0.11}$  found in Sec. 4.7.1 to  $N(\geq M_{\rm h})=0.6^{+4.2}_{-0.6}$  or, in terms of probabilities of detecting an integer number of galaxies,  $\{P(0),P(1),P(2+)\}=\{55^{+42}_{-54},33^{+29}_{-29},12^{+21}_{-2}\}\%$ . That is, although this still implies that a non-detection is the most likely outcome, the prospects of finding a few are less dire.

#### 5.3. Field galaxies vs. cluster galaxies

The fact that the galaxies are taken from a proto-cluster region might be a concern, since they could evolve differently from a "typical" galaxy. However, although cluster galaxies form earlier, and peak earlier in star formation, than field galaxies, the two have comparable specific SFRs (Muldrew et al. 2017). Since our model assigns a brightness to a galaxy based on its mass, but the mass distribution itself is taken from the HMF which is unrelated to the simulated galaxies, we do not consider this to be an issue.

#### 5.4. Ionization state of the IGM

The largest uncertainty in our forecast is arguably the ionization state of the IGM. Although the UV RT is treated accurately, it hinges on the assumed evolution of the UVB field. The global neutral fraction in our hydro-simulation is  $x_{\rm HI} \simeq 0.13$ , but in the IGM the fraction is much lower, of the order  $10^{-4}$  to  $10^{-3}$ . This is still enough to erase the blue part of the Ly $\alpha$  line, and the CGM and residual neutral clumps cause the damping wing to erase a large part of the red wing as well.

Even if we have overestimated the impact of the CGM/IGM, it is hard to imagine that even a small fraction of the blue wing escape; although some galaxies are surrounded by highly ionized bubbles, galaxy and quasar spectra show complete Gunn-Peterson troughs (e.g. Fan et al. (2005); see however Hu et al. (2016) and Matthee et al. (2018) for a counterexample at z=6.6) If we redo our analysis simply removing the blue half of the spectrum — thus neglecting the effect of the damping wing — the expected number of detected LAEs increases to  $1.0^{+2.9}_{-1.0}$ . Only if we completely neglect the IGM do we predict a large success rate, with  $N=4.5^{+10.8}_{-4.1}$ .

#### 5.5. Starburst-driven outflows

When massive stars explode as supernovae, they heat up the ISM, causing it to expand and form bubbles. If the SN explosion rate is sufficiently high, the SN remnants overlap before they can cool radiatively, in which case these bubbles — assisted by super-Eddington photon pressure — may extend beyond galactic scales, manifesting themselves as outflowing superwinds (see e.g. Powell et al. 2011, and references therein).

Such winds have been observed at lower redshifts, mainly through blueshifted absorption lines (e.g. Kunth et al. 1998; Pettini et al. 2001; Shapley et al. 2003), and are usually thought to be the explanation for the often-observed asymmetric Ly $\alpha$  line profiles (e.g. Verhamme et al. 2006; Tapken et al. 2007;

Yamada et al. 2012), where the red peak is enhanced with respect to the blue. One of the largest uncertainties in hydrosimulations in general is arguably how the feedback from stellar energy output affects the surrounding gas. Although many cosmological simulations have employed various implementations of feedback that are able to generate outflows, when it comes to Ly $\alpha$  RT in general the predicted line profiles tend to be rather symmetric or even have an increased *blue* peak (e.g. Laursen et al. 2009a; Barnes et al. 2011; Yajima et al. 2012). That is, despite gas being ejected from the galaxies, infalling gas accreting onto the galaxies dominate the kinematics, leading to the opposite effect. Only in simulations of isolated disc galaxies has a prominent red peak been successfully reproduced, and only when observed face-on where the wind is strongest (Verhamme et al. 2012).

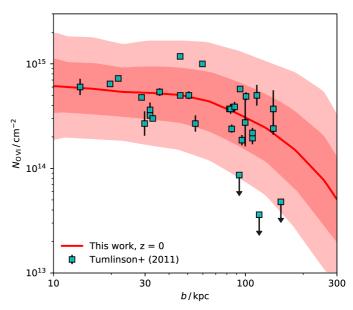
Observations based primarily on O vI absorption lines indicate that the CGM around star-forming galaxies at  $z\sim0$  contains considerable amounts of oxygen (e.g. Tumlinson et al. 2011; Prochaska et al. 2011). Also lower-ionization species such as Si II, Si III, and N II are detected (e.g. Prochaska et al. 2017, and references therein). Based on observations of potential O vII absorption in the hot CGM of the Milky Way, Gupta et al. (2012) infer the presence of large amounts of oxygen in the CGM as well (see however Wang & Yao 2012).

