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Understanding cosmic reionization:
the escape fraction of Lyman-continuum and
Lyman-alpha photons in high-redshift
galaxies

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The Epoch of Reionization (EOR) represents one of the most exciting frontiers of research in astronomy and astrophysics. This era occurred within the first billion years of the Universe’s history and it is characterised by the large-scale transformation of hydrogen gas in the Universe from fully neutral to almost entirely ionized. This dramatic change was propelled by the young galaxies and black holes forming in the early Universe that emitted vast amounts of ionizing photons into their surrounding environment, called the intergalactic medium (IGM).

One of the fundamental aims in studies of galaxy formation and evolution is to understand the detailed role played by galaxies in ionizing the Universe, and in turn, how this rapidly evolving environment shaped galaxy evolution. There are a number of key unknowns that astronomers are tackling, using the latest, space-based observatories such as the James Webb Space Telescope (JWST), in order to piece together our understanding of this important epoch in the Universe’s history.

The goal of my research is to help tackle some of these unknowns so that a clearer picture of the reionization epoch can be assembled. Specifically, as outlined in this thesis, I use data collected from some of the most advanced telescopes in the world, including JWST and the Very Large Telescope (VLT), to better measure the number of ionizing photons produced by the young, hot stars forming in early galaxies. Crucially, I focus on deciphering the fraction of the ionizing photons that escape their galaxy into the wider Universe.

One might expect, given the vast amount of empty space between stars, that all the ionizing light produced by a galaxy easily escapes into the IGM. However, researchers studying galaxies much closer to our own Milky Way find very little, if any at all, of the ionizing photons leak into the surrounding space. This is due
to absorption by both hydrogen gas and dust that is comprised of tiny grains of carbon and silicon. It is therefore very important to measure the fraction of photons that escape galaxies like those that were present during reionization. In Chapter 3, I measure the escape fraction of galaxies which existed only a short time after the end of the EOR using VANDELS, one of the deepest spectroscopic surveys of its kind ever carried out. I find that approximately 7 per cent of the ionizing photons produced by the stars in these galaxies can escape, and that the galaxies with smaller amounts of stars, and less dust, have higher escape fractions than large galaxies. This work needed images taken from ground-based telescopes like the VLT, and it was one of the first successful measurements of the amount of ionizing photons escaping galaxies using this type of method.

In Chapter 4, I extend my investigations of the escape of ionizing photons from galaxies. Specifically, I explore how this is connected with observations of Ly\(\alpha\) emission, which is light emitted from hydrogen gas that has been illuminated by newly formed stars. Astronomers have a keen interest in Ly\(\alpha\) emission as both Ly\(\alpha\) and ionizing photons are stopped by dust and gas in a similar way, meaning that they should escape galaxies down the same pathways. From this work I learned that galaxies with more powerful Ly\(\alpha\) emission can signpost the types of galaxies that ionizing photons can escape from, which is in good agreement with previous research. I also find evidence suggesting that the pathways by which Ly\(\alpha\) photons escape from a galaxy do not change over approximately 90 per cent of the Universe’s history.

In Chapter 5, to compliment my measurements of the fraction of ionizing photons that can escape galaxies, I explore how the number of ionizing photons generated by galaxies changes over the course of the first \(\approx 25\%\) of the Universe’s history. My research demonstrates that galaxies that formed early in the Universe’s history generate substantially more ionizing photons than their later-forming counterparts.

The measurements in this thesis of the numbers of ionizing photons produced in galaxies, along with the fraction of the photons that can escape into the surrounding gas environment, confirm that galaxies can provide the necessary supply of ionizing photons to propel reionization. What is more, my research supports the picture in which the abundant population of smaller, fainter galaxies are the main drivers of reionization in the Universe.
Abstract

The quest to gain a full understanding of the Epoch of Reionization (EOR) is hampered by our incomplete knowledge of the ionizing properties of the young star-forming galaxies (SFGs) that drive this phase transition of the Universe. A key limitation is the uncertainty in the fraction of hydrogen ionizing (Lyman continuum) photons that escape galaxies ($f_{\text{esc}}^{\text{LyC}}$) into the intergalactic medium (IGM). In this thesis I provide measurements of $f_{\text{esc}}^{\text{LyC}}$, and examine its connection with other key galaxy properties such as the escape fraction of Ly$\alpha$ photons, UV luminosity and stellar mass. Another crucial component required in piecing together the timeline of reionization is the ionizing photon production rate of high-redshift galaxies. Complimentary to constraints on LyC escape, I therefore explore the redshift evolution of the average ionizing photon production rate using the [O III]+H$\beta$ nebular emission of galaxies over the redshift range $2 \leq z \leq 8$.

Direct measurements of $f_{\text{esc}}^{\text{LyC}}$ must be made at $z \leq 4$ as a result of the highly opaque IGM at higher redshifts. To measure $f_{\text{esc}}^{\text{LyC}}$ as close to the EOR as possible, I use a spectroscopically confirmed sample of SFGs at $3.35 \leq z_{\text{spec}} \leq 3.95$ from the VANDELS survey, together with ultra-deep ground-based $U$-band imaging directly probing the rest-frame ionizing flux. For the first time based on ground-based imaging, I place statistically significant ($\gtrsim 3.5\sigma$) constraints on $f_{\text{esc}}^{\text{LyC}}$, measuring an average of $\langle f_{\text{esc}}^{\text{LyC}} \rangle \approx 0.07 \pm 0.02$ across the sample of $N=148$ SFGs. Moreover, I find $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ correlates strongly with Ly$\alpha$ equivalent width ($W_{4}(\text{Ly}\alpha)$), and anti-correlates with the intrinsic UV luminosity and UV dust attenuation. These results support the scenario that the low-dust, low-metallicity galaxies commonly found at $z > 6$ are likely to dominate the reionization photon budget.

Motivated by the clear LyC–Ly$\alpha$ connection shown in these results, I analyse the Ly$\alpha$ emission properties of VANDELS galaxies further using a sample of $3.85 \leq z_{\text{spec}} \leq 4.95$ SFGs, only $\approx 300$ Myr after reionization was completed. Comparing the H$\alpha$ luminosity derived from robust SED fitting, with the Ly$\alpha$
luminosities measured directly from the VANDELS spectra, I place individual constraints on the Ly\(\alpha\) escape fraction \(f^{\text{Ly}\alpha}_{\text{esc}}\) for each galaxy. In agreement with lower-redshift literature results, I uncover a positive \(W_{\lambda}(\text{Ly}\alpha) - f^{\text{Ly}\alpha}_{\text{esc}}\) correlation at \(z \approx 4 - 5\). This analysis provides new evidence that the \(W_{\lambda}(\text{Ly}\alpha) - f^{\text{Ly}\alpha}_{\text{esc}}\) relation for SFGs at \(z \approx 4 - 5\) is remarkably consistent with that observed in high-redshift galaxy analogues at \(z \leq 0.3\). This implies that the physical processes determining the production and escape of Ly\(\alpha\) photons from low metallicity, high ionizing photon production efficiency galaxies do not vary significantly over \(\approx 90\%\) of cosmic time.

Using the low-ionization-state, FUV absorption lines present in composite VANDELS spectra, I investigate the relationship between \(f^{\text{Ly}\alpha}_{\text{esc}} - f^{\text{LyC}}_{\text{esc}}\), a first at \(z = 4 - 5\), and show that \(f^{\text{LyC}}_{\text{esc}}\) rises monotonically with \(f^{\text{Ly}\alpha}_{\text{esc}}\), following an approximate relation of the form \(f^{\text{LyC}}_{\text{esc}} \approx 0.15 f^{\text{Ly}\alpha}_{\text{esc}}\). The observed correlation is in good qualitative agreement with theoretical predictions and strengthens the case for using proxies that trace the neutral gas geometry and dust attenuation to infer \(f^{\text{LyC}}_{\text{esc}}\).

Lastly, assembling data from VANDELS at \(z \sim 3\) and taking advantage of revolutionary imaging from the CEERS JWST program, I measure the evolution of the \([\text{O}\text{III}]+H\beta\) equivalent width distribution \(W_{\lambda}(\text{[O}\text{III}]+H\beta)\) over the redshift range \(z \approx 2 - 8\). In agreement with literature results, I find that strong \([\text{O}\text{III}]+H\beta\) emission becomes common at the highest redshifts, with the \(W_{\lambda}(\text{[O}\text{III}]+H\beta)\) distribution becoming narrower and more peaked at higher values of \(W_{\lambda}(\text{[O}\text{III}]+H\beta)\) with increasing redshift. This result indicates that galaxies within the reionization epoch display ionizing photon production efficiencies of up to \(\log(\xi_{\text{ion}}) \approx 25.8\), a factor of \(\approx 3\) higher than typically assumed in pre-JWST models of reionization.

The analysis presented in this thesis focuses primarily on exploring the Lyman continuum escape fraction and ionizing photon production rate, along with how these quantities vary with key galaxy properties. The measurements of the average \(f^{\text{LyC}}_{\text{esc}}\) presented here, and its anti-correlations with UV luminosity and dust attenuation, provide robust evidence that the types of galaxies found during the EOR can be expected to display \(f^{\text{LyC}}_{\text{esc}} \gtrsim 5\%\). Taken together with the confirmation that high-redshift galaxies also become more efficient producers of ionizing photons, the results of this thesis strongly supports the scenario that SFGs can comfortably provide the necessary ionizing photon budget to drive reionization.

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I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

Parts of this work have been published in Begley et al. (2022) and Begley et al. (2023).

(R. A. Begley, November 2023)
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Chapter 1

Introduction

The beginning of extragalactic astrophysics can arguably be dated to 1926 with the seminal paper by Hubble (1926) on the characterisation of ‘nebulae’ in the sky. Using observations of Cepheid variable stars, he established that these ‘nebulae’ were at vast extragalactic distances, proving the existence of so-called ‘island Universes’ beyond our own Milky Way for the first time. A few years prior, Friedmann (1922) had derived solutions of the recently published General Theory of Relativity (Einstein, 1915) describing an expanding Universe, which were independently discovered by Lemaître (1927). By this time, Hubble had taken another fundamental step in providing observational evidence for the cosmologies being explored by theorists at the time. In 1929, Hubble established a velocity-distance relation now known as Hubble’s Law, which when combined with an Isotropic Universe, implied a uniform expansion of the Universe (Hubble, 1929).

Rapid progress followed in the decades from this early 1910’s to 1930’s era, with a number of critical breakthroughs in our understanding of the Universe being made, which led to our current understanding of cosmology.

In the 1940’s, George Gamow presented some of the earliest work explaining the origin of elements in the Universe through a process called primordial nucleosynthesis (Gamow, 1946), inspired by the realisation that at early times an expanding Universe must have been a very hot and dense environment. During this period the Universe was ‘radiation-dominated’, as the majority of the energy density was thermal. Expanding on this work, Ralph Alpher and Robert Herman had built-up a detailed history of the thermal properties of the Universe, leading to the first prediction that a diffuse remnant of this radiation-dominated era must
still permeate the Universe as cool blackbody radiation (Alpher, Bethe & Gamow, 1948).

The technology to investigate the presence of this background signal was first realised in the 1960’s, and it was ultimately detected by Penzias & Wilson (1965). This signal was termed the Cosmic Microwave Background (CMB), and allowed theorists to continue their work on the formation of structure in the very early Universe guided by observational constraints.

Leading on from this era, in the 1990’s a key breakthrough came from the use of Type Ia supernovae as ‘standard candles’ to accurately estimate cosmic distances. Observations of Type Ia supernovae allowed independent measurements of the expansion of the Universe to be made (Riess et al., 1995), and subsequently provided the first evidence for an accelerating expansion (Riess et al., 1998).

By the early 2000’s, a coherent concordance model of cosmology known as ΛCDM had emerged, supported by a wealth of observational and theoretical evidence (e.g., see Section 1.1.2). A series of space-based telescopes beginning with the Cosmic Background Explorer (Smoot et al., 1992), followed by the Wilkinson Microwave Anisotropy Probe (Bennett et al., 2003), and then lastly the Planck spacecraft (Tauber et al., 2010; Planck Collaboration et al., 2020), had allowed a remarkably detailed picture of the CMB and its power spectrum to be pieced together. Complementary to explorations of the very early Universe, optical and near-infrared instruments were used to carry out large-scale galaxy surveys such as 2dF (Cole et al., 2005) and SDSS (York et al., 2000), and to build up large samples of known Type Ia supernovae (Riess et al., 2004). Together these were used to establish the structure of the Universe locally, providing evidence that the geometry of the Universe is flat to a high level of precision (<1%), and that the expansion of the Universe is accelerating.

1.1 The cosmological framework

1.1.1 ΛCDM

The Lambda cold dark matter (ΛCDM) cosmological model is a physical framework through which the origin and evolution of the large-scale structure of the Universe is understood. This framework has been developed iteratively from
the ~1930’s to date, as theory was challenged by ever-improving observations. Although not without some criticisms and remaining challenges (see Section 1.1.2), it is widely accepted that ΛCDM (often known as The Standard Model of Cosmology) has had success in explaining a significant number of observed phenomenon. These include, but are not limited to: the precise structure of temperature fluctuations in the CMB characterised by its power spectrum, the large-scale distribution of galaxies and the abundances of the primordial elements Hydrogen, Helium (and trace amounts of Lithium).

Summarising the key features of ΛCDM cosmology, the Universe was in a high-temperature, high-density state immediately after the Big Bang. This was followed by a rapid inflationary phase in which small quantum fluctuations in the otherwise homogeneous and isotropic Universe were exponentially amplified (Guth, 1981). These over-dense regions then became the backbone for structure growth under the force of gravity, leading to the eventual formation of stars and galaxies, which we then study as they evolve over > 13 Gyr of cosmic time. Importantly, the baryons (and leptons such as electrons and neutrinos) that make up everything observed in the Universe such as stars, interstellar gas, and planets, only constitute approximately 4.9% of the total mass-energy density. In ΛCDM, the remaining mass-energy density consists of 26.2% dark matter and and 68.9% dark energy (Planck Collaboration et al., 2020); these two components providing the origin for the name of this cosmological theory. Current evidence indicates that dark matter is non-baryonic (not made up of fermions or bosons in the current standard model of particle physics) “cold” (with $v \ll c$), dissipationless (do not radiate photons), and is collisionless (interacting only via gravity) (Peebles, 1982; Trimble, 1987; Bertone et al., 2005). Although not visible directly, dark matter imprints clear signatures on the observed dynamics of galaxies and clusters of galaxies (Blumenthal et al., 1984), and forms the vital scaffolding upon which galaxies first formed and then evolved (Kauffmann et al., 1993).

Dark energy, currently synonymous with the cosmological constant and denoted as Λ, is yet more elusive than Dark Matter. Large surveys of Type 1a supernova (e.g., see The Dark Energy Survey; Dark Energy Survey Collaboration et al., 2016; Abbott et al., 2018) that have shown that the expansion of the Universe is accelerating, provide evidence that an additional, large component of energy density in the Universe is required. This dark energy component is further justified by the observed geometrical flatness of the Universe ascertained from CMB observations by Planck and WMAP. The current most favourable
explanation of dark energy is that it is a fundamental property of space-time, and provides a negative pressure term in Einstein’s mass-energy equations, thus accelerating the expansion of space (Albrecht et al., 2006).

The foundations of ΛCDM

The foundations of ΛCDM originate from two key observational leads - the expansion of the Universe seen through the velocity-distance relation \( v = H_0 r \), where \( H_0 \) is Hubble’s constant (sometimes quoted as the dimensionless Hubble constant \( h \), where \( h = H_0 / 100 \text{km s}^{-1} \text{Mpc}^{-1} \)), and the apparent isotropy and homogeneity of galaxies on the largest scales. Detailed investigations of the CMB probing the Universe at early-times, and extensive observations of the large-scale distribution of galaxies at late times, enabled by spectroscopic redshift surveys such as 2dF (Cole et al., 2005) and SDSS (e.g., York et al., 2000), have validated these foundations. Before detailing the collated evidence in support of a ΛCDM Big Bang cosmology, below I provide a brief overview of the key quantities in this framework.

In cosmological model frameworks, it is common to define the scale factor \( a(t) \), which relates the current distance \( r_0 \) at time \( t_0 \) between two observers, and the distance \( r(t) \) measured at a cosmological time \( t \) in an expanding Universe;

\[
r(t) = a(t) \cdot r_0
\]  

(1.1)

The scale factor takes a value \( a(t_0) = 1 \) at the present time \( t_0 \approx 13.8 \) Gyr, and becomes \( a(t) < 1 \) at \( t < t_0 \). In this formulation, \( r(t) \) is denoted as the proper radial distance representing the physical distance between any two observers at time \( t \). For two observers fixed in space relative to each other, the proper distance will increase as the Universe expands. However \( r_0 \), referred to as the comoving radial distance, will be constant as the scale factor \( a(t) \) (assuming no local factors are at play such as gravitational attraction) accounts for the expansion of space.

In this framework, the Hubble constant \( H_0 \), defined at present time, can be generalised as the Hubble parameter \( H(t) \) at time \( t \), and is written in terms of the scale factor:

\[
\frac{d}{dt} r(t) = H(t) \cdot r(t) \quad \overset{\text{Eq.1.1}}{\longrightarrow} \quad H(t) = \frac{\dot{a}}{a}
\]

(1.2)
Figure 1.1  The distribution of galaxies from large spectroscopic galaxy surveys (Left: 2dF Galaxy Redshift Survey, Top: Sloan Digital Sky Survey and CfA2 survey), out to distances of approximately $2 \times 10^9$ light-years. These galaxy maps trace out the large-scale structure of the Universe, with a number of nodes, filaments and voids clearly visible. Equivalent large-scale structure maps from the $\Lambda$CDM dark-matter only Millennium simulations are shown in the bottom/right. Significant agreement between the large-scale distribution of matter in the Universe is present between observations and simulations. Figure taken from Desjacques et al. (2018).
The comoving distance can be defined as;

\[ d_C(z) = \int \frac{c}{H(z')} dz' \tag{1.3} \]

as a function of redshift (z) - a key observable in extragalactic studies commonly used as a proxy for distance. Cosmological redshift occurs as a result of photon wavelengths becoming ‘stretched’ by the expansion of the Universe as they travel from a distant galaxy to the observer. For a photon emitted with \( \lambda_{\text{emit}} \) at time \( t_{\text{emit}} \), by the time it is observed at \( t_{\text{obs}} \), the wavelength will be redshifted to \( \lambda_{\text{obs}} = \lambda_{\text{emit}} \times a(t_{\text{obs}}) / a(t_{\text{emit}}) \) with the redshift then defined as;

\[ z \equiv \frac{\lambda_{\text{obs}} - \lambda_{\text{emit}}}{\lambda_{\text{emit}}} = \frac{\lambda_{\text{obs}}}{\lambda_{\text{emit}}} - 1 = \frac{a(t_{\text{obs}})}{a(t_{\text{emit}})} - 1 \tag{1.4} \]

The most commonly adopted distance in observational cosmology is the luminosity distance, \( d_L \). In a standard Euclidean geometry, the observed flux \( F \), intrinsic luminosity \( L \) and the distance \( d_C \) to an object are related through the inverse square law, which is then augmented in an expanding Universe;

\[ F = \frac{L}{4\pi d_C^2 (1 + z)^2} \rightarrow F = \frac{L}{4\pi d_L^2} \tag{1.5} \]

where the luminosity distance is defined as \( d_L = (1 + z) d_C \).

As the scale factor accounts for the impact of expansion on distance measurements, it can used to trace the dynamics of the Universe’s expansion over cosmological time. This expansion history is represented through the Friedmann equation which expresses the time evolution of the scale factor as a function of the matter and radiation density \( \rho \), the space-time curvature \( k \) and the vacuum energy density parameterised by the cosmological constant \( \Lambda \);

\[ H^2(t) = \left( \frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \rho - \frac{k c^2}{a^2} + \frac{\Lambda c^2}{3} \tag{1.6} \]

where \( c \) is the speed of light and \( G \) is the gravitational constant.

The density term \( \rho \) represents the combined mass-energy density of the Universe, and can be expressed in terms of its constituent parts, including non-relativistic matter, radiation, and the vacuum energy density \( \rho_\Lambda = \Lambda^2 c^4 / 8\pi G \), at the present time;
\[ \rho = \rho_{m,0} \left( \frac{a_0}{a} \right)^3 + \rho_{r,0} \left( \frac{a_0}{a} \right)^4 + \rho_{\Lambda,0} \]  

(1.7)

From the Friedmann equation, there is a clear link between the geometrical curvature and the density of the Universe. It is useful to define the critical density \( \rho_{\text{crit}} \), which is the density at which the Universe will have a flat geometry. Specifically, if \( \rho > \rho_{\text{crit}} \), the Universe is **closed**, and if \( \rho < \rho_{\text{crit}} \), the Universe is **open**. The critical density is calculated from Eq. 1.6 after setting \( k = 0 \) (and assuming \( \Lambda = 0 \)) as: \( \rho_{\text{crit}}(t) \equiv 3H^2(t)/8\pi G \). Using \( \rho_{\text{crit}} \), the density components in the Friedmann equation (Eq. 1.6) can be redefined in terms of the dimensionless quantity \( \Omega \) (e.g., \( \Omega_{m,0} \equiv \rho_{m,0}/\rho_{\text{crit},0} \)) at time \( t_0 \) as:

\[ \Omega_{k,0} \equiv -\frac{kc^2}{H_0^2a_0^2} = 1 - \Omega_0 \]  

(1.8)

where \( \Omega_0 \) is the total density given by \( \Omega_0 = \Omega_{m,0} + \Omega_{r,0} + \Omega_{\Lambda,0} \). In the present day (or more generally at \( t > 10^5 \) years), the radiation contribution is negligible, and so the ultimate history and fate of the dynamics of the Universe is closely tied to \( \Omega_{m,0} \) and \( \Omega_{\Lambda,0} \).

### 1.1.2 Observational evidence in support of \( \Lambda \)CDM

**The Cosmic Microwave Background**

The CMB is ‘relic radiation’ from the epoch of recombination. During this epoch the Universe had cooled enough such that the plasma of protons and electrons could form into the first Hydrogen atoms, and photons became decoupled. This allowed photons to travel freely, imprinted with information about the structure and conditions \( \sim 380,000 \) years after the Big Bang. We see this radiation today at microwave wavelengths (\( T \approx 2.7 \) K), cooled from its original \( T \sim 3000 \) K due to expansion of the Universe, as shown in the top-panel of Fig. 1.2. The temperature angular power spectrum, shown in the bottom panel of Fig. 1.2, characterises the structure of temperature fluctuations, namely the CMB anisotropies. The various peaks and features in this power spectrum encode information about cosmological parameters such as the mass density, the cosmological constant and the geometry of space-time (e.g., Hu & Dodelson, 2002). Alongside more subtle details of the CMB, including its polarisation and the impact of foreground matter such as
intracluster gas, the power spectrum provides unparalleled constraining power for the ΛCDM cosmological model (e.g., see Durrer, 2015).

The large-scale structure of galaxies and dark matter

Significant observational campaigns such as the 2dF Galaxy Redshift Survey (Cole et al., 2005) and the Sloan Digital Sky Survey (York et al., 2000) have unveiled the 3-dimensional structure of galaxies on approximately Gpc scales. This large-scale structure of galaxies grew from seeds of over-densities in place from the early Universe (e.g., seen in the CMB as shown in Fig. 1.2), now forming a cosmic web of sheets, nodes, filaments and voids within which no galaxies are present. An example of such a structure in the observable Universe is the Pisces–Cetus Supercluster Complex. This is the filament that our own Milky Way galaxy resides in, and is estimated to be ~ 300 Mpc long and ~ 45 Mpc wide. The clustering distribution of galaxies is often described statistically through the two-point correlation function (e.g., Desjacques et al., 2018), which quantifies the excess probability of seeing a galaxy within some distance $r$, compared with a random distribution. Using SDSS in a pivotal study, Eisenstein et al. (2005) found a characteristic separation scale of $\sim 100 h^{-1}$ Mpc, an imprint leftover from the acoustic oscillations of baryons in the early Universe. These surveys mapping the distribution of galaxies on large scales have provided independent evidence in support of the ΛCDM cosmology with matter-energy densities of $\Omega_m,0 \sim 0.3$, in agreement with the studies of the CMB and large-scale N-body simulations of the Universe (Springel et al., 2005a).

Elemental abundances of light elements

George Gamow, inspired by the suggestion that the Universe was once extremely hot and dense, suggested that the chemical elements were created in this early Universe by primordial nucleosynthesis in the 1940’s. This theory initially faced opposition due to the challenge of creating elements heavier than Lithium, however subsequent developments in our understanding of the role that stars play in element synthesis, led by Hoyle (1946) and followed by Burbidge et al. (1957), again provided support for the BBN model. A significant body of observational evidence has been assembled to-date, including CMB measurements by Planck and spectroscopic studies of near-pristine quasar absorption systems (Cooke et al.,
Figure 1.2  **Upper Panel:** The earliest view of the Universe - the cosmic microwave background (CMB) temperature map measured by Planck, showing an average temperature of $T \sim 2.74 \text{ K}$, with anisotropies of the order $\sim 10^{-5}$ at $z \sim 1100$, approximately 380,000 years after the Big Bang. The structure of these anisotropies are predicted by the $\Lambda$CDM model, and originate from the quantum fluctuations that underwent inflation in the Universe’s first moments.

**Lower Panel:** The associated temperature angular power spectrum (top, and residuals, bottom) from the Planck 2018 results, with the best-fitting $\Lambda$CDM model plotted as a blue line. The positions and heights of various peaks contain information about the geometric shape of the Universe and provides evidence that it is consistent with being flat ($\Omega_k = 1$). Figure taken from Planck Collaboration et al. (2020).
As a result of the BBN mechanism within ΛCDM, after primordial nucleosynthesis in the first 10 seconds to 20 minutes after the Big Bang, the baryon abundances were ∼ 75% $^1$H, ∼ 25% $^4$He, and trace amounts (∼ 0.01%) of $^2$H, $^3$He and $^7$Li.

**Other key successes of ΛCDM**

Beyond the temperature anisotropy distribution characterised by the power spectrum, in 2002 the CMB polarisation was discovered (Kovac et al., 2002), a feature predicted by ΛCDM. Another key prediction of ΛCDM is the presence of baryon acoustic oscillations. These oscillations, created by the interplay between gravity and pressure in the early Universe, left an imprint on the galaxy power spectrum corresponding to the characteristic distance of the sound horizon, that is, the distance baryon sound waves could have travelled before recombination (after which, gravity was able to dominate over the pressure due to more effective cooling, which froze this feature into the large-scale structure). Finally, the accelerating expansion of the Universe, inferred through observations of Type 1a supernovae, is explained through a negative pressure mass-energy density. This observed acceleration is provided by the dark energy term, Λ, in the current iteration of the ΛCDM cosmological model.

**Remaining challenges and open questions for Cosmology**

Currently, the ‘Hubble tension’ is one of the leading uncertainties in ΛCDM cosmology (e.g., see Di Valentino et al., 2021; Perivolaropoulos & Skara, 2022). This tension describes the current statistically significant (≥ 5σ) discrepancy between $H_0$ measurements in the late Universe, for example from the cosmological distance ladder (e.g., Cepheid variable stars, SN1a observations etc), that suggest $H_0 \approx 73$ km s$^{-1}$ Mpc$^{-1}$, with early Universe $H_0$ measurements (e.g., from the CMB power spectrum) that favour values of $H_0 \approx 67$ km s$^{-1}$ Mpc$^{-1}$. Many solutions to, and causes of the Hubble tension have been explored, including systematic errors in the local Universe distance ladder (Efstathiou, 2020), the possibility that our Milky Way galaxy is situated in a statistically large underdensity (e.g., the KBC void; Keenan et al., 2013), and updated cosmological models that include new physics (Di Valentino et al., 2021) such as modified gravity (Clifton et al., 2012).

Another key challenge faced by the current cosmological paradigm is the ongoing
lack of direct dark matter detections, which lead to uncertainties about the exact properties of dark matter and therefore in ΛCDM predictions (Arbey & Mahmoudi, 2021). Related to uncertainties about the nature of dark matter, the potential existence of galaxies without dark matter (van Dokkum et al., 2018), and the cusp-core problem (regarding the unexpected dark matter density profiles in some galaxies, e.g., see; Navarro et al., 1996; de Blok, 2010; Bullock & Boylan-Kolchin, 2017) also warrant explanation in the ΛCDM framework.

As outlined in Perivolaropoulos & Skara (2022) (see also; Bullock & Boylan-Kolchin, 2017; Di Valentino et al., 2021), there are other remaining challenges facing ΛCDM (although less significant than the Hubble tension), including the ‘Lithium problem’, the ‘missing satellite problem’, and possible hints that parts of the Universe violate the homogeneity and isotropy principles. Nonetheless, the ΛCDM model remains a remarkable success and to-date is the best theory of cosmology in our Universe, providing an accurate framework within which a robust timeline of the Universe has been pieced together, as outlined below in Section 1.1.3.

1.1.3 The timeline of the Universe in ΛCDM

With ΛCDM established as a leading and successful cosmological theory (albeit with some remaining challenges outlined above), it is useful to briefly summarise the key events and epochs in the Universe’s 13.787 ± 0.020 Gyr timeline.

Figure 1.3 Schematic highlighting a number of key epochs in the timeline of the Universe. The study of the Epoch of Reionization, marked in yellow, represents a frontier of extragalactic research. A key uncertainty in understanding this era is the Lyman continuum photon escape fraction, the measurement of which is a core topic of this thesis. Figure courtesy of NAOJ.
Immediately after the Big Bang, the Universe was a hot, dense, soup of primordial energy and matter. The physics of this era is not currently known due to the need for a unified theory of the fundamental forces within the extremely high-energy regime of the early Universe. Approximately $10^{-36}$ seconds after the Big Bang, cosmic inflation occurred, causing a rapid expansion of the Universe by a factor $>10^{26}$ over the next $\sim 10^{-32-33}$ seconds. The details and historical controversies of inflation are beyond the scope of this thesis, however it is important to note that the inflationary $\Lambda$CDM model (Guth, 1981) solved a number of problems facing Big Bang cosmology, i.e. explaining the observed flatness and isotropy of the Universe, in addition to manifesting the seeds of large-scale structure from quantum fluctuations in the Early Universe.

After inflation, from $\sim 1$ second to $\sim 3$ minutes after the Big Bang, the Universe continued to expand, but much slower, and cooled sufficiently to allow the four fundamental forces, and a series of subatomic particles including hadrons and leptons, to emerge. From this point the important stage of Big Bang Nucleosynthesis occurred. As predicted by $\Lambda$CDM, and with decades of observational, experimental and theoretical supporting evidence, during BBN $\sim 75\%$ of the protons and most of the neutrons in existence were fused into deuterium and then into Helium-4, and trace amounts of Lithium-7.

The continued cooling of the Universe resulted in BBN only lasting $\sim 17$ minutes, after which the primordial abundances of $^1$H, $^4$He, $^2$H, $^3$He and $^7$Li were constant until the formation of the first stars. In the ensuing era, known as the ‘Photon epoch’, the Universe consisted of a dense plasma of electrons, neutrinos and positive nuclei, in addition to an abundance of photons. Thomson scattering between the ionized gas and photons produced a completely opaque Universe during this time, lasting of the order $\sim 10^{4-5}$ years.

Over the ensuing $\sim 18,000 - 370,000$ years after the Big Bang leading into recombination epoch, the Universe significantly cooled from nucleosynthesis temperatures of $\gtrsim 10^8$ K, to $\sim 10^3$ K, crossing a number of key temperature milestones. First, He$^+$ is able to form, followed by HeH$^+$, and then importantly, neutral Hydrogen at the end of the recombination epoch at $z \sim 1100$. The formation of neutral Hydrogen marks the transition from an opaque to a transparent Universe, where the optical depth due to Thomson scattering rapidly dropped and the photons ‘decoupled’ from the matter. These photons, able to travel freely across the Universe, are what we now observe as the Cosmic Microwave Background. The recombination epoch also marks a crucial transition
point in the cosmological history of the Universe, evolving from radiation to matter-energy density dominated.

Between the recombination epoch and the formation of the first stars is the so-called Dark Ages, the longest period in the timeline so far. In the dark ages, the beginnings of the large-scale structure we see today began to form through a process called gravitational instability. The force of gravity allowed the remnant over-densities from inflation to grow preferentially over the less dense regions. Unaffected by radiation pressure, dark matter in overdensities was able to coalesce and gravitationally collapse, thereby growing into large dark-matter haloes. Eventually, as the gravitational pull of the dark-matter haloes increased, large gas clouds composed of Hydrogen and Helium were able to coalesce, forming the first stars in the Universe around 100 Myr after the Big Bang at \( z \approx 30 \), marking the end of the dark ages and the beginning of the Epoch of Reionization (EOR).

The epoch of reionization is particularly important to the contents of this thesis and is discussed in detail in Section 1.4. Briefly, the birth of the first stars and subsequent galaxies produced large amounts of ionizing radiation (\( E_\gamma \geq 13.6 \text{ eV} \)). Over the course of the next \( \sim 1 \text{ Gyr} \) (approximately \( 6 \lesssim z \lesssim 30 \)), the cumulative ionizing radiation output from the emerging young galaxy populations completely (re-)ionized the neutral hydrogen formed during recombination.

From the end of the EOR until the present day, a time spanning \( \sim 12 \text{ Gyr} \), there was a significant evolution in the populations of stars and galaxies in the Universe. The large-scale structure of the Universe continues to become more defined, with galaxies progressively forming larger structures such as clusters from the cosmic web of nodes and filaments. Until \( z \sim 2 \) (\( t_{\text{age}} \sim 10 \text{ Gyr} \)), the star-formation rate per unit volume increases, leading to the significant increases in the amount of metals in the Universe through stellar nucleosynthesis. This material is then recycled into further populations of stars and eventually into the planets like our own planet Earth, which formed \( \sim 4 \text{ Gyr} \) ago. The largest galaxies, become passive and stop forming stars, in addition to evolving morphologically into ellipsoidal behemoths as large as 150 kpc in diameter and with stellar masses in excess of \( 10^{11} \text{ M}_\odot \).
1.2 Galaxy Fundamentals

Observationally, galaxies have been studied in detail for ~ 100 years, since it was first realised by Hubble and others in the 1920’s that a large fraction of the nebulae then discovered were in fact beyond our own ‘Island Universe’ the Milky Way, and were themselves, galaxies.

Over this time frame, populations of galaxies have been observed and investigated across a range of wavelengths and physical scales; from galaxies in our local neighbourhood, to the most distant spectroscopically confirmed to date with a redshift $z = 13.2$ (designated JADES-GS-z13-0, Robertson et al., 2023), observed when the Universe was only a few hundred Myr old; and from faint dwarf galaxies with as little as $\approx 10^{3-4}$ stars (Belokurov et al., 2009; Kirby et al., 2013), to large and bright monsters containing hundreds of millions of stars (Bernardi et al., 2010).

Galaxies are massively complex gravitationally-bound systems, primarily consisting of (up ~ $10^{11}$) stars within a dark-matter halo, and often with a super-massive black hole (SMBH) at the centre. Stars themselves are vastly diverse objects, with a detailed classification system (e.g., see Morgan & Keenan, 1973) characterising their luminosity, mass and surface temperature which are governed by their initial mass, chemical composition and evolutionary stage. Gas in an assortment of forms, dust, and stellar remnants, such as white dwarf and neutron stars, are also all vital components of a galaxy.

The formation and evolution of galaxies, and all the components they contain, is governed by an extensive amalgam of physical processes. These include, but are not limited to: gravitational interactions in massive cluster environments including mergers, quenching on large scales due to active SMBHs, and feedback on small scales from stars injecting radiation and matter via stellar winds into the interstellar medium (ISM). Moreover, a near-constant cycle of star-formation fueled by pristine gas inflows and subsequent gas recycling leads to the ISM becoming metal enriched as well as the growing presence of older stellar populations as a result of the younger, more massive stars moving towards the later stages of stellar evolution, such as supernova and the formation compact objects (white dwarfs, neutron stars, and black holes), much more rapidly.

Constructing a coherent, detailed framework within which galaxy formation and
evolution can be accurately understood is a key goal in astrophysics research. The progress towards this goal has been immense and decades, if not centuries, in the making, relying on a huge array of observations, theoretical investigations and large-scale simulations, all bringing in a variety of physics disciplines to piece together this framework.

**Observations**

Stars, which can be approximated as black bodies, have effective temperatures ranging from a few $\sim 10^3$ K to $\sim 10^5$ K, and therefore emit the bulk of their emission at wavelengths $0.1 \mu m \lesssim \lambda \lesssim 5 \mu m$. Being the most abundant component, stellar populations dominate the total integrated light of a galaxy’s spectral energy distribution over this wavelength regime. Significant amounts of our understanding of galaxies has come from observing this stellar component using telescopes and instrumentation capable of imaging in the FUV-optical-NIR regime.

Spectroscopy covering the same wavelength regime has allowed a number of key emission line and absorption features to be observed including; Ly$\alpha$, H$\alpha$ and [O$\text{III}$] from ionized H$\text{II}$ regions; Balmer breaks (and Ca, Na, Mg absorption lines) from the atmospheres of evolved stellar populations; and high ionization lines indicating the presence of an AGN. The Sloan Digital Sky Survey (York et al., 2000) has been particularly vital in combining imaging and spectroscopy to revolutionize our understanding of the low-redshift galaxy population.

**Simulations and modelling**

Simulations and detailed numerical modelling have played a vital role in progressing our knowledge of galaxy evolution, bringing together complex physical processes from less than sub-pc to greater than Mpc scales (e.g., Somerville & Davé, 2015). Cosmological simulations primarily come in two main forms; semi-analytic and hydrodynamical models, which are both underpinned by the same large-scale N-body dark-matter simulation framework. Semi-analytic models are excellent for folding-in simplified prescriptions of physical processes that may be too computationally expensive to directly compute (e.g., see Somerville & Primack, 1999), while hydrodynamic simulations can allow the aspects of the gas physics to be solved numerically in a self-consistent fashion within the dark-matter
structure (e.g., see Springel, 2005; Mitchell et al., 2018).

These large-scale simulations such as the Millennium Simulation (Springel et al., 2005b), have been vital tools in testing theories of galaxy formation and evolution. Another more recent example is the THESAN project (Kannan et al., 2022a, see Fig. 1.4), a suite of large-volume simulations folding in radiative transfer as well as magnetic fields and hydrodynamics, which have allowed the EOR to be studied self-consistently within galaxy evolution frameworks.

1.2.1 The formation of stars

In all galaxies, the onset of star-formation is governed by the accretion and subsequent cooling of gas. At high redshift, and in low-mass dark-matter haloes, ‘cold mode accretion’, whereby cold dense gas from cosmic filaments flows into the galaxy, is the primary mode of gas accretion (e.g., Kereš et al., 2005; Benson, 2010). Mergers and other similar galaxy-galaxy interactions also provide a mechanism for gas accretion, often producing subsequent ‘starburst’ activity (e.g., Barnes & Hernquist, 1991).

Gas cooling is vital for the formation of stars as it allows the thermal pressure within gas clouds to be reduced. Once the thermal gas pressure has sufficiently reduced and the Jeans mass has been reached, the onset of cloud collapse and subsequent star-formation can begin. The cooling of accreted gas is primarily driven through collisional excitation and subsequent decay and radiative recombination. If the gas becomes very cold ($T_{\text{vir}} < 10^4$ K), further cooling by traditional atomic processes is suppressed due to the low-energy state of the gas. In these scenarios, molecular H$_2$ (and other trace element species) driven cooling is the primary mechanism (Abel et al., 1997) and as such, is important for the formation of the first population III stars forming from cool gas after the epoch of recombination (Abel et al., 2002; Bromm et al., 2009). In the hotter, ionized environments within higher mass haloes ($T_{\text{vir}} > 10^7$ K), Bremsstrahlung emission is the primary cooling mode (Benson, 2010).

As cooling is more efficient in denser environments (Yoshida et al., 2002), and cooling leads to an increase in gas density, an accelerating cooling effect occurs. This induces the collapse of gas clouds into Giant Molecular Clouds that subsequently fragment into dense regions ($n_{\text{H}_2} > 10^4$ cm$^{-3}$, Chevance et al., 2022) that can then go on to form (clusters of) stars after further cooling and collapse.
Figure 1.4 Kaleidoscopic snapshot from the THESAN project demonstrating the range of physical properties traced self-consistently in this radiation-magneto-hydrodynamic cosmological simulation. Two insets show mock images of a large simulated galaxy, containing > $10^5$ particles, with JWST and ALMA. Figure courtesy of the THESAN Collaboration.
Furthermore, beginning with the first generation of stars, metals begin to pollute the interstellar medium (ISM) which again enhances the cooling efficiency (Silk & Wyse, 1993).

### 1.2.2 The spectral energy distributions of galaxies

The spectral energy distribution (SED) of a galaxy shows its emitted energy as a function of wavelength, as illustrated in Fig. 1.5. Inferring the SEDs of galaxies has been a key goal of astronomy for decades, as it offers a unique insight into the composition of the galaxy, in addition to the physical processes at play acting on its constituent parts. The SED of a galaxy, particularly from ultraviolet to infrared wavelengths, is dominated by three primary components: stellar light from the various populations of stars, nebular emission from gas, and emission and absorption from dust - each of which are reviewed below.

#### Stellar populations

The ultraviolet (UV), optical, and near-infrared (NIR) regimes of a galaxy’s SED are primarily shaped by the light emitted from its stellar populations. Notably, in the case of high-redshift star-forming galaxies, the young stellar populations with ages of less than 100 million years play a dominant role at UV/optical wavelengths. Among these, the most massive O/B stars, characterised by effective temperatures exceeding $T_{\text{eff}} > 10^4$ K, emit significant quantities of UV photons (as exemplified in Fig. 1.5). As the stellar populations within the galaxy age, older components gradually contribute the majority of the optical and NIR emission.

The stellar light observed from a galaxy therefore holds crucial information about the properties of the underlying stellar population, including the age and metallicity (e.g., Bruzual & Charlot, 2003). When exclusively looking at the UV/optical light of a galaxy, these two properties are degenerate along with a third parameter, the level of dust attenuation – creating the age-metallicity-dust degeneracy (Worthey, 1994; Maraston, 2005). The presence of older populations, higher metallicity and increased dust attenuation all reduce the relative amount of light at shorter wavelengths and ‘redden’ the SED. The challenge of accurately measuring these parameters is eased by the inclusion of longer wavelength photometry providing a larger dynamic range in wavelength. At high-redshift, where populations are generally younger and have less dust and metals (Stark,
Figure 1.5  Schematic galaxy spectral energy distribution taken from Galliano (2017). Massive, short-lived O/B stars dominate UV wavelengths (blue line), whilst the more long-lived stars with masses $< 10 M_\odot$ emit most strongly at optical-NIR wavelengths (red line). The hatched areas indicate the amount of flux attenuated my dust. Strong nebular emission lines (and the nebular continuum) is shown in green. Re-processed UV photons absorbed by dust are radiated predominantly at $\lambda > 5 - 10 \mu$m (purple line).
2016), the age-metallicity-dust degeneracy is also less important.

Particularly relevant for the subject of this thesis is the stellar populations that dominate the ionizing photon production (i.e., $E_{\gamma} = h\nu \geq 13.6$ eV, named Lyman-continuum photons), and in doing so, also drive the nebular emission properties of a galaxy (see Section 1.2.2). As noted previously, the relevant stars are the massive O/B stars produced in recent episodes of star-formation. Due to their mass, they are short-lived and on the main sequence for as little as 5–10 Myr in the case of stars with masses in excess of $> 10 M_\odot$. As a result of the short lifetimes, the ionizing flux output of a stellar population drops rapidly after $\approx 20$ Myr, as shown in Bruzual & Charlot (2003, Fig. 9). Lower metallicities (producing hotter stellar atmospheres) boost the ionizing flux, while a ‘bursty’ star-formation history will produce more O/B stars periodically and hence increase the amount of time over which a galaxy will emit significant amounts of ionizing flux compared to ‘constant’ star-formation histories.

The goal of achieving a better understanding of the UV spectra of high-redshift star-forming galaxies has driven a number of recent developments in stellar population synthesis models. Two such examples are the Starburst99 (Leitherer et al., 1999a, later updated in Leitherer et al. 2016) and BPASS (Eldridge et al., 2017) SPS models, which include the impact of stellar rotation and binary interactions, respectively. In particular, these models can 1) boost the ionizing output of a stellar population, and 2) extend the time over which galaxies can produce considerable numbers of Lyman-continuum (LyC) photons. These developments help explain the elevated ionizing photon production values observed in high-redshift low-metallicity galaxies (Bouwens et al., 2015; Stark, 2016; Maseda et al., 2020), that were often poorly matched by BC03 stellar population models.

The Initial Mass Function (IMF), characterising the mass distribution of stars formed, is another key influence on the ionizing photon output, and more generally also for the star formation and subsequent evolution within a galaxy. The IMF is an important assumption that is made in a variety of analyses including SPS modelling for SED fitting and star-formation rate (SFR) conversion factors. Much of the early work investigating star-formation assumed a Salpeter (1955) (power-law) IMF, with more recent work including a broader range of stellar masses and more sophisticated stellar modelling leading to the Kroupa (2001) (broken power-law) and Chabrier (2003) (log-normal) IMF prescriptions which are widely used in the modern literature.
A common assumption employed widely in the literature is that the IMF is roughly universal. However, there is still substantial ongoing debate, fuelled by significant observational and theoretical challenges, aiming to establish if the IMF evolves with redshift, becoming increasingly ‘top-heavy’ at high-redshift (Davé, 2008; van Dokkum, 2008) or in starbursts where there is a higher SFR, higher gas density and lower metallicity (Kroupa, 2002; Marks et al., 2012). Importantly, regarding the influence of galaxies on the IGM during the EOR, IMFs that are more ‘top-heavy’ produce more massive O/B stars that dominate the ionizing photon budget.

**Nebular Emission**

The next major component of a galaxy’s UV-to-IR spectral energy distribution is nebular emission, particularly in those that are star-forming. Nebular emission originates from ionized H\textsubscript{II} regions in the ISM that are created by the intense UV radiation from short-lived, massive O/B stars. Emission lines produced in the H\textsubscript{II} regions from radiative recombination; such as Ly\textalpha and the Balmer series (e.g., H\textalpha, H\beta), and from (forbidden) collisional de-excitation (e.g., [O\textsc{iii]},[N\textsc{ii}]) dominate the nebular emission contribution to a galaxy SED. There is also nebular continuum emission generated from free-free, free-bound and two-photon processes.

In addition to star-forming regions, AGN, post-AGB stars, and shocks can induce nebular emission, as they also create ionized regions in galaxies. Establishing whether the nebular emission is dominated by young stellar populations, or otherwise, can be accomplished from line-ratio diagnostic diagrams (Veilleux & Osterbrock, 1987). The most well-known is the ‘BPT diagram’ (Baldwin, Phillips & Terlevich, 1981), which shows that the nebular emission line ratios powered by star-formation and AGN occupy different regions in the [N\textsc{ii}]/H\textalpha − [O\textsc{iii}]/H\beta parameter space. Moreover, various combinations of emission lines and their ratios can be employed as ‘diagnostics’ to measure physical properties of the ISM gas, such as electron density and temperature, gas pressure and the ionization state (e.g., see Kewley et al. 2019 for a review).

An important caveat in the use of line-ratio diagrams is that they need accurate calibrations, particularly at high-redshift. Data from the MOSDEF survey (Kriek et al., 2015) has shown that \(z \sim 2\) SFGs are displaced on BPT diagrams relative to local star-forming galaxies observed in SDSS (Shapley et al., 2015; Sanders
et al., 2016; Strom et al., 2018). Additionally, low-metallicity AGN at \( z > 6 \) fall in the star-forming region of the BPT diagram, limiting its use at the highest redshifts. This evolution in the line-ratio diagnostics is likely a result of the larger ionization parameters, evolving gas densities and harder ionizing spectra more commonly found in \( z \gtrsim 2 \) galaxies (e.g., see Kewley et al., 2013; Hirschmann et al., 2017), and therefore motivates direct calibrations of line-ratio diagnostics at high-redshift (Sanders et al., 2023).

Linking the physical properties of the ISM gas through its nebular emission, with the underlying stellar populations and global star-formation properties is generally not possible analytically, and so relies on the use of photoionization models. The most modern of these are MAPPINGS-III (Sutherland et al., 2018) and CLOUDY (Ferland et al., 2013), which self-consistently model the nebular, dust and ionization physics of HII regions based on an input ionizing spectrum. Importantly, a number of recent SED fitting codes (e.g., BAGPIES; Carnall et al., 2018, and BEAGLE; Chevallard & Charlot 2016) directly fold in processing of the stellar light using these photoionization codes. Accounting for the impact of nebular emission is often vital when constraining galaxy SEDs using broadband photometry, which can be significantly boost the observed flux (e.g., see Chapter 4). This impact on broadband photometry from nebular emission can cause misidentification between passive galaxies, star-forming galaxies and possibly AGN (e.g., see Merlin et al., 2018; Santini et al., 2021), can impact photometric redshift measurements (Wilkins et al., 2013), and can generally bias estimates of galaxy physical properties such as SFR (e.g., see Stark et al., 2013). Alternatively, the nebular contamination can be used to empirically measure the equivalent widths of emission lines, whilst avoiding potential biases, degeneracies and limitations of a full SED plus photoionization modelling approach (e.g., see Chapter 5).

**Dust**

Dust also plays a vital role in determining the SED of a galaxy, particularly at UV/optical (\( \lambda \lesssim 0.5 \mu m \)) wavelengths where significant dust attenuation can occur, and in the IR regime (\( \lambda \gtrsim 10 \mu m \)), where dust emission becomes the dominant component of a galaxy SED.
Dust is particulate in nature, and forms as a by-product of stellar population evolution in supernova ejecta and the stellar winds of massive evolved stars (Morgan & Edmunds, 2003; Leśniewska & Michalowski, 2019). The growth of dust grains in the ISM, as well as their destruction, are both also key processes regulating dust in galaxies (e.g., see Jones, 2004; Draine, 2009). Dust grains primarily consist of either silicates, or are carbonaceous, for example graphite or Polycyclic Aromatic Hydrocarbons (PAHs) (see below). They generally have a mixture of sizes between 5–250 nm with the exact size distribution governed by the complex interplay between the production, growth and destruction processes as well as the chemical makeup of the ISM itself.

When considering a galaxy’s SED at UV-to-NIR wavelengths, a key action of dust is the ‘reddening’ it produces as a consequence of preferential absorption and scattering at bluer wavelengths. This is clearly seen in dust attenuation curves, such as the Calzetti dust attenuation law (Calzetti et al., 2000) shown in Fig. 1.6, derived from local starburst galaxies. Dust attenuation laws are commonly parameterised as $A_\lambda/A_V$, quantifying the amount of attenuation at a given wavelength $\lambda$ in magnitudes relative to the level of $V$–band ($\lambda \sim 5000\,\text{Å}$) attenuation.

As a brief aside, it is worth highlighting the important distinction between a dust extinction and a dust attenuation curve. The former is the correct terminology if light is scattered / absorbed from a singular source, typically a nearby star or possibly a distant quasar or Gamma Ray Burst (GRB), by a foreground dust screen. In contrast, the term attenuation is valid when a more complex inhomogeneous geometry of stellar populations and dust is present, as is the case in a galaxy. It then follows that a dust attenuation curve folds in the effects of absorption and scattering as well as light scattering back into the line of sight (e.g., see Salim & Narayanan, 2020). This results in dust attenuation curves, like the Calzetti curve, becoming flatter (‘grayer’) than the comparatively steep extinction curves (e.g., for the SMC).

Determining the exact form of the dust attenuation curve for high-redshift galaxies remains a key open question. For example, Scoville et al. (2015) and Cullen et al. (2018) infer dust attenuation laws consistent with the ‘grayer’ Calzetti attenuation law for spectroscopically confirmed SFG samples at $z > 2$. In contrast, using a $z \sim 2$ sample from the MOSDEF survey (Kriek et al., 2015), Reddy et al. (2015) measure a dust attenuation law intermediate between the shallower Calzetti law and steeper SMC extinction curve (e.g., see Fig. 1.6).
Figure 1.6  A subset of literature dust attenuation curves (grey/black lines) shown as $A_{\lambda}/A_V$, including the Calzetti et al. 2000 (solid), Charlot & Fall 2000 (dash-dotted) and Reddy et al. 2015 (dotted) attenuation curves, as well as the SMC extinction curve (dashed; Gordon et al., 2003). An example dust attenuation curve derived for an individual $z \approx 3 - 4$ galaxy from VANDELS is also shown (red line). On average, VANDELS star-forming galaxies show ‘flatter’ dust attenuation curves, in good agreement with the Calzetti attenuation curve. Figure courtesy of Cullen et al. (2018).
A significant body of evidence now exists in support of large individual galaxy-to-galaxy variations in the dust attenuation law (Buat et al., 2012), regardless of redshift (Salim & Narayanan, 2020), which can result in biased measurements of key galaxy properties (e.g., stellar mass) when a universal dust law is assumed (Kriek & Conroy, 2013).

An additional complexity is that nebular emission produced by H\textsc{ii} regions surrounding recently formed stars undergoes increased attenuation relative to that of the stellar continuum (Calzetti et al., 2000). This is consistent with the physical picture in which the young O/B stars dominating the production of nebular emission remain embedded in their denser ‘birth clouds’, leading to elevated reddening (Charlot & Fall, 2000). The exact dust attenuation law governing this additional nebular attenuation may be distinct from that for describing stellar attenuation (Reddy et al., 2020), and metallicity also likely plays a key role in the steepness of the attenuation law (Shivaei et al., 2020).

Lastly, it is the exact composition and properties of the dust grains (Draine & Li, 2007) that set the underlying extinction curve. Small dust grains scatter and absorb bluer wavelengths more efficiently compared to larger grains, producing a steeper dust curve. One of the more complex constituents of dust is PAHs (Polycyclic aromatic hydrocarbons) which, aside from their important role in regulating thermal and chemical processes taking place in the ISM (Tielens, 2008), also attenuate UV light in a galaxy.

Although initially discovered via the large emission features at rest-frame $\sim 10\mu$m (Gillett et al., 1973; Allamandola et al., 1985), they are now attributed with giving rise to the 2175 Å feature frequently seen in dust extinction laws (most famously in that of the Milky Way; Cardelli et al., 1989). This so-called ‘UV-bump’ varies from galaxy to galaxy, appearing strongly in the our own galaxy, but not at all in the SMC extinction curve. Its presence in high-redshift galaxies seems equally as uncertain. Evidence from JWST suggests that individual galaxies at $z \sim 6$ (Witstok et al., 2023) can have this feature in their dust attenuation law. Nonetheless, it is clear that no consensus has been reached regarding the typical strength of the UV bump and its potential variation with galaxy properties (Scoville et al., 2015; Shivaei et al., 2020; Salim & Narayanan, 2020), if present at all (Calzetti et al., 2000).
1.2.3 Galaxy morphology

The classification of galaxies based on their morphological features was one of the earliest steps taken in extragalactic astronomy. The ‘Hubble Sequence’ (Hubble, 1926, 1927) classified galaxies primarily as ellipticals or spirals, whereby the former have smooth stellar distributions, and the latter have disk like structures with spiral arms.

There are also irregular (peculiar) galaxies, that alongside spiral galaxies become increasingly common at higher redshifts relative to the passive, elliptical population (Conselice, 2014; Huertas-Company et al., 2023). Star-forming galaxies tend to be spirals and irregular, whereas the older more massive galaxies that are commonly found in large overdense environments (e.g., in large clusters) and have therefore undergone multiple mergers, are typically elliptical (Blanton & Moustakas, 2009).

High-redshift star-forming galaxies can also display significant ‘star-forming clumps’, particularly in rest-frame UV imaging. These clumps arise from localised regions of particularly young and/or intense recent star-formation episodes, leading to the presence of O/B stars which massively outshine the more evolved stars which primarily radiate at longer optical wavelengths. This morphological distinction with wavelength is also noticeable, for example, in narrow band imaging which targets nebular emission lines such as H\(\alpha\) that signposts recent < 10 Myr stellar populations (e.g., see Best et al., 2013; Tadaki et al., 2014).

It is also worth noting that image resolution, in addition to the wavelength probed (discussed above), can pose challenges to morphologically classifying high-redshift galaxies (Conselice, 2014). This has become more evident in the apparent discrepancies between HST and JWST classifications of the same galaxies, and also by the inconsistencies in the observed redshift evolution of different morphological classes (Huertas-Company et al., 2023; Kartaltepe et al., 2023).

1.2.4 The star-forming main sequence

A major early success of SDSS was the confirmation of a clear bimodality in the galaxy population (Strateva et al., 2001; Kauffmann et al., 2003; Baldry et al., 2006), a feature first hinted at by the classification system presented by Hubble
Figure 1.7  The bimodality of the galaxy population is evident in the distinct regions occupied by star-forming galaxies and passive galaxies in the star-formation rate versus stellar-mass (SFR–$M_*$) plane. Star-forming galaxies exist along a relatively tight SFR–$M_*$ sequence, whereas more massive quiescent galaxies are isolated in the ‘red’ cloud. Example colour images showing the typical morphology of star-forming and passive galaxies are also shown in the top-right and bottom-right, respectively. Figure taken from Longair (2023).
This bimodality appears in a number of linked characteristics including the morphology, the observed colour and the star-formation rate, where ‘blue’ galaxies are star-forming and ‘red’ galaxies are passive (quiescent).

Star-forming galaxies (SFG) form a tight, relatively low scatter ($\approx 0.3$ dex) sequence in the SFR − $M_*$ plane (e.g., Daddi et al., 2007; Speagle et al., 2014; Schreiber et al., 2015), separate from the region of parameter space occupied by the massive passive galaxy population, as shown in Fig. 1.7. This ‘star-forming main sequence’ (SFMS) continues out to at least $z \approx 4 – 6$ with smooth monotonic evolution (Schreiber et al., 2015), as shown in the Fig. 1.8. The SFMS also has a characteristic mass turnover, beyond which the SFMS begins to flatten (e.g., see Lee et al., 2015), with growing, but still uncertain evidence that the turnover increases to higher masses with increasing redshift or perhaps disappears altogether (e.g., Schreiber et al., 2015, see also Fig. 1.8).

As a result of the SFMS evolution, star-formation increases with redshift at a fixed stellar mass. This corresponds to a $\sim 1.5 – 2$ dex increase in the average specific star-formation rate ($\text{SSFR} = \text{SFR}/M_*$) from $z \sim 0 – 4$, with further increases into the EOR (Stark et al., 2013). The overall increase in global SSFR is in accordance with theoretical expectations that SSFR is regulated by the gas accretion rate onto a galaxies host dark-matter halo which is higher in the early universe (Davé et al., 2011), however some discrepancies between theory and observations clearly remain (e.g., see right panel of Fig. 1.8).

The exact relation of the SFMS is likely a result of the correlation between the stellar mass of a galaxy and its molecular gas mass, which itself fuels star-formation (Lin et al., 2019). This underlying correlation similarly provides a sound explanation of the characteristic mass turnover, as the fraction of cold molecular gas mass to total decreases with stellar mass (e.g., Popping et al., 2014; Saintonge et al., 2016) likely as a result of mass-quenching feedback in high-mass galaxies (e.g., see Peng et al., 2010).

Passive galaxies inhabit a less well-defined region on the SFR − $M_*$ plane, although are still clustered in a ‘red cloud’. Galaxies that are undergoing quenching, and thus transitioning from star-forming to passive, can exist in-between in the so-called ‘green valley’. Lastly, there is also a population of galaxies with extreme SFRs, lying above the SFMS. These ‘starburst’ galaxies are undergoing an intense burst of star-formation activity in contrast to the steadier rate seen in standard SFMS galaxies. The starburst events are likely triggered by mergers, or possibly
Figure 1.8  **Left:** Evolution of the star-formation main sequence across redshifts $z \sim 0 - 4$ (coloured lines), using a sample of $N > 10^5$ galaxies with imaging spanning $0.35 \mu m < \lambda < 500 \mu m$. Figure taken from Schreiber et al. (2015). **Right:** Redshift evolution of the specific star-formation rate (SSFR), showing a rapid evolution until cosmic noon followed by a more gradual increase into the EOR. Figure taken from Popesso et al. (2023).
by accretion of cold, dense gas and can play a critical role in the subsequent quenching of these systems (Rodighiero et al., 2011).

It should be noted that there are a number of observational challenges in measuring the star-forming main sequence, including the systematic uncertainties faced when estimating accurate SFRs (see Section 1.3.3), and the issue of obtaining representative, mass-complete samples (Sparre et al., 2015; Matthee & Schaye, 2019; Leja et al., 2022).

1.3 The high-redshift galaxy population

Given the vast distances involved to high-redshift galaxies, and the resulting very faint magnitudes, studies of galaxies at high redshift only properly began in the 1990’s. The presence of high-redshift galaxies was investigated theoretically in the 20-30 years prior, but the first of these galaxies were discovered serendipitously. Since then, 1000’s at $z > 5$, 100’s at $z > 7$ and 10’s at $z > 9$ have been identified, primarily by observations with HST, with the numbers further accelerating in the past year with JWST.

Overall, the identification of large samples of high-redshift galaxies is driven by photometry, with spectroscopy then playing a vital role in the confirmation of these candidates, in addition to detailed studies of their physical properties.

1.3.1 Initial searches for high-redshift galaxies

Beyond redshifts of $z \gtrsim 4$, any flux short-wards of the Lyman limit ($\lambda_{\text{rest}} = 912 \, \text{Å}$) in the spectra of galaxies and quasars has been almost entirely attenuated by neutral Hydrogen along the line of sight (e.g., see Madau, 1995). Searches for this feature, named the ‘Lyman break’, formed the foundation of the initial explorations seeking to uncover populations of high-redshift galaxies (e.g., see Steidel & Hamilton, 1992; Madau et al., 1996; Steidel et al., 1996).

A key early demonstration of the success of this method, often called the ‘colour-selection’ or ‘drop-out’ technique, can be found in Steidel et al. (1999), who selected galaxies for spectroscopic follow-up using the $UGR$ filter set. As a result of the Lyman break, there is a very strong ‘drop’ in the broadband flux in the $U$-band filter situated blueward of the break at $z \sim 3$, which when combined with
another filter placed on the break to detect the bright UV continuum of a young star-forming galaxy (e.g., \(G\)-band), will produce a characteristic strong red colour (positive \(U - G\)). Accompanying these two filters straddling the Lyman break, at least one additional filter redward is typically necessary to confirm the presence of the break feature itself, as well as the UV continuum flux blueward of the break (e.g., see Dunlop, 2013). In their pioneering work, Steidel et al. (1999) (see also; Steidel & Hamilton, 1992; Steidel et al., 1996) successfully photometrically selected, and then spectroscopically confirmed galaxies at \(3.0 \leq z_{\text{spec}} \leq 3.5\), thus paving the way for the characteristics of high-redshift galaxy populations as a whole to be measured.

It is worth highlighting that by \(z \gtrsim 5 - 6\), the compounding impact of neutral Hydrogen along the line of sight (particularly entering the highest-redshifts during the EOR) leads to the Ly\(\alpha\) forest becoming a full ‘Gunn-Peterson trough’ (e.g., Gunn & Peterson, 1965) in which all the flux blueward of Ly\(\alpha\) (\(\lambda_{\text{rest}} = 1216\) Å) has been attenuated. The break feature at \(\lambda_{\text{rest}} = 1216\) Å in the highest-redshift galaxies, and the \(\lambda_{\text{rest}} = 912\) Å break seen at intermediate redshifts are both commonly referred to as the ‘Lyman-break’ and galaxies selected using this feature are referred to as ‘Lyman-break galaxies’ (LBGs) - a term almost synonymous with ‘star-forming high-redshift galaxy’ in the modern literature.

**Selection of strong Ly\(\alpha\) emitters**

A complimentary technique used in parallel with ‘drop-out’ surveys is to search for the Ly\(\alpha\) emission in high-redshift SFGs. The Ly\(\alpha\) emission line is expected to be intrinsically strong in high-redshift SFGs as a result of young stellar populations photoionizing their surrounding ISM (Charlot & Fall, 1993).

This technique provided the first success in breaking the \(z > 5\) barrier (Dey et al., 1998) after years of attempts (Koo & Kron, 1980; Pritchet & Hartwick, 1990). Subsequently, deep, wide-area narrowband (NB) imaging with facilities such as Subaru or Keck enabled searches for Ly\(\alpha\) emitters (LAEs) on a scale not yet seen, producing large (\(N \geq 10^3\)) samples of high-redshift galaxy candidates (Ouchi et al., 2005; Murayama et al., 2007; Ouchi et al., 2008). Testimony to the effectiveness of NB-based LAE searches, they are still widely used today to establish large samples of SFGs out to high-redshifts and even during the EOR (e.g., SILVERRUSH, Ouchi et al., 2018; Konno et al., 2018; Goto et al., 2021).
The modern approach: photometric redshifts from SED fitting

With the growth of multi-band imaging datasets, an SED fitting-based approach has become widely used in searches for measuring galaxy redshifts. This approach typically uses a statistical comparison, such as a $\chi^2$ fit, between synthetic photometry derived from a model (template) spectral energy distribution and the observed photometry (e.g., see McLure et al., 2010, 2011) to derive ‘photometric redshifts’. Spectral templates are most commonly constructed from stellar population synthesis models (e.g., Bruzual & Charlot, 2003) with a range of physically motivated ages, metallicities and star-formation histories, followed by accounting for potential dust attenuation or nebular emission (although see Koo, 1999, for examples using empirically-derived templates). By virtue of this approach, in addition to redshift estimates for individual galaxies, important quantities such as stellar mass and star-formation rates can be estimated.

There are a number of distinct benefits in using SED-fitting compared with more traditional ‘drop-out’ methods for high-redshift galaxy searches. Most importantly, it utilises the full photometric information available in contrast to the 3-filter colour-selection method, and as a result can obtain more robust samples with less contaminants. This is shown clearly by Finkelstein et al. (2010), who demonstrate that a pure colour-selection methodology using HST/WFC3 filters (e.g., see Yan et al., 2010) would likely include low-redshift ($z < 6$) contaminants as well as galactic brown dwarfs in a sample of $z \approx 6.5 - 7.0$ SFGs. It is worth noting that extending the colour-selection criteria to utilise a wider suite of filters can be used to alleviate some of the contamination in high-redshift galaxy samples (e.g., Bouwens et al., 2015).

Another advantage offered by template SED fitting is the capacity for a more statistically rigorous procedure. In the maximum likelihood comparisons, a redshift probability distribution is often produced (e.g., EAZY, Brammer et al., 2008), which allows robust errors to be placed on photometric redshifts (and the derived physical properties). Secondary redshift solutions, potentially indicative that an object is a low-redshift contaminant, can also be visible in the redshift PDF and therefore be considered fully. Moreover, a large parameter space of physical properties can also be explored to assess the probability of alternative, but rarer solutions.

There are a number of important considerations to make when SED fitting, some of which can potentially introduce biases into photometric redshift estimates. An
example is the choice of templates to use, which requires assumptions about the stellar population synthesis models and dust attenuation law to be made. Another factor to acknowledge is the growing number of SED-fitting codes available, each with their own set of advantages and drawbacks to consider. A detailed discussion about the advances in SED template-fitting, the specific approach taken with SED-fitting in this thesis, and the associated uncertainties are presented in Chapter 2.

1.3.2 Galaxy luminosity functions

The galaxy luminosity function (LF) is a key statistical distribution describing the galaxy population through its luminosity.

In principle the LF can be measured at any wavelength (e.g., using Hα, Sobral et al. 2016; Lyα, Ouchi et al. 2010; Goto et al. 2021, IR, Reddy et al. 2008; Goto et al. 2019; or at 1.4 GHz radio frequencies, Pracy et al. 2016), but it is much more typical to measure the UV luminosity function (UVLF) in high-redshift galaxies studies, describing the number of galaxies per unit volume, per unit UV magnitude (measured at rest-frame $\lambda \approx 1500$ Å), for example as done in: McLure et al. (2010), McLure et al. (2013), Finkelstein et al. (2015), Bouwens et al. (2015), Bowler et al. (2020).

The UVLF has most commonly been fit using a ‘Schechter function’ parameterisation shown below in Eq. 1.9, which features a power-law slope $\alpha$ describing the number density of galaxies at faint luminosities and a characteristic luminosity $L_*$, with higher luminosity galaxies ($L > L_*$) having an exponential decline in number density. Lastly, there is an overall normalisation of the Schechter function given by $\phi_*$ (Schechter, 1976). This form of the LF was originally derived within the framework of models describing early structure formation (e.g., Press & Schechter, 1974), augmented with the addition of the faint-end slope parameter to better fit the available data;

$$\phi(L) = \phi_* \left( \frac{L}{L_*} \right)^\alpha e^{-L/L_*}$$  \hspace{1cm} (1.9)

Aided massively by HST and other large ground-based surveys, the UVLF has been routinely established up to $z \sim 8$, revealing significant evolution over cosmic time, as shown in Fig 1.9 (Finkelstein et al., 2015). From high-to-low redshift,
the number density of $M_{UV} \sim M_*$ galaxies increases whilst the exponential cut-off of bright galaxies becomes more pronounced and the relative proportion of faint galaxies rises. These changes are evident in the UVLF Schechter fits of Finkelstein et al. (2015) whereby from $z \sim 7$ to $z \sim 4$, $\phi_*$ decreases by a factor $\simeq 9\times$, $M_*$ becomes fainter by $\simeq 0.4$ magnitudues, and $\alpha$ evolves from $\alpha = -2.03$ to $\alpha = -1.56$, respectively. This progression of the UVLF with cosmic time offers a unique insight into the processes governing galaxy evolution, revealing the hierarchical growth of galaxies (increase in $\phi_*$ and flattening of $\alpha$) as well as the early stages of significant AGN-driven and stellar feedback in high- and low-mass galaxies, respectively.

**Uncertainties in the UV luminosity function**

Determining the exact form and evolution of the UVLF still drives an extremely active field of research as it offers unique insight into a number of key open questions regarding the evolution of the earliest galaxies during the EOR and beyond.

Firstly, there has been growing evidence (Finkelstein et al., 2015; Ono et al., 2018; Bowler et al., 2020) that a Schechter function UVLF is in conflict with the excess of bright $M_{UV} \leq -21$ galaxies recently uncovered at $z \geq 7$ (Stefanon et al., 2017, 2019; Donnan et al., 2022). Instead, a double power-law with a steepening bright-end slope has been found to provide a good description of the high-redshift UVLFs across a wide UV magnitude dynamic range ($-23 \leq M_{UV} \leq -17$) (e.g., see Bowler et al., 2020). As first postulated in Bowler et al. (2015), this evolution is consistent with a decrease in dust attenuation and AGN feedback efficiency (see also Bowler et al., 2020). It is worth highlighting here, that such changes in the galaxy population at high-redshift offers a crucial window into the physical processes operating in this epoch (Dayal et al., 2014; Paardekooper et al., 2015).

Secondly, there is still active debate on the faint-end slope $\alpha$ of the UVLF, particularly towards the highest redshifts $z \geq 9$. McLure et al. (2013) show a modest steepening of faint-end slope from $\alpha = -1.9$ to $\alpha = -2.02$ from $z \sim 7 - 8$, consistent with the steady redshift evolution observed at $z \geq 4$ (Bouwens et al., 2015). Beyond $z \sim 8$, the uncertainty in measurements of $\alpha$ is significant and as a result it is unclear if the redshift evolution observed at $4 \leq z \leq 8$ continues to values of $\alpha \simeq -2.4$ at $z \sim 9 - 11$ (Bowler et al., 2020; McLeod et al., 2023). The exact value of $\alpha$ critically impacts the expected number densities of UV-
Figure 1.9 UV luminosity functions at $z = 4, 5, 6, 7$ from Finkelstein et al. (2015), using an ensemble of the deepest available HST imaging surveys, including CANDELS and the UDF12 (e.g., see also McLure et al., 2013), alongside several robust literature UVLF measurements. The best-fitting Schechter (single power-law) function parameterisation is shown as a solid (dashed) red line. Figure taken from Finkelstein et al. (2015).

faint SFGs that may be the dominant sources of ionizing photons in the EOR, and consequently, small changes in $\alpha$ can have important ramifications for reionization models (see Section 1.4).