Computer simulations indicate that models based on inefficient stellar feedback ("low"-feedback models) cannot reproduce the level of O vi column densities observed in the CGM to impact parameters of 150–200 kpc (e.g. Stinson et al. 2012, 2013; Hummels et al. 2013). The simulations presented in this work were stopped at z=8.8, but in another project (Sommer-Larsen & Laursen 2018, in prep.), the same code was used to simulate the formation and evolution of eight field disk galaxies to z=0 in a cosmological context using the zoom-in technique. At z=0, the galaxy luminosities, stellar masses, and specific SFRs span the ranges  $L\sim0.2-0.6$   $L^\star$ ,  $M_\star\sim3-6\times10^{10}M_\odot$ , and sSFR  $\sim0.04-0.1$  Gyr $^{-1}$ , respectively.

For each of the eight galaxies, 6800 LOSs are shot through the galaxy in random directions and with impact parameters bspanning the range b = 2-500 kpc. Along each LOS the total O vi column density  $N_{\text{OVI}}$  is determined. Averaging over the eight galaxies, Fig. 12 shows the median  $N_{OVI}$  as a function of impact parameter b, compared to the observational data from Tumlinson et al. (2011) for "star-forming" galaxies (sSFR  $\gtrsim 0.01 \, {\rm Gyr}^{-1}$ ) of luminosities in the range  $L \sim 0.1$ –1  $L^{\star}$ . As can be seen from the figure, the match between simulations and observations is quite acceptable, indicating that the simulations capture at least these outflow properties correctly — see also Sommer-Larsen & Fynbo (2017) for the case of the high-impact parameter and high-metallicity DLA towards Q0918+1636, at z = 2.58; this system is very well reproduced by simulations based on a code similar to the one utilized in this work, and it is shown that by far the majority of the  $\alpha$ -element absorption seen in this system at galacto-centric distances  $\gtrsim 20-30$  kpc is caused by metals that have been produced in the inner part of the galaxy, and subsequently transported outwards by galactic winds.

#### 6. Summary and conclusions

We have explored numerically the prospects of detecting Ly $\alpha$ -emitting galaxies on the verge of the Epoch of Reionization. To ensure both good number statistics and high resolution, we employed a combination of a semi-analytical halo mass funtion matched to a large-scale N-body simulations and zoom-in simulations of hydrodynamical, cosmological simulations. This was



**Fig. 12.** Median O vi column density  $N_{\rm OVI}$  (red) as a function of impact parameter b, averaged over LOSs through eight z=0 disk galaxies simulated using the same code as the one utilized in this work. Shaded region indicate the  $1\sigma$  and  $2\sigma$  deviations from the median, respectively. The observations of "star-forming" galaxies by Tumlinson et al. (2011) are shown by cyan squares.

combined with accurate RT schemes of both ionizing UV and  $\text{Ly}\alpha$ .

Physical uncertainties such as variance in the escape of  $Ly\alpha$  in different directions — both out through the ISM of the galaxies and further through the IGM — galaxy-to-galaxy variation, and statistical number variance, as well as observational uncertainties such as differing filter shapes and varying detector exposure, were taken into account. In general, such uncertainties are asymmetrical, and a numerical scheme for adding asymmetrical errors is described (in App. B) and made public.

With these simulations we have been able to predict a number of physical characteristics of galaxies at redshift z=8.8. Our stellar mass—halo mass relation is consistent with the observationally based model by Behroozi et al. (2013), extrapolated to z=8.8. At the investigated redshift the Ly $\alpha$  LF is largely unconstrained, but the predicted UV LF is shown to be consistent with observations. Predicting Ly $\alpha$  LFs at lower redshifts where observations are less sparse is beyond the scope of this work, but will be addressed in future work based on the simulation code presented here and in Sommer-Larsen & Fynbo (2017).