Moreover, only a limited number of studies have been able to measure the UVLF down to faint magnitudes of $M_{UV} \approx -17$ at $z \approx 6–9$ (e.g., see McLure et al., 2013; Oesch et al., 2018b; Bouwens et al., 2021), which adds significant uncertainty in $\alpha$. The impact of the uncertain faint-end slope is apparent when it is realised that reionization modelling requires integration of the UVLF to $M_{UV} \approx -13$ or fainter to provide the necessary numbers of ionizing photons (e.g., Finkelstein et al., 2019, see also Section 1.4.3).
1.3.3 The cosmic star-formation rate density

Tracking historical levels of star-formation through cosmic time has been a central undertaking in extragalactic astronomy. The most recognisable observational signature of this is perhaps the Madau et al. (1996) (and; Lilly et al., 1996) ‘cosmic star-formation history’ plot that traces the redshift evolution of the cosmic star-formation rate density (CSFD) $\rho_{SFR} (\equiv \psi)$. A more recent version of the cosmic star-formation history from Madau & Dickinson (2014), collating decades of UV- and IR-based observational measurements of $\rho_{SFR}$ is shown in Fig 1.10. These results show a clear rise in the global star-formation rate density over the first 10 Gyr of the Universe’s history, consistent with a $\rho_{SFR} \propto (1 + z)^{-2.9}$ power-law. Following a peak of $\log (\rho_{SFR}/M_\odot yr^{-1}Mpc^{-3}) \approx -0.9$ at $z \approx 2$, there is a steady decline by a factor $\gtrsim 10$ until present day, approximately following the relation $\rho_{SFR} \propto (1 + z)^{2.7}$.

UV-based tracers of star-formation-rate density

At redshifts $z > 2$, beyond the peak of star-formation, $\rho_{SFR}$ is typically inferred from rest-frame UV-based observations (as a result of the superior sensitivity to star-formation of optical / NIR instruments compared with those in the FIR regime). In practice, this is done by first integrating the UV luminosity function to measure the UV luminosity density $\rho_{UV}$, which is then converted into $\rho_{SFR}$ using assumptions about the underlying stellar populations that produce the UV light.

This method can inherently introduce a number of potentially systematic biases. Firstly, integrating the UVLF to infer $\rho_{UV}$ requires an assumption about the upper and lower UV luminosity limits to adopt. The rapid decline in the bright galaxy population alleviates any significant biases introduced by the choice of the $L_{UV,upper}$ (which is commonly set to $L_{UV,upper} = \infty$), however the same is not true for $L_{UV,lower}$ due to the rising abundance of faint galaxies. The steeper, and more uncertain, UVLF faint-end slopes ($\alpha \leq -2$) seen at $z \gtrsim 6$, combined with the relatively arbitrary choice of $L_{UV,lower}$ can introduce significant correction factors (Mesinger et al., 2016).

For $z > 6$ measurements of $\rho_{UV}$ it has been convention to set a lower integration limit equivalent to $M_{UV} = -17$, corresponding to the approximate detection limits of ultra-deep HST galaxy surveys (McLeod et al., 2016, 2023). Future
Figure 1.10  Redshift evolution of the cosmic star formation rate density ($\psi \equiv \rho_{\text{SFR}}$), compiling SFR tracers based on FUV ($\lambda \sim 1500$Å, green, blue and magenta markers) and IR ($\lambda \sim 70-160$µm, orange and red markers) wavelength regimes. All measurements have been corrected for systematic biases, and calibrated using a Salpeter IMF (e.g., see Section 1.3.3). The CSFD history can be described by a rise from $z \sim 8$ to $z \sim 3$ given as $\rho_{\text{SFR}} \propto (1+z)^{-2.9}$, with a turnover at $z \sim 2$, followed by a decline to present day following $\rho_{\text{SFR}} \propto (1+z)^{2.7}$. Figure taken from Madau & Dickinson (2014).
analyses utilising of JWST’s deeper imaging will be required to extend UVLF measurements to fainter magnitudes (see also Livermore et al., 2017), a necessary step to reduce uncertainties on reionization models, as discussed in Section 1.4.2.

The impact of dust attenuation is also particularly acute for measurements of $\rho_{UV}$. Typical dust attenuation at $z \sim 2$ can reach $\approx 1$ dex (Reddy et al., 2008; Bouwens et al., 2012), which if uncorrected, would result in values of $\rho_{SFR}$ underestimated by $\sim 1$ dex due to the intrinsic UV light being attenuated by dust. Although robust dust corrections can be made (evident from the UV- and FIR-based $\rho_{SFR}$ consensus; Madau & Dickinson, 2014), there are still practical challenges. In particular, dust corrections based on UV slopes (Reddy et al., 2018a; McLure et al., 2018a) are often limited by photometric-filter coverage (Rogers et al., 2013), and those derived from SED-fitting can additionally be biased by the age-dust-metallicity degeneracy.

Reassuringly, the challenge of correcting for dust attenuation lessens beyond $z \gtrsim 3$ due to the decreasing levels of attenuation with redshift (Bogdanoska & Burgarella, 2020).

The challenge of measuring star formation rates

The conversion of $\rho_{UV}$ to $\rho_{SFR}$ necessitates various assumptions about the underlying young stellar population that dominates the UV continuum of galaxies. In fact, this challenge of choosing appropriate assumptions whilst avoiding systematic biases is mirrored more generally in making estimates of SFRs for individual galaxies as a whole.

The conversion is usually calculated as $\text{SFR} \approx K_{UV} \times L_{UV}$, where $K_{UV}$ is derived for a stellar population of a given age ($t_{age}$), star-formation history, IMF, and metallicity ($Z_*$) (Kennicutt, 1998; Kennicutt & Evans, 2012). Fundamentally, UV-based SFR tracers measure the rate at which more massive stars are formed as these are the stars that dominate the total UV output. This is then converted to a global, integrated SFR representing the full star-formation dictated by the IMF. A more top-heavy (or bottom-light) IMF (producing a greater proportion of stars with larger masses) will therefore have a lower value of $K_{UV}$, as a higher proportion of the stellar population is ‘represented’ in the total UV emission of the galaxy (e.g., see Fig. 4 in Madau & Dickinson, 2014).
Similar differences in $K_{UV}$ are seen in stellar populations of various ages and metallicities. In the latter case, lower $Z_*$ stars produce relatively more UV light (due to hotter stellar atmospheres), resulting in differences of up to $\Delta(K_{UV}) \sim 0.4$ between a solar metallicity ($Z_* = Z_\odot$) stellar population and one with $Z_* = 0.1 Z_\odot$.

The value of $K_{UV}$ will vary with $t_{\text{age}}$, particularly if $t_{\text{age}} \lesssim 20$ Myr as the most massive O-type stars will still be present and significantly boost the galaxy UV luminosity. Adding further complexity, the exact SFH can significantly alter the age-dependence of $K_{UV}$. An example of this is presented in Madau & Dickinson (2014), whereby a constant SFH produces a relatively steady $L_{UV}$ at $t_{\text{age}} \gtrsim 100$ Myr after an initial rise, in comparison with an initial burst (simple stellar population) SFH which has a steadily declining $L_{UV}$ after only 2–3 Myr.

It is worth reiterating that each of these factors influence measurements of a galaxy SFR due to their connection with the numbers and properties of the young O/B stars producing the bulk of the UV photons. It is therefore true that they will also impact the estimated number of ionizing photons produced, and as such, will be a factor of uncertainty in measurements of LyC $f_{\text{esc}}^{\text{LyC}}$ and models of the reionization history more generally (see Section 1.4.3).

### 1.3.4 The ultra-high redshift frontier

**Pushing the limits of HST**

With the deepest HST data available, the UVLF and subsequently the evolution in $\rho_{\text{SFR}}$ was inferred out to redshifts $z \sim 8$ with minimal controversy (McLure et al., 2013; Bouwens et al., 2015; McLeod et al., 2016; Oesch et al., 2018b; Bouwens et al., 2021). Before the recent first light of JWST, gathering robust statistical samples of galaxies beyond this redshift limit was extremely difficult due to the 1.6 $\mu$m wavelength cutoff of HST. Additionally, due to the extreme faintness of such galaxies, any searches at these redshifts demanded huge telescope time commitments (e.g., HUDF, Ellis et al. 2013; HFF, Lotz et al. 2017) to obtain sufficient imaging depth and coverage for photometric redshifts, and more again if these objects were to be spectroscopically confirmed.

A specific observational challenge that arose was the lack of mid-infrared capabilities with HST and the current generation of 8–10m class ground-based observatories. Specifically, due to the lack of cooling on HST and subsequent high
background noise, imaging at wavelengths beyond $\lambda \approx 1.6 \mu m$ is not feasible, leaving only $2-3$ filters of deep, high-resolution, space-based imaging fully redward of the Lyman-break in $z \gtrsim 8$ galaxies. Longer wavelength constraints then relied on ground-based imaging (e.g., using MOSFIRE/Ks or HAWK-I/Ks imaging; Brammer et al. 2016), or lower-resolution, shallower Spitzer/IRAC imaging spanning $\lambda \sim 3.6-4.5 \mu m$ (e.g., Ashby et al., 2013; Stefanon et al., 2021).

This combination of limited wavelength coverage and/or inhomogeneous depths and resolution hampered the search for higher-redshift samples, and consequently led to a number of disagreements regarding the evolution of $\rho_{SFR}$ at the highest redshifts. Specifically, the limited data available was unable to distinguish between a rapid exponential decline in $\rho_{SFR}$ at $z > 8$, as favoured by Oesch et al. (2013, 2018b), or a more gradual decline (continuing the trend seen at $z \sim 6-8$), advocated by McLeod et al. (2015, 2016) (see also Section 1.3.2 for uncertainties at both the bright- and faint-end of the UVLF). It is interesting to note that such discrepancies are similarly present among a range of galaxy simulation and theoretical model predictions (e.g., Paardekooper et al. 2015; Mason et al. 2015; Yung et al. 2019; Kannan et al. 2022b in favour of a rapid decline, and Behroozi & Silk 2015; Wilkins et al. 2023 supporting a gradual fall-off beyond $z \sim 8$, see also Fig. 8 in McLeod et al. 2023).

The first year of progress with JWST

With JWST/NIRCam (Rieke et al., 2023) alone, the wavelength regime beyond the $\lambda \sim 1.6 \mu m$ limit of HST has been transformed, granting orders of magnitude improvements over the best surveys carried out using Spitzer/IRAC, in both imaging depth and resolution. Using NIRCam imaging taken in its first year of operation, a significant number of $z > 10$ galaxy candidates have rapidly been identified (e.g., see Castellano et al., 2022; Donnan et al., 2022; Finkelstein et al., 2022a; Harikane et al., 2022; Naidu et al., 2022; Adams et al., 2023; Donnan et al., 2023) - a subset of which have already been confirmed spectroscopically (Arrabal Haro et al., 2023a,c; Harikane et al., 2023; Robertson et al., 2023).

Accompanying progress on pushing the $z > 10$ ultra-high redshift frontier, an important accomplishment of JWST is the discovery of $\gtrsim 10^2$ galaxy candidates at $z > 8$ (Hainline et al., 2023; Harikane et al., 2023; McLeod et al., 2023), allowing the debate about the evolution of $\rho_{SFR}$ to be settled for the first time. Using a combination of wide-area, ground-based UltraVISTA DR5 data with ERO+ERS
NIRCam imaging, Donnan et al. (2022); Harikane et al. (2023) provide the first JWST-derived evidence for a smooth, gradual decline in $\rho_{SFR}$. This result was then conclusively confirmed by McLeod et al. (2023), using a large ensemble of 13 public JWST/NIRCam datasets spanning $> 250$ arcmin$^2$.

Interestingly, the JWST-enabled improvements of the UVLF have allowed the transition from a Schechter to a double power-law parameterisation, first postulated by Bowler et al. (2015, 2020), to be confirmed (see also; McLeod et al., 2023). Moreover, in addition to strengthening evidence for a lack of evolution in the bright-end slope, a steep faint end slope ($\alpha \leq -2$) now appears to be favoured.

1.4 The frontier of extragalactic research: The Epoch of Reionization

The Epoch of Reionization (EOR) is one of the major phase transitions that occurred in the Universe’s history, during which the neutral gas that permeated the Universe became ionized by the first generations of stars and the emerging galaxy population. Reionization likely started at $z \sim 10-15$ (Robertson, 2021), with the first generation of so-called ‘Population III’ stars that formed at $z \sim 20-30$ likely playing an initial role as the earliest sources of ionizing photons and metals (Sokasian et al., 2004; Karlsson et al., 2013). Observations of the Ly$\alpha$ forest in high-redshift quasars, as discussed in Section 1.4.2, confidently place the end of reionization at $z \simeq 5-6$, with the highly-ionized state of the IGM persisting to the present day (Fan et al., 2006; Bosman et al., 2021; Goto et al., 2021).

1.4.1 The link between the EOR and galaxy evolution

The Epoch of the Reionization marks the era in which nascent galaxies, for the first time, significantly shape the IGM. At first, the intense UV emission from the dust and metal-free stellar populations of young SFGs would have created small, localised ionized regions defined by their Strömgren spheres. These ‘bubbles’ would initially grow relatively slowly as early sources would have formed in locations of cosmic over-densities with correspondingly faster than average recombination timescales (e.g., Barkana & Loeb, 2001; Hayes & Scarlata, 2023, however see also Section 1.4.3).
Figure 1.11  THESAN simulation snapshots centered on three different mass haloes (top to bottom), visualising the evolution of the IGM from mostly neutral (red) at $z = 9$ to almost entirely ionized (blue) at $z = 6$ (left to right). The progress of reionization by ionizing photons can be clearly seen. Figure courtesy of the THESAN Collaboration.
As star-formation ramped up, fueled by the abundance of gas in early dark-matter haloes (Finlator et al., 2011), so too did the net ionizing emissivity of the young galaxy population, driving the expansion of the ionized bubbles. Eventually, these bubbles began to overlap and merge, a process that accelerated the global transition from neutral to ionized. The EOR ends when the vast majority of the IGM is highly ionized, with only small pockets of neutral Hydrogen in dense, self-shielded regions remaining ($\ll 1\%$; e.g., see Keating et al., 2020; Bosman et al., 2021, 2022), some of which persist to low redshift as evidenced by the existence of Damped Ly$\alpha$ systems (DLAs) and the Ly$\alpha$ forest (McQuinn, 2016).

A key goal of reionization studies has been piecing together the timeline of reionization, or in other words; what is the redshift evolution of the global neutral Hydrogen fraction ($Q_{\text{HI}}$)? There has been progress in answering this question as detailed in Section 1.4.2, with significant constraints placed on the endpoint of reionization (Bosman et al., 2021; Goto et al., 2021) and its approximate mid-point (Planck Collaboration et al., 2020). Nevertheless, no clear consensus has been reached on the reionization timeline between $z \approx 6 - 9$, with either a rapid, late reionization, or an earlier starting, more gradual reionization both plausible scenarios.

Additional complexities are introduced as a result of the expected ‘patchy’ reionization process, leading to sizeable spatial variations in the evolution of the neutral Hydrogen fraction. Furthermore, the exact properties of the galaxies that contributed most to the ionizing photon budget is not agreed upon (see Section 1.4.2).

These uncertainties and complexities shed light on the interconnected co-evolution of the IGM and young galaxy population during the EOR. The IGM served as the vital reservoir of gas that fueled star-formation, subsequently propelling forward the early stages of galaxy evolution. Conversely, star-formation fueled by the IGM in this era was the driving force of its reionization and chemical enrichment, which then impacted future waves of star-formation - highlighting the intricate relationship of feedback processes between the IGM and young galaxies during the EOR.
1.4.2 The sources of ionizing photons during the EOR

The dominant role of SFGs over quasars during the EOR

Since the end of the epoch of reionization at \( z \sim 5 - 6 \), the IGM has remained in a highly ionized state, (McQuinn, 2016). At redshifts \( z \leq 3 \) quasars supply the vast majority of ionizing photons needed, whilst a combined contribution from both quasars and star-forming galaxy population at \( z > 3 \) provide the required ionizing emissivity (Becker & Bolton, 2013).

During the EOR the relative roles of AGN and SFGs in producing the bulk of the LyC (\( E_\gamma \gtrsim 13.6 \) eV) photon budget has historically been contested (Madau et al., 1997; Madau, 1998; Ricotti & Shull, 2000; Miralda-Escudé et al., 2000; Volonteri & Gnedin, 2009; Robertson et al., 2010; Finkelstein et al., 2019). However, recent progress investigating the high-redshift quasar population has shown the number density of quasars (and fainter AGN) drop rapidly at higher redshifts (Aird et al., 2015; Parsa et al., 2018; McGreer et al., 2018; Kulkarni et al., 2019; Faisst et al., 2019; Maiolino et al., 2023). Compounded with measurements of low AGN LyC escape fractions (e.g., \( f_{\text{esc}}^{\text{LyC}} \sim 1\% \); Iwata et al., 2022), there is now a general consensus that star-forming galaxies at \( z > 6 \) are the principal source of LyC photons driving reionization (Chary et al., 2016; Robertson, 2021).

Democratic versus oligarch-driven reionization?

Although the SFG versus quasar contribution debate has somewhat settled, a number of new questions have arisen. Specifically, to gain a full picture of the epoch of reionization, it is vital that the properties of the underlying galaxy population are established and fully understood in the context of their connection to the timeline of reionization (e.g., their LyC escape fraction, see Section 1.5).

Promisingly, studies have shown these galaxies tend to be highly-star-forming, relatively dust-poor and low metallicity (McLure et al., 2011; Dunlop et al., 2013; Stark, 2016; Endsley et al., 2022; Cullen et al., 2023). Nonetheless, the quantity of ionizing photons produced by the young stellar populations and the fraction of these LyC photons that are able to go on to ionize the surrounding IGM (i.e., \( \xi_{\text{ion}} \) and \( f_{\text{esc}}^{\text{LyC}} \), see Section 1.5) are a source of significant uncertainty in the process of reionization and how it is interlinked with galaxy evolution.
Moreover, the contributions of various sub-populations of galaxies remains unclear. The analytical study by Robertson et al. (2010) (building on earlier work by Madau et al., 1999) suggested that a significant amount of the UV photon budget must come from very faint galaxies (with a moderately high LyC escape fraction of $f_{\text{LyC}}^{\text{esc}} \approx 0.2$), beyond the detection limit of existing surveys to magnitudes as faint as $M_{\text{UV}} \approx -13$ (a ‘democratic’ reionization). More recent literature, for example by Naidu et al. (2020), suggest that massive ‘oligarchs’ (with $M_{\text{UV}} \leq -18$) produce the bulk of the ionizing photon budget – highlighting the ongoing debate surrounding the identity of the galaxies that powered reionization.

The details of the relative contributions to the ionizing photon budgets from various populations of galaxies play a crucial role in the redshift evolution of the neutral Hydrogen fraction. Combining constraints from Planck Collaboration et al. (2020) and $\rho_{\text{SFR}}$ results from the deepest HST imaging campaigns (e.g., McLure et al., 2013; Bouwens et al., 2015; McLeod et al., 2015), Robertson et al. (2015) produced a reionization timeline in which the faint galaxy population down to magnitudes $M_{\text{UV}} \lesssim -13$ with $f_{\text{LyC}}^{\text{esc}} \approx 0.2$ were required to complete reionization by $z \sim 5.5 - 6$. Similarly, Finkelstein et al. (2019) show that such a faint population of galaxies is required to alleviate the need for $f_{\text{LyC}}^{\text{esc}} \gtrsim 20\%$ that is not currently favoured in direct measurements of $f_{\text{LyC}}^{\text{esc}}$ in SFGs at $z \leq 4$ (e.g., Pahl et al., 2021; Begley et al., 2022; Meštrič et al., 2021, see also Section 3).

In models with the faint, more numerous population of galaxies dominating the total ionizing photon budget, there tends to be a more gradual, steady evolution of the volume-averaged neutral Hydrogen fraction over $6 \leq z \leq 10$, sometimes with the early stages (i.e., up to $Q_{\text{HII}} \sim 0.1 - 0.2$) extending to $z \gtrsim 10$ (e.g., Robertson et al., 2015; Finkelstein et al., 2019). A gradual, steady reionization history is in reasonable agreement with neutral Hydrogen fraction constraints based on a number of Ly$\alpha$ emitter fraction studies (Pentericci et al., 2014; Schenker et al., 2014a; Tilvi et al., 2014; Pentericci et al., 2018b) that infer $Q_{\text{HI}}$ based on comparing the number of galaxies expected to produce strong intrinsic Ly$\alpha$ emission with the number actually observed.

Contrary to this picture, Mason et al. (2019) (see also: Mason et al., 2018a; Hoag et al., 2019) place a (1$\sigma$) lower limit of $Q_{\text{HI}} > 0.76$ at $z \sim 7.9$ using the distribution of observed Ly$\alpha$ equivalent widths (describing the relative intensity of the Ly$\alpha$ emission relative to the underlying stellar continuum flux), which supports an alternative, more rapid but later reionization history. Such a reionization history
Figure 1.12  Redshift evolution of the neutral Hydrogen fraction from Mason et al. (2019), showing their Bayesian inference constraints, based on Lyα observations (see also Mason et al., 2018a), in red. The inferred $Q_{\text{HI}}$ values from a variety of literature tracers are also shown (i.e., Lyα emitter fraction, LAE clustering, quasar dark pixel fraction and damping wings, and the $\tau$-based Planck Collaboration et al. (2020) constraint). Model reionization histories from Mason et al. (2015) are shown as coloured lines.
can still occur when the ionizing photon budget is dominated by fainter galaxies (e.g., see Mason et al., 2019; Lewis et al., 2022; Rosdahl et al., 2022; Umeda et al., 2023), however the possibility of UV-bright ‘oligarchs’ taking this role has recently gained some traction (Naidu et al., 2020).

The primary assumption of this ‘oligarch’ driven model is the inferred correlation \( f_{\text{esc}}^{\text{LyC}} \propto \Sigma^{0.42} \) (see Naidu et al., 2020, for details), that was initially motivated by the high SSFR’s seen among confirmed LyC emitters (e.g., Flury et al., 2022a, see also Yoo et al. (2020); Pahl et al. (2022) for less optimistic \( f_{\text{esc}}^{\text{LyC}} \propto \Sigma_{\text{SFR}} \) results), as well as the drop in \( \rho_{\text{SFR}} \) predicted by Oesch et al. (2018b). The resultant model favours a late, rapid reionization history consistent with \( Q_{\text{HI}} \) constraints at \( z \sim 7 – 8 \) from Ly\( \alpha \) equivalent width distributions (Mason et al., 2019; Hoag et al., 2019) and quasar Ly\( \alpha \) forests (McGreer et al., 2015).

In spite of this apparent agreement with a number of \( Q_{\text{HI}} \) constraints, the oligarch model appears to be inconsistent with mounting evidence that the abundant faint population of galaxies significantly contribute to, or dominate, the total ionizing photon budget required to power reionization. Both SPHINX and CoDa III, which are two independent state-of-the-art radiation-hydrodynamical simulations of the EOR, predict that faint \( M_{\text{UV}} \gtrsim -18 \) galaxies produce the bulk of LyC photons at \( z > 6 \) (Rosdahl et al., 2022; Lewis et al., 2022, respectively, see also Hutter et al. 2021; Ocvirk et al. 2021; Trebitsch et al. 2023; Mutch et al. 2023).

Moreover, a ‘democratic’ reionization is in accordance with the \( M_\ast – f_{\text{esc}}^{\text{LyC}} \) anti-correlations shown in some simulations (Paardekooper et al., 2015; Xu et al., 2016; Yoo et al., 2020). The drop in \( f_{\text{esc}}^{\text{LyC}} \) with mass is also consistent with the low \( f_{\text{esc}}^{\text{LyC}} \) constraints on a small sample of bright JWST \( z \sim 7 \) galaxies by Witten et al. (2023), and tentative \( M_\ast – f_{\text{esc}}^{\text{LyC}} \) anti-correlations uncovered from direct LyC measurements at \( z \sim 3 – 4 \) (Begley et al., 2022; Pahl et al., 2022).

A complicating factor in this apparently simple \( M_\ast – f_{\text{esc}}^{\text{LyC}} \) relation is that feedback is expected to significantly disrupt star-formation (and hence limit LyC production) in low-mass regimes (e.g., see Hutter et al., 2021), and so a turnover in this relation is likely (e.g., at \( M_\ast \approx 10^7 M_\odot \) Rosdahl et al., 2022). Such a turnover is also found by Ma et al. (2020) in the FIRE-2 simulation suite, albeit with more equitable contributions to the ionizing photon budget across the galaxy population. A more balanced contribution from both faint and brighter galaxies is a likely scenario, backed by evidence that low (high) mass galaxies are the primary source of LyC photons earlier (later) in the reionization history (Lin et al., 2023; Yeh et al., 2023)
The topology of reionization

In addition to ‘first order’ constraints on the global volume-averaged $Q_{\text{HI}}$ evolution, early steps have been taken in probing the ‘second order’ spatial structure (and timing) of reionization observationally (Pentericci et al., 2018a; Tang et al., 2023; Umida et al., 2023), building on previous theoretical predictions (Barkana & Loeb, 2001; Iliev et al., 2009; Friedrich et al., 2011). Constraining the topology of reionization is vital to inform the level of variance (Gnedin & Kaurov, 2014) on certain neutral fraction estimates (e.g., quasar or GRB sightlines and Ly$\alpha$ visibility Leonova et al. 2022; Jung et al. 2022). Furthermore, the topology (as well as the local reionization history) is closely tied to the properties of the sources that drove reionization (Qin et al., 2021; Larson et al., 2022; Lu et al., 2023; Witstok et al., 2023; Whiter et al., 2023). A number of simulations (Ocvirk et al., 2020; Rosdahl et al., 2022), and observational probes (e.g., higher visibility of brighter galaxies; see Jung et al., 2022), show that reionization likely played out in an ‘inside-out’ topology, whereby the largest haloes ionized earlier (Katz et al., 2019). Many of the models described above, and indeed the large-scale simulations, take as input, or are tuned to reproduce, the latest constraints on the neutral Hydrogen fraction evolution (see Fig. 1.12).

1.4.3 The physics of reionization

The reionization timeline from both models and observations has mainly been tracked through the evolution of the globally-averaged ionized hydrogen fraction. Treating the IGM as a two-phase medium, with an ionized fraction $Q_{\text{HII}}$, and a neutral fraction $Q_{\text{HI}}$ (related as $Q_{\text{HII}} = 1 - Q_{\text{HI}}$), the evolution of $Q_{\text{HI}}$ can be approximately modelled using the equation below that encapsulates the balance between the sources of ionizing photons and the recombination of HII (Madau et al., 1999);

$$\dot{Q}_{\text{HI}} = \frac{n_{\text{ion}}}{\langle n_H \rangle} - \frac{Q_{\text{HII}}}{t_{\text{rec,HI}}}$$  \hspace{1cm} (1.10)

where $n_{\text{ion}}$ is the ionizing photon density, $\langle n_H \rangle$ is the mean cosmic Hydrogen density, and $t_{\text{rec}}$ is the Hydrogen recombination timescale.

In reality the EOR is governed by a range of physically complex and interlinked processes, in contrast to the apparent simplicity of Equation 1.10. Firstly, gas
in the IGM is highly inhomogeneous due to hierarchical structure formation
and therefore contains significant density variations. Denser regions of gas have
shorter recombination timescales, and can lead to ‘self-shielded’ regions of the
IGM which remain neutral for an extended time. The impact of an inhomogenous
IGM is usually characterised through the ‘clumping factor’, \( C_{\text{HII}} \equiv \langle n_{\text{H}}^2 \rangle / \langle n_{\text{H}} \rangle^2 \),
such that the average recombination timescale at redshift \( z \) is given as;

\[
\bar{t}_{\text{rec}} = [C_{\text{HII}} \alpha_B(T)(1 + 2\chi)n_{\text{H}}(1 + z)^3]^{-1}
\] (1.11)

where \( \alpha_B(T) \) is the case B recombination coefficient (assuming temperatures of \( T \sim 10^5 \) K) and \( \chi \) is the cosmic He-to-H abundance ratio. The exact value (and
potential evolution) of \( C_{\text{HII}} \) adopted, which depends heavily on photoheating of
the IGM by the UV background (e.g., see Pawlik et al., 2009; Finlator et al., 2012),
can have a considerable impact on the end stages of reionization, as outlined
in Robertson et al. (2013). Although it remains an uncertainty in reionization
modelling, values of \( C_{\text{HII}} \approx 3 \) produce \( Q_{\text{HII}} \) evolution histories consistent with
observations (Robertson et al., 2013, 2015).

Much like the clumpiness of the IGM, the ionizing flux distribution produced by
young star-forming galaxies traces the structure of the cosmic web, and is also
highly spatially inhomogeneous (e.g., see Fig.1.11). Furthermore, the physical
properties and population statistics of SFGs, now widely assumed to be the
dominant drivers of reionization (Chary et al., 2016; Mason et al., 2018a; Faisst
et al., 2021; Robertson, 2021), are the main source of uncertainty in \( n_{\text{ion}} \), and
therefore in the reionization equation. Based on this assumption, the source term
\( n_{\text{ion}} \) in Eq.1.10, can be written as;

\[
n_{\text{ion}} = f_{\text{esc}}^{\text{LyC}} \cdot \xi_{\text{ion}} \cdot \rho_{\text{UV}}
\] (1.12)

where \( f_{\text{esc}}^{\text{LyC}} \) is the escape fraction of (ionizing) LyC photons, \( \xi_{\text{ion}} \) is the ionizing
photon production efficiency, and \( \rho_{\text{UV}} \) is the UV luminosity density. The ionizing
photon production efficiency \( \xi_{\text{ion}} \), describes the number of ionizing photons
produced per unit UV luminosity, and is defined as the ratio \( \xi_{\text{ion}} = N(H^0) / L_{\text{UV}} \),
with \( L_{\text{UV}} \) being the UV luminosity at \( \sim 1500\text{Å} \) and \( N(H^0) \) is the absolute rate
of production of ionizing (LyC) photons. The UV luminosity density \( \rho_{\text{UV}} \) is
calculated from the UV luminosity function, which can now be measured out to
early EOR redshifts (see Section 1.3.4).
The UV luminosity density $\rho_{UV}$

Reionization timeline models (e.g., see Robertson et al., 2015; Finkelstein et al., 2019) commonly use empirical measurements of $\rho_{UV}$, derived from compilations of UVLFs (e.g., Bouwens et al., 2015) when calculating $\dot{n}_{ion}$.

As discussed in Section 1.3.3, the conversion from a UVLF to $\rho_{UV}$ requires a number of assumptions about the underlying stellar population (e.g., Madau & Dickinson, 2014), including metallicity, the star-formation history and the IMF. These assumptions can contribute uncertainties in $\rho_{UV}$ and therefore in $\dot{n}_{ion}$ estimates.

Additional uncertainties on $\rho_{UV}$ arise due to open questions about the UVLF faint-end slope $\alpha$ - does it become significantly steeper at the highest redshifts (Bouwens et al., 2023) and does it remain steep at the faintest magnitudes (Livermore et al., 2017; O'Shea et al., 2015)?

The latter is particularly relevant for reionization models showing a dominant contribution to the ionizing photon budget from faint galaxies (see also Section 1.4.2). For example, Finkelstein et al. (2019) demonstrate a relatively low $f_{esc}^{LyC} \approx 5\%$ galaxy population can complete reionization by $z \sim 6$, if UVLF integration limits as faint as $M_{UV} \approx -13 \rightarrow -11$ are used. However, if the UVLF faint-end has a turnover at $M_{UV} \sim -15$ (e.g., due to feedback in the low-mass halo regime), as suggested by O'Shea et al. (2015) (see also; Yue et al., 2016; Bouwens et al., 2017), other reionization model assumptions would need to be explored.

The ionizing photon production efficiency $\xi_{ion}$

In Eq.1.12, $\xi_{ion}$ converts the UV luminosity density measurable through the UVLF to a number of LyC photons produced by the underlying galaxy population.

Canonically, values in the range $\log(\xi_{ion} / \text{erg s}^{-1} \text{Hz}) \sim 25.2 - 25.3$ have been adopted in models of the reionization timeline (e.g., Robertson et al., 2013), which has been backed up by observational constraints from Stark et al. (2015) and Bouwens et al. (2015), although these observational measurements have found significant scatter in $\xi_{ion}$ across the galaxy population (e.g., Robertson et al., 2013, see also Wilkins et al. 2016).
The large variation in $\xi_{\text{ion}}$ is likely a result of its high sensitivity to the properties of the underlying stellar population, varying dramatically with metallicity and the IMF, as well as the stellar population age, SFH and the degree of binarity (Eldridge et al., 2017; Stanway & Eldridge, 2018; Eldridge & Stanway, 2022).

These properties can all lead to elevated $\xi_{\text{ion}}$ values. For example, Schaerer et al. (2016) (see also: Emami et al., 2020a; Maseda et al., 2020; Saxena et al., 2023; Simmonds et al., 2023) find $\xi_{\text{ion}}$ values $\sim 2 - 5\times$ higher than those canonically assumed in reionization models (e.g., Robertson et al., 2013) for a sample of known Lyman continuum emitters (LCEs) with low metallicity and young stellar populations. Naturally, an increase in the typical $\xi_{\text{ion}}$ boosts the net LyC photon budget, relieving the need for a strong redshift evolution to higher $f_{\text{esc}}^{\text{LyC}}$ values during EOR (e.g., Khaire et al., 2016), and potentially easing the reliance on an extremely faint, currently undetected, population of galaxies.

### 1.5 The Lyman continuum escape fraction

**The importance of the LyC escape fraction during reionization**

Of the three main components for calculating $n_{\text{ion}}$ in Eq. 1.12, the LyC escape fraction $f_{\text{esc}}^{\text{LyC}}$ is the most challenging to measure, and therefore represents a significant uncertainty for reionization models (e.g., Robertson et al., 2015).

Based on the current best $\rho_{\text{UV}}$ constraints and adopting canonical values for $\xi_{\text{ion}}$ in EOR galaxies, values as high as $\langle f_{\text{esc}}^{\text{LyC}} \rangle \approx 20\%$ or greater have been found to be necessary for reionization to have been completed by $z \approx 6$ (Ouchi et al., 2010; Bunker et al., 2010; Haardt & Madau, 2012; Finkelstein et al., 2012). Despite arguments for an elevated average $\xi_{\text{ion}}$ in EOR galaxies and suggested reionization models with less stringent requirements (e.g., $f_{\text{esc}}^{\text{LyC}} \approx 5 - 10\%$; Finkelstein et al., 2019), there are still major uncertainties surrounding the value of $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ across the galaxy population below $z \sim 3.5$ where direct measurements are possible (e.g., see Mestrić et al., 2021).

As discussed in Section 1.4.2, variations in $f_{\text{esc}}^{\text{LyC}}$ with galaxy properties can drastically influence the reionization history. The relative contributions to the ionizing photon budget reaching the IGM from either faint, or UV-bright early star-forming galaxies, is heavily modulated by $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ in these sub-
populations. Recent observational and theoretical progress aimed at establishing which properties are correlated with higher $f_{\text{esc}}^{\text{LyC}}$, and can therefore be used as indicators of LyC leakage is discussed in Section 1.5.4.

1.5.1 Direct measurements of the LyC escape fraction

The opacity of the IGM to ionizing photons increases rapidly with redshift (Madau, 1995; Inoue et al., 2014) making direct detections of LyC photons challenging at $z = 3 - 4$, and practically impossible at higher redshifts. Observations of LyC emission in the local Universe are equally as challenging. As a consequence of the Earth’s atmosphere, rest-frame FUV observations at low-redshift must be carried out with space-based instruments (e.g., GALEX, Martin et al. 2003 and HST/COS, Green et al. 2003; in addition to facing other observational challenges, see Leitherer et al., 2016). Moreover, the properties of the evolved galaxy population at $z \sim 0$ are not generally conducive to high LyC production and escape (e.g., Razoumov & Sommer-Larsen, 2010), although analogues of high-redshift galaxies can be found (see Section 1.5.2).

Regardless of these challenges, direct constraints are needed to properly calibrate models of the reionization history and the sources that powered it, and as such the various spectroscopic and photometric campaigns aimed at measuring $f_{\text{esc}}^{\text{LyC}}$ in $z \lesssim 3.5$ galaxies are vital.

Initial successes in measuring $f_{\text{esc}}^{\text{LyC}}$ were found in individual LCE galaxies such as Haro 11 (Bergvall et al., 2016), Q1549-C25 (Shapley et al., 2016), the Sunburst galaxy (Rivera-Thorsen et al., 2019; Vanzella et al., 2021) and Ion 1–3 (Vanzella et al., 2010a, 2012, 2016a; de Barros et al., 2016; Ji et al., 2020), with escape fractions ranging from $f_{\text{esc}}^{\text{LyC}} \sim 3\%$ to $f_{\text{esc}}^{\text{LyC}} \gtrsim 50\%$. These galaxies are rare and often display extreme properties (e.g., with $\beta \approx -2.5$ Vanzella et al., 2018). As a result, the typical $f_{\text{esc}}^{\text{LyC}}$ was still elusive, as was the properties that correlated with $f_{\text{esc}}^{\text{LyC}}$ across the SFG population as a whole.