Our main findings — that all apply to z = 8.8 — are:

- Scattering in the CGM prevents Lyα from escaping a galaxy until large distance from its emission site. This results in of the order of half of the flux falling outside standard apertures. However, since larger apertures also implies more noise, it does not help to enlarge it, and in fact we find that, for the UltraVISTA, an aperture of 1".4 results in a slightly larger probability of detecting a galaxy.
- Scattering in the IGM erases completely the blue part of the spectrum, and a large fraction (~ 25%) of the red half. This means that, on average, the Lyα line is suppressed to continuum level.
- The escape of  $Ly\alpha$  is, however, very dependent on the direction from which a galaxy is observed. Both the anisotropy of the ISM, and inhomogeneities in the transmittance of the IGM, results in the spectra exhibiting prominent peaks in a

- significant fraction of directions, enabling us to see them in some cases (see Fig. 5).
- Accurate treatment of the Ly $\alpha$  RT and the halo number statistics enables of to predict the expected number of LAEs in the UltraVISTA survey; the probabilities of detecting 1, 2, or two or more LAEs are roughly 90%, 10%, and 1%, respectively (see Eq. 14).
- Since the Ly $\alpha$  break lies far to the blue in the J broadband filter, and since the damping wing of the IGM absorption extends far into the red wing of Ly $\alpha$ , the IGM suppresses a much smaller fraction in BB than in the NB. Thus, a colour selection criterion of NB BB  $\lesssim 0$  will miss many possible LAEs. Simulating the colours of our galaxies without the Ly $\alpha$  emission lines, we show that the lower  $1\sigma$  limit lies approximately at NB BB = +0.85, which we argue is a better criterion
- Using that criterion, we find that even if a galaxy is detectable in the NB, its has only ≤ 35% chance of being selected as a LAE.
- We investigated what might lead to a larger probability of success. Using a Planck cosmology rather than a WMAP7 increases the predicted number of detections from  $\sim 0.12$  to  $\sim 0.61$ . Assuming an unrealistically less aggressive IGM (simply removing the blue wing of the Ly $\alpha$  line) further increase the expected number to 1, while neglecting the IGM altogether would result in a handful of detections.

On the whole, while the UltraVISTA (broadband) survey has already resulted more than 100 papers directly using the data<sup>5</sup> and many more papers using the data via the photometric, photoz and stellar mass catalogues (Ilbert et al. 2013; Muzzin et al. 2013; Laigle et al. 2016), the hunt for LAEs seems unprofitable.

According to our simulations, increasing the probable number of detections to 1 (2) would require roughly another 500 (1000) hours of observations with UltraVISTA. However, as the analysis is still in progress, and as our simulations show that galaxies sufficiently bright for being detected with UltraVISTA do indeed exist, hoping is still allowed.

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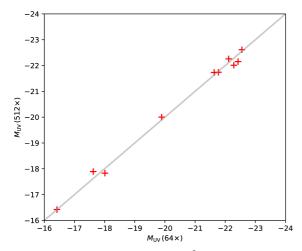
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**Fig. A.1.** Absolute UV magnitudes at 1600 Å  $M_{\rm UV}$  for the very high-res simulations (512×) vs. production runs (64×). No dust-correction has been performed. To guide the eye, the *grey* line shows a unit slope.

# Appendix A: Convergence studies

As described in Sec. 3.1.2, for convergence study purposes, seven simulations were carried out at eight times higher mass resolution and twice better linear resolution than the production simulations described and utilized in this work. Unfortunately, the HR regions for these simulations turned out to be too small to robustly carry out  $\text{Ly}\alpha$  RT, which by nature is non-local. Nevertheless, other properties of the galaxies formed can be compared to the results of the production runs.

Figure A.1 shows the absolute, dust-uncorrected 1600 Å AB magnitudes  $M_{\rm UV}$  for ten galaxies at 512× vs. 64× resolution. As can be seen from the figure, the correspondence between the 512× and 64× magnitudes is quite good, with differences being  $\lesssim 0.2$  mag.

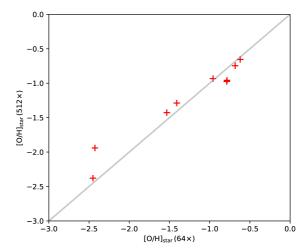
Figure A.2 shows the median stellar metallicity [O/H] for nine of the galaxies at  $512\times$  vs.  $64\times$  resolution. For eight of the galaxies, there is reasonable agreement between  $512\times$  and  $64\times$  values, with differences being  $\lesssim 0.2$  dex. For the ninth galaxy, the difference is somewhat larger,  $\sim 0.5$  dex. This galaxy is small, however, with the  $64\times$  version consisting of 69 star particles, so stochastic effects are significant.

These results indicate that convergence has been successfully achieved.

#### Appendix B: Adding asymmetric uncertainties

On several occasions during this work, it was necessary to add numbers with uncertainties, or errors, not governed by Gaussian probability density functions (PDFs). That is, numbers that are written not as  $\mathbf{X} = x_0 \pm \sigma$ , but as  $\mathbf{X} = x_0^{+\sigma_+}$ , where  $x_0$  is the central value, and  $\sigma_-$  and  $\sigma_+$  are the lower and upper error, respectively. If the full PDFs are known, the result  $\mathbf{X}+\mathbf{Y}$  can simply be obtained by convolution or Monte Carlo sampling. In many cases, however, they are not. When only the set  $\{x_0, \sigma_-, \sigma_+\}$  is known, there cannot be a unique solution, since infinitely many PDFs can be described by the same three numbers.

A widespread approach to this problem is to let the sum of two such numbers be equal to the sum of the central values, with the errors given by the upper and lower errors added in quadra-



**Fig. A.2.** Median stellar metallicity [O/H] for nine galaxies: very high-resolution simulations  $(512\times)$  vs. production runs  $(64\times)$ . To guide the eye, the *grey* line shows a unit slope.

ture separately. That is, to set

$$\mathbf{X} + \mathbf{Y} \equiv x_{0-\sigma_{x-}}^{+\sigma_{x+}} + y_{0-\sigma_{y-}}^{+\sigma_{y+}}$$

$$= (x_0 + y_0)_{+\sqrt{\sigma_{x-}^2 + \sigma_{y-}^2}}^{-\sqrt{\sigma_{x+}^2 + \sigma_{y-}^2}} \quad \text{(wrong!)}$$
(B.1)

This procedure has no statistical justification. That it must be wrong can be seen from considering the central limit theorem: In the limit of many distributions of the same asymmetry, the combined PDF should approach a Gaussian. In contrast, errors added according to Eq. B.1 never decrease in asymmetry.

Part of the confusion arises from the ambiguity in what represents "the central value". A common interpretation is the most probable value of the distribution, i.e. the mode. An unwary scientist may then think that mode[X + Y] = mode[X] + mode[Y]. But if X and Y are both skewed in the same direction, say towards negative values such that  $\sigma_{-} > \sigma_{+}$ , the mode will be skewed in the same direction. If  $x_0$  represents the mean  $\mu$ , the combined mean will be the sum of the two means, but errors added in quadrature will be even more off. We argue that, for asymmetric errors, a more natural estimator of the central value is the median, and a natural estimator of a CI is the 68% range that is given by the 16th and 84th percentiles. In this case there is equal probability that a number drawn from the PDF lies above and below the central value and, more importantly, one can be sure that the central value lies between the lower and the upper values, which is not necessarily the case for the mode and the mean when dealing with asymmetric PDFs.

A further argument for using the {50, 16, 84} percentiles is that — in contrast to other estimators — they do not care whether the variable in question in linearly or logarithmically distributed (for instance, the median of an ensemble of measured fluxes picks out the same data point as the median of the magnitudes).

A statistical error on x can be thought of as deriving from a nuisance parameter a. If a itself has an uncertainty  $\sigma_a$ , then in the "normal", linear case that uncertainty propagates to x as  $\sigma_x^2 = (dx/da)^2 \sigma_a^2$ . Asymmetric errors arise when the relationship between  $\sigma_x$  and  $\sigma_a$  is non-linear. As mentioned above, if the full PDFs of  $\mathbf{X}$  and  $\mathbf{Y}$  are not known, there is no "correct" solution to the problem. Nevertheless, as will be described in the following it is possible to construct a method that is a significant improvement over the (standard) quadrature adding. This method is simply a numerical implementation of

the technique described by Barlow (2003). A Python function capable of performing such additions can be downloaded from github.com/githyankipela/add\_asym.