A number of deep $U$–band imaging campaigns on larger scales have allowed samples of potential LCE candidates to be identified (Meštric et al., 2020; Fletcher et al., 2019) at $z \gtrsim 3$, however these samples have generally been dominated by LyC non-detections, which typically only allow upper limits on $f_{\text{esc}}^{\text{LyC}}$ to be calculated (Guaita et al., 2016; Grazian et al., 2017; Saxena et al., 2021).
Deep rest-frame FUV spectroscopy has had more success. First presented in Steidel et al. (2018), the Keck Lyman Continuum Survey (hereafter KLCS) identified new samples of LyC candidates, and constrained the sample-averaged escape fraction to be $⟨f_{\text{LyC}}^\text{esc}⟩ = 0.09 \pm 0.01$ for a large sample of $N \approx 120$ SFGs at $z \sim 3$. This estimate was later revised by Pahl et al. (2021) to $⟨f_{\text{LyC}}^\text{esc}⟩ = 0.06 \pm 0.01$, after the removal of low-redshift contaminants.

A major issue faced in these studies generally is contamination, in which low-redshift interlopers masquerade as LyC leaker detections (e.g., the $\lambda_{\text{rest}} > 1500$ Å flux of a $z \sim 1.5$ galaxy, misidentified as a $z \sim 3.5$ galaxy with significant LyC flux). This problem was acutely demonstrated by Mostardi et al. (2015), who obtained follow-up, high-resolution HST imaging of 16 LyC candidates originally selected from ground-based NB imaging. In this study, > 90% of their sample (15/16) contained foreground objects giving a false LyC signal.

The origin of contamination in LyC samples can be either foreground objects unresolved in ground-based imaging or galaxies with incorrect redshifts. Both these problems are alleviated by obtaining high-resolution imaging of the targets (for example using HST), in addition to having spectroscopic confirmation of the galaxy redshift (Siana et al., 2015; Shapley et al., 2016; Begley et al., 2022). Spectroscopic samples with UV (non-ionizing) HST imaging have now produced contamination free samples of LyC candidates at high-redshift (Steidel et al., 2016; Naidu et al., 2017; Meštrić et al., 2020).

**Overcoming the high-opacity IGM**

Measuring $f_{\text{LyC}}^\text{esc}$ for individual objects can be subject to systematic biases and large uncertainties, even with a high signal-to-noise LyC detection, due to the high stochasticity of the IGM (Inoue et al., 2014; Steidel et al., 2018; Bassett et al., 2021, 2022). Nevertheless, $⟨f_{\text{LyC}}^\text{esc}⟩$ constraints can still be made using statistical samples that allow large fluctuations in sightline opacity to be averaged over.

Using a narrow-band imaging stack consisting of $N \approx 100$ galaxies, Guaita et al. (2016) set an upper limit of $⟨f_{\text{LyC}}^\text{esc}⟩ \lesssim 0.05$, a typical result from stacking $U$–band imaging, which has provided mostly upper limits. Stacking has been more successful in samples comprised of LyC detections (e.g., see Fletcher et al., 2019, measuring $⟨f_{\text{LyC}}^\text{esc}⟩ \approx 0.2$ for a sample of $N \approx 10$ strong [OIII] emitters at $z \approx 3.1$). However, these $⟨f_{\text{LyC}}^\text{esc}⟩$ constraints are not representative of typical
galaxy samples which are dominated by LyC non-detections (either due to lack of imaging depth and/or intrinsically low $f_{\text{esc}}^{\text{LyC}}$). Moreover, sample size itself is not sufficient to provide robust constraints on $\langle f_{\text{esc}}^{\text{LyC}} \rangle$, as demonstrated by Meštrić et al. (2021) in a meta-analysis of more than two decades of collated data. They show that the vast majority of studies, even those based on deep spectroscopy, have returned $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ only upper limits.

Both the apparent very low average intrinsic $\langle f_{\text{esc}}^{\text{LyC}} \rangle$, and the high opacity of the IGM have been, and remain, challenges on the path to understanding how $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ varies across the full galaxy population. A method to help overcome some of these challenges centres around a statistical treatment of the IGM, primarily in the form of simulating a large number of model sightlines through the IGM (Inoue et al., 2014) and the circumgalactic medium (CGM; e.g., see Steidel et al., 2018). From these sightlines, an average transmission through the IGM based on the sightline statistics can then be calculated (e.g., as in Steidel et al., 2018; Pahl et al., 2021), or these sightlines can be included individually through a Monte Carlo and/or Bayesian approach (e.g., Begley et al., 2022, see Chapter 3). It is worth highlight that including the contribution of the CGM in attenuating the LyC flux from a galaxy is important, as it can impact the overall transmissivity by up to $\sim 10\%$ (Steidel et al., 2018). It should be noted that a statistical treatment of this sightline approach can still cause biases in $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ constraints for small sample sizes of galaxies with LyC detections, given they are inherently more likely to correspond to more transmissible sightlines (Bassett et al., 2021, 2022).

**Alternative measurements of the Lyman-continuum escape fraction**

Complimentary to direct rest-frame LyC emission imaging of galaxies, there are a number of alternative methods for assessing $f_{\text{esc}}^{\text{LyC}}$ that have recently been explored. One such method assesses the impact of SFGs on the IGM itself as a means to measure $f_{\text{esc}}^{\text{LyC}}$. Developed initially by Kakiichi et al. (2018), and extended by Meyer et al. (2020), cross correlations between SFGs and sightlines with low opacity (measured via distant quasars) were used to place constraints of $f_{\text{esc}}^{\text{LyC}} = 0.23^{+0.46}_{-0.12}$ at $z = 5.5 - 6.4$, significantly beyond the $z \sim 4$ upper limit for direct LyC detections and importantly, during the end stages of reionization.

Another alternative technique involves exploiting the distinct emission characteristics of Gamma-Ray Burst (GRB) events, which have intrinsic afterglow spectra consistent with a power-law. As a consequence, GRB bursts offer an avenue for
Figure 1.13  Top: Three examples of the HST/COS NUV acquisition images used in the Low-redshift Lyman Continuum Survey (LzLCS). The 2.5 arcsec COS spectroscopic apertures, and 5 kpc scale lines are also plotted. The left, middle, and right galaxies are examples of a non-emitter, a marginally detected LCE and a strongly detected LCE, respectively. Bottom: The FUV COS spectra for the same three objects as the top panel, generally showing the $800 \lesssim \lambda_{\text{rest}} \lesssim 1200$ Å rest-frame wavelength range. the LyC flux wavelengths, and a number of key FUV emission line features are marked. Figure taken from Flury et al. (2022a).

quantifying $f_{\text{LyC}}^{\text{esc}}$ within their host galaxies, as explored by Tanvir et al. (2019), by searching for observed deviations in their power-law spectra.

Anticipating future prospects, several other probes of the IGM will become available over the coming years. These include leveraging 21 cm radio emission, that originates from neutral gas, using future state-of-the-art observatories such as HERA (DeBoer et al., 2017), LOFAR (van Haarlem et al., 2013; Best et al., 2023), and SKA (Braun et al., 2015). These observations will enable the direct measurements of the the neutral Hydrogen fractions, thereby allowing more precise constraints of the timeline on reionization and the typical $\langle f_{\text{esc}}^{\text{LyC}} \rangle$ of the underlying galaxy population.
1.5.2 Local analogues

Motivated in-part by the increasing opacity of the IGM at higher-redshifts, a significant number of investigations have been carried out aiming to establish the LyC properties of low-redshift \((z \lesssim 0.5)\) galaxies, including \(f_{\text{esc}}^{\text{LyC}}\) and its correlations with other key galaxy properties. Low-redshift studies also present the opportunity for more spatially resolved observations that can allow the detailed intricacies of LyC escape mechanisms to be more closely scrutinised.

Observations using the HST Cosmic Origins Spectrograph (COS) instrument have produced small samples of low-redshift LCEs (e.g., see Izotov et al., 2016b,a, 2018b, 2021; Wang et al., 2020). A more comprehensive exploration of potential LCEs was carried out within the Low Redshift Lyman Continuum Survey (LzLCS) (Flury et al., 2022a,b). Notably, the selection criteria for galaxies targeted by LzLCS are based on distinctive properties that typically indicate more highly-ionizing conditions including: blue UV slopes, elevated star-formation rate surface densities \(\Sigma_{\text{SFR}}\) and high \([\text{O} \, \text{iii}]/[\text{O} \, \text{ii}]\) ratios. These properties, while rare across the broader low-redshift galaxy population, crucially make these low-redshift samples analogues of high-redshift galaxies. Additionally, selecting galaxies based on these properties has proven to be a successful strategy for identifying LyC leakers within the LzLCS dataset.

Using the LzLCS sample at \(z \approx 0.3\), Flury et al. (2022b) find a robust correlation between the escape fraction of Ly\(\alpha\) and LyC photons. This finding aligns with the simulations using an idealized clumpy geometry by Dijkstra et al. (2016) and the detailed hydrodynamical simulations of Kimm et al. (2019), in addition to a suite of other observational studies (e.g., Vanzella et al., 2016b; Verhamme et al., 2017; see also Section 1.5.4).

The LzLCS survey, facilitated by its deep FUV spectroscopy, has further enabled the exploration of various proxies and potential indicators that shed light on the mechanisms underlying the common escape of Ly\(\alpha\) and LyC photons. In particular, the findings emphasise the pivotal roles of neutral gas and dust properties in regulating these escape processes (Flury et al., 2022b; Saldana-Lopez et al., 2022a, see also; Chisholm et al. 2018; Gazagnes et al. 2020a), offering valuable guidance for future observations.

Additionally, observations at low redshifts have highlighted the potential significance of so-called ‘green pea’ (GP) galaxies exhibiting strong nebular \([\text{O} \, \text{iii}]\)
emission. These GPs share properties more commonly associated with high-redshift counterparts and have garnered attention as promising candidates for LyC emitters (e.g., see Cardamone et al., 2009; Schaefer et al., 2016; Izotov et al., 2018a).

1.5.3 The physics of LyC escape

Both simulations and detailed observations (primarily with spectra) have informed our understanding of the conditions that facilitate LyC escape. The simplest physical scenario in which LyC photons can escape is described by a ‘density-bounded’ geometry, in which the stellar population producing LyC photons is encased in a shell of ISM gas that has been fully photoionized by the stars within (Zackrisson et al., 2013). Any photons leftover from ionizing the surrounding ISM can then escape the region and travel (potentially) onward into the IGM. This is known as the ‘density-bounded’ H II region model (Nakajima & Ouchi, 2014). An obvious simplification made in this model picture is that a galaxy is highly unlikely to consist simply of a population of stars surrounded by a uniform shell of gas, whereas in reality it will be a collection of gas and stars spatially mixed, with differing properties of both. This geometrical set-up appears to be rare in reality, with little observational evidence, beyond possibly the most extreme $f_{\text{LyC}}$ (Gazagnes et al., 2020a; Ramambason et al., 2020) and it is generally inconsistent with inferences about the gas distribution inferred from UV metal lines as well as H I lines (e.g., see Reddy et al., 2018a).

A more realistic physical scenario relative to the density-bounded, is the an ‘ionization-bounded’ geometry with holes. In this scenario LyC photons only escape through ‘channels’ in the ISM, thought to be created by stellar feedback from supernova, stellar winds, or potentially by turbulence (photoionization regions during a starburst, Kakiichi & Gronke 2021), or perhaps an (intrinsically) already-present low-density ISM regime (Jaskot et al., 2019). In the ionization-bounded scenario, $f_{\text{esc}}^{\text{LyC}}$ is simply given by $(1 - f_c)$, where $f_c$ is the covering fraction, which describes the fraction of the galaxy obscured by a screen of non-ionized gas. Again this model geometry is certainly oversimplified by lacking an inhomogeneous mixing of gas and stars.

Both of these geometrical scenarios are only valid simplifications for galaxies with no dust, which even for galaxies during the EOR is relatively rare. Accounting for dust is important as even small amounts of dust can significantly attenuate
UV and LyC photons alike. To account for dust in the ionization-bounded model, a simple dust screen coincident with HI regions can be included in the modelling of this system, commonly known in the literature as the ‘holes’ model (e.g., see Reddy et al., 2016; Steidel et al., 2018; Pahl et al., 2021). The model is parameterised as below:

\[ S_{\nu,\text{obs}} = S_{\nu,\text{intr}} \left[ (1 - f_c) + f_c \cdot e^{-\tau_1} \cdot 10^{-A_\lambda/2.5} \right] \]  

(1.13)

where \( S_{\nu,\text{obs}} \) and \( S_{\nu,\text{intr}} \) are the observed and intrinsic spectra, respectively, \( f_c \) is the covering fraction of H I gas, \( \tau_1 \) is the optical depth due to H I gas and \( A_\lambda \) is the attenuation (in magnitudes) due to dust. This model is physically motivated and supported by correlations observed between Ly\( \alpha \) emission and the low-ionization-state (LIS) absorption lines (which traces neutral HI). An alternative model to this, also including the impact of dust, is an ionization-bounded ‘screen-model’, or simply ‘screen model’ (Steidel et al., 2018) in which the dust also impacts the regions with HII coverage (rather than just tracing the fraction screened with HI gas), modelled as:

\[ S_{\nu,\text{obs}} = 10^{-A_\lambda/2.5} \cdot S_{\nu,\text{intr}} \left[ (1 - f_c) + f_c \cdot e^{-\tau_1} \right] \]  

(1.14)

The latter has been shown to explain the relatively low \( f^{\text{LyC}}_{\text{esc}} \) seen in low-redshift SFGs (Chisholm et al., 2018; Gazagnes et al., 2020a), however it is not fully clear if one model or the other should take preference, with evidence supporting both (Steidel et al., 2018; Saldana-Lopez et al., 2022b).

The ‘holes’ and ‘screen’ models are the two models currently explored in detail in the literature. It is worth noting that distinguishing between the two, and more generally between any of the potential geometries, requires deep, rest-frame UV continuum spectra with high enough resolution to measure absorption line features. Obtaining such spectra for significant sample sizes is observationally very expensive, compared with obtaining LyC-target imaging that enables direct \( f^{\text{LyC}}_{\text{esc}} \) constraints. It is therefore clear that a combination of both will be required to gain a full understanding of \( f^{\text{LyC}}_{\text{esc}} \), both for tracing the changes in global galaxy properties such as \( M_{\text{UV}} \), dust and UV slope (\( \beta \)), and investigating the detailed processes that regulate LyC escape through UV line-diagnostics.
1.5.4 Links between galaxy properties and LyC escape

Establishing if reionization was dominated by a large population of UV faint, low-mass galaxies, or by a minority of rare ‘oligarchs’ will require robust inferences of the $f_{\text{LyC}}^{\text{esc}}$ of these galaxies during the EOR. Due to the opacity of the IGM at $z \gtrsim 3.5$, $f_{\text{LyC}}^{\text{esc}}$ measurements will have to be through robustly calibrated ‘tracers’ of high LyC leakage. Uncovering which galaxy properties correlate with $f_{\text{esc}}^{\text{LyC}}$ also offers a unique insight into the physical mechanisms that facilitate LyC escape, as well as the complex interplay between star-formation and the ISM conditions.

Correlations between global galaxy properties, such as stellar mass ($\log(M_*/M_\odot)$), UV magnitude ($M_{\text{UV}}$), or UV slope ($\beta$) and $f_{\text{esc}}^{\text{LyC}}$ are potentially the most desirable, if present, given they can be readily measured at EOR redshifts (e.g., Bouwens et al., 2012; McLure et al., 2013; Dunlop et al., 2013; Rogers et al., 2013; McLeod et al., 2016; Bhatawdekar & Conselice, 2021; Cullen et al., 2022). Large-scale simulations (Kimm & Cen, 2014; Wise et al., 2014; Paardekooper et al., 2015) generally suggest that $f_{\text{esc}}^{\text{LyC}}$ decreases towards higher masses, owing primarily to the increase in dust (the increased gravitational potential in more massive galaxies also makes the formation of transparent channels in ISM more difficult e.g., see Section 1.5.3). This aligns well with the significant relations seen between $f_{\text{esc}}^{\text{LyC}}$ and the level of dust attenuation $E(B-V)$ (Steidel et al., 2018; Pahl et al., 2022; Saldana-Lopez et al., 2022c) as well as the UV slope $\beta$ which indirectly probes dust attenuation (Begley et al., 2022).

Tentative evidence of a relatively weak $\log(M_*/M_\odot) - f_{\text{esc}}^{\text{LyC}}$ correlation was found by Begley et al. (2022, see also Chapter 3). This was later shown to be in agreement with Pahl et al. (2022), who find a $\approx 2\times$ decrease in $f_{\text{esc}}^{\text{LyC}}$ over $\log(M_*/M_\odot) \approx 9 - 10$ in KLCS. This observed mass-dependence disfavours the ‘oligarch’ model suggested in Naidu et al. (2020).

In practice, it is unlikely that stellar-mass alone could be used as a robust indicator of high $f_{\text{esc}}^{\text{LyC}}$. Using detailed zoom-in radiation-hydrodynamical simulations (FIRE-2), Ma et al. (2020) find a similar anti-correlation between stellar mass and $f_{\text{esc}}^{\text{LyC}}$ at $\log(M_*/M_\odot) \gtrsim 8$, however they also show a similar decrease in $f_{\text{esc}}^{\text{LyC}}$ towards low stellar masses. In low-mass galaxies, the reduced star-formation efficiency impacts the formation of low-density photoionized sightlines in the ISM through which LyC escapes. The predicted drop in $f_{\text{esc}}^{\text{LyC}}$ at lower stellar masses has not yet been tested observationally, owing to current limits on the dynamic
range of masses observed (e.g., $M_\ast/M_\odot \approx 10^{8-10}$ in Begley et al., 2022; Pahl et al., 2022).

All simulations predict that there should be substantial scatter in $f_{\text{esc}}^{\text{LyC}}$ with global galaxy properties (e.g., stellar-mass) as a whole (Ma et al., 2020), indicating that LyC escape is governed by processes that play out on smaller scales within local regions of the ISM with active star-formation. To this end, a number of authors have investigated the nebular emission properties of galaxies showing strong and weak $f_{\text{esc}}^{\text{LyC}}$ alike. One promising connection has been with strong [O III] emission, measured through high equivalent widths $W_\lambda([\text{O III}])$ or high $[\text{O III}] / [\text{O II}]$ ratios ($O_{32}$). More extreme [O III] properties are associated with higher $\xi_{\text{ion}}$ in high-redshift analogues locally (Vanzella et al., 2016c; Izotov et al., 2018c), and indeed for $z > 2$ galaxies (Tang et al., 2019, 2021b) and during the EOR itself (Endsley et al., 2021, 2023). Kewley et al. (2019) attribute these extreme [O III] conditions to the presence of density-bounded H II regions, which can enable high $f_{\text{esc}}^{\text{LyC}}$ (e.g., see Zackrisson et al., 2013; Jaskot et al., 2019).

In fact, it may be the case that high $O_{32}$ is a prerequisite for significant LyC leakage as put forward by Nakajima & Ouchi (2014). However, establishing $O_{32}$ as a clear-cut $f_{\text{esc}}^{\text{LyC}}$ indicator has proven evasive, with conflicting results between in independent observations (Naidu et al., 2020; Saxena et al., 2021).

The most promising indicator, backed by observations showing relatively robust correlations with $f_{\text{esc}}^{\text{LyC}}$, is the Ly$\alpha$ emission line. Mostardi et al. (2013) demonstrated that LAEs are more likely to have higher $f_{\text{esc}}^{\text{LyC}}$ than their LBG counterparts (see also Marchi et al., 2017; Begley et al., 2022). This finding was robustly confirmed by Steidel et al. (2018) and Pahl et al. (2021), showing a relatively tight relation given by $f_{\text{esc}}^{\text{LyC}} \approx 0.53 W_\lambda(\text{Ly} \alpha)$.

The connection between LyC escape and Ly$\alpha$ has been extensively studied from a simulation and theoretical perspective. Radiative transfer simulations by Kimm & Cen (2014) and Wise et al. (2014), capturing the complex physics of the resonant Ly$\alpha$ emission line, demonstrate that both Ly$\alpha$ and LyC escape through the ‘cleared-out’ channels in the ISM. This has been confirmed observationally by Chisholm et al. (2018) using deep rest-frame-FUV spectra to show that the escape of LyC/Ly$\alpha$ is closely linked with the geometry of the ISM (see also Shapley et al. 2003; Gazagnes et al. 2020a). This is further backed-up by observations demonstrating that the peak separation of the Ly$\alpha$ emission is an excellent indicator of $f_{\text{esc}}^{\text{LyC}}$ (Verhamme et al., 2017; Izotov et al., 2020; Hu et al., 2023).
It is worth highlighting that accurately interpreting Lyα observations is challenging due to its resonant nature and sensitivity to the underlying ionization conditions (e.g., see Smith et al., 2019; Hayes et al., 2023). Firstly, star-forming galaxies have been shown to possess significantly extended Lyα ‘haloes’ (Hayes et al., 2013). In these cases, a non-negligible proportion of the total Lyα emission has escaped through repeated absorption and scatterings, rather than through channels in the ISM (Marchi et al., 2019; Rasekh et al., 2022). Secondly, Lyα escape is also sensitive to gas kinematics (Hayes, 2015), such as outflows (Dijkstra et al., 2016) or turbulence (Kimm et al., 2019). It is therefore not a guarantee that intense Lyα emission is accompanied by high $f_{\text{esc}}^{\text{LyC}}$. As a result, there will undoubtedly be scatter in any correlation between LyC escape and the escape of Lyα photons, as shown in simulations by Dijkstra et al. (2016); Maji et al. (2022) and observationally (e.g., Verhamme et al., 2017; Chisholm et al., 2018; Flury et al., 2022b; Saldana-Lopez et al., 2022b).

Establishing the Lyman-continuum escape fraction (and the ionizing photon production rate) is vital for accurately tracing the timeline of reionization. Significant progress has been made, with direct estimates of $f_{\text{esc}}^{\text{LyC}}$ being made in high-redshift SFGs at $z \gtrsim 3$ (Pahl et al., 2021; Begley et al., 2022, see Chapter 3), and explorations of properties that can indicate non-zero $f_{\text{esc}}^{\text{LyC}}$ being carried out (e.g., Flury et al., 2022b; Pahl et al., 2022; Begley et al., 2023, see Chapter 4). Nonetheless, a number of key uncertainties remain. Measurements of $f_{\text{esc}}^{\text{LyC}}$ are restricted to relatively small samples of galaxies, and its connection with a wide dynamic range of physical properties is limited, which motivates deeper, and more extensive studies into the ionizing properties of star-forming galaxies.

### 1.6 Thesis outline

As referenced throughout this introduction, the core theme of this thesis is on obtaining a better understanding of the Lyman-continuum escape fraction from high-redshift star-forming galaxies. In Chapter 2, I summarise the VANDELS survey which is a key observational dataset that forms the backbone of the work throughout the entirety of this thesis. I also discuss the key analysis methods used in both imaging and spectroscopic data, including photometry and SED modelling to infer galaxy properties. Lastly, this chapter describes the JWST Cosmic Evolution ERS Survey (CEERS), a public program released in the first year of JWST’s operations which we utilise in the final chapter.
The subsequent three chapters comprise the scientific contents of the thesis. In Chapter 3, I present the body of work published in Begley et al. (2022) in which I measure the average Lyman-continuum escape fraction ($\langle f_{\text{LyC}}^{\text{esc}} \rangle$) of a sample of spectroscopically confirmed star-forming galaxies at $z \approx 3.5$, selected from VANDELS. Combining observations from ultra-deep, ground-based $U$–band imaging and high resolution HST $V$–band imaging, with a novel, empirically motivated model, I place robust constraints on $\langle f_{\text{LyC}}^{\text{esc}} \rangle$ and its correlations with stellar-mass, UV luminosity and importantly, Lyman-alpha emission.

Motivated by the correlation between Lyman-alpha ($\text{Ly} \alpha$) and Lyman-continuum ($\text{LyC}$) emission properties in Chapter 3, I explore the $\text{Ly} \alpha$–$\text{LyC}$ connection further in a sample of $z \approx 4–5$ SFGs in Chapter 4 (Begley et al. 2023). By comparing the observed $\text{Ly} \alpha$ emission strength measured directly using VANDELS rest-frame far-ultraviolet spectra, to the predicted intrinsic $\text{Ly} \alpha$ production from robust photometric SED modelling, I place constraints on the $\text{Ly} \alpha$ escape fraction ($f_{\text{esc}}^{\text{Ly} \alpha}$) for individual galaxies. This chapter concludes with inferences on $f_{\text{esc}}^{\text{LyC}}$, based on the strength of low-ionization-state absorption lines detected in stacked spectra of the VANDELS sample, and how it is connected with the escape of $\text{Ly} \alpha$ photons.

In addition to uncertainties about the Lyman continuum escape fraction of SFGs, there are questions remaining about the production rate of ionizing photons in galaxies, and more specifically, which galaxies dominate the bulk of the ionizing photon budget necessary to drive the reionization epoch. To this end, in Chapter 5 I investigate redshift evolution of the $[\text{O III}]+\text{H} \beta$ equivalent width of SFGs across the redshift range $2 \lesssim z \lesssim 8$, combining galaxy samples from VANDELS, CEERS and the wider literature. Within this analysis, I also explore trends between galaxy physical properties and their $W_\lambda([\text{O III}]+\text{H} \beta)$ that can provide key insight into the ionizing photon production efficiency of high-redshift SFGs.

To conclude, Chapter 6 summarises the main findings and implications of the research presented in the thesis. I also include details of future avenues of exploration that I will pursue to further our understanding of galaxy evolution during the Epoch of Reionization.
Chapter 2

Observational datasets and techniques

In this Chapter, I briefly highlight the key observational datasets and analysis techniques used in this thesis. The VANDELS survey is used throughout the entirety of the thesis, forming the backbone of the work presented in Chapters 3, 4 and 5, and is outlined below. I also summarise the key aspects of the JWST CEERS survey, which I use to measure the [O III] + Hβ emission properties of high-redshift galaxies during the EOR (see Chapter 5). Following this, I introduce the key imaging and spectroscopic data analysis methods used throughout the thesis, including photometry and spectral energy distribution modelling.

2.1 Key datasets

2.1.1 The VANDELS survey

The VANDELS dataset formed the backbone of the observational data used throughout this thesis, providing a vital sample of spectroscopically confirmed galaxies, accompanied by robust multi-wavelength photometry that was used across the three main science chapters.

In Chapter 3 (e.g., see Begley et al., 2022), I use a VANDELS star-forming galaxy sample selected in the redshift range $3.35 \leq z_{\text{spec}} \leq 3.95$, where ground-
based VIMOS/\textit{U}–band imaging probes the ionizing emission. In this work VANDELS provided the necessary spectroscopic confirmation to help produce a contamination-free sample, in addition to allowing vital measurements of the Ly\textalpha\ equivalent width and the UV spectral slope, both of which are found to correlate with LyC escape.

Following on from this work in Chapter 4 (e.g., see Begley et al., 2023) I further investigate the Ly\textalpha–LyC connection, where again, VANDELS provides the vital observed Ly\textalpha flux properties that are needed to infer the Ly\textalpha escape fraction in a sample of SFGs at $4.85 \leq z_{\text{spec}} \leq 4.95$. Moreover, with the deep far-ultraviolet spectra from VANDELS, the FUV absorption features can be measured allowing indirect constraints on $f_{\text{esc}}^\text{LyC}$ to be placed.

Lastly, in Chapter 5 (Begley et al. 2023b, in prep.) I combine a sample of VANDELS SFGs at $3.2 \leq z_{\text{spec}} \leq 3.6$ with a sample of high-redshift $z_{\text{phot}} \approx 7.0–7.6$ galaxies selected from the JWST/CEERS (see Section 2.1.2) survey to measure the redshift evolution of the [O\textsc{iii}]+H\textbeta\ equivalent width distribution. Combined with robust spectral energy distribution fits enabled by the VANDELS multi-wavelength photometry, I also able to investigate how [O\textsc{iii}]+H\textbeta emission line properties vary across the galaxy population.

VANDELS is an ESO public spectroscopic survey (Programme ID 194.A-2003, Co-PIs: R. J. McLure, L. Pentericci), primarily described in McLure et al. (2018b); Pentericci et al. (2018a) and Garilli et al. (2021). The final data release of VANDELS (DR4; Garilli et al., 2021) comprises of $N = 2087$ spectroscopic redshifts in the range $1.0 \leq z_{\text{spec}} \leq 7.0$, based on ultra-deep optical spectra ($0.48 \mu m < \lambda_{\text{obs}} < 1.0 \mu m$) taken with the Visible MultiObject Spectrograph (VIMOS; Le Fèvre et al., 2003) on the ESO Very Large Telescope (VLT). The survey primarily targeted galaxies in three categories; 1) a bright ($i_{\text{AB}} < 25$) star-forming galaxy sample in the redshift range $2.4 \leq z \leq 5.5$ 2) a large statistical sample of $3.0 \leq z \leq 7.0$ faint SFGs ($25 \leq H_{\text{AB}} \leq 27$, $i_{\text{AB}} \leq 27.5$), and 3) a sample of massive, passive galaxies at redshifts $1.0 \leq z \leq 2.5$ with $H_{\text{AB}} \leq 22.5$. Lastly, a small sample of AGN and FIR \textit{Herschel}-detected sources were also observed. Throughout the thesis, I focus specifically on the star-forming galaxy sample.

These targets were selected within the Chandra Deep Field South (CDFS) and UKIDSS Ultra Deep Survey (UDS) fields, which have central footprints covered extensively by deep optical and NIR HST imaging taken by the CANDELS survey (Grogin et al., 2011; Koekemoer et al., 2011), as shown in Fig. 2.1. Targets in
Figure 2.1  Schematic of the VANDELS footprint, observed in 8 VIMOS pointings split evenly between the CDFS and UDS fields (overlaid quadrants). The central background region in each field is deep HST $H$-band imaging from the CANDELS survey (Koekemoer et al., 2011; Grogin et al., 2011), while the wider-area region is ground-based $H$-band imaging from the UKIDSS (UDS; Almaini, 2005) and VISTA VIDEO (CDFS; Jarvis et al., 2013) surveys. Figure taken from McLure et al. (2018b).
Figure 2.2  The filter profiles for the imaging used to construct multi-wavelength photometry catalogues in the four VANDELS regions (CDFS-HST, CDFS-GROUND, UDS-HST, UDS-GROUND, top to bottom panels). The CANDELS survey photometric catalogues (Guo et al., 2013; Galametz et al., 2013) were used for the central regions (see Fig. 2.1). On the other hand, newly constructed catalogues based on a variety of deep publicly available ground-based imaging were used for the wider VANDELS footprint (McLure et al., 2018b). Each region has $N_{\text{band}} = 13 - 20$ photometric bands, with wavelength coverage spanning $0.35 \mu m \lesssim \lambda \lesssim 4.5 \mu m$. In addition to the CANDELS HST coverage, wide-area imaging from a range of ground-based observatories was assembled and used to select target galaxies across the entire VIMOS footprint (McLure et al., 2018b), leading to four VANDELS regions spanning a total area of $\approx 0.2 \text{deg}^2$; CDFS-HST, CDFS-GROUND, UDS-HST, UDS-GROUND. As the full VANDELS area also benefits from deep Spitzer/IRAC imaging (Ashby et al., 2013), each target galaxy benefitted from photometry spanning the wavelength range $0.35 \mu m \lesssim \lambda_{\text{obs}} \lesssim 4.5 \mu m$, in at least $N \gtrsim 13$ filters (e.g., as shown in Fig. 2.2).

Each VANDELS galaxy was observed for $t_{\text{int}} \approx 20 - 80 \text{hrs}$, designed to achieve an approximately uniform signal-to-noise ratio of at least $\gtrsim 5 - 10$ per resolution.
element across the entire sample, with a SNR $\gtrsim 7$ for $\approx 80\%$ of the galaxies achieved in the DR4 release (Garilli et al., 2021). The depth of the VANDELS spectra allowed redshift measurements for almost all of the targets (each with a redshift quality flag), and enabled detailed measurements of physical properties for the bright star-forming and massive, passive galaxy samples, often an individual galaxy basis.

In addition to the of the multi-wavelength catalogues and spectroscopic redshifts, VANDELS DR4 also included physical properties (e.g., stellar mass, SFR and dust attenuation) derived from robust SED fitting using BAGPIPES (Carnall et al., 2018). The details of the SED fitting procedure are outlined in Garilli et al. (2021), however it should be noted that throughout this thesis I have performed my own SED-fitting procedures designed specifically for the science goals I have pursued.

**Key successes of VANDELS**

VANDELS is the deepest high-redshift, ground-based spectroscopic program ever undertaken, thus enabling state-of-art studies on the properties of high-redshift galaxies.

The high SNR spectra have allowed UV absorption and emission lines to be measured on individual galaxies as well as in stacked spectra of continuum-faint sources. Both Marchi et al. (2017) and Calabrò et al. (2022) investigated the ISM gas kinematics of $z \gtrsim 3$ VANDELS SFGs, finding direct evidence that the emerging Ly$\alpha$ is heavily influenced by H$\text{I}$ gas densities and outflows, and that inflows as well as gas turbulence play a vital role in the overall gas kinematics seen at $z > 2$.

Using VANDELS rest-frame FUV spectra combined with novel stellar metallicity inferences, Cullen et al. (2019) measured the stellar mass-metallicity relation (MZR) for the first time at $z > 2$, revealing significant evolution from the local MZR, in addition to establishing a robust Ly$\alpha$--$Z_*$ correlation (Cullen et al., 2020). When combined with NIRVANDELS, a rest-frame optical spectroscopic follow-up program, the VANDELS FUV spectra enabled the gas-phase and stellar metallicities to be measured concurrently (Cullen et al., 2021). This subsequently provided the first direct evidence of $\alpha$--enhancement in $z > 3$ SFGs, building on independent work at lower redshifts (Steidel et al., 2016; Topping et al., 2020).
Accurate reconstructions of the SFHs of massive, quiescent galaxies at $z \approx 1$ using VANDELS data (Carnall et al., 2019) have provided vital observational tests of the AGN-feedback models in cosmological simulations. Moreover, the SFHs have been used to measure formation and quenching redshifts, with the oldest VANDELS galaxy estimated to have formed during the EOR at $z_{\text{form}} \approx 7.02^{+3.06}_{-2.07}$ (Hamadouche et al., 2023).

Lastly, and importantly for the goals of this thesis, VANDELS has provided a significant legacy dataset with a large number of spectroscopic redshifts as well as continuum spectroscopy. As detailed in Begley et al. 2022 (see also Chapter 3 & Section 1.5), spectroscopic confirmation is vital for robust decontamination of the galaxy samples used in $f_{\text{esc}}$ measurements. Spectroscopic redshifts across large samples also help eliminate systematic uncertainties in SED fitting, and thus improve physical property measurements. As highlighted in Begley et al. (2022, 2023) (see also; Saldana-Lopez et al., 2022b), the VANDELS spectroscopic Ly{$\alpha$} measurements (as well as the FUV absorption features and continuum) have been indispensable in piecing together the physics of LyC escape in SFGs.

### 2.1.2 CEERS - The Cosmic Evolution ERS Survey

The Cosmic Evolution Early Release Science Survey (CEERS; Finkelstein et al., 2023, see also Bagley et al. (2023) for a detailed discussion of the NIRCam Epoch 1 data release) is a JWST early release science program (ID 1345, PI: S. Finkelstein) over the Extended Groth Strip (EGS) field - one of the legacy HST CANDELS fields.

In Chapter 5, the CEERS imaging provides one of the two key datasets (along with VANDELS) used to measure the evolution of the [O{III}]$+$H{$\beta$} equivalent width distribution from redshift $z \approx 3.2 - 7.6$. The CEERS NIRCam imaging, specifically at $\lambda_{\text{obs}} \gtrsim 2\mu$m, offers a significant improvement over the deepest Spitzer/IRAC imaging available prior to the launch of JWST. In turn, I am able to both uncover, and measure the physical properties of galaxies in the EOR (and beyond) more efficiently than ever before. As detailed in Chapter 5, I use photometry measured from the CEERS data to first select galaxies at $7.0 \leq z \leq 7.6$ using robust photometric redshift measurements. For this sample, the deep F410M medium-band imaging enables accurate photometric measurements of the [O{III}]$+$H{$\beta$} emission lines to be measured.
CEERS consists of 10 JWST/NIRCam pointings, totaling an area of $\approx 100$ arcmin$^2$, and parallel observations using both the NIRSpec (MSA spectroscopy; 6/10 pointings) and MIRI (imaging; 4/10 pointings) instruments. In addition, 4 pointings of MIRI imaging are taken, in parallel with Wide Field Slitless Spectroscopy (WFSS) using NIRCam. The observations for CEERS were taken in two ‘Epochs’ due to the scheduling constraints imposed by the survey design (to maximise the CANDELS HST imaging overlap). NIRCam imaging from epoch 1 ($\approx 40$ arcmin$^2$) was used in Chapter 5 of this thesis specifically, which consisted of pointing IDs 1, 2, 3 and 6 in the CEERS survey layout shown in Fig. 2.3.

Each of the NIRCam pointings consist of six broadband filters (F115W, F150W, F200W, F277W, F356W and F444W) and the F410M medium-band filter, providing deep ($m_{AB} = 28.0 - 28.6$; McLeod et al., 2023), high resolution imaging across a $1.0 \, \mu m \leq \lambda \leq 5.0 \, \mu m$ wavelength range. The CEERS imaging used in this work was reduced (courtesy of D. Magee) using the PRIMER Enhance NIRCam Image Processing Library (PENCIL; Magee et al., in preparation) software tool.
The PENCIL package is based on the standard JWST NIRCam reduction pipeline (v1.6.2, pmap >0989), with additional functionality added to tackle a number of the artifacts commonly seen in NIRCam imaging; namely to remove ‘snowballs’ and ‘wisps’, correcting for 1/f noise striping, and a robust background subtraction procedure.

The deep HST CANDELS imaging available in the EGS footprint provides all-important wavelength coverage in the optical regime, with an updated reduction of the F606W and F814W imaging data made available courtesy of the CEERS team (HDR1; Koekemoer et al., 2011). Moreover, the filter coverage of the CEERS footprint was extended to blue wavelengths thanks to deep F435W imaging taken by the UVCANDELS survey (GO 15647, PI Teplitz; DOI: 10.17909/8s31-f778; see also Wang et al., 2020).

The first JWST extragalactic science driver of CEERS is to improve our understanding of First Light and Reionization (Finkelstein et al., 2017), with significant progress already made. The detection of 10’s of galaxies at \( z > 9 \) with NIRCam have enabled robust constraints on the UVLF out to the highest-redshifts probed by HST and beyond (Donnan et al., 2022; McLeod et al., 2023), while simultaneously testing the different star-formation efficiency predictions of cosmological models (e.g., Bouwens et al., 2023; Finkelstein et al., 2023). Moreover, deep NIRSpec observations have enabled measurements of the ionizing properties and metallicities of galaxies over \( 3 \leq z \leq 9 \) (Sanders et al., 2023; Shapley et al., 2023), with a particular efficacy for galaxies during the EOR (Endsley et al., 2022; Jung et al., 2023; Umeda et al., 2023; Whitler et al., 2023).

The high-resolution JWST imaging allows robust measurements of galaxy structure and morphology to made across \( z \approx 1 - 7 \) as demonstrated by Ferreira et al. (2022) and Kartaltepe et al. (2023). Additionally, the mid-IR imaging from MIRI has allowed a unique insight into dust-obscured star-formation (Akins et al., 2023; Magnelli et al., 2023; Zavala et al., 2023) and the growth of SMBH / AGN (Barro et al., 2023; Kocevski et al., 2023; Yang et al., 2023) over much of cosmic time.

As highlighted previously, the CEERS imaging offers the perfect opportunity to photometrically select strong nebular-line emitting galaxies based on their \([\text{O}\text{III}]+\text{H}\beta\) emission which contaminates the F410M medium-band filter at \( z \approx 7.0 - 7.6 \). When combined with VANDELS data at \( z \approx 3 - 4 \) and literature measurements at lower redshifts, the evolution of the \([\text{O}\text{III}]+\text{H}\beta\) equivalent width
distribution can be traced from $z \approx 2 - 8$, enabling a key insight into the ionizing properties of galaxies across cosmic time. This measurement forms the basis of the work presented in Chapter 5.

### 2.2 Key methodology and analysis techniques

The observational data used in extragalactic research primarily comes in two forms; imaging and spectroscopy, each with their own distinct set of advantages and disadvantages. Imaging has allowed large statistical samples of galaxies across all redshifts to be assembled such that the population statistics, and key physical properties such as stellar mass and star-formation rates can be measured, thus offering a unique perspective on the growth and evolution of galaxies across cosmic time.

Complimentary to imaging and photometric datasets, spectroscopy provides a much deeper insight into the physical processes at play within galaxies. With deep spectra of galaxies, the swathe of emission lines from interstellar gas as well as the subtle signatures in the stellar continuum light can be measured to uncover the detailed properties of the stellar populations and surrounding gas, in addition to enabling accurate star-formation histories to be determined.

In the following sections, I outline a number of the key methods commonly used when handling both imaging and spectroscopic data. In each chapter, multi-wavelength photometry (e.g., for VANDELS and CEERS galaxy samples, measured mainly from broadband imaging) are used in SED-fitting to measure galaxy stellar masses, dust attenuation, and UV magnitudes, to name a few physical properties. The key processes used to prepare robust and accurate photometry and the associated errors are detailed below in Section 2.2.1.

Then in Section 2.2.2, I summarise the Ly$\alpha$ emission line and spectroscopic redshift measurements for VANDELS galaxies from their rest-frame UV spectra, which are used in Chapters 3, 4 and 5. Additionally, I detail the method employed to estimate the equivalent widths of the emission and absorption line features present in the VANDELS spectra.

Finally, in Section 2.3 I discuss the SED modelling carried out throughout the work presented in this thesis.
2.2.1 Imaging

Photometry

Photometry is the measurement of an object’s flux density (hereafter referred to as flux for simplicity), or more precisely the amount of energy received per second, per unit area, per unit frequency $f_\nu$ (or wavelength $f_\lambda = \frac{c}{\nu} f_\nu$). The flux density is commonly measured in micro-Jansky units for high-redshift galaxies, where $1 \mu\text{Jy} \equiv 1 \times 10^{-32} \text{ W m}^{-2} \text{ Hz}^{-1}$, or in AB magnitudes where $m_{\text{AB}} = -2.5 \log_{10}(f_\nu[\mu\text{Jy}]) + 23.9$. Measuring the flux of a galaxy in a variety of filters centred on different wavelength allows a low-resolution galaxy SED to be constructed. Subsequently, SED-fitting can then be used to infer key physical properties of the galaxy.

Aperture photometry is one of the most common techniques used to measure the flux of high-redshift galaxies, as they are often unresolved (see below for discussion of this assumption). In its most basic form, this is carried out by summing the counts of a galaxy on a CCD image within a circular aperture of radius $r$, centred on the galaxy. When observing an unresolved (or point source) object, its image light profile is dictated by the point spread function (PSF) which is a function of the telescope optics and atmospheric seeing (for ground-based imaging). The PSF is often approximated by a Gaussian and therefore apertures with $r \approx 2 \times$ FWHM will enclose $> 90\%$ of the object’s flux. Using an accurate reconstruction of the PSF (see below), the measured flux of a given aperture size can then be scaled to the total flux using an aperture correction factor. An optimal signal-to-noise ratio (for a Gaussian PSF) is achieved when using a $r_{\text{opt}} \approx 1.34 \times$ FWHM, corresponding to $\sim 70\%$ of the total flux (although for seeing-limited imaging, a Moffat profile, in which a greater proportion of light is at larger radii, is a more accurate PSF, and therefore $r_{\text{opt}} \approx 1.5 \times$ FWHM). Another factor to consider in choosing an aperture size is the spatial extent of the galaxy. In particular, with the resolution of JWST (and HST), an aperture larger than the ‘optimal aperture’ (assuming a given PSF for a point source) may be needed to accurately measure the flux of an extended galaxy.

In practice, the exact aperture correction needed is calculated using a curve-of-growth plot, showing the enclosed flux as a function of aperture radius. This can be constructed by measuring the photometry of the empirical PSF, created
by isolating a sample of true point sources (stars) on an image, and stacking their normalised light profiles. However, this curve-of growth is unique to the instrumentation and the filter used, as the PSF varies as a function of wavelength, becoming larger with increasing wavelength (e.g., for the JWST NIRCam PSF, see Rigby et al., 2023). To avoid biases in the galaxy SED due to variations in the percentage of enclosed flux within each filter, the individual flux values must correspond to a constant percentage enclosed. This can be achieved using PSF-matched photometry, in which a variable aperture size is used, with a constant percentage enclosed flux for each (as defined per the curves of growth of each band) (e.g., as in Dunlop et al., 2013; McLure et al., 2013). Alternatively, PSF homogenization can be carried out to produce images with a uniform PSF, which then allows a constant aperture choice across the imaging set. This can reduce potential systematics that may be introduced by the wavelength-dependent aperture correction factor, and moreover, avoids having to make the point source assumption. The homogenization is carried out by convolving each image with a kernel to achieve a common PSF, typically that of the broadest PSF, across the images. PSF-homogenized fluxes typically achieve band-to-band enclosed flux percentages that are consistent at the \( \approx 1 - 2\% \) level (e.g., see McLeod et al., 2016; Donnan et al., 2023).

Aperture photometry and the associated curve of growth corrections are relatively accurate for compact galaxy sources, but it can introduce systematic biases in extended sources as a result of flux extending beyond the aperture radius. At high redshifts, these biases will only affect the largest galaxies and can usually be alleviated by using a larger aperture size. Although not used in this work, at lower-redshifts an alternative to aperture-based photometry is isophotal photometry, in which an objects flux is measured from its ‘isophotal footprint’ (i.e., the surface of pixels above a specified detection threshold relative; e.g., see SExtractor Bertin, 2013, discussed below).

Throughout this thesis, I adopt aperture-based photometric fluxes measured from PSF-homogenised images, unless otherwise stated, to produce accurate and robust photometry. The exception is in the measurement of the \( U \)-band flux in Chapter 3, in which the aperture size is chosen to maximise the potential signal-to-noise of any detected ionizing flux signatures - a vital step for measurements of faint LyC emission (e.g., as described in Chapter 3).
Throughout this thesis, the SExtractor (Source Extractor; Bertin & Arnouts, 1996; Bertin et al., 2022) software is routinely used for source detection and photometry measurements. A brief outline of methods used in SExtractor (hereafter SE) is detailed below, beginning with background estimation procedure.

Within a localised region of an image defined by the `back_size` parameter, SE will estimate the background as the mean of the distribution of pixel (flux) values, after an iterative $3\sigma$ clipping process. The `back_size` value should be larger than the most extended source on the image, while still small enough to capture spatial variations in the background across the image. If a background region is too small, the flux from bright extended objects will likely bias the background estimation. The global mesh of localised regions can then be smoothed using a median filtering across `BACK_FILTERSIZEx` regions to suppress overestimates of the mean background. After a bi-linear interpolation is applied across the smoothed background estimates, the final output of this process is a background map (e.g., top-right panel Fig. 2.4).

SE will then automatically detect objects as groups of adjacent pixels, with a minimum number specified by `DETECT_MINAREA` and with a value above `DETECT_THRESH` relative to the background map. The detection step can be carried out on the image directly, but more commonly after the image has been filtered, for example with a Gaussian filter to smooth the image. This step may aide in detecting fainter objects in the image, such as high-redshift galaxies.

It may be the case that multiple, close objects are classified as part of the same group of adjacent pixels (particularly if a low `DETECT_THRESH` is used). The deblending procedure carried out by SE, controlled by `DEBLEND_NTHRESH` and `DEBLEND_MINCONT`, can be used to separate out the ‘pixel islands’ that may be a separate, neighbouring object (Bertin & Arnouts, 1996). SE deblending can be leveraged to test whether different local structures are simply clumpy regions in a given galaxy, or if there two galaxies are overlapping on the image (e.g., see Pahl et al., 2021). From these steps, a segmentation map is produced, showing the detected objects, including those that have been deblended (e.g., bottom-left in Fig. 2.4).

Lastly, SE will perform aperture photometry on a background subtracted image, placing apertures on each (deblended) detected object. For this thesis,
Figure 2.4 Demonstration of the various check-images that are output by SExtractor. The background map, used for defining source detection thresholds and background correcting aperture photometry (e.g., see Source Extraction in Section 2.2.1) is shown in the top-right panel. The segmentation map, highlighting the pixel areas detected as part of an object is shown in the bottom-left panel. Figure courtesy of the SExtractor manual Bertin & Arnouts (1996).
photometry is carried out using circular apertures, however other variations are available (e.g., with an elliptical Kron aperture, see bottom-right panel Fig. 2.4). The photometry measurements for each object, along with their positions and other optional quantities; including shape parameters (e.g., half-light radii), flags (e.g., for bad pixels), and classification (between stars and galaxies based on a simple neural network) are all output in a catalogue, in addition to the important ‘check images’.

**Image depths**

Photometric flux errors throughout this thesis are assigned using the *photometric depths* of the relevant measurement image. Robust estimates of the image depth are vital for assessing the validity of SED fits in addition to characterising the significance of any analysis results (e.g., see the $\langle f_{\text{esc}} \rangle$ measurement in Chapter 3).

To calculate the photometric depth, a grid of apertures (with the same size used in the photometry measurement) is first placed on empty (‘blank’) regions of an image. Here empty regions are defined using the segmentation map created by SE, such that the blank aperture must not overlap with any source pixels highlighted in the map (e.g., the coloured regions shown in the bottom-left panel of Fig. 2.4). Commonly, the segmentation map is first dilated to remove any residual flux low surface-brightness flux.

From the distribution of fluxes measured within the empty background apertures $f_{\text{empty}}$, one can define the *global depth* of the image $\sigma_{\text{global}}$, which assesses the large-scale noise levels of the image, as follows;

$$
\sigma_{\text{global}} = 1.4826 \times \sigma_{\text{MAD}}
= 1.4826 \times \text{Median}( | f_{\text{empty}} - \text{Median}(f_{\text{empty}}) | )
$$

(2.1)

Here, the scaled median absolute deviation is the preferred estimator of the width of the empty background flux distribution over the standard deviation, as it is more robust against outliers. In the analysis of high-redshift galaxy samples, it is common to quote the image $5\sigma$ global depth in magnitudes (e.g., McLure et al., 2013; Donnan et al., 2022; McLeod et al., 2023) as;

$$
m_{5\sigma} = -2.5 \log(5\sigma_{\text{global}}) + ZP
$$

(2.2)
However, in this thesis local depths are adopted as the photometric error for galaxy photometry measurements. The local depth better accounts for spatial variations in depth across the image which may occur as a result of high source density regions in the image (e.g., in cluster fields, see McLeod et al., 2016) or near the edges of imaging mosaics (e.g., see Fig 3.1; and Begley et al., 2022).

The local depth $\sigma_{\text{local}}$ for each galaxy (in each filter) is calculated from Eq. 2.1, using the distribution of measured fluxes from the nearest $N \approx 200$ empty background apertures, rather than the full blank field.

**Visual inspection**

A key step in assembling robust samples of high-redshift galaxies is a thorough visual inspection procedure. For example, as discussed in McLeod et al. (2016); Donnan et al. (2022); McLeod et al. (2023), visually inspecting bands blueward of the Lyman break suggested by a photometric redshift fit for marginal detections is essential to eliminate potential low-redshift interlopers. Moreover, as discussed in Begley et al. (2022) (see Chapter 3), visual inspection of potential LyC leaking candidates is essential to remove line-of-sight contamination and produce a robust, clean sample of galaxies.

The visual inspection of candidate galaxy samples involves looking for nearby neighbours that may contaminate any aperture centered on the object, as
well as assessing the object’s proximity to imaging artifacts including star diffraction spikes, or ‘hot’ pixels. To aide the visual inspection process, a custom PYTHON+MATPLOTLIB GUI, as shown in Fig. 2.6, was used. The tool enabled users to pan, zoom and adjust the colour scale simultaneously for galaxies across multiple image cutouts. In addition, the user adds a flag and comment to each object in the input catalogue, with the results output into a catalogue for reference and further analysis.

2.2.2 Spectroscopy

Throughout this thesis, spectroscopy, in particular from VANDELS (e.g., see Section 2.1.1), has been used to provide valuable spectroscopic redshifts, in addition to robust measurements of Ly$\alpha$ and rest-frame FUV absorption features (e.g., see Chapter 4). The VANDELS spectroscopic redshifts and Ly$\alpha$ equivalent width measurements were primarily performed by the VANDELS core team and F. Cullen, respectively. The methodologies employed for these measurements are described below, along with the FUV line feature measurements carried out for this thesis.
Figure 2.7  Example 2D spectrum, extracted 1D spectrum, sky counts spectrum, and RMS noise spectrum (top to bottom) for VANDELS galaxy CDFS-202794. This galaxy is a relatively bright ($H_{AB} = 24.1$) LBG, with a robust $Q_z = 4$ spectroscopic redshift of $z_{spec} = 4.4266$. A number of the key emission and absorption lines present in the spectrum are labelled, including the relatively strong Ly$\alpha$ emission line with $W_\lambda(Ly\alpha) = 20.87\pm1.45$ Å. Figure courtesy of Pentericci et al. (2018b).

Spectroscopic redshifts

The spectroscopic redshift of each VANDELS galaxy was initially measured independently by two VANDELS core team members, primarily using EZ (Easy Redshift; Garilli et al., 2010), a tool that is part of Pandora software suite initially developed for the VIMOS VLT Deep Survey (Le Fèvre et al., 2005).

The EZ tool is a decisional tree, allowing a custom set of routines to be performed in order to measure the spectroscopic redshift including emission-line finding and a correlation measurements between the observed spectrum and a reference template (e.g., see Garilli et al., 2010). The software also allows the user to display both the 1D and 2D spectrum, alongside those from the RMS noise and sky, as shown in Fig. 2.7.

A template-fitting method was used by each of the two team members, alongside
manual estimates of the line centres for multiple line features when appropriate (Pentericci et al., 2018b; Garilli et al., 2021). The redshift determinations were performed without prior knowledge of the photometric redshift of the given target galaxy, and then subsequently combined. The two VANDELS PIs reanalysed each VANDELS spectrum as an additional check, ensuring any discrepancies were rectified.

Lastly, each VANDELS spectroscopic redshift measurement has a corresponding quality flag $Q_z$ following the literature standard scheme set out in (Le Fèvre et al., 2005). The flags were initially assigned by the core-team members, and later consolidated by the PIs. Throughout the work in this thesis using VANDELS, sample galaxies were required to have $Q_z = 4, 3$ indicating highly reliable redshifts with $> 99\%$ probability of being correct (e.g., see Garilli et al., 2021). The $Q_z = 4$ galaxies have a high SNR spectrum, with multiple unambiguous absorption or emission line features, and a strong reference template match in EZ. Similarly, a $Q_z = 3$ galaxy will have multiple clear spectral features providing a reliable redshift measurement, albeit with relatively lower SNR compared with the galaxies having the most secure redshifts.

VANDELS galaxies with $Q_z = 2, 1, 0$ have less reliable redshifts, or none at all, and were not used throughout this thesis. There is also a classification system used to define if an object was found to be a Broad Line AGN, or if a serendipitous object appeared in the same slit as a primary target galaxy. Galaxies classified as AGN or serendipitous objects were also not included in the samples used in this thesis.

Ly$\alpha$ equivalent width measurements

The VANDELS galaxies Ly$\alpha$ equivalent width $W_{\lambda}(\text{Ly} \alpha)$ measurements were carried out by F. Cullen following the procedure outlined in Kornei et al. (2010) (see also; Cullen et al., 2020), and briefly detailed below.

Firstly, each galaxy is visually classified as ‘emission’, ‘absorption’, ‘combination’ or ‘noise’, based on the morphology of the Ly$\alpha$ line in the spectra as shown in Fig 2.8, courtesy of Cullen et al. (2020).

The method described in Kornei et al. (2010) is a numerical integration technique, with a robust determination of the limits over which the line profile should be integrated to measure the Ly$\alpha$ line flux.
Figure 2.8  Figure from Cullen et al. (2020) demonstrating the four classifications (a: ‘Emission’, b: ‘Combination’, c: ‘Absorption’, d: ‘Noise’) outlined in Kornei et al. (2010) based on the Ly$\alpha$ spectral shape.
For each spectrum the ‘red’ continuum \( (c_{\text{red}}) \) and ‘blue’ continuum \( (c_{\text{blue}}) \) are calculated as the median flux density value over the 1120 Å \( \leq \lambda_{\text{rest}} \leq 1180 \) Å and 1228 Å \( \leq \lambda_{\text{rest}} \leq 1255 \) Å wavelength ranges, respectively. These two regions are chosen to avoid strong absorption line features (e.g., SiII) in the vicinity of the Ly\( \alpha \) line.

For the ‘emission’, ‘absorption’ and ‘combination’ spectra, the wavelengths at which the Ly\( \alpha \) feature intersects (either moving from the emission peak or absorption minimum outwards) with \( c_{\text{red}} \) and \( c_{\text{blue}} \) are used as the integration limits in the line flux calculation. In the ‘absorption’ and ‘combination’ cases, the spectra are first smoothed with a boxcar filter to minimise any biases in the wavelength limits as a result of potential noise spikes. For the ‘noise’ category, where no clear feature is visible, fixed limits of 1199.9 – 1228.8 Å are adopted. In all cases, the rest-frame \( W_\lambda (\text{Ly}\alpha) \) is then calculated by dividing the integrated line flux by \( c_{\text{red}} \times (1 + z) \), while the \( c_{\text{blue}} \) flux value is discarded as a result of the impact of IGM attenuation blueward of \( \lambda_{\text{rest}} = 1216 \) Å. When the galaxy continuum is not significantly \( (\leq 2\sigma) \) detected, the continuum levels are adopted from the best-fitting SED (e.g., see Chapter 4).

The Ly\( \alpha \) measurement process is repeated \( N = 500 \) times for each galaxy, perturbing its spectrum by the corresponding error spectrum on a pixel-by-pixel basis each time. From the resulting distribution of \( W_\lambda (\text{Ly}\alpha) \) measurements, the median and scaled median absolute deviation \( (\sigma_{\text{MAD}} \approx 1.4826 \times \text{MAD}) \) are adopted as the measured \( W_\lambda (\text{Ly}\alpha) \) and uncertainty, respectively.

**FUV line feature measurements**

The low-ionization-state (LIS) absorption lines in the rest-frame FUV of the VANDELS spectra, such as SiII\( \lambda 1260 \) and CII\( \lambda 1334 \), allow estimates of the LyC \( f_{\text{esc}} \) to be made, as shown in Chapter 4 (e.g., Begley et al., 2023, see also Saldana-Lopez et al. 2022b). More generally, as comprehensively explored in Shapley et al. (2003), the absorption and emission features in the FUV yield unique insights into the ionizing and gas properties of SFGs. Specifically, the LIS features measured in this thesis trace the distribution of neutral Hydrogen, which in turn governs the LyC escape fraction (e.g., see Section 1.5.3).

In general, most spectra for the \( z_{\text{spec}} \geq 3 \) star-forming galaxy samples used in this thesis are not detected in the continuum at high enough SNR to facilitate
LIS absorption line measurements on a galaxy-by-galaxy basis. To overcome this shortcoming in SNR, the VANDELS spectra are stacked as described in Section 4.4.2, before measuring the LIS spectral features.

In a similar fashion to the \( W_\lambda (\text{Ly} \alpha) \) measurements described above, the FUV features in the VANDELS stacks are calculated numerically using the following equation:

\[
W_{\text{LIS}} = \int_{\Delta \lambda} \left(1 - \frac{f_{\text{obs}}}{f_{\text{cont}}} \right) d\lambda \quad (2.3)
\]

where \( f_{\text{obs}} \) is the flux density of the observed VANDELS spectrum, \( f_{\text{cont}} \) is the underlying stellar continuum flux density, and \( \Delta \lambda \) is the width of the region over which the numerical integration is performed. By default, the adopted integration region \( \Delta \lambda \) corresponds to a velocity interval \( \Delta v = \pm 500 \text{ km s}^{-1} \), however \( \Delta \lambda \) and the central wavelength \( \lambda_0 \) may be adjusted for individual line measurements to account for velocity offsets or noise spikes impacting the flux calculation.

To calculate the stellar continuum \( f_{\text{cont}} \) underlying the LIS absorption features, a \( f_\lambda \propto \lambda^\beta \) power-law is fitted to the continuum blue- and red-ward of the line, over a region spanning \( \pm 4500 \text{ km s}^{-1} \) (\( \gtrsim 20 \text{ Å} \)). Robust errors for the \( W_{\text{LIS}} \) measurements were assigned in a Monte Carlo procedure, where the numerical integration was carried out on a large number of realisations of the (stacked) VANDELS spectrum, with each realisation generated by perturbing the spectrum with its associated error spectrum. As with the Ly\( \alpha \) line measurements, this method produces a \( W_{\text{LIS}} \) distribution for each line, from which the 16th and 84th percentiles were used as the \( \pm 1\sigma \) errors (\( \sigma_{W_{\text{LIS}}} \)) (rather than the \( \sigma_{\text{MAD}} \) to account for potential asymmetric errors).

**VANDELS spectroscopic redshifts versus systemic redshifts**

Throughout this thesis, the redshifts of galaxies selected from the VANDELS survey are the *spectroscopic redshifts* (\( z_{\text{spec}} \)) presented in VANDELS DR4 (Garilli et al., 2021, see also Section 2.1.1).

As discussed above, these spectroscopic redshifts are derived from template-fitting and emission line-based measurements, and therefore they are primarily driven by the strongest features present in the spectrum; for example Ly\( \alpha \) which is typically redshifted relative to \( z_{\text{spec}} \), and low-ionization-state absorption lines which are
tend to be blueshifted from $z_{\text{spec}}$. As a consequence, an important caveat is that these redshifts are generally not representative of the ‘true’ systemic redshift ($z_{\text{sys}}$) of each galaxy.

Ideally, $z_{\text{sys}}$ would be derived from (stellar) photospheric absorption lines (e.g., O\textsc{iv}\,$\lambda$1343, Si\textsc{ii}\,$\lambda$1417 and S\textsc{v}\,$\lambda$1500), however these features are extremely faint and not detected even in the ultra-deep VANDELS spectra. Alternatively, non-resonant nebular emission lines such as C\textsc{iii}\,$\lambda$1909 and He\textsc{ii} $\lambda$1640 could be used to estimate $z_{\text{sys}}$, but these lines are beyond the wavelength range covered by VANDELS spectroscopy for the $z \approx 4 - 5$ sample assembled in Chapter 4.

Deviations between the true underlying systemic redshift and the measured VANDELS spectroscopic redshift can potentially introduce additional uncertainties in the composite spectra created to measure faint LIS lines in Chapter 4 (that are first shifted to the rest-frame using their spectroscopic redshift). Using VANDELS spectroscopy to infer the ISM properties in SFGs at $z \approx 2 - 5$, Calabrò et al. (2022) measure the median velocity of low-ionization-state gas to be very close the systemic velocity ($v_{\text{LIS}} \approx -60$ km s$^{-1}$, see also Marchi et al., 2017). In turn, this implies a wavelength shift at the level of $\Delta \lambda \lesssim 0.3$ Å for the FUV low-ionization-state absorption lines measured, which is below the spectral resolution achieved by VANDELS ($R \approx 600$, see Section 2.1.1) for galaxies at $z \approx 4 - 5$.

2.3 SED modelling and galaxy property measurements

Fitting the spectral energy distribution of a galaxy is a powerful tool for obtaining photometric redshifts and measuring galaxy physical properties such as stellar mass, dust attenuation, and star-formation rate. Moreover, SED fitting enables the types of stellar populations present within a galaxy to be constrained.

The majority of SED-fitting codes are template-based, whereby a spectral energy distribution model is statistically compared to the observed photometry. The main ingredients that are required in practice to construct these templates are outlined in Fig. 2.9 (see also Section 1.2.2 for a more pedagogical discussion of galaxy spectral energy distributions).

Typically the starting point of an galaxy SED template is the simple stellar
population (SSP, centre panel in Fig. 2.9) which describes the flux density as a function of wavelength and age for a collection of stars that formed at the same time and with the same metallicity. The initial distribution of masses of the stars formed is dictated by the choice of IMF (top left panel). Subsequently, their evolutionary stages and lifespan is controlled by stellar isochrones (usually from detailed stellar evolution codes). These two components combined with empirical (or model) stellar spectra are used construct the SSP template spectral energy distributions.

Multiple SSPs are then combined according to prescriptions for the star-formation history and resulting chemical evolution, with the impact of dust attenuation and emission also accounted for. As shown in Fig. 2.9 (bottom panel), these steps allow detailed, physically motivated galaxy SEDs to be constructed and then compared with photometry to infer the properties of observed galaxies.

In this thesis, in addition to making robust measurements of photometric redshifts and galaxy properties, I also use SED fitting to obtain accurate estimates of the stellar continuum flux density to make photometric inferences of strong nebular lines (e.g., Hα and [OIII]+Hβ as outlined in Chapters 3 & 5, respectively). The specific SED codes used in this thesis, along with a brief description of the key features of each is detailed below.

**FAST++**

FAST++ is a template-based SED fitting code (rewritten in C++ by Schreiber et al., 2018, based on the original FAST code by Kriek et al. 2009). The code fits composite template models to the observed photometry based on a $\chi^2$ minimisation routine, with errors calculated from a Monte Carlo simulation in which the observed fluxes are scattered by their corresponding errors. The FAST++ code implements a flexible analytical star-formation history (SFH), which along with the choice of input simple stellar population (SPS) model and IMF, allows custom SED templates to be constructed. Throughout this thesis, unless otherwise stated, the BC03 (updated 2016 version; Bruzual & Charlot, 2003) SPS models (with ~20% solar metallicities) are used with a Chabrier (2003) IMF. A constant SFH is generally used, although other options including a delayed exponentially decaying SFH are explored (e.g., see Chapter 5). A redshift grid spanning $z_{\text{min}}$ to $z_{\text{max}}$, with a spacing $\Delta z$, is specified by the user, with the option to fit a fixed spectroscopic redshift when available (e.g., from VANDELS).
Figure 2.9  Schematic overview of the ‘ingredients’ that form a composite SED template. The base simple stellar population (SPS, centre) models are constructed assuming an IMF (top-left), stellar evolution pathways through isochrones (top-centre), and stellar spectra (top-right). The SPS models are combined according to the star-formation history (and chemical evolution) of the galaxy (left-center), alongside the impact of dust attenuation and emission (and also nebular emission when relevant, but not shown), to create a composite stellar population template representative of a galaxy (bottom). The final template shows both the dust-free, and dust-attenuated SEDs. Figure courtesy of Conroy (2013)
Lastly, a variety of dust parameterisations are implemented, including the ‘grey’ Calzetti et al. (2000) dust attenuation law, a steeper SMC-like dust curve (e.g., see Gordon et al., 2003), and the Noll et al. (2009) dust law that modifies the Calzetti dust law with a power-law slope and the addition of a UV bump.

In addition to best-fitting stellar masses, stellar ages and the optical dust attenuation $A_V$, FAST++ can compute non-parametric physical quantities such as the average SFR over a specified time-frame, the star-formation duration and the time taken to form a given fraction of the current mass. These quantities are generally more physically meaningful than the SFH history parameters.

An important caveat is that FAST++ does not model nebular emission lines (or continuum), and so the resulting SED fits only include emission from the stellar continuum. It is therefore important to exclude broadband photometry that may be significantly contaminated by the presence of strong nebular emission lines (e.g., Hα or [OIII]). However, this feature can also be used advantageously to empirically measure emission lines from stellar continuum-only SED fits to broadband photometry (e.g., see Begley et al., 2023, and Chapters 4 & 5).

**EAZY**

Another template-based SED fitting code is EAZY (Brammer et al., 2008). EAZY is primarily designed to provide robust photometric redshifts, using a linear combination of $N$ composite stellar population templates. By default EAZY is run in ‘principle component analysis’ (PCA) mode, using a minimal template basis set derived from semi-analytical modelling. Both the PCA mode, and the more traditional single composite template mode (with the provided PÉGASE models Fioc & Rocca-Volmerange 1997, 2019) are used as part of the strategy outlined in Chapter 5 to obtain a robust photometric redshift sample of $z \approx 7$ galaxies.

EAZY includes a novel ‘template error function’ to address potential unaccounted uncertainties arising from limitations of the composite stellar templates (e.g., due to uncertain stellar isochrones), and therefore provides more realistic estimates of the redshift errors, and subsequent redshift probability density functions $P(z)$. 87
LePhare

Similar to both fast++ and eazy, LePhare is also an SED template fitting code (Arnouts et al., 1999; Ilbert et al., 2006). The code pre-computes model magnitudes for a large grid of templates, with the stellar population synthesis models, dust attenuation law, and SFH specified by the user (as with fast++). The best-fitting model is then found through a $\chi^2$ comparison to the input photometric catalogue. Uncertainties on the photometric redshift and physical properties are calculated from bootstrapping the template $\chi^2$ grid.

LePhare also outputs a $P(z)$ for each galaxy fit, which is combined the with eazy redshift $P(z)$ in Chapter 5 to select a robust sample of high-redshift galaxies from the CEERS JWST ERS program.

![Figure 2.10](image)

**Figure 2.10** Example $z = 7.3$ model galaxy (black) generated with bagpipes to test and calibrate the $\mathrm{[O_{III}] + H\beta}$ recovery method for the CEERS $z \sim 7$ galaxy sample assembled in Chapter 5. The model galaxy has a stellar mass of $\log(M_*/M_\odot) \approx 8.9$, and is generated using a $Z = 0.2Z_\odot$ metallicity BC03 SPS model (Bruzual & Charlot, 2003) with a Chabrier (2003) IMF and $\approx 50$Myr CSFH. The model uses a Calzetti et al. (2000) dust attenuation law with $A_V = 0.2$, and no nebular emission, which is added separately (e.g., see Chapter 5). The model photometry calculated using the JWST NIRCam bands observed with CEERS (in addition to the available HST/ACS imaging) is shown in blue.

BAGPIPES

The final SED fitting code used in this thesis is bagpipes (Bayesian Analysis of Galaxies for Physical Inference and Parameter ESTimation Carnall et al., 2018, 2019), which implements a Bayesian fitting methodology using MultiNest nested sampling (Feroz et al., 2009).
BAGPIPES first generates realistic model galaxy spectra from the FUV to beyond IR wavelengths, using a user-defined number of components. With this functionality, galaxy SED templates ranging from simple burst populations to complex, multi-faceted stellar populations with a variety of metallicities and ages, can be constructed. The code also enables flexible prescriptions to account for the impact of dust and the addition of nebular-emission self-consistently.

Having generated physically motivated, customised SED templates, BAGPIPES then has the ability to statistically fit these models to observational data (both photometric and spectroscopic, or a combinations), using a Bayesian framework as outlined in Carnall et al. (2018).

Specifically, in the context of this thesis, BAGPIPES is used in Chapter 5 to generate physically realistic model galaxy spectra representative of the $z \approx 3.4$ and $z \approx 7.5$ galaxies observed in VANDELS and CEERS respectively (e.g., as shown in Fig. 2.10). These physically motivated model spectra as then used to robustly test and calibrate the [O III]+H$\beta$ measurements made in Chapter 5.
Chapter 3

The VANDELS survey: a measurement of the average Lyman-continuum escape fraction of star-forming galaxies at $z = 3.5$

The material in this chapter was originally published in Begley et al. (2022).

3.1 Introduction

During the "Epoch of Reionization" (EoR), the Universe underwent a phase change in which the hydrogen gas in the intergalactic medium (IGM) was transformed from its early cold neutral state into the largely ionized IGM we see around us today. Current data indicate that the EoR spanned the approximate redshift range from $z \approx 10–15$ down to $z \approx 5–6$ (Robertson et al. 2015; Robertson 2021; Bosman et al. 2021; Goto et al. 2021). However, the detailed progress and physical drivers of reionization currently remain highly uncertain and somewhat controversial, with some evidence supporting a late, short-lived, rapid reionization process (e.g. Mason et al., 2018b), while other indicators favour a more gradual evolution of the IGM, commencing at much higher redshift (e.g Wu et al., 2021).

Historically, the two main candidates for producing the bulk of the LyC photon budget required to achieve hydrogen reionization have been active galactic nuclei
(AGN) and/or star-forming galaxies. However, with the number density of quasars and lower-luminosity AGN now known to fall rapidly at high redshift (Aird et al. 2015; Parsa et al. 2018; McGreer et al. 2018; Kulkarni et al. 2019; Faisst et al. 2021), and recent constraints limiting the escape fraction of LyC photons in AGN to $f_{\text{esc}} \ll 1$ (Iwata et al., 2022), early star-forming galaxies are now thought to be the primary source of ionizing photons (Chary et al., 2016).

With ever improving measurements of the galaxy luminosity function at high redshift (Bowler et al., 2020; Harikane et al., 2021), it is becoming possible to track the progress of galaxy-driven reionization. However, doing so accurately requires reliable estimates of the production rate of LyC photons from early galaxies (e.g. Tang et al., 2019), and the average escape fraction ($\langle f_{\text{esc}} \rangle$) of such photons into the IGM (e.g. Ocvirk et al., 2021).