#### Appendix B.1: Piecewise linear error propagation

In the simplest non-linear approach, propagating the uncertainty from a to x knowing only the set  $\{x_0, \sigma_-, \sigma_+\}$  can be achieved assuming a piecewise linear dependency. A similar method using a quadratic relationship (not to be confused with "addition of errors in quadrature") has also been implemented in the public code. There is no a priori reason to favor on over the other; the piecewise linear transformation has an unphysical kink, while the quadratic one has a turnover somewhere outside of the 68% CI, but their results are comparable nonetheless (and both much better than the "standard" method).

First, the nuisance parameter a is transformed to a variable u given by a unit Gaussian, while as the dependent variable we will consider X(u) = x(u) - x(0). The function propagating the PDF of the nuisance parameter is then

$$X = \begin{cases} \sigma_{-}u & \text{for } u \leq 0 \\ \sigma_{+}u & \text{for } u \geq 0. \end{cases}$$
 (B.2)

A consequence of this transformation is that the expectation value, or the average, of *X* no longer is equal to the most likely value, but instead given by:

$$\langle X \rangle = \mu = \int_{-\infty}^{0} du \, \sigma_{-} u \frac{e^{-u^{2}/2}}{\sqrt{2\pi}} + \int_{0}^{+\infty} du \, \sigma_{+} u \frac{e^{-u^{2}/2}}{\sqrt{2\pi}}$$
$$= \frac{1}{\sqrt{2\pi}} (\sigma_{+} - \sigma_{-}). \tag{B.3}$$

Thus, if X(u) is a non-linear function of u, its expectation  $\langle X \rangle$  is not  $X(\langle u \rangle)$ , and if X(0) is quoted as the central value, it is not the mean. It will still be the median, though, and could as such still be quoted as the central value. The error propagation is illustrated in Fig. B.1.

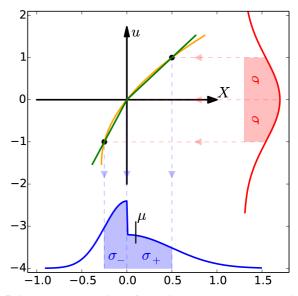
With this transformation we obtain PDFs corresponding to the three-number set, which can then be convolved with the PDF of another three-number set. But convolving two non-Gaussians does not necessarily result in a PDF of the same form as the original functions, as is the case for Gaussians. However, even though the form is not preserved, some things are; the Thiele semi-invariant cumulants (Thiele 1889) still add under convolution. The first three of these are the usual mean (Eq. B.3), the variance

$$V = \frac{1}{2}(\sigma_{-}^{2} + \sigma_{+}^{2}) - \frac{1}{\sqrt{2\pi}}(\sigma_{+} - \sigma_{-}), \tag{B.4}$$

and the unnormalized skewness

$$\gamma = \langle x^{3} \rangle - 3 \langle x \rangle \langle x^{2} \rangle + 2 \langle x \rangle^{3} 
= \frac{1}{\sqrt{2\pi}} \left[ 2(\sigma_{+}^{3} - \sigma_{-}^{3}) - \frac{3}{2}(\sigma_{+} - \sigma_{-})(\sigma_{+}^{2} + \sigma_{-}^{2}) \right. 
\left. + \frac{1}{\pi} (\sigma_{+} - \sigma_{-})^{3} \right].$$
(B.5)

Now the problem of adding n PDFs has been reformulated so as to find the distribution that has mean, variance, and unnormalized skewness equal to the sums of the indvidual distributions:  $\{\mu_{\text{tot}}, V_{\text{tot}}, \gamma_{\text{tot}}\} = \{\sum_{i}^{n} \mu_{i}, \sum_{i}^{n} V_{i}, \sum_{i}^{n} \gamma_{i}\}$ , i.e. to revert Eqs. B.3, B.4, and B.5, which express these quantities in terms of  $\sigma_{-}$  and  $\sigma_{+}$ .