A number of studies have attempted to use measurements of the evolving UV luminosity density produced by the early star-forming galaxy population to estimate what the $\langle f_{\text{esc}} \rangle$ from young galaxies must be in order to deliver hydrogen reionization within the required time-frame (Bouwens et al., 2015, 2021; Finkelstein et al., 2015, 2019; Robertson et al., 2013, 2015). For example, Robertson et al. (2013) suggested that $\langle f_{\text{esc}} \rangle$ in the range 10 – 20 per cent is required, whereas the modelling of Finkelstein et al. (2019) concluded that $\langle f_{\text{esc}} \rangle \approx 5$ per cent may suffice (helped by the gradual reduction in the optical depth $\tau$ to electron scattering derived from successive releases of data from Planck: now $\tau = 0.056 \pm 0.007$; Planck Collaboration et al. 2020).

The inferred values for average $\langle f_{\text{esc}} \rangle$ quoted by such studies are inevitably dependent on a number of empirical results and model assumptions, such as the assumed ionizing photon production efficiency of early galaxies (e.g. Eldridge et al., 2017). One common additional assumption is that the production of LyC photons is dominated by the more numerous faint (and presumably metal poor) galaxies at such early times, however alternative assumptions can be explored.

An example is presented in Naidu et al. (2020), who propose a model allowing $f_{\text{esc}}$ to vary based on star-formation rate surface density. In contrast to requiring a low-to-moderate $\langle f_{\text{esc}} \rangle$ across the entire galaxy population, their work suggests that $\gtrsim 80$ per cent of the ionizing photon budget may be accounted for by rarer, more massive galaxies with higher than average $f_{\text{esc}}$. Such uncertainties over the production and escape of LyC photons from EoR galaxies arise because direct measurements of the LyC emission from these objects are impossible. Therefore,
with the aim of studying galaxies that are most directly analogous to those that
drove reionization, many studies have focused on searching for LyC leakers at
$3 \leq z \leq 4$, where the level of IGM transmission still allows the direct detection of
LyC emission (Inoue et al., 2014).

Some of the earliest successes in such searches have come from deep rest-frame
UV spectroscopy, both through targeted surveys such as KLCS (Steidel et al.,
2018) and from serendipitous discoveries. The former has resulted in 13 secure
detections of LyC emission (Pahl et al., 2021), including the LyC leaker Q1549-
C25 first reported in Shapley et al. (2016). Other discoveries, both serendipitous
and targeted, include such notable objects as Ion 1-3 (Vanzella et al. 2012, 2016c;
de Barros et al. 2016; Vanzella et al. 2018; Ji et al. 2020) and the Sunburst
galaxy (Rivera-Thorsen et al. 2019; Vanzella et al. 2021). However, with less than
20 spectroscopically confirmed LyC leakers discovered to date at intermediate
redshifts, the available sample of such sources remains small.

Constraints on the average escape fraction can also be derived from detailed
analyses of larger samples that do not feature significant individual LyC
detections, for example $\langle f_{\text{esc}} \rangle = 0.06 \pm 0.01$ (Pahl et al., 2021). However, even with
relatively large samples of galaxies, it is still difficult to achieve robust constraints
on the typical level of LyC flux at intermediate redshifts, as shown in the meta-
analysis by Meštrić et al. (2021). Their work collates literature results from the
last $\sim 20$ years, finding that many studies were only able to derive upper limits
on $\langle f_{\text{esc}} \rangle$, even from deep spectroscopic observations.

As a potentially efficient alternative to spectroscopic searches, a growing number
of studies have sought to use narrow and/or broadband imaging to hunt for LyC
emitting galaxies. The main observational requirement for such searches is the
availability of deep $U$-band imaging, which a number of studies have obtained
via programmes such as CLAUDS (Meštrić et al., 2020), and LACES (Fletcher
et al., 2019), resulting in a number of likely LyC emitting candidates. As with
spectroscopic studies, high angular-resolution imaging (effectively from $HST$) is
required to robustly decontaminate samples of potential LyC leakers (Siana et al.,
2015). Regardless of their ability to unveil new candidate LyC emitting galaxies,
these deep $U$-band imaging surveys have generally only been able to place upper
limits on $\langle f_{\text{esc}} \rangle$ across their full galaxy samples (e.g. Guaita et al. 2016; Grazian

In the past decade a significant amount of effort has also been directed towards
exploring which galaxy properties are correlated with, and therefore can be utilised as indirect indicators of, the level of leaking ionizing radiation. To date, the most promising such indicators for $f_{\text{esc}}$ are tied to Ly$\alpha$ emission. Most recently, Pahl et al. (2021) confirmed the positive correlation between increased $f_{\text{esc}}$ and Ly$\alpha$ equivalent width ($W_{\lambda}(\text{Ly}\alpha)$), previously found by Steidel et al. (2018). This statistical link is physically supported by simulations, which show that both ionizing continuum flux and Ly$\alpha$ line emission can escape through the same ionized channels in the interstellar medium (ISM) (e.g. Kimm & Cen 2014; Wise et al. 2014).

However, the case for $W_{\lambda}(\text{Ly}\alpha)$ as a clean proxy for LyC leakage is not clear cut (e.g. Mostardi et al. 2013). With a host of properties able to alter the transmission of both Ly$\alpha$ and ionizing continuum photons, such as geometry and gas kinematics (Dijkstra et al., 2016), any relationship between $W_{\lambda}(\text{Ly}\alpha)$ and $f_{\text{esc}}$ is undoubtedly complex. Conflicting results also exist for the connection between other galaxy properties and $f_{\text{esc}}$, such as galaxy stellar mass and UV magnitude (e.g. Fletcher et al. 2019; Izotov et al. 2021; Pahl et al. 2021), both of which are particularly important in the ongoing debate over which galaxies provided the bulk of the ionizing photon budget in the EoR.

In addition to Ly$\alpha$, a number of other rest-frame UV/optical spectral features, accessible by JWST for galaxies within the EoR, have also been scrutinised as potential indicators of LyC leakage (Nakajima & Ouchi 2014; Ramambason et al. 2020; Katz et al. 2020; Mauerhofer et al. 2021). In particular, the usefulness of $[\text{O} \, \text{III}]$ line emission from galaxies ($W_{\lambda}([\text{O} \, \text{III}])$ and the $[\text{O} \, \text{III}]/[\text{O} \, \text{II}]$ ratio, hereafter O32), has been much explored, due to their association with recent bursts of star-formation activity and increased ionizing photon production efficiency (Vanzella et al. 2016a; Izotov et al. 2018c; Tang et al. 2019, 2021c; Endsley et al. 2021; Tang et al. 2021a). Indeed, more extreme $[\text{O} \, \text{III}]$ properties are usually attributed to the presence of density-bounded H$\upiota$ regions (Kewley et al., 2019), from which LyC photons are thought to escape (Jaskot et al., 2019). However, as with other proposed proxy indicators of LyC leakage, the link between $W_{\lambda}([\text{O} \, \text{III}])$, O32, and $f_{\text{esc}}$ is not conclusive (e.g. Naidu et al. 2020; Saxena et al. 2021).

The analysis by Nakajima et al. (2020) suggests that high O32 is a requirement for high $f_{\text{esc}}$, but that not all galaxies with high O32 are necessarily LyC leakers (a situation that is mirrored by the relationship between O32 and Ly$\alpha$ emission; Tang et al. 2021c). That no single measure has proven to be a clear and universal
indicator of LyC leakage highlights the complexity of the underlying physics, in which anisotropic or time-evolving leakage may play a significant role, potentially explaining apparently inconsistent results (Cen & Kimm 2015; Steidel et al. 2018; Fletcher et al. 2019). The lack of a clear consensus further bolsters the case for studying larger sample sizes with varied and complete datasets and/or using alternative methodologies (see also Tanvir et al., 2019; Meyer et al., 2020, for constraints derived using gamma-ray bursts and galaxy-IGM cross-correlations, respectively).

To try to advance this situation, in this study we have assembled a large sample of star-forming galaxies at $3.35 \leq z_{\text{spec}} \leq 3.95$ from the ultra-deep VANDELS spectroscopic survey (McLure et al. 2018b; Pentericci et al. 2018a; Garilli et al. 2021). We utilise deep VLT/VIMOS $U$-band imaging to probe LyC emission ($\lambda_{\text{rest}} \approx 820$ Å), along with high resolution HST imaging to measure non-ionizing UV fluxes ($\lambda_{\text{rest}} \approx 1300$ Å) and effectively clean the sample from line-of-sight contamination. We have calibrated the imaging with additional astrometric corrections, and have undertaken sophisticated depth determinations to ensure that our derived photometric uncertainties are robust. We compare the observed distribution of ionizing to non-ionizing flux ratios with simulated ratios from a realistic model which is based on physically motivated and/or empirically measured inputs, and includes an accurate treatment of both IGM and circumgalactic medium (CGM) transmission via Monte Carlo sightline simulations. From this thorough analysis, for the first time via a broadband imaging-based approach, we provide a statistical measurement ($\geq 3\sigma$) of the sample-averaged absolute escape fraction at $z \approx 3.5$.

### 3.2 Data and sample selection

The constraints on $\langle f_{\text{esc}} \rangle$ derived in this work fundamentally rely on accurately measuring the observed ratio of LyC to non-ionizing UV flux in a sample of star-forming galaxies at $z \approx 3.5$.

The three key datasets necessary to perform this experiment are all publicly available. A suitable sample of spectroscopically confirmed star-forming galaxies has recently been provided in the CDFS by the final data release (DR4) of the VANDELS ESO public spectroscopic survey (Garilli et al., 2021). Moreover, the necessary measurements of the observed LyC flux are provided by the publicly...
available, ultra-deep, $U$–band imaging of the CDFS presented by Nonino et al. (2009). Finally, the necessary measurements of the non-ionizing UV flux are provided by the $HST$ ACS F606W, hereafter $V_{606}$, imaging of the CDFS, released as part of version 2.0 of the Hubble Legacy Field programme\(^1\) (Whitaker et al. 2019). In this section we fully describe the sample selection process, together with the steps taken to extract robust photometry from the ground-based and $HST$ imaging.

### 3.2.1 The VANDELS survey

The sample of star-forming galaxies utilized in this work is drawn exclusively from the final data release (DR4) of the VANDELS ESO public spectroscopy survey (McLure et al. 2018b; Pentericci et al. 2018a; Garilli et al. 2021). The VANDELS survey obtained ultra-deep (20-80 hours of integration), red optical ($4800 < \lambda_{\text{obs}} < 10200$ Å) spectra for a sample of 2087 galaxies with the VIMOS spectrograph on the VLT. The primary VANDELS sample, accounting for 83 per cent of the spectroscopic targets, consisted of galaxies on the star-forming main sequence (e.g. Daddi et al., 2007) within the redshift interval $2.4 \leq z_{\text{phot}} \leq 6.4$. Full details of the survey design can be found in McLure et al. (2018b) and a detailed description of the data reduction, data quality assurance and spectroscopic redshift determinations can be found in Pentericci et al. (2018a) and Garilli et al. (2021).

The initial sample selected for this work consists of 242 VANDELS DR4 star-forming galaxies within the CDFS\(^2\), with high-quality spectroscopic redshifts ($z_{\text{flag}} = 3$ or 4) within the interval $3.35 \leq z_{\text{spec}} \leq 3.95$. We note here that the spectroscopic redshifts for VANDELS galaxies with quality flags $z_{\text{flag}} = 3$ or 4 are derived from multiple spectral features and the analysis presented by Garilli et al. (2021) confirms that they are reliable at the 99 per cent level. Each galaxy had an associated stellar mass derived from multi-wavelength broad band photometry using the SED-fitting code BAGPIPES (Carnall et al., 2018, 2019) as described in Garilli et al. (2021), and a measured Ly$\alpha$ equivalent width ($W_{\lambda}(\text{Ly}\alpha)$) following the method outlined in Cullen et al. (2020) (following Kornei et al., 2010). The UV magnitude ($M_{\text{UV}}$) of each galaxy is calculated based on the VANDELS spectra and available photometry, following the method outlined in Section 3.3.3.

\(^1\)https://archive.stsci.edu/prepds/hlf/

\(^2\)A similar number of suitable VANDELS DR4 galaxies are available in the UDS survey field, however the UDS currently lacks the necessary ultra-deep $U$–band imaging data.
Figure 3.1  Depth map for the CDFS $U$–band mosaic, as measured within photometric apertures with a diameter of 1.2 arcsec. The locations of the 148 galaxies within our final star-forming galaxy sample are shown as filled red circles. Mapping the spatially varying depth allows robust photometric uncertainties to be allocated to each galaxy, based on its position.

The low-redshift limit at $z_{\text{spec}} = 3.35$ was imposed to ensure that the $U$–band filter used for the VIMOS imaging only samples rest-frame wavelengths shortward of the Lyman limit. In contrast, the high-redshift limit was determined based on a simulation of the combined impact of the IGM and CGM on the transmission of LyC photons. This indicated that $z_{\text{spec}} = 3.95$ was the redshift at which the increasing opacity of the IGM+CGM outweighed the improved signal-to-noise provided by a larger sample size. Moreover, at $z > 3.95$ the $\lambda_{\text{rest}} \sim 800 - 900$ Å regime begins to shift redward of the wavelength range probed by the VIMOS/$U$–band transmission profile. We note that Vanzella et al. (2010a) reached the same conclusion regarding the optimal redshift window for detecting potential LyC emission in an earlier study using the same $U$–band imaging data.
3.2.2 Imaging data

This study makes use of the $U$-band imaging of the CDFS field obtained with VLT+VIMOS by Nonino et al. (2009) and the coincident $V_{606}$ imaging obtained with HST. Fitting with the psfex software package (Bertin, 2013) demonstrated that the PSF of the $U$-band mosaic shows little spatial variation. Over the area of the mosaic where the VANDELS star-forming galaxies are located, we find a median FWHM of 0.79 arcsec and a maximum FWHM of 0.80 arcsec. As a result, throughout this paper we measure photometry within circular apertures with a diameter of 1.2 arcsec, in order to maximize the signal-to-noise ratio for compact sources (e.g. Brammer et al., 2016).

PSF homogenisation

Our adopted method for determining $\langle f_{\text{esc}} \rangle$ relies on an accurate measurement of the LyC to non-ionizing UV flux ratio; effectively the $U-V_{606}$ colour. This measurement clearly relies on the $U$-band and $V_{606}$-band aperture photometry capturing the same fraction of total flux for each object. To meet this requirement, the $V_{606}$ image was PSF-homogenised to the $U$-band image using a convolution kernel generated by Photutils, based on stacks of isolated stars. Following PSF homogenisation, a curve of growth analysis confirmed that the enclosed relative flux within an 1.2-arcsec diameter aperture on the $U$-band and $V_{606}$-band images matched to within $\pm$2 per cent.

Astrometry calibration

In addition to PSF homogenisation, the measurement of an accurate $U-V_{606}$ colour requires any astrometric shifts between the $U$-band and $V_{606}$-band images to be minimised. To address this issue we selected a catalogue of bright sources, detected in both images with S/N $\geq 8 \sigma$, with positions that matched within a tolerance of 0.5 arcsec. This catalogue revealed that the median astrometry offset between the two images was $\Delta \alpha = 0.133$ arcsec.

By applying a spatially varying correction to the $U$-band astrometry, based on the median off-sets of the nearest 200 bright objects, it was possible to reduce the median astrometry offset to $\Delta \alpha = 0.08$ arcsec. This improvement in astrometric accuracy allowed us to extract robust $U$-band photometry at the measured $V_{606}$
centroids, without astrometric shifts contributing significantly to the uncertainty in the $U - V_{606}$ colours.

**Sky subtraction and depth analysis**

We adopted a two-step process to address the issues of sky subtraction and the positionally varying depth of the $U$–band imaging. The first step was to subtract a low-order, two-dimensional, sky-background fit to the $U$–band image with photutils, using a dilated segmentation map to exclude objects from the fit. Following this global sky-subtraction, a second step was employed to deal with any remaining local variations. This step involved creating a dense grid of non-overlapping blank-sky apertures, each with a diameter of 1.2 arcsec. For each galaxy in our final sample, the $U$–band photometry was measured within an aperture with a diameter of 1.2 arcsec, centred on the measured $V_{606}$ centroid, with the median flux of the nearest 200 blank-sky apertures taken as the local sky-background estimate. The corresponding value of $\sigma_{\text{MAD}}$ measured from the flux distribution of the nearest 200 blank-sky apertures was adopted as the local 1$\sigma$ depth estimate. An identical procedure was followed to measure and quantify the $V_{606}$–band photometry extracted from the PSF-homogenised $V_{606}$ image.

A depth map, illustrating the spatial variation in sensitivity of the $U$–band image, is shown in Fig. 3.1. Within the region occupied by our final galaxy sample, we calculate a global median 1$\sigma$ depth of $m_{1\sigma} = 30.4$. Although there is clearly spatial variation in the depth of the $U$–band image, $\geq 90$ per cent of our final galaxy sample lie in regions with $m_{1\sigma} \geq 30.1$. Having an accurate measurement of the spatially varying depth allows us to allocate robust flux errors to each object as a function of their position.

**3.2.3 Final sample selection**

Unfortunately, the whole initial sample of 242 star-forming galaxies is not suitable for constraining the escape fraction of LyC photons, primarily due to the potential for significant contamination of the ground-based $U$–band photometry by flux from nearby companion objects. It was therefore necessary to clean our initial sample for potential contaminants, as described below.
Figure 3.2  Corner plot showing the distribution of stellar mass (top), Ly\(\alpha\) equivalent width (middle), and spectroscopic redshift (bottom), for our final sample of 148 star-forming galaxies. The scatter plots show the relations between each physical parameter. The median values of the three properties shown are \(\log(M_*/M_\odot) = 9.5\), \(W_{\lambda}(\text{Ly}\alpha) = -6\ \text{\AA}\) and \(z_{\text{spec}} = 3.58\) (see \S\ 3.4.3).
Line-of-sight contamination in the imaging data

As discussed above, based on the ≃ 0.8 arcsec FWHM of the $U$–band PSF, we adopt photometric apertures with a diameter of 1.2 arcsec. Therefore, the first stage in cleaning the sample involved visually inspecting $U$–band cutouts of each object and removing all objects that displayed any level of contaminating flux from nearby companion objects within a radius of 0.6 arcsec. From the initial sample, 23 objects were excluded due to having $U$–band photometric apertures that were unambiguously contaminated by flux from nearby objects, leaving a sample of 219 remaining objects.

The second stage of the cleaning process exploited the high-spatial-resolution $V_{606}$ imaging to identify small angular separation contaminants ($r < 0.6$ arcsec) that could not be identified from the low-spatial resolution $U$–band imaging. The third stage of the cleaning process made use of true-colour images constructed from the other available HST ACS imaging data (i.e. F435W, F775W, F850LP)\(^3\) in order to exclude those extended objects that visually displayed strong colour gradients, potentially indicative of line-of-sight projections of objects at different redshifts. In total, based on the high-spatial resolution HST imaging, we excluded a further 34 objects, leaving a sample of 185 objects.

For a further 32 galaxies, it was not possible to state unambiguously that they contain no contaminating flux within the photometric aperture through a combination of the three previous cleaning stages. As a result, these galaxies were classed as potentially contaminated, and given our conservative approach, we also excluded these objects, leaving a sample of 153.

AGN contamination

The final stage of cleaning the sample involved excluding potential AGN. This process was based on the identification of sources within the 7Ms Chandra X-ray catalogue of the E-CDFS (Luo et al., 2017), which covers an area including the full VANDELS sample in the CDFS. We excluded a further five objects as potential AGN, all of which could be associated with high SNR detections in the 7Ms X-ray catalogue, within an angular separation of 1.1 arcsec.

\(^3\)ACS F850LP and F606W imaging was available for all galaxies, with additional F775W and F435W imaging available for 70 per cent of the sample.
Figure 3.3  The $\mathcal{R}_{\text{obs}}$ distribution of our final sample of 148 star-forming galaxies, derived in Section 3.2. It is the centroid and overall shape of this distribution that provides the fundamental observational constraint on $\langle f_{\text{esc}} \rangle$. 
Final galaxy sample

Following the exclusion of potential AGN, the final sample of galaxies consists of 148 star-forming galaxies within the redshift interval $3.35 \leq z_{\text{spec}} \leq 3.95$. Our conservative approach to cleaning excluded a total of 94 objects from the initial sample (39 per cent), primarily on the basis of potential photometric contamination from nearby objects. The redshift, stellar mass and $W_\lambda$(Ly$\alpha$) distributions of our final sample are shown in Fig. 3.2.

The LyC to non-ionizing UV flux ratio

As discussed previously, the observational constraint on $f_{\text{esc}}$ for a given galaxy is derived from the the LyC to non-ionizing UV flux ratio:

$$ R_{\text{obs}} = \frac{L_{\text{LyC}}}{L_{\text{UV}}} = \frac{\langle f_U \rangle}{\langle f_V \rangle} \text{obs}, \quad (3.1) $$

where $\langle f_U \rangle$ and $\langle f_V \rangle$ are the flux densities per unit frequency measured within 1.2-arcsec diameter apertures on the $U$–band and PSF-homogenised $V_{606}$–band images, respectively. In the next section, we describe the technique we have adopted to model the $R_{\text{obs}}$ distribution of the final sample (see Fig. 3.3), and thereby measure the value of $\langle f_{\text{esc}} \rangle$. However, it is worth noting that it is $R_{\text{obs}}$ that is the fundamental observable and that, after correcting for the effects of the IGM and CGM, it is $R_{\text{obs}}$ that is directly related to a galaxy’s total ionizing emissivity. The subsequent conversion between $R_{\text{obs}}$ and $f_{\text{esc}}$ is inevitably more model dependent, a fact that is worth remembering when comparing the values of $f_{\text{esc}}$ derived from different studies.

3.3 Modelling the $R_{\text{obs}}$ probability distribution

Armed with the $R_{\text{obs}}$ distribution we can then proceeded to estimate $\langle f_{\text{esc}} \rangle$ for the final sample of 148 star-forming galaxies. To do this we first constructed a generative model to predict the probability distribution of $R_{\text{obs}}$ for a given object, as a function of $f_{\text{esc}}$. The basic equation relating $R_{\text{obs}}$ to $f_{\text{esc}}$ is:

$$ R_{\text{obs}} = f_{\text{esc}} \times R_{\text{int}} \times e^{-r_{H\text{i}}} \times 10^{0.4A_{\text{UV}}}, \quad (3.2) $$
Figure 3.4  To accurately account for the fluctuating optical depth facing ionizing photons from a combination of the IGM and CGM, we generated a large number of individual sight-line transmission curves as a function of redshift, as detailed in Section 3.3.2. Left panel: Nine random IGM+CGM transmission curves generated at $z=3.4$ (black) over the observed wavelength range for LyC flux (the Lyman-limit lies at $\lambda_{\text{obs}} = 4013\ \text{Å}$ at $z = 3.4$), illustrating the strong variation across different sight lines. The blue shading in the background of each panel shows the transmission of the $U$-band filter. Right panel: Histograms showing the average transmission from 10,000 sight lines generated at $z = 3.55$, calculated by integrating the transmission curve for each sight line through the $U$-band filter. The filled grey histogram corresponds to sight lines accounting for both the IGM and CGM, while the red histogram shows IGM-only sight lines. The importance of incorporating the CGM contribution is highlighted by the significant increase in the relative number of sight lines with $\langle e^{-\tau_U} \rangle \approx 0$. The inset panel shows the $\langle e^{-\tau_U} \rangle$ distribution of sight lines at $z=3.4$ (green) and $z=3.9$ (blue), highlighting the increasing optical depth at higher redshifts.
where $R_{\text{int}}$ is the intrinsic LyC to non-ionizing UV flux ratio, $e^{-r_{\text{HI}}}$ is the line-of-sight transmission through the IGM and CGM, and $A_{\text{UV}}$ is the UV dust attenuation\(^4\).

While $R_{\text{int}}$ and $A_{\text{UV}}$ can be estimated using standard stellar population fitting and/or empirical methods, the crucial complicating factor is the value of $e^{-r_{\text{HI}}}$, which is strongly sight-line dependent and can take a range of values drawn from a highly non-Gaussian distribution (e.g. Steidel et al., 2018). As a result, there is no unique mapping between $f_{\text{esc}}$ and $R_{\text{obs}}$ for individual objects, and one must account for the full distribution of possible $R_{\text{obs}}$ values at a given $f_{\text{esc}}$. In this section we describe in detail how our model for $R_{\text{obs}}(f_{\text{esc}})$ was constructed, focusing on each of the three key quantities ($R_{\text{int}}, e^{-r_{\text{HI}}}, A_{\text{UV}}$) in turn.

### 3.3.1 Intrinsic LyC to non-ionizing UV flux ratio

The intrinsic LyC to non-ionizing UV flux ratio is determined by the properties of the underlying stellar population, which sets the shape of the intrinsic SED, and the galaxy redshift, which fixes the specific rest-frame wavelength regions covered by the $U$ and $V_{606}$-band filters.

In order to define an intrinsic SED that is representative of the average properties of our sample, we first constructed a stack of the VANDELS spectra, following the method described in Cullen et al. (2019). The best-fitting stellar metallicity of this stacked spectrum was then determined by fitting the Binary Population and Spectra Synthesis version 2.2 (BPASSv2.2) SPS models (Eldridge et al., 2017; Stanway & Eldridge, 2018) following the full spectral fitting approach outlined in Cullen et al. (2019), assuming a constant star-formation history over a 100 Myr timescale, binary stellar evolution, and a standard Kroupa (2001) IMF with an upper mass limit of $100 M_\odot$. Our choice of the BPASS models was motivated by observations that suggest these models yield the best predictions for the ionizing continuum spectra of high-redshift stellar populations (e.g. Steidel et al., 2016; Reddy et al., 2021).

The best-fitting BPASS model had a metallicity of $Z_\star \approx 0.001 \approx 0.07 Z_\odot$ (assuming Asplund et al., 2009), consistent with previous estimates of the average stellar metallicity of galaxies at similar redshifts and stellar masses (Cullen et al.,

\(^4\)As measured at the rest-frame effective wavelength of the F606W filter, which is typically $\approx 1300 \, \text{Å}$ for our sample.
2019, 2021; Kashino et al., 2021). This best-fitting model was adopted as the representative intrinsic SED for our sample, and the individual $R_{\text{int}}$ values were then calculated by integrating through the $U$ and $V_{606}$-band filters at the redshift of each galaxy. Across our final galaxy sample the individual values of $R_{\text{int}}$ range from 0.17 to 0.20 with a median value of $R_{\text{int}} = 0.19$ \(^5\). It is worth noting that this is essentially the same intrinsic SED used to infer $\langle f_{\text{esc}} \rangle$ and other related parameters in the recent KLCS spectroscopic analyses at $z \sim 3$ (e.g. Steidel et al., 2018; Pahl et al., 2021).

### 3.3.2 IGM and CGM transmission

At the redshift of our sample, the nuisance parameter with the largest influence on the derived value of $\langle f_{\text{esc}} \rangle$ is the optical depth of the IGM and CGM, which determines the transmitted fraction of ionizing photons through the intervening H\textsc{i} along the line-of-sight to each galaxy ($e^{-\tau_{\text{H}\textsc{i}}}$). The optical depth can vary significantly with sight line, depending on the exact distribution of neutral clouds (as a function of column density and redshift), and therefore must be accounted for in a probabilistic sense.

In many previous studies, it has been common to only consider the contribution of the IGM when accounting for H\textsc{i} optical depth (e.g Vanzella et al., 2010a). However, as galaxies exist in regions of gas overdensities, and are known to be surrounded by significant quantities of H\textsc{i} in their CGM (out to $\approx 700$ physical kpc; e.g. Rudie et al., 2012, 2013), sight lines to galaxies are not representative of random sight lines through the Universe. As a result, it is more accurate to account for both the IGM and CGM when considering the optical depth of H\textsc{i} towards galaxies (e.g. Steidel et al., 2018; Pahl et al., 2021).

To account for the IGM and CGM contribution we generated transmission curves ($e^{-\tau_{\text{H}\textsc{i}}}$) using the parameterization for the column density and redshift distribution of H\textsc{i} clouds given in Steidel et al. (2018). Specifically, we generated 10,000 individual sight lines in six separate redshift bins ($z = 3.4, 3.5, 3.6, 3.7, 3.8, 3.9$),

\(^5\)Although the adopted intrinsic SED model is representative of the average galaxy in our sample, the range of $R_{\text{int}}$ values is expected to be slightly broader in reality as variations on a galaxy-by-galaxy basis in properties such as the star-formation history and metallicity, are not included. However, we highlight that the scatter in our model $R_{\text{obs}}$ distribution is dominated by the stochasticity of the IGM+CGM sightline opacity. We also note that the use of a fixed intrinsic SED model will also influence the calculations of the UV dust attenuation for each individual galaxy (e.g., see Section 3.3.3).
covering the full redshift range of our sample. Full details of the method used to generate the individual sight lines are provided in Appendix 1 of Begley et al. (2022), and examples of nine random sight lines at \( z = 3.4 \) are shown in the left-hand panel of Fig. 3.4, highlighting the significant variation.

For a given galaxy, a value of \( e^{-r_{\text{HI}}} \) is obtained by selecting a random sight line at the nearest redshift and integrating through the \( U \)-band filter. The right-hand panel of Fig. 3.4 illustrates how the resulting distribution of \( e^{-r_{\text{HI}}} \) is strongly peaked at zero, with a highly non-Gaussian shape.

### 3.3.3 UV dust attenuation

After the IGM+CGM transmission, the model parameter that has the largest systematic influence on the derived value of \( \langle f_{\text{esc}} \rangle \) is the UV dust attenuation. In this study, we have taken advantage of the rest-frame UV VANDELS spectra to adopt an empirical approach to calculating the level of UV attenuation on a galaxy-by-galaxy basis. By comparing to our adopted intrinsic SED model (see §3.3.1), which has a UV spectral slope of \( \beta_{\text{int}} = -2.44 \pm 0.02 \), we calculated the value of \( A_{\text{UV}} \) for each object by measuring the observed UV spectral slope (\( \beta_{\text{obs}} \)) from its VANDELS spectrum.

The first step in this process was fitting a power-law \( (f_{\lambda} \propto \lambda^{\beta}) \) to each of the VANDELS spectra over the wavelength range 1300 – 1800 Å, within the continuum windows specified by Calzetti et al. (1994). Fitting \( \beta \) in this fashion, the final galaxy sample has \( \langle \beta_{\text{spec}} \rangle = -1.26 \pm 0.04 \), with a median value of \( \beta_{\text{spec}} = -1.29 \). The average of these individual \( \beta \) estimates is fully consistent with the value derived from the stacked spectrum of the full sample \( \beta_{\text{stack}} = -1.24 \pm 0.03 \).

Armed with the individual values of \( \beta_{\text{obs}} \), it was then possible to calculate individual determinations of \( A_{1600} \) based on the value of \( \Delta \beta = \beta_{\text{obs}} - \beta_{\text{int}} \). However, making this conversion requires a decision to be made on the form of the UV attenuation curve. Unfortunately, the average form of the UV attenuation curve at high redshift is still a matter of debate, with no consensus having been reached in the literature (e.g. Cullen et al., 2018; McLure et al., 2018b; Reddy et al., 2018a; Shivaei et al., 2020), and we therefore chose to employ a dust curve that is at least consistent with both the VANDELS spectra and our choice of intrinsic SED model. To do this, we fitted the stacked VANDELS spectrum using the BPASS intrinsic SED model, attenuated by a dust curve parameterized following Salim
et al. (2018). According to this formulation, the Calzetti et al. (2000) attenuation curve is modified by a power-law exponent (δ), such that δ = 0.0 corresponds to the Calzetti starburst curve and δ ≃ −0.5 is close to the SMC extinction curve (e.g. Gordon et al., 2003). Fitting the stacked spectrum over the wavelength range 1300 – 1800 Å returned a best-fitting dust slope of δ = −0.25^{+0.37}_{−0.27}, with no 2175 Å dust bump.

Based on this dust curve, we proceeded to convert the individual values of Δβ measured for each galaxy into attenuation at 1600 Å, using the relation: $A_{1600} = 1.28 \times \Delta\beta$. For each object, we then calculated the value of $A_{UV}$ at the effective wavelength of the $V_{606}$ filter using $A_{UV} = 1.2 \times A_{1600}$, where the constant has a slight redshift dependence. The error on $A_{UV}$ ($\sigma_{A_{UV}}$) was estimated by propagating the error on $\Delta\beta$.

### 3.3.4 Constructing model $R_{obs}(f_{esc})$ distributions

Combining these three components, it is possible to construct the expected distribution of $R_{obs}$ as a function of $f_{esc}$. The model distribution can then be statistically compared to the observed $R_{obs}$ distribution, to place constraints on $\langle f_{esc} \rangle$ for any given sample. We adopted a Monte Carlo procedure for producing
model $R_{\text{obs}}$ distributions as a function of $f_{\text{esc}}$. For a set of $N$ galaxies drawn from the full galaxy sample, we performed the following steps:

1. For each galaxy, select a random IGM+CGM sight line at the appropriate redshift and calculate the value of $e^{-\tau_{\text{HI}}}$ integrated through the $U-$ band filter.

2. Set the value of $A_{\text{UV}}$ by perturbing the measured value assuming a Gaussian scatter of $\sigma_{A_{\text{UV}}}$ and ensuring that $A_{\text{UV}} \geq 0$.

3. Using these two values, and the adopted value of $R_{\text{int}}$, calculate the expected $R_{\text{obs}}$ using Equation 3.2.

4. Perturb $R_{\text{obs}}$ according to the depth of the $U$ and $V_{606}-$ band mosaics at the position of the galaxy.

These steps yield $N$ model $R_{\text{obs}}$ values. The process was then repeated 10,000 times in order to build-up the average model distribution that could then be directly compared to the observed data, as shown in Fig. 3.5. It is worth highlighting that the underlying $R$ distribution before considering the effect of finite image depth, is strictly positive, and only becomes Gaussian-like when the imaging noise is accounted for. It then follows that the information in $R_{\text{obs}}$ constraining $\langle f_{\text{esc}} \rangle$ primarily derives from the positive skew in $R_{\text{obs}}$ that increases with increasing $\langle f_{\text{esc}} \rangle$ (e.g., see left-to-right panels in Fig. 3.5).

### 3.4 Results

In this section we describe how we estimated $\langle f_{\text{esc}} \rangle$ for our final galaxy sample, using two approaches: (i) a binned maximum likelihood method and (ii) a Bayesian framework for combining individual $f_{\text{esc}}$ estimates. We also explore whether trends in $\langle f_{\text{esc}} \rangle$ can be identified by splitting our sample on the basis of properties that are expected to correlate with $f_{\text{esc}}$; such as the equivalent width of Ly$\alpha$, UV continuum slope $\beta$ (a proxy for dust attenuation), galaxy stellar mass and intrinsic UV luminosity.
3.4.1 Maximum likelihood

The maximum likelihood technique is based upon a comparison between the observed and model $R_{\text{obs}}$ distributions. Model $R_{\text{obs}}$ distributions were built for a grid of $\langle f_{\text{esc}} \rangle$ values between 0 and 1 with an interval of $\Delta \langle f_{\text{esc}} \rangle = 0.001$, following the procedure outlined in Section 3.3. The fitting procedure was to maximize the following log-likelihood function:

$$\ln L = \sum_i n_i \ln p_i,$$

(3.3)

where the summation runs over the $i$ bins of the $R_{\text{obs}}$ histogram (see Fig. 3.3), $n_i$ is the number of galaxies in bin $i$ and $p_i$ is the probability of finding a galaxy within bin $i$ for a given value of $f_{\text{esc}}$. The probability $p_i$ is naturally defined as $n_i^m / N$, where $n_i^m$ is the number of galaxies in bin $i$ predicted by the model, for a given $f_{\text{esc}}$, and $N$ is the total number of galaxies in the sample ($N = 148$). The $1\sigma$ confidence interval can be estimated via:

$$\Delta \chi^2 = -2 \ln (L/L_{\text{max}}) = 1,$$

(3.4)

Figure 3.6  The result of the maximum likelihood fit to the $R_{\text{obs}}$ distribution of the full sample of 148 star-forming galaxies. The best-fitting value is found to be $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$ and $f_{\text{esc}} = 0.0$ is excluded at $\geq 3\sigma$ confidence (i.e. $\Delta \chi^2 \geq 9$).
where $L_{\text{max}}$ is the maximum likelihood value. Applying this technique we find clear evidence for a non-zero $\langle f_{\text{esc}} \rangle$ at the $> 3\sigma$ level, with a best-fitting value of $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$ (see Fig. 3.6).

Fig. 3.5 provides a visual illustration of this result. It can be seen from the middle panel that the model distribution corresponding to $\langle f_{\text{esc}} \rangle = 0.07$ provides an excellent description of the data. In contrast, the $\langle f_{\text{esc}} \rangle = 0$ model predicts too many galaxies with $R_{\text{obs}} < 0$, while the $\langle f_{\text{esc}} \rangle = 0.15$ model predicts a positive tail in excess of what is observed and underestimates the $R_{\text{obs}} = 0$ peak.

### 3.4.2 Bayesian inference

To complement the maximum likelihood fitting, we adopted a second approach for estimating $\langle f_{\text{esc}} \rangle$ that utilises the individual posterior probabilities for $f_{\text{esc}}$ of each galaxy. Using Bayes’ theorem, the posterior probability for $f_{\text{esc}}$ is given by:

$$p(f_{\text{esc}} | R_{\text{obs}}) \propto \int p(R_{\text{obs}} | f_{\text{esc}}, \Theta) p(f_{\text{esc}}) p(\Theta) d\Theta$$

(3.5)

where $\Theta = (R_{\text{int}}, e^{-\tau_{\text{HI}}}, A_{\text{UV}})$ and $p(R_{\text{obs}} | f_{\text{esc}}, \Theta)$ is the likelihood for $R_{\text{obs}}$, $p(f_{\text{esc}})$ is the prior on the escape fraction, and $p(\Theta)$ is the prior on the additional free parameters. For a given galaxy, we can write the log-likelihood as,

$$\ln p(R_{\text{obs}} | f_{\text{esc}}, \Theta) = \frac{-(R(f_{\text{esc}}, \Theta) - R_{\text{obs}})^2}{2\sigma_{\text{obs}}^2} - \ln(\sqrt{2\pi}\sigma_{\text{obs}}),$$

(3.6)

where $\sigma_{\text{obs}}$ is the error on $R_{\text{obs}}$ and $R(f_{\text{esc}}, \Theta)$ is the predicted value of $R$ for a given set of input parameters, according to Equation 3.2.

The crucial aspect of the Bayesian approach then becomes determining the priors for each parameter. For simplicity, we assumed a fixed value for $R_{\text{int}}$ for each galaxy (see Section 3.3.1). We adopted the following priors for each of the other three free parameters: (i) for $f_{\text{esc}}$ we assume a uniform prior between 0 and 1; (ii) for $A_{\text{UV}}$ we assume a Gaussian prior with mean and standard deviation given by the individual fits to the UV continuum slope of each galaxy (Section 3.3.3); (iii) finally, to generate a prior on $e^{-\tau_{\text{HI}}}$ we perform a kernel density estimation to turn the distribution of sight lines (see Section 3.3.2) into a smooth probability distribution. The resulting prior distributions for $e^{-\tau_{\text{HI}}}$ as a function of redshift
are shown in Fig. 3.7.

Armed with the likelihood and prior distributions we determined the posterior of \( f_{\text{esc}} \) for each galaxy using an MCMC sampling technique (Foreman-Mackey et al., 2013). Examples of the posterior distributions for a detected (S/N \( \geq 5\sigma \)) and non-detected galaxy in the \( U- \) band are shown in the left-hand panel of Fig. 3.8. The value of \( \langle f_{\text{esc}} \rangle \) can then be obtained by multiplying the individual posteriors:

\[
p(\langle f_{\text{esc}} \rangle | \{ R_{\text{obs}} \}) \propto \prod_i^{N_{\text{gal}}} p_i(f_{\text{esc}}).
\] (3.7)

In the right-hand panel of Fig. 3.8 we show the resulting \( p(\langle f_{\text{esc}} \rangle | \{ R_{\text{obs}} \}) \) for our full sample. It is important to note that equation 3.7 is only valid under that assumption that each galaxy has the same value of \( f_{\text{esc}} \). Therefore, \( \langle f_{\text{esc}} \rangle \) should be interpreted as the most likely value of \( f_{\text{esc}} \) assuming a uniform value across the sample, rather than the average of 148 individual (potentially different) values. In this way, \( \langle f_{\text{esc}} \rangle \) has the same physical interpretation as \( \langle f_{\text{esc}} \rangle \) derived from the maximum likelihood fitting above. Using this method, we infer a best-fitting value of \( \langle f_{\text{esc}} \rangle = 0.05 \pm 0.01 \), fully consistent (within 1\( \sigma \)) with the value inferred from the maximum likelihood approach, and inconsistent with \( \langle f_{\text{esc}} \rangle = 0 \) at the \( \geq 3\sigma \) level.

### 3.4.3 Escape fraction dependence on galaxy physical properties

Having established that \( \langle f_{\text{esc}} \rangle \) for the full sample is non-zero, it is clearly of interest to investigate whether or not there is any indication that \( f_{\text{esc}} \) correlates with other galaxy properties. As discussed in the introduction, reliable proxies for LyC escape are required in order to infer \( f_{\text{esc}} \) during the reionization era, where direct measurements are not possible.

One of the most prominent amongst potential \( f_{\text{esc}} \) indicators is the equivalent width of the Ly\( \alpha \) line (\( W_\lambda(\text{Ly}\alpha) \)), which is expected to correlate with LyC escape since both are sensitive to the column density and distribution of H\( \text{I} \) within galaxies (e.g. Verhamme et al., 2015; Gronke et al., 2015; Dijkstra et al., 2016). Observational evidence in support of this connection has recently been reported via spectroscopic analyses of galaxies at \( z \approx 3 \), which find strong evidence for a
Figure 3.7  Probability density functions for $e^{-\tau_{HI}^U}$, used as priors in our Bayesian inference methodology (Section 3.4.2). To generate the smooth probability density functions we performed a kernel density estimation of the distribution of 10,000 sight lines at each redshift (examples of these can be seen in Fig. 3.4). The increase in probability density at low transmission (i.e., high IGM+CGM optical depth) with increasing redshift can clearly be seen.
Figure 3.8  Left: A corner plot showing the 1D and 2D marginalised posteriors for $f_{\text{esc}}$, $A_{\text{UV}}$ and $e^{-\tau_{\text{HI}}}$ for two example galaxies drawn from our final sample. The blue posteriors show one of the two galaxies in our full sample with a robust ($\geq 5\sigma$) individual $R_{\text{obs}}$ detection. The red posteriors show an example of a typical galaxy that is not individually detected. To calculate the average $\langle f_{\text{esc}} \rangle$ for a given galaxy sample, the individual $f_{\text{esc}}$ posteriors (i.e., curves in the upper left panel) were multiplied together. Right: The posterior probability $p(\langle f_{\text{esc}} \rangle | \{R_{\text{obs}}\})$ for the full galaxy sample, corresponding to $\langle f_{\text{esc}} \rangle = 0.05 \pm 0.01$. 

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correlation between $f_{\text{esc}}$ and $W_\lambda(\text{Ly}\alpha)$ (Marchi et al., 2017; Steidel et al., 2018; Pahl et al., 2021), as well as $W_\lambda(\text{Ly}\alpha)$ and the covering fraction of H\textsc{i} (Reddy et al., 2016; Gazagnes et al., 2020b; Reddy et al., 2021; Saldana-Lopez et al., 2022a). Other likely indirect tracers of the neutral H\textsc{i} column density of galaxies include the dust content (traced by the UV continuum slope, $\beta$) and stellar mass ($M_*$); indeed, both of these quantities are known to be linked to the escape of Ly\textalpha{}photons (Du et al., 2018; Cullen et al., 2020).

Finally, it is also of interest to investigate whether $f_{\text{esc}}$ and UV luminosity are correlated, given that calculating the global ionizing background during the EoR typically relies on integrating down the UV galaxy luminosity function with an assumption that $f_{\text{esc}}$ is constant (e.g. Robertson et al., 2015). Below we explore the correlation between $f_{\text{esc}}$ and each of these galaxy properties ($W_\lambda(\text{Ly}\alpha)$, $\beta$, $M_*$, $L_{\text{UV}}$), in turn.

### $W_\lambda(\text{Ly}\alpha)$

To investigate the link between $f_{\text{esc}}$ and $W_\lambda(\text{Ly}\alpha)$, we split the full sample in half at the median value of $W_\lambda(\text{Ly}\alpha)=-6$ Å. After excluding two galaxies with unreliable $W_\lambda(\text{Ly}\alpha)$ measurements due to artefacts in the VANDELS spectra, the resulting low- and high-$W_\lambda(\text{Ly}\alpha)$ sub-samples had median equivalent widths of $W_\lambda(\text{Ly}\alpha)=-14.2$ Å and $W_\lambda(\text{Ly}\alpha)=4.9$ Å, respectively. Fitting the two sub-samples using the maximum likelihood technique returned best-fitting values of $\langle f_{\text{esc}} \rangle = 0.02^{+0.02}_{-0.02}$ for the low-$W_\lambda(\text{Ly}\alpha)$ sub-sample and $\langle f_{\text{esc}} \rangle = 0.12^{+0.06}_{-0.04}$ for the high-$W_\lambda(\text{Ly}\alpha)$ sub-sample (Fig. 3.9). Using the Bayesian inference methodology, the constraints for the low and high-$W_\lambda(\text{Ly}\alpha)$ sub-samples were $\langle f_{\text{esc}} \rangle < 0.03$ (2\sigma) and $\langle f_{\text{esc}} \rangle = 0.08^{+0.02}_{-0.02}$ (Fig. 3.10). These results represent significant evidence ($>3\sigma$) for an increase in $f_{\text{esc}}$ with increasing $W_\lambda(\text{Ly}\alpha)$, in broad agreement with recent spectroscopic studies (Steidel et al., 2018; Pahl et al., 2021).

### UV continuum slope

Next, we looked for a link between $f_{\text{esc}}$ and the observed UV continuum slope $\beta_{\text{obs}}$ (a proxy for dust attenuation at UV wavelengths). A $f_{\text{esc}}-\beta_{\text{obs}}$ correlation is expected due to the sensitivity of LyC photon escape to the dust and H\textsc{i} column density of the ISM.
Figure 3.9  The constraints on $⟨f_{\text{esc}}⟩$ returned by the maximum-likelihood technique for the four sample splits described in Section 3.4.3. In each panel the red and blue curves show the $⟨f_{\text{esc}}⟩$ constraints when the full sample is split in two at the median value of the physical parameter in question. The red and blue curves can be identified by the labels in the top-right corner of each panel. For reference, the grey curve in each panel shows the constraint on $⟨f_{\text{esc}}⟩$ for the full galaxy sample.
Figure 3.10 The constraints on \( \langle f_{\text{esc}} \rangle \) returned by the Bayesian inference technique for the four sample splits described in Section 3.4.3, in the same format as Fig. 3.9. The red and blue curves show the posterior probability distributions for the sample splits, whereas the grey curve in each panel shows the posterior probability distribution of \( \langle f_{\text{esc}} \rangle \) for the full sample. As before, the red and blue curves can be identified by the labels in the top-right corner of each panel.
Table 3.1  Summary of the best-fitting \( (f_{\text{esc}}) \) values of the various samples discussed in Section 3.4. Results are quoted for both the maximum likelihood and Bayesian inferences methods. Upper limits represent 2\( \sigma \) constraints.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Maximum Likelihood</th>
<th>Bayesian Inference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full Sample</td>
<td>0.07^{+0.02}_{-0.02}</td>
<td>0.05^{+0.01}_{-0.01}</td>
</tr>
<tr>
<td>Low ( W_{\Delta}(\text{Ly}\alpha) )</td>
<td>0.02^{+0.02}_{-0.02}</td>
<td>&lt; 0.03</td>
</tr>
<tr>
<td>High ( W_{\Delta}(\text{Ly}\alpha) )</td>
<td>0.12^{+0.06}_{-0.04}</td>
<td>0.08^{+0.02}_{-0.02}</td>
</tr>
<tr>
<td>Red ( \beta )</td>
<td>0.04^{+0.01}_{-0.02}</td>
<td>&lt; 0.03</td>
</tr>
<tr>
<td>Blue ( \beta )</td>
<td>0.22^{+0.04}_{-0.06}</td>
<td>0.14^{+0.06}_{-0.04}</td>
</tr>
<tr>
<td>High-( M_\star )</td>
<td>0.06^{+0.02}_{-0.02}</td>
<td>0.05^{+0.02}_{-0.01}</td>
</tr>
<tr>
<td>Low-( M_\star )</td>
<td>0.09^{+0.05}_{-0.04}</td>
<td>0.05^{+0.02}_{-0.01}</td>
</tr>
<tr>
<td>Intrinsic UV-bright</td>
<td>0.03^{+0.02}_{-0.01}</td>
<td>0.04^{+0.01}_{-0.01}</td>
</tr>
<tr>
<td>Intrinsic UV-faint</td>
<td>0.18^{+0.06}_{-0.05}</td>
<td>0.10^{+0.04}_{-0.03}</td>
</tr>
</tbody>
</table>

Again, the full galaxy sample was split in half at the median value of \( \beta_{\text{obs}} \) = −1.29, producing low attenuation (‘blue’, with median \( \beta_{\text{obs}} = −1.62 \)) and high attenuation (‘red’, with median \( \beta_{\text{obs}} = −0.92 \)) sub-samples. Applying the maximum likelihood approach returned best-fitting values of \( \langle f_{\text{esc}} \rangle = 0.22^{+0.04}_{-0.06} \) and \( \langle f_{\text{esc}} \rangle = 0.04^{+0.01}_{-0.02} \) for the low- and high-attenuation sub-samples, respectively (Fig. 3.9). Similarly, the Bayesian inference approach returned \( \langle f_{\text{esc}} \rangle = 0.14^{+0.06}_{-0.04} \) for the low-attenuation sub-sample and \( \langle f_{\text{esc}} \rangle < 0.03 \) (2\( \sigma \)) for the high-attenuation sub-sample (Fig. 3.10). Taken together, these results again represent significant evidence in favour of a picture in which galaxies with lower levels of UV dust attenuation display higher values of \( \langle f_{\text{esc}} \rangle \).

**Stellar mass**

Although \( W_{\Delta}(\text{Ly}\alpha) \) and \( \beta_{\text{obs}} \) are two galaxy properties with a clear and direct link to \( f_{\text{esc}} \), it is also interesting to examine any correlation between \( f_{\text{esc}} \) and stellar mass, a property that is already known to correlate with both \( W_{\Delta}(\text{Ly}\alpha) \) and UV dust attenuation (e.g McLure et al., 2018b; Cullen et al., 2020). Splitting the sample into low-\( M_\star \) (median = \( 10^{8.72}M_\odot \)) and high-\( M_\star \) (median = \( 10^{9.22}M_\odot \)) sub-samples, the maximum likelihood approach returned best-fitting values of \( \langle f_{\text{esc}} \rangle = 0.09^{+0.05}_{-0.04} \) and \( \langle f_{\text{esc}} \rangle = 0.06^{+0.02}_{-0.02} \), respectively (Fig. 3.9). With our Bayesian inference approach, we derive corresponding constraints of \( \langle f_{\text{esc}} \rangle = 0.05^{+0.02}_{-0.01} \) and
\( \langle f_{\text{esc}} \rangle = 0.05^{+0.02}_{-0.01} \) (Fig. 3.10). In either case, we find that any dependence of \( f_{\text{esc}} \) on \( M_* \), if one exists, is not a strong as the dependence on \( W_\lambda(\text{Ly}\alpha) \) and \( \beta \), suggesting that \( M_* \) is at best a secondary indicator of \( f_{\text{esc}} \).

**Intrinsic UV luminosity**

Finally, we divided the full galaxy sample at the median intrinsic (i.e. dust corrected) UV magnitude \( (M_{\text{UV}} = -21.8) \), into UV-faint (median \( M_{\text{UV}} = -21.3 \)) and UV-bright (median \( M_{\text{UV}} = -22.4 \)) sub-samples, spanning intrinsic UV luminosities in the range \( 0.05 \lesssim (L_{\text{UV}}/L^*_{\text{UV}}) \lesssim 2.5 \). The maximum likelihood fitting technique returned values of \( \langle f_{\text{esc}} \rangle = 0.18^{+0.06}_{-0.05} \) for the UV-faint galaxies and \( \langle f_{\text{esc}} \rangle = 0.03^{+0.02}_{-0.01} \) for the UV-bright galaxies (Fig. 3.9). The constraints returned by the Bayesian inference approach are consistent, with \( \langle f_{\text{esc}} \rangle = 0.10^{+0.04}_{-0.03} \) and \( \langle f_{\text{esc}} \rangle = 0.04^{+0.01}_{-0.01} \), respectively (Fig. 3.10). We note that the decision to focus on the intrinsic UV magnitude rather than observed UV magnitude was taken because the latter is heavily dust-attenuation dependent, especially at the bright end, complicating the physical interpretation.

A summary of the \( \langle f_{\text{esc}} \rangle \) constraints for the full galaxy sample and the four sample splits considered here is presented in Table 3.1. The constraints derived from the two fitting approaches are consistent to at least the 2\( \sigma \) level, across all sample splits investigated. Taken together, these results form a consistent picture, in which LyC photons preferentially escape from the same UV-faint, dust-free galaxies that are also the primary sources of Ly\( \alpha \) escape. Across the range of physical properties probed by our sample, the typical escape fraction appears to roughly encompass \( f_{\text{esc}} \approx 0 - 0.2 \), with a full sample average of \( \langle f_{\text{esc}} \rangle \approx 0.07 \). While our current sample is limited in terms of statistics and dynamic range, our analysis clearly demonstrates the ability of our adopted technique to recover \( \langle f_{\text{esc}} \rangle \) trends from broad-band photometry.

### 3.4.4 Individual \( R_{\text{obs}} \) detections

The analysis presented here is primarily focused on constraining \( \langle f_{\text{esc}} \rangle \) for our galaxy sample based on modelling the shape of the \( R_{\text{obs}} \) distribution. However, it is worth noting that two objects in our sample could be considered as robust LyC detections, having individual \( U \)-band flux measurements with \( \geq 5\sigma \) significance.
Both of these objects have been previously reported in the literature (Vanzella et al., 2010b; Ji et al., 2020; Saxena et al., 2021).

In fact, the number of objects within our sample with a positive $U$-band flux detection provides a useful additional sanity check on the $\langle f_{\text{esc}} \rangle$ value we derived for the full sample. We performed a simple test in which we constructed simulated samples as a function of average escape fraction, using the method described in Section 3.3. For each value of $\langle f_{\text{esc}} \rangle$ in the range $0 \leq \langle f_{\text{esc}} \rangle \leq 0.2$ ($\Delta \langle f_{\text{esc}} \rangle = 0.01$) we produced 5000 simulated samples of 148 galaxies, and calculated the predicted number of $U$-band flux detections. As can be seen from Fig. 3.11, the number of $\geq 2\sigma$ and $\geq 5\sigma$ $U$-band flux detections we see in the real data is in good agreement with the model prediction for $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$. 

Figure 3.11 The expected number of $U$-band flux detections in our sample as a function of $\langle f_{\text{esc}} \rangle$ (see Section 3.4.4). The expected number of $U$-band flux detections at $\geq 2\sigma$ and $\geq 5\sigma$ based on our model are shown as the solid black lines, with the $1\sigma$ uncertainties indicated by the shaded regions. The two data points indicate the observed number of $\geq 2\sigma$ and $\geq 5\sigma$ detections in our final sample. It can be seen that for our best-fitting value of $\langle f_{\text{esc}} \rangle \approx 0.07$, the expected and observed number of $U$-band flux detections are in good agreement.
3.5 Discussion

The results presented above clearly demonstrate that meaningful constraints on $\langle f_{\text{esc}} \rangle$ at $z \approx 3 - 4$ can be obtained from broadband photometric measurements of the emergent LyC flux in the $U$-band. In this section we begin by comparing our results to previous measurements in the literature at similar redshifts, before briefly considering the physical picture suggested by our results. We finish with a quantitative discussion of the various systematic uncertainties present in our study, suggesting avenues for future improvement.

3.5.1 Literature comparison

In Fig. 3.12 we show a comparison between the $\langle f_{\text{esc}} \rangle$ constraints presented in this work and a selection of comparable studies of star-forming galaxies at $z \sim 2 - 4$ from the literature. The literature compilation includes estimates of $\langle f_{\text{esc}} \rangle$ derived from both spectroscopy and photometry. It can be seen that, prior to this work, the only statistical ($\geq 3\sigma$) measurements of $\langle f_{\text{esc}} \rangle$ have come from deep spectroscopic analyses (e.g. Marchi et al., 2017; Steidel et al., 2018; Pahl et al., 2021).

The relative success of spectroscopic studies versus photometric studies indicated by Fig. 3.12 is primarily due to the fact that spectroscopy enables a measurement of the LyC flux across a narrow bandpass, close to the intrinsic Lyman limit, where the optical depth to H\textsc{i} is minimized (e.g. the 880 – 910 Å window used by Steidel et al., 2018). For example, at $z = 3.6$, the average IGM+CGM transmission integrated across the $U$-band filter is $\langle e^{-\tau_{\text{H}i}} \rangle = 0.07$, compared to an average of $\langle e^{-\tau_{\text{H}i}} \rangle = 0.28$ across the 880 – 910 Å bandpass\(^6\).

Despite this, the analysis presented here clearly demonstrates that it is possible to derive constraints from broad-band imaging that move beyond upper limits, and are comparable to those achieved from spectroscopy. However, to achieve this, large statistical samples, ultra-deep $U$-band imaging, accurate treatment of the

\^6At the median redshift of our sample ($\langle z_{\text{spec}} \rangle = 3.58$), the $U$-band imaging probes $\lambda_{\text{rest}} \approx 750 - 870$ Å, which is marginally bluer than the wavelength range used to constrain $\langle f_{\text{esc}} \rangle$ in Steidel et al. (2018). However, given the relatively flat intrinsic SED across the $\lambda_{\text{rest}} \approx 700 - 900$ Å wavelength regime, and the fact that we take a robust statistical approach to account for the impact of the highly stochastic IGM+CGM opacity, we are confident that the $\langle f_{\text{esc}} \rangle$ measurement derived here are can be compared against the spectroscopic results of Steidel et al. (2018) (see also Pahl et al., 2021) without significant systemic biases.
IGM+CGM optical depth, and an analysis that exploits the full $R_{\text{obs}}$ distribution, are all required.

It can be seen from Fig. 3.12 that our best-fitting value of $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$ is fully consistent with the latest estimates from the VIMOS Ultra Deep Survey presented in Marchi et al. (2017), and the Keck Lyman Continuum Spectroscopic Survey presented in Steidel et al. (2018) and Pahl et al. (2021). Moreover, these results are in quantitative agreement with the majority of previous upper limits reported from broadband imaging studies, which typically find $\langle f_{\text{esc}} \rangle \lesssim 0.1$ at the 2σ level.

### 3.5.2 A physical picture

Our results point towards a surprisingly simple physical picture, in which the observed distribution of the ionizing to non-ionizing UV flux ratio for our galaxy sample can be modelled as population with a single value of $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$. However, we have also found evidence that $\langle f_{\text{esc}} \rangle$ varies as a function of galaxy properties; increasing with $W_d(\text{Ly} \alpha)$ and decreasing with UV dust attenuation and intrinsic UV luminosity. These trends are in good agreement with recent results from spectroscopic studies at similar redshifts (Steidel et al., 2018; Pahl et al., 2021), and have a number of important implications. Most importantly, our result suggest that low-dust, UV-faint galaxies at $z \geq 6$ are plausibly capable of displaying the $\langle f_{\text{esc}} \rangle \geq 0.1$ required to drive reionization (Robertson et al., 2013; Finkelstein et al., 2019).

As far as our sample is concerned, it is clear from Fig. 3.5 and Fig. 3.11 that the observed data is fully consistent with our simple model. Indeed, based on our sample alone, there is no indication that the more complex pictures that have been suggested in the literature, in which Lyman-continuum emission is switched either ‘on’ or ‘off’ due to anisotropic dust/ISM distributions leading to line-of-sight effects, and/or stochastic star-formation histories (e.g. Fletcher et al., 2019), are required to explain the data.

However, although our current sample does not justify a more complex physical model statistically, it is clear that the true underlying $f_{\text{esc}}$ distribution is likely to be significantly more complicated. In the future, larger sample sizes and deeper photometry should make it possible to fit more complex underlying
Figure 3.12 A comparison between the results presented here and \( \langle f_{\text{esc}} \rangle \) measurements for \( z \approx 3 \) galaxy samples in the literature. Results based on photometry are shown in red and results based on spectroscopy are shown in blue. The circular markers represent studies that report a \( \geq 2\sigma \) constraint on \( \langle f_{\text{esc}} \rangle \), while the triangular markers represent studies that report upper limits (\( 2\sigma \)). Where necessary, we have converted relative escape fraction estimates to absolute escape fraction estimates assuming \( E(B-V) = 0.1 \) and the Calzetti et al. (2000) attenuation curve, as in Meštrić et al. (2021). For Grazian et al. (2017), who derive constraints on \( \langle f_{\text{esc}} \rangle \) as a function of \( M_{\text{UV}} \), we plot the result for their \( M_{\text{UV}} \sim -19.7 \) stack, closest to the median of our sample (\( M_{\text{UV}} \sim -20.2 \)).
$f_{\text{esc}}$ distributions and quantitatively compare them to our simple model using Bayesian model selection techniques.

Interestingly, in contrast to the clear correlations between $f_{\text{esc}}$ and $W_A(\text{Ly}\alpha)$, $\beta$ and $M_{\text{UV}}$, our results do not show evidence for a strong trend between $f_{\text{esc}}$ and galaxy stellar mass. The lack of a clear $f_{\text{esc}}-M_*$ trend is perhaps surprising given the known correlations between $M_*$, $W_A(\text{Ly}\alpha)$ and $\beta$ (e.g. McLure et al., 2018a; Cullen et al., 2020); however, our results suggest while strong Ly$\alpha$ emission, low dust attenuation, and faint intrinsic UV luminosity can be considered primary indicators of $f_{\text{esc}}$, any $f_{\text{esc}}$ trend with $M_*$, if present, is secondary and ‘washed-out’ by the scatter in the $M_*-W_A(\text{Ly}\alpha)$, $M_*-\beta$ and $M_*-M_{\text{UV}}$ relations. This apparent lack of a clear $f_{\text{esc}}-M_*$ correlation is in good agreement with recent results for galaxies at $z \approx 0.4$ reported in Izotov et al. (2021). However, it is important to note that of the four properties physical properties considered here, $M_*$ is the most model-dependent, and therefore subject to the largest number of systematic uncertainties.

Finally, we note that our results are qualitatively in agreement with the results of Reddy et al. (2016), who found that the ionizing escape fraction is driven predominantly by changes in the covering fraction of H$\text{i}$ ($f_{\text{cov}}(\text{H} \text{i})$), with lower $f_{\text{cov}}(\text{H} \text{i})$ corresponding to higher $f_{\text{esc}}$ (see also; Gazagnes et al., 2020b; Reddy et al., 2021; Saldana-Lopez et al., 2022a). Crucially, Reddy et al. (2016) showed that dust covering fraction increases with $f_{\text{cov}}(\text{H} \text{i})$, implying that $f_{\text{esc}}$ will decrease towards galaxies with lower dust attenuation, consistent with our findings. Indeed, a fundamental correlation between $f_{\text{esc}}$ and $f_{\text{cov}}(\text{H} \text{i})$ (or dust) is well-motivated from a theoretical point of view, and naturally explains the resulting $f_{\text{esc}}$ trends with $W_A(\text{Ly}\alpha)$ and $\beta$.

### 3.5.3 Systematic uncertainties

Before concluding, it is worth considering the systematic impact of some of the key choices made in our analysis and understanding the effect that they have on our results.

One simplifying assumption we made was the choice of a single underlying SPS model for the full sample, which fixes the intrinsic ratio of ionizing to non-ionizing UV flux (Section 3.3.1). Although this single model is physically motivated, being derived from a full-spectrum fit to the stacked VANDELS spectrum of
our full galaxy sample, other choices for the intrinsic underlying SED would systematically alter the value of $R_{\text{int}}$, and hence $\langle f_{\text{esc}} \rangle$. However, it is important to note that our choice of the BPASS binary models yields larger values of $R_{\text{int}}$ than most other available SPS models, and in that sense most alternative models would result in marginally larger $\langle f_{\text{esc}} \rangle$ estimates. However, this is a relatively small systematic effect, for example, assuming the Starburst99 models (Leitherer et al., 1999b), with the same star-formation history and IMF, increases $\langle f_{\text{esc}} \rangle$ by a factor of $\approx 1.1$.

We have also assumed constant star-formation histories on a 100 Myr timescale, a common assumption when modelling the stellar populations of $z \approx 2 - 3$ star-forming galaxies (e.g., Steidel et al., 2016; Cullen et al., 2019). Alternative choices for the star-formation history have only a minor effect on $R_{\text{int}}$ (< 10 per cent), as long as the assumption of a constant star-formation rate is valid on timescales $\gtrsim 50$ Myr. Systematically younger ages would increase $R_{\text{int}}$ and hence decrease the resulting $\langle f_{\text{esc}} \rangle$ (at the $\gtrsim 20$ per cent level). However, there is currently no strong observational evidence for star-formation timescales $< 50$ Myr at the typical stellar mass of our sample.

Another simplifying assumption we made was to adopt a single dust law, with a slope of $\delta = -0.25$, motivated by a comparison between the intrinsic model and the stacked spectrum of the full sample (Section 3.3). A $\delta = -0.25$ slope is intermediate between the commonly-adopted Calzetti ($\delta = 0$) and SMC curves ($\delta = -0.5$). Adopting a dust curve as steep as the SMC extinction curve would increase our derived $\langle f_{\text{esc}} \rangle$ values by a factor of $\approx 1.5$. In contrast, adopting an attenuation curve as grey as the Calzetti et al. (2000) starburst law would decrease our derived $\langle f_{\text{esc}} \rangle$ values by a factor of $\approx 1.7$.

In reality, each galaxy in our sample has a unique metallicity, star-formation history and dust attenuation curve, which could in principle be incorporated directly into the determination of $\langle f_{\text{esc}} \rangle$ in a future analysis. Nevertheless, first-order estimates of the potential systematic effects suggest the range of $\langle f_{\text{esc}} \rangle$ for the full sample would remain within the range $0.03 \leq \langle f_{\text{esc}} \rangle \leq 0.1$. 

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3.6 Conclusions

We have presented the results of a study aimed at constraining the average Lyman-continuum escape fraction $\langle f_{\text{esc}} \rangle$ of star-forming galaxies at $z \approx 3.5$. After performing a careful selection against line-of-sight contamination and AGN interlopers, we assembled a sample of 148 galaxies at $3.35 \leq z_{\text{spec}} \leq 3.95$ from the VANDELS spectroscopic survey (McLure et al., 2018b; Garilli et al., 2021).

Using a combination of ultra-deep, ground-based, $U$-band imaging and Hubble Space Telescope $V$-band imaging, we were able to robustly measure $R_{\text{obs}} = (L_{\text{LyC}}/L_{\text{UV}})_{\text{obs}}$ for each galaxy. By fitting the $R_{\text{obs}}$ distribution of our full sample, we were able to derive consistent constraints on $\langle f_{\text{esc}} \rangle$, using two different fitting techniques. Both techniques were based upon the assumption that a single value of $f_{\text{esc}}$ could be applied to the full sample and utilised accurate Monte Carlo simulations to trace the full distribution of $H_{\text{i}}$ optical depths through the intervening IGM and CGM.

Splitting the sample in two, we investigated the evidence for trends between $\langle f_{\text{esc}} \rangle$ and a number of physical properties, namely $W_d(\text{Ly}\alpha)$, $\beta_{\text{obs}}$, $M_\star$ and intrinsic $M_{\text{UV}}$. The main results of this study can be summarised as follows:

1. Fitting the $R_{\text{obs}}$ distribution for the full sample using a maximum-likelihood technique returns a best-fitting value of $\langle f_{\text{esc}} \rangle = 0.07 \pm 0.02$ (Fig. 3.6). Models with $\langle f_{\text{esc}} \rangle = 0$ and $\langle f_{\text{esc}} \rangle \geq 0.15$ are rejected at the $\geq 3\sigma$ level. Using an independent Bayesian inference approach, we obtain a fully consistent value of $\langle f_{\text{esc}} \rangle = 0.05 \pm 0.01$ (Fig. 3.8). This result represents the first significant measurement ($\geq 3\sigma$) of $\langle f_{\text{esc}} \rangle$ from ground-based broadband imaging at $z > 3$.

2. Splitting the full sample into sub-samples based on various physical properties, we find evidence that $\langle f_{\text{esc}} \rangle$ positively correlates with $W_d(\text{Ly}\alpha)$, but anti-correlates with intrinsic UV luminosity and UV dust attenuation. We find that the high $W_d(\text{Ly}\alpha)$, low intrinsic UV luminosity and low dust attenuation sub-samples all return best-fitting $\langle f_{\text{esc}} \rangle$ values in the range $0.12 \leq \langle f_{\text{esc}} \rangle \leq 0.22$ (see Fig. 3.9 and Fig. 3.10).

3. In contrast, splitting the sample by $M_\star$ yields a weak/non-existent trend between $M_\star$ and $f_{\text{esc}}$. Our results suggest that $M_\star$ is, at best, a secondary indicator of $f_{\text{esc}}$. Therefore, any trend between $f_{\text{esc}}$ and $M_\star$ is likely...
the result of the known correlations between $M_*$ and the other stronger indicators: $W_\lambda$($\text{Ly}\alpha$), $\beta_{\text{obs}}$ and $M_{\text{UV}}$.

4. Overall, the results of the sub-sample splits suggest that the young, low metallicity, dust-free galaxies expected to be common at $z \geq 6$ are likely to display $\langle f_{\text{esc}} \rangle \geq 0.1$, the threshold often quoted as necessary for them to drive cosmic reionization.

5. The agreement between our simple model and the observed data (Fig. 3.5 and Fig. 3.11) suggests that, at least for our sample, a more complicated model of the underlying $f_{\text{esc}}$ distribution is not statistically justified. Nevertheless, it is clear that the true underlying $f_{\text{esc}}$ distribution is likely to be significantly more complicated than our simple model. Therefore, it would clearly be desirable to expand the modelling performed here to larger galaxy samples with deeper photometry, in order to explore more complicated $f_{\text{esc}}$ distributions and to improve the significance of the correlations between $f_{\text{esc}}$ and various galaxy properties.
Chapter 4

Connecting the escape fraction of Lyman-alpha and Lyman-continuum photons in star-forming galaxies at $z \approx 4 - 5$

The contents of this chapter has been accepted for publication in Begley et al. (2023).

4.1 Introduction

The formation of the first stars and the growth of galaxy progenitors in the early Universe signalled the beginning of the Epoch of reionization (EOR), during which the fully neutral Hydrogen gas in the intergalactic medium (IGM) became completely ionized (e.g., Robertson et al., 2015). Although it is generally acknowledged that reionization was completed between $z \sim 5 - 6$, based primarily on measurements of the Lyα forest from distant quasars (e.g., Fan et al., 2006; McGreer et al., 2015; Goto et al., 2021), key details of the process of reionization and the nature of the sources responsible remain a matter of debate (e.g., Mason et al., 2019; Naidu et al., 2020).

One fundamental reason for the continued debate is that the progress of reionization is intimately linked to the physical properties of the sources that are
responsible for it, as well as their location within the large-scale structure of the Universe (Robertson, 2021). It is now widely accepted that active galactic nuclei are simply too rare at high redshift to contribute significantly to reionization (e.g., Matsuoka et al., 2023) and that the dominant contribution to the ionizing photon budget must come from star-forming galaxies (SFGs) (e.g, Robertson et al., 2015; Chary et al., 2016; Iwata et al., 2022).

A key component needed to quantify the ionizing photon budget is the abundance of star-forming galaxies during the EOR, most commonly parameterised through the UV luminosity density ($\rho_{UV}$), that is now being established with increasing accuracy out to $z \approx 12$ by JWST (e.g., Donnan et al., 2022; Finkelstein et al., 2022b; Harikane et al., 2022). The latest JWST results indicate that $\rho_{UV}$ displays a smooth, steady decline through the EOR (e.g., Donnan et al., 2023; McLeod et al., 2023) indicating, in principle, the availability of more ionizing photons than some pre-JWST studies (e.g., Oesch et al., 2018b; Ishigaki et al., 2018) had suggested.

Another essential element is the ionizing photon production efficiency $\xi_{\text{ion}}$, a measure of the number of ionizing photons produced per unit UV luminosity of the star-forming galaxy population. Recent evidence has suggested that the faint, blue population of galaxies commonly found at $z > 6$ (i.e. with UV spectral slope $\beta \lesssim -2.3$; Cullen et al., 2022) display log($\xi_{\text{ion}}$) in the range $\sim 25.5 - 25.8$ (Stark et al., 2015; Bouwens et al., 2016), a factor of $\geq 2 - 3$ higher than canonically assumed in models of reionization (e.g., Bouwens et al., 2012; Finkelstein et al., 2012; Duncan & Conselice, 2015).

Although the abundance of SFGs and the elevated values of $\xi_{\text{ion}}$ at $z > 6$ indicate that sufficient numbers of ionizing photons are being generated within the EOR, whether or not these Lyman-continuum (LyC) photons escape their source galaxies and ionize the IGM is ultimately determined by the escape fraction ($f_{\text{esc}}^{\text{LyC}}$).

Due to the near-total attenuation of UV photons below the Lyman break by the IGM at $z \geq 4$ (e.g., Steidel et al., 2018), direct observational constraints on $f_{\text{esc}}^{\text{LyC}}$ are only possible up to $z \approx 3.8$. At the highest redshifts where such observations are possible, recent estimates from deep photometric and spectroscopic studies have typically constrained the average $f_{\text{esc}}^{\text{LyC}}$ to be $\approx 5 - 10\%$ (e.g., Steidel et al., 2018; Pahl et al., 2021; Meštrić et al., 2021; Begley et al., 2022; Saldana-Lopez 2022).
et al., 2022b). Generally, these studies have also found that the fainter, less-dust-obscured galaxies that are expected to be numerous during the EOR are more likely to display high \( f_{\text{LyC}}^{\text{esc}} \). Promisingly, these trends are in accordance with the assumptions that are often made in reionization models (Robertson et al., 2010; Wise et al., 2014; Robertson et al., 2015; Finkelstein et al., 2019) where \( \langle f_{\text{LyC}}^{\text{esc}} \rangle \geq 5\% \) is typically required for reionization to be completed by \( z \approx 5 – 6 \).

In spite of these encouraging results, we still lack a comprehensive understanding of exactly how LyC photons escape galaxies. To this end, a number of studies have attempted to link \( f_{\text{LyC}}^{\text{esc}} \) to nebular emission-line features, such as Mgii (Katz et al., 2022), CIV (Schaerer et al., 2022) and [OIII] (e.g., Verhamme et al., 2015; Wang et al., 2019; Izotov et al., 2020; Nakajima et al., 2020), which are modulated by the same interstellar medium (ISM) and stellar-population properties that ultimately determine \( f_{\text{LyC}}^{\text{esc}} \).

One of the most promising and closely investigated indicators is the Ly\( \alpha \) emission line, with a number of studies showing that strong Ly\( \alpha \) emission (i.e., identified by a high Ly\( \alpha \) equivalent width, \( W_\lambda (\text{Ly} \alpha) \)) is an excellent indicator of high \( f_{\text{esc}}^{\text{LyC}} \) (Marchi et al., 2018; Pahl et al., 2021; Begley et al., 2022). Furthermore, a clear correlation between \( f_{\text{esc}}^{\text{Ly} \alpha} \) and \( f_{\text{esc}}^{\text{LyC}} \) has been found by Flury et al. (2022b), using galaxies at \( z \approx 0.3 \) selected from the Low Redshift Lyman Continuum Survey (LzLCS; Flury et al. 2022a); a finding consistent with simulation results (e.g., Dijkstra et al., 2016; Kimm et al., 2019).

This Ly\( \alpha \)–LyC connection is expected given that \( f_{\text{esc}}^{\text{Ly} \alpha} \) and \( f_{\text{esc}}^{\text{LyC}} \) are both modulated by the geometry and nature of the gas in the vicinity of young star-forming regions (e.g., Shapley et al., 2003; Chisholm et al., 2018; Gazagnes et al., 2020a; Maji et al., 2022). Furthermore, the characteristics of the young stellar populations themselves influence both LyC and Ly\( \alpha \) photon production, with low-metallicity stellar populations having higher \( \xi_{\text{ion}} \) and therefore producing more LyC and Ly\( \alpha \) photons for a given star-formation rate (e.g., Trainor et al., 2015; Erb et al., 2016; Trainor et al., 2016; Cullen et al., 2020).

The main escape path for ionizing photons is likely through channels of low-column-density, and/or high-ionization-state gas in the ISM, through which Ly\( \alpha \) photons can also escape in significant quantities (e.g., Atek et al., 2008; Dijkstra et al., 2016; Jaskot et al., 2019). Gazagnes et al. (2020a) presented strong observational evidence for LyC leakage via this mechanism, finding significant correlations between the presence of low H\textsc{i} covering fractions and the observed...
LyC escape fraction. Similar correlations have been found in several other independent observational studies (e.g., Verhamme et al., 2017; Chisholm et al., 2018; Saldana-Lopez et al., 2022c).

This argument is further bolstered by the well-established links between Lyα and the ISM properties of galaxies. Shapley et al. (2003) showed that the observed range of $W_1$(Lyα) in Lyman break galaxies at $z \approx 3$ is accounted for by variations in the covering fraction of neutral outflowing H I gas and dust (see also; Atek et al., 2008; Kornei et al., 2010; Berry et al., 2012; Reddy et al., 2016). More-recent literature studies have uncovered a relationship between $W_1$(Lyα) and the covering fraction of neutral gas, as traced by the strength of low-ionization-state ISM absorption lines (Henry et al., 2015; Du et al., 2018; Steidel et al., 2018; Jaskot et al., 2019; Trainor et al., 2019).

In this study, we explore the connection between Lyα and LyC escape in galaxies only $\approx 300$ Myr after reionization was completed, using a sample of galaxies in the range $3.85 \leq z_{\text{spec}} \leq 4.95$ drawn from the VANDELS ESO public spectroscopic survey. We combine direct Lyα line measurements from the VANDELS spectra with H α luminosity constraints based on robust SED fitting, allowing us to individually estimate $f_{\text{esc Lyα}}$ for each galaxy. Using composite spectra formed from sub-samples of Lyα emitters, we then investigate how $f_{\text{esc LyC}}$, as estimated from FUV LIS ISM line strengths, varies with $f_{\text{esc Lyα}}$ and $W_1$(Lyα).

### 4.2 Data and sample selection

Our sample of star-forming galaxies is drawn from the VANDELS ESO public spectroscopic survey final data release (DR4, Garilli et al. 2021). The VANDELS survey used the VIMOS spectrograph (Le Fèvre et al., 2003) installed on the ESO Very Large Telescope (VLT) to obtain ultra-deep spectra of 2087 galaxies at red-optical wavelengths ($4800 \, \text{Å} < \lambda < 10000 \, \text{Å}$) in the Chandra Deep Field South (CDFS) and UKIDSS Ultra Deep Survey (UDS) fields (McLure et al., 2018b; Pentericci et al., 2018a). The vast majority of VANDELS targets were main-sequence star-forming galaxies at $2.4 \leq z \leq 7.0$, for which the ultra-deep ($20 – 80$ hour integration) VIMOS spectra\(^1\) cover the rest-frame far-ultraviolet (FUV), enabling measurements of the Lyα line (e.g., Cullen et al., 2020). Full

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\(^{1}\)The VANDELS observations used the MR grism+GG475 order sorting filter with 1 arcsec slit widths. Approximately 90% of the observations had seeing of $\leq 1$ arcsec.
details of the survey design and target selection can be found in McLure et al. (2018b).

All galaxies targeted in VANDELS benefit from deep, multi-wavelength imaging data covering the observed wavelength range $0.38 \mu m \leq \lambda_{\text{obs}} \leq 4.5 \mu m$. Approximately half of the VANDELS sample lies within the CANDELS GOODS-S and UDS Hubble Space Telescope (HST) imaging footprint (Koekemoer et al., 2011; Grogin et al., 2011), for which we adopt the photometry from Guo et al. (2013) and Galametz et al. (2013), respectively. The other half of the sample lies outside the CANDELS footprint, but benefits from wider-area, primarily ground-based optical/nearIR imaging. For this study we adopt the updated VANDELS photometry catalogues described in Garilli et al. (2021) and publicly released as part of DR4. Crucially, in addition to optical/near-IR data, the full VANDELS sample benefits from deep, deconfused Spitzer IRAC photometry at 3.6 $\mu m$ and 4.5 $\mu m$. As discussed below, it is the photometric excess at 3.6 $\mu m$ that provides our measurement of H$\alpha$ line flux, with the 4.5 $\mu m$ photometry providing a long-wavelength (emission-line free) anchor for the SED fitting.

Our initial sample consists of all VANDELS galaxies in the redshift range $3.85 \leq z_{\text{spec}} \leq 4.95$, within which the IRAC 3.6 $\mu m$ filter is contaminated by the H$\alpha$ emission line. In addition, to ensure the redshifts are robust, we restricted the sample to the $N = 263$ galaxies in this redshift range with redshift quality flags of $z_{\text{flag}} = 3, 4$ or 9, corresponding to a $\geq 95\%$ probability of being correct (Garilli et al., 2021). Finally, in order to measure Ly$\alpha$ escape fractions, we restricted the sample to galaxies which displayed Ly$\alpha$ in emission (i.e., an equivalent width $> 0$ Å; see below), resulting in a sample of $N = 152$ galaxies with a median redshift of $\langle z \rangle = 4.36$.

### 4.3 Emission line flux measurements

Our principal aim is to determine Ly$\alpha$ escape fractions for the galaxies in our sample. To do this we combine measurements of the observed Ly$\alpha$ flux (measured directly from the VANDELS spectra) with estimates of the intrinsic flux derived from the observed H$\alpha$ flux (measured using the IRAC 3.6 $\mu m$ flux excess). In this section, we describe each stage in the process of deriving our Ly$\alpha$ escape fraction measurements for our sample of $3.85 \leq z_{\text{spec}} \leq 4.95$ galaxies.
Figure 4.1  The distribution of rest-frame Lyα equivalent width for our final sample of \( N = 152 \) star-forming galaxies at \( 3.85 \leq z_{\text{spec}} \leq 4.95 \) showing Lyα in emission. The median rest-frame equivalent width is \( \langle W_{\lambda}(\text{Ly} \alpha) \rangle = 11.9 \, \text{Å}. \)

4.3.1 Observed Lyα fluxes and equivalent widths

Observed Lyα fluxes and rest-frame equivalent widths, \( W_{\lambda}(\text{Ly} \alpha) \), are measured from the VANDELS spectra following the method described by Kornei et al. (2010) and adopted in our previous analysis of the correlation between \( W_{\lambda}(\text{Ly} \alpha) \) and stellar metallicity (Cullen et al., 2020). Briefly, the line flux is measured by integrating the spectrum around the peak of the Lyα emission line, between limits defined as the wavelengths where the spectrum intersects the ‘red’ and ‘blue’ continuum levels, defined as the median flux between \( 1120 \, \text{Å} \leq \lambda_{\text{rest}} \leq 1180 \, \text{Å} \) (\( c_{\text{blue}} \)) and \( 1228 \, \text{Å} \leq \lambda_{\text{rest}} \leq 1255 \, \text{Å} \) (\( c_{\text{red}} \)), respectively\(^2\). The rest-frame equivalent width is then simply obtained by dividing the integrated Lyα line flux by \( c_{\text{red}}(1+z) \).

For each galaxy, the above process is repeated 500 times, each time perturbing the galaxy spectrum on a pixel-by-pixel basis by its corresponding error value. From the resulting distribution, the median and scaled median absolute deviation (\( \sigma_{\text{MAD}} \approx 1.4826 \times \text{MAD} \)) are calculated and adopted as the final rest-frame \( W_{\lambda}(\text{Ly} \alpha) \) and uncertainty. The equivalent width distribution of our final sample of \( N = 152 \) galaxies showing Lyα emission is shown in Fig. 4.1.

\(^2\)For three objects no continuum was detected in the spectra and continuum levels were estimated from the best-fitting SED model (Section 4.3.2).
4.3.2 Observed H\textalpha{} fluxes and equivalent widths

To estimate the intrinsic Ly\alpha{} flux we first obtain an estimate of the observed H\alpha{} flux and nebular dust attenuation (see also; Section 4.3.3) from SED fitting the available multi-wavelength photometry. When fitting the photometry we exclude the IRAC 3.6 \textmu{}m filter containing the H\alpha{} line, which enables a robust estimate of the \(W_d(H\alpha)\) and H\alpha{} line flux, via the well-known photometric excess technique (Fig. 4.2; e.g., Stark et al., 2013; Bouwens et al., 2016; Máról-Queraltó et al., 2016; Smit et al., 2016). Below we give details of the stellar population modelling and our method for deriving \(W_d(H\alpha)\).
Stellar population modelling

In this analysis we use the fast++ code (Kriek et al., 2009; Schreiber et al., 2018) to perform SED fitting for each galaxy, using Bruzual & Charlot (2003) stellar population synthesis models with a Chabrier (2003) IMF and a metallicity range of $0.2 - 0.4 \times Z_\odot$. We assume a constant star-formation history, with the age allowed to vary within the range $6.7 \leq \log(t/\text{yr}) \leq 10.0$ in steps of $\Delta(\log(t/\text{yr})) = 0.2$. We adopt the Calzetti et al. (2000) dust attenuation law and allow the absolute attenuation $A_V$ to vary within the range $0.0 \leq A_V \leq 4.0$. All photometric data points are included in the SED fitting, except for the IRAC 3.6 $\mu$m filter, and we do not include nebular emission in the SED fits (see Fig. 4.2 for an example). Our final sample has a median stellar mass of $\langle \log(M/\text{M}_\odot) \rangle = 9.08$ and a median star-formation rate of $\langle \log(\text{SFR}/\text{M}_\odot\text{yr}^{-1}) \rangle = 1.12$, fully consistent with being located on the star-forming main sequence at $z \approx 4 - 5$.

H $\alpha$ equivalent widths

For each galaxy in our sample the H $\alpha$ equivalent width is estimated by comparing the observed IRAC 3.6 $\mu$m flux to the stellar population model prediction (see Fig. 4.2). For each galaxy we determine

$$\Delta[3.6\mu m] = m_{3.6\mu m}^{\text{obs}} - m_{3.6\mu m}^{\text{mod}},$$

where $m_{3.6\mu m}^{\text{obs}}$ and $m_{3.6\mu m}^{\text{mod}}$ are the observed and model apparent magnitudes in the IRAC 3.6$\mu$m filter, respectively. The resulting distribution of $\Delta[3.6\mu m]$ is shown in Fig. 4.3. The distribution shows a clear systematic shift from $\Delta[3.6\mu m] = 0$ towards negative values (median $\Delta[3.6\mu m] = -0.31$), signifying the presence of H$\alpha$ emission in the majority of our sample. Based on the IRAC 3.6 $\mu$m excess, we estimate the rest-frame H$\alpha$ equivalent width using

$$W_A(\text{H}\alpha) = f_{\text{H}\alpha} \times \frac{W_{3.6\mu m}^{\text{eff}}}{1 + z_{\text{spec}}} \times \left(10^{-0.4 \Delta[3.6\mu m]} - 1\right),$$

where $W_{3.6\mu m}^{\text{eff}} = 6844$ $\text{Å}$ is the effective width of the 3.6 $\mu$m filter and $f_{\text{H}\alpha}$ is the fraction of the total contaminating line flux attributed to the H$\alpha$ line alone (i.e. excluding $[\text{N}\ II] \lambda 6584$ $\text{Å}$ and $[\text{S}\ II] \lambda \lambda 6717,6731$ $\text{Å}$). The value of $f_{\text{H}\alpha}$ is often cited to be in the range $f_{\text{H}\alpha} = 0.71 - 0.9$ (e.g., Shim et al., 2011; Stark et al., 2013; Már mol-Queraltó et al., 2016; Smit et al., 2016). In this analysis, we use a
The median value of $\Delta[3.6\mu m] = -0.31$ corresponds to $W_d(H\alpha) = 365$ Å at the median redshift of $z = 4.36$. This value is in excellent agreement with previous estimates at similar redshifts. For example, Smit et al. (2016) find $W_d(H\alpha) = 325 \pm 22$ Å for a sample of $N = 80$ spectroscopically confirmed galaxies at $3.8 \leq z \leq 5.0$. In the same redshift range, Stark et al. (2013) report values of $W_d(H\alpha) \approx 280 - 410$ Å (assuming $f_{H\alpha} = 0.76$). Finally, we note that our constraints are also in good agreement with the redshift evolution for $W_d(H\alpha)$ derived by Mármol-Queraltó et al. (2016) across the redshift range $1 \leq z \leq 5$.

### Null Sample Verification

As a sanity check of our method, we perform the same analysis on a sample of $N = 119$ VANDELS star-forming galaxies selected in the redshift range $3.6 \leq z_{\text{spec}} \leq 3.8$, within which the H$\alpha$ emission line does not contaminate the IRAC 3.6 μm photometry and a photometric excess signature should not be detected\(^3\). We apply the same procedures discussed above to this 'null' sample, deriving the blue histogram in Fig. 4.3. The null sample distribution is fully consistent with $\Delta[3.6\mu m] = 0$, as expected. The median of the distribution is $\Delta[3.6\mu m] = 0.05$ with $\sigma_{\text{MAD}} = 0.20$. For the remainder of this paper, we adopt $\sigma = 0.20$ as the typical uncertainty on $\Delta[3.6\mu m]$.

### 4.3.3 Dust attenuation

To determine the intrinsic Ly$\alpha$ flux we first need an estimate of the intrinsic H$\alpha$ flux. The observed H$\alpha$ flux values are simply determined by multiplying $W_d(H\alpha)$ by the continuum flux derived from the best-fitting SED. To dust-correct the observed fluxes we use the prescription of Wuyts et al. (2013):

$$A_{H\alpha,\text{nebular}} = A_{H\alpha,\text{cont}} + 0.9A_{H\alpha,\text{cont}} - 0.15A_{H\alpha,\text{cont}}^2,$$

where $A_{H\alpha,\text{cont}}$ is the continuum attenuation at $\lambda_{\text{rest}} = 6563$ Å determined from the fast++ SED fitting to the VANDELS DR4 photometry (see Section 4.3.2). The additional attenuation is physically motivated by the increased dust

\(^3\)We note that this redshift range has been chosen such that none of the photometric filters are affected by nebular emission line contamination.
Figure 4.3 The distribution of $\Delta[3.6\mu m]$, defined as the difference between the observed magnitude in the 3.6 $\mu$m filter and the predicted magnitude from the best-fitting SED model (see text for details). The red histogram shows the distribution of the $N = 152$ galaxies with Ly$\alpha$ in emission. The median value of $\Delta[3.6\mu m] = -0.31$, corresponds to $\langle W_\lambda(\text{H}\alpha) \rangle \approx 365$ $\AA$ at the median redshift of the sample. The blue histogram shows the distribution for the null sample, for which the IRAC 3.6 $\mu$m filter is free from H$\alpha$ contamination. As expected, the null distribution is consistent with no flux excess. The $\Delta[3.6\mu m]$ typical error is denoted by the black error bar.
obscuration surrounding young star-forming regions (e.g., Wuyts et al., 2013; Reddy et al., 2020). We note that this conversion explicitly assumes a Calzetti et al. (2000) attenuation law, which our previous work has shown to provide a good description of the average dust attenuation in VANDELS galaxies down to stellar masses of $\log(M_*/M_\odot) \approx 9.0$ (Cullen et al., 2018). We discuss the implications of assuming a steeper dust attenuation curve in Section 4.5.

As a further sanity check on our approach we compare the star-formation rates inferred from the dust-corrected H$\alpha$ emission and dust-corrected FUV stellar continuum in Fig. 4.4. Assuming that our SED-fitting and $W_\lambda$(H$\alpha$) estimates are robust, there should be good agreement between these two star-formation-rate indicators that are both sensitive to star-formation on $< 100$ Myr timescales. To calculate the FUV-based star-formation rates we assume the Madau & Dickinson (2014) calibration

$$\text{SFR}_{\text{UV}}(M_\odot\text{yr}^{-1}) = 6.58 \times 10^{-29} L_{1500}(\text{erg s}^{-1}\text{Hz}^{-1}),$$

where the dust-corrected $L_{1500}$ is calculated from the best-fitting SED template determined in Section 4.3.2 using a 100 Å wide top-hat filter centered on $\lambda_{\text{rest}} = 1500$ Å. To calculate the H$\alpha$-based star-formation rate, we use the Reddy et al. (2018b) calibration

$$\text{SFR}_{\text{H}\alpha}(M_\odot\text{yr}^{-1}) = 3.24 \times 10^{-42} L_{\text{H}\alpha}(\text{erg s}^{-1}),$$

where $L_{\text{H}\alpha}$ is the dust-corrected H$\alpha$ luminosity. It can be seen from Fig. 4.4 that the two estimates are qualitatively in excellent agreement. Fitting a fixed 1:1 relationship we find that the log(SFR$_{\text{H}\alpha}$) estimates are $+0.05$ dex ($\approx 10\%$) larger than the corresponding log(SFR$_{\text{UV}}$) estimates. However, we note that this systematic shift is much smaller than the statistical uncertainty on any individual measurement and globally decreasing the H$\alpha$ fluxes by $\approx 10$ per cent does not affect any of the conclusions of this work.

### 4.3.4 Ly$\alpha$ escape fractions

The Ly$\alpha$ escape fraction is defined as the ratio between the observed and intrinsic Ly$\alpha$ flux. We determine intrinsic Ly$\alpha$ fluxes from the dust-corrected H$\alpha$ fluxes under the assumption of Case-B recombination (i.e., $F_{\text{Ly}\alpha,\text{int}} = 8.7 \times F_{\text{H}\alpha,\text{int}}$;
Figure 4.4  A comparison of the star-formation rates derived from our dust-corrected Hα and UV (L_{1500}) luminosities. The one-to-one relation is shown as the dashed line. The broad agreement between the two estimates demonstrates the relative robustness of the L_{Hα} measurements.

Osterbrock & Ferland, 2006, see also; Henry et al. 2015) which yields,

\[ f_{\text{esc} \, \text{Ly} \alpha} = \frac{F_{\text{Ly} \alpha, \text{obs}}}{8.7 \times F_{\text{H} \alpha, \text{int}}}. \]  

(4.6)

For the objects in our sample with \( W_{\lambda}(\text{H} \alpha) < 0 \) (\( N = 20 \)) we calculate a 3\( \sigma \) upper limit on \( f_{\text{esc} \, \text{Ly} \alpha} \).

4.4 Results

In this section we use our estimates of the observed Ly\( \alpha \) and H\( \alpha \) line fluxes to place constraints on the Ly\( \alpha \) escape fraction and explore the relationship between \( f_{\text{esc} \, \text{Ly} \alpha} \) and \( W_{\lambda}(\text{Ly} \alpha) \). At the end of the section we investigate whether the scatter around the \( f_{\text{esc} \, \text{Ly} \alpha} - W_{\lambda}(\text{Ly} \alpha) \) relation is in part driven by an underlying correlation between \( f_{\text{esc} \, \text{Ly} \alpha} \) and \( f_{\text{esc} \, \text{Ly} \beta} \).
Figure 4.5  The left-hand panel shows the relationship between \( f_{\text{esc}}^{\text{Ly}\alpha} \) and \( W_\lambda(\text{Ly}\alpha) \) for the final sample of \( N = 152 \) VANDELS galaxies at 3.85 \( \leq z_{\text{spec}} \leq 4.85 \) with \( W_\lambda(\text{Ly}\alpha) > 0 \) \( \AA \). The best-fitting relation is shown as the dashed line and \( f_{\text{esc}}^{\text{Ly}\alpha} \) upper limits are shown as triangles (see text for details). The right-hand panel shows a comparison between our new results and those of previous literature studies. The best-fitting relation from Sobral \\& Matthee (2019), based on the combined sample of lower-redshift \( z \sim 0-0.3 \) ‘high-redshift analogue’ galaxies and \( z \sim 2.2-2.6 \) Lyman-alpha emitters (LAEs) (see Sobral et al. 2017 using stacks; and Trainor et al. 2015 using binning; red squares and circles, respectively), is shown as a red dashed line. A compilation of literature results based on LAE samples, including those from Harikane et al. (2018) (LAE stacks, blue circles) at comparable redshifts (\( z \sim 4.9 \)), and constraints on individual \( z \sim 2.6 \) (purple diamonds) and \( z \sim 3.0 - 6.0 \) (orange pentagons) LAEs from Pucha et al. (2022) and Roy et al. (2023), respectively, are also plotted. A sample of low-redshift (\( z \sim 0.3 \)) Green Pea galaxies (Yang et al., 2017) are shown as green crosses. The magenta square indicates the predicted \( f_{\text{esc}}^{\text{Ly}\alpha} \) value at the median redshift of the sample, \( \langle z_{\text{spec}} \rangle \approx 4.36 \), according to the \( f_{\text{esc}}^{\text{Ly}\alpha} - z \) relation of Hayes et al. (2011).
4.4.1 A non-evolving $f_{\text{esc}}^{\text{Ly}\alpha} - W_\lambda (\text{Ly} \alpha)$ relation out to $z = 5$

In the left-hand panel of Fig. 4.5 we plot $f_{\text{esc}}^{\text{Ly}\alpha}$ versus $W_\lambda (\text{Ly} \alpha)$ for our final sample of $N = 152$ galaxies displaying Ly\alpha in emission, along with our best-fitting relation (dashed line). Assuming the standard form of $f_{\text{esc}}^{\text{Ly}\alpha} = A \times W_\lambda (\text{Ly} \alpha) + B$, we determine the best-fitting relation to be:

$$f_{\text{esc}}^{\text{Ly}\alpha} = (3.8 \pm 0.3) \times 10^{-3} W_\lambda (\text{Ly} \alpha) - (1.0 \pm 0.7) \times 10^{-3},$$

(4.7)

using the nested sampling algorithm DYNESTY (Speagle, 2020) with flat parameter priors. Here, the best-fitting slope and intercept are given by the median of the posterior distribution, with the 1\sigma errors designated as the 16\th and 84\th (68\%) percentiles. We find evidence for a correlation at the $\approx 10\sigma$ level, with $f_{\text{esc}}^{\text{Ly}\alpha}$ increasing monotonically from $\approx 4\%$ to $\approx 19\%$ over the range $10 \leq W_\lambda (\text{Ly} \alpha) \leq 50 \text{ Å}$. As expected, our best-fitting relation is consistent with $f_{\text{esc}}^{\text{Ly}\alpha} \approx 0$ at $W_\lambda (\text{Ly} \alpha) = 0 \text{ Å}$.

In the right-hand panel of Fig. 4.5 we compare our new results to those of previous studies in the literature. Our results are in good agreement with the relation (red dashed line) derived by Sobral & Matthee (2019) for a combined sample of $z \approx 2.2 - 2.6$ Ly\alpha emitters and lower-redshift $z \sim 0 - 0.3$ ‘high-redshift analogue’ galaxies (including Green Pea galaxies, LyC leakers, and H\alpha emitters; e.g., Hayes et al., 2013; Henry et al., 2015; Verhamme et al., 2017; Yang et al., 2017). Our results are also consistent with the stacking-based analysis of $N = 99$ Ly\alpha emitters at a similar redshift to our sample ($z \approx 4.9$) presented by Harikane et al. (2018). It can be seen from Fig. 4.5 that our best-fitting relation has a somewhat lower normalisation than both the Sobral & Matthee (2019) relation, and the binned Harikane et al. (2018) data. However, the relations are consistent at the $< 2\sigma$ level and, given the different selection and analysis techniques applied in these other studies (i.e., stacking), we do not consider the offset to be significant. Indeed, the normalisation and scatter of our individual measurements seem fully consistent with the $z = 2.6$ Ly\alpha emitters presented in Pucha et al. (2022) and the $z = 0 - 0.3$ sample of Green Pea galaxies from Yang et al. (2017). We also show measurements from a sample of $z \approx 3.0 - 6.0$ LAEs analysed in Roy et al. (2023) that are broadly consistent within the observed scatter.

As discussed in Sobral & Matthee (2019) (see also Harikane et al., 2018) the observed $f_{\text{esc}}^{\text{Ly}\alpha} - W_\lambda (\text{Ly} \alpha)$ relation will be influenced by $\xi_{\text{ion}}$ and dust attenuation,
both of which are linked to metallicity. Given that these properties are known to evolve with redshift (Emami et al., 2020b; Matthee et al., 2016), the apparent non-evolution of the $f_{\text{esc}}^{\text{Ly}\alpha} - W_A(\text{Ly}\alpha)$ relation shown in Fig. 4.5 is worthy of further consideration.

Crucially, the $z \sim 0 - 0.3$ galaxy samples we compare to in Fig. 4.5 have been deliberately selected to be analogues of high-redshift SFGs, such as those comprising our $z \approx 4 - 5$ sample from VANDELS. Using follow-up rest-frame optical spectroscopy of $N = 33$ VANDELS SFGs at $z \gtrsim 3$, Cullen et al. (2021) measured metallicites spanning $12 + \log(O/H) = 7.6 - 8.2$, comparable to the range displayed by the Yang et al. (2017) Green Pea galaxy sample (also included in the $z \sim 0.3$ sub-sample of Sobral & Matthee, 2019). We can further deduce that the low-redshift samples and our own $z \approx 4 - 5$ sample will have comparable $\xi_{\text{ion}}$ as a result of their similar metallicities (Cullen et al., 2020). Consequently, the lack of evolution in the $f_{\text{esc}}^{\text{Ly}\alpha} - W_A(\text{Ly}\alpha)$ relation shown in Fig. 4.5, simply indicates that the physical processes regulating the production and escape of Ly$\alpha$ photons in high-redshift SFGs are comparable to those in low-redshift analogues, deliberately selected to be a close match in terms of metallicity, $\xi_{\text{ion}}$ and dust attenuation.

We note that, due to the depth of the VANDELS spectroscopy, we are able to trace the $f_{\text{esc}}^{\text{Ly}\alpha} - W_A(\text{Ly}\alpha)$ relation for individual objects for the first time at these redshifts, as well as extending the relation to $W_A(\text{Ly}\alpha) \lesssim 20$ Å, a regime previously only accessible to low-redshift studies. Our analysis demonstrates that at $z \gtrsim 4$ the $f_{\text{esc}}^{\text{Ly}\alpha} - W_A(\text{Ly}\alpha)$ relation extends down to $W_A(\text{Ly}\alpha) \approx 2 - 3$ Å, with our $f_{\text{esc}}^{\text{Ly}\alpha}$ constraints at these low $W_A(\text{Ly}\alpha)$ values directly comparable to those derived in the low-redshift Universe (Fig. 4.5).

Overall, our analysis indicates that the $f_{\text{esc}}^{\text{Ly}\alpha} - W_A(\text{Ly}\alpha)$ relation for SFGs at $z = 4 - 5$ is indistinguishable from that followed by their low-redshift analogues. This implies that the physical processes determining the production and escape of Ly$\alpha$ photons from low metallicity, high $\xi_{\text{ion}}$ galaxies do not vary significantly over $\approx 11$ Gyr (i.e., $\approx 90$ per cent) of cosmic time.

**Average $f_{\text{esc}}^{\text{Ly}\alpha}$ of Ly$\alpha$ emitters**

It is interesting to compare our results for individual objects to previous constraints on the population averaged Ly$\alpha$ escape fraction. Based on a
compilation of Ly$\alpha$, UV, and H$\alpha$ luminosity functions, Hayes et al. (2011) determined that the redshift evolution of $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle$ is well-described by a power law of the form $\propto (1+z)^{2.57}$, with $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle$ evolving from $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle \approx 0.01$ at $z \approx 0.3$ up to $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle \approx 0.4$ at $z \approx 6$. At the median redshift of our final sample ($\langle z_{\text{spec}} \rangle = 4.36$), the Hayes et al. (2011) relation predicts $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle \approx 0.13$ which is indicated by the purple data point in the right-hand panel of Fig. 4.5.

This average value is clearly in good agreement with the high $W_A$(Ly$\alpha$) objects in our sample, consistent with the fact that the galaxies used to derive the Hayes et al. (2011) relation were typically Ly$\alpha$ emitters with $W_A$(Ly$\alpha$) > 20 Å. Restricting our sample to objects with $W_A$(Ly$\alpha$) > 20 Å we find a median value of $\langle f_{\text{esc}}^{\text{Ly}\alpha} \rangle \approx 0.12$, in excellent agreement with the Hayes et al. (2011) prediction. This consistency is encouraging, given that the two estimates originate from completely independent methods.

### 4.4.2 Connecting Ly$\alpha$ and LyC escape

Although the results presented in Fig. 4.5 show a strong correlation between $f_{\text{esc}}^{\text{Ly}\alpha}$ and $W_A$(Ly$\alpha$), there is clearly a large amount of associated scatter ($\approx 0.5$ dex). Some fraction of this scatter is attributable to measurement uncertainties, given that our individual estimates of $f_{\text{esc}}^{\text{Ly}\alpha}$ are undoubtedly noisy. However, at a given value of $W_A$(Ly$\alpha$) we also expect intrinsic scatter in $f_{\text{esc}}^{\text{Ly}\alpha}$ due to variations in the stellar populations and dust/gas properties. One way of exploring the range of $f_{\text{esc}}^{\text{Ly}\alpha}$ at a given value of $W_A$(Ly$\alpha$) is to investigate the link between $f_{\text{esc}}^{\text{Ly}\alpha}$ and $f_{\text{esc}}^{\text{LyC}}$.

A growing body of literature has empirically established a strong positive correlation between $W_A$(Ly$\alpha$) (i.e., $f_{\text{esc}}^{\text{Ly}\alpha}$) and $f_{\text{esc}}^{\text{LyC}}$ in high-redshift star-forming galaxies, either via direct measurements of LyC emission (e.g., Marchi et al., 2018; Steidel et al., 2018; Pahl et al., 2021; Begley et al., 2022), or via indirect studies characterising the H$\text{I}$ covering fraction (Shapley et al., 2003; Gazagnes et al., 2020a; Saldana-Lopez et al., 2022b). A similarly strong connection is also observed at low redshifts (e.g., Vanzella et al., 2016b; Verhamme et al., 2017; Flury et al., 2022b). This link can be explained by the similar escape path of LyC and Ly$\alpha$ photons through low dust/H$\text{I}$ column-density channels (e.g., Dijkstra et al., 2016; Jaskot et al., 2019), a picture supported by detailed radiative transfer simulations (e.g., Cen & Kimm, 2015; Kimm et al., 2019).
Below, we use composites of our VANDELS spectra to explore this connection further. Rather than using $W_1(\text{Ly}\alpha)$ as a proxy for $f_{\text{esc}}^{\text{Ly}\alpha}$, we can take advantage of our individual $f_{\text{esc}}^{\text{Ly}\alpha}$ escape estimates to trace the connection between $f_{\text{esc}}^{\text{Ly}\alpha}$ and the properties of the ISM measured from deep rest-frame FUV spectra. This in turn allows us to connect the escape of Ly$\alpha$ and LyC photons using the correlation established between the equivalent width of low-ionization-state FUV ISM absorption lines and $f_{\text{esc}}^{\text{LyC}}$ by Saldana-Lopez et al. (2022b).

**Constructing VANDELS composite spectra**

To maximise the available signal-to-noise of our VANDELS spectra we create stacked FUV composites following a similar procedure to that outlined in Cullen et al. (2019). To create the composite spectra of a given ensemble of galaxies, we first shift each individual spectrum to the rest-frame using its spectroscopic redshift$^4$ and normalise to the median flux in the range $1420 \leq \lambda_{\text{rest}} \leq 1480$ Å. The individual flux elements of each spectra are then binned onto the desired wavelength grid of the final stack (1 Å/pix). The flux of each pixel in the composite spectrum is given by the median of the individual fluxes after $3\sigma$ outliers have been sigma clipped. The associated error spectrum is estimated by bootstrap re-sampling of the fluxes in each wavelength bin, taking the standard deviation of each as the $1\sigma$ uncertainty.

$^4$As discussed in Section 2.2.2, deviations of the measured VANDELS spectroscopic redshift from the systemic redshift may introduce uncertainties in the stacked composite spectra, and thus in the $W_{\text{LIS}}$ measurements. As previously highlighted, this effect is expected to minimal as a result of the relatively low-resolution VANDELS spectra in addition to the fact the typical LIS velocity shift is close to the systemic velocity ($\approx -60$ km s$^{-1}$). Nonetheless, to confirm that our composite spectra, and in turn our $W_{\text{LIS}}$ measurements are robust against redshift-based systematics, we carry out a number of additional tests outlined below.

Firstly, we recreate the stacks based on galaxies from three equally occupied bins split on $f_{\text{esc}}^{\text{Ly}\alpha}$ ($