**Fig. B.1.** Error propagation of a nuisance parameter u (red with transparent  $1\sigma$  confidence interval) to a variable X (blue with  $1\sigma_-1\sigma_+$ confidence intervals) through a piecewise linear relationship (green line). Here,  $\sigma_-=0.25$  and  $\sigma_+=0.50$ . A quadratic relationship between u and X is also shown (orange). The mean  $\mu$  differs from the central value by a factor  $(\sigma_+-\sigma_-)/\sqrt{2\pi}\simeq 0.1$ .

This must be done numerically. Defining  $D \equiv \sigma_+ - \sigma_-$  and  $S \equiv \sigma_-^2 + \sigma_+^2$  the equations

$$S = 2V + \frac{D^2}{\pi} \tag{B.6}$$

$$D = \frac{2}{3S} \left( \sqrt{2\pi} \gamma - D^3 (\frac{1}{\pi} - 1) \right)$$
 (B.7)

are solved iteratively, starting with D=0 (takes only a handful of iterations). The resulting PDF is then given by

$$x_0 = \mu - \frac{D}{\sqrt{2\pi}} \tag{B.8}$$

$$\sigma_{-} = \bar{\sigma} - \frac{D}{2} \tag{B.9}$$

$$\sigma_{+} = \bar{\sigma} + \frac{D}{2} \tag{B.10}$$

where the (biased) mean is calculated through

$$\mu = \sum_{i}^{n} x_{0,i} + \frac{\sigma_{+,i} - \sigma_{-,i}}{\sqrt{2\pi}},\tag{B.11}$$

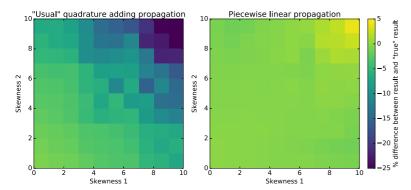
and

(B.5) 
$$\bar{\sigma} = \sqrt{V - \frac{D}{2}(1 - \frac{2}{\pi})}$$
 (B.12)

is the mean uncertainty.

# Appendix B.2: Testing the scheme

In order to test the method, we carry out a series of additions of PDFs. The tested functions are of various functional forms (lognormal, loglogistic, Fréchet, and Weibull), and for each pair the value of their parameters are drawn randomly in intervals such that their skewness ranges from 0 (symmetric) to 10 (highly



**Fig. B.2.** Offset of the central value  $x_0$  from the "true" value  $x_{0,\text{true}}$  obtained through convolution, in the case of the "usual", but wrong, method of adding errors in quadrature (*left*), and a piecewise linear error propagation (*right*), as a function of the skewness of the two addends. Here, offset is defined as  $(x_0 - x_{0,\text{true}})/x_{0,\text{true}}$ . The former method is off by a large fraction for relatively small skewnesses, whereas the latter method is correct on the <1% level even out to skewnesses of 8–9.

asymmetric). Their central values and lower and upper uncertainties are calculated, and compared to their "true" values obtained through a convolution of their full PDFs. The result is shown in Fig. B.2 for the central values of the "usual" (left) and the piecewise linear error propagation (right) method. The colour shows the offset of  $x_0$  of the two methods from the true result, defined as  $(x_0 - x_{0,true})/x_{0,true}$ , as a function of the normalized skewnesses of the two PDFs (defined as the third moment about the mean, divided by the cube of the second moment about the mean). The "usual" method causes an unwanted bias of  $x_0$  of >1% already for small skewnesses of  $\sim 0.5$ , and for moderate skewnesses of  $\simeq 5$  and above, the bias is >10%! This is for adding only two PDFs.; if multiple PDFs are added, the bias accumulates, leading to unacceptably large inaccuracies. In contrast, propagating errors through a piecewise linear transformation is accurate on the <1% level even out to large skewnesses

Similar figures can be constructed for the offset of  $\sigma_-$  and  $\sigma_+$  and for the quadratic relationship. For the PDFs tested, the piecewise linear method performs slightly better than the quadratic with regards to  $x_0$ , while the opposite is true for  $\sigma_-$  and  $\sigma_+$  (with both methods performing much better than the "usual" method). In this work, we have chosen to apply the piecewise linear error propagation throughout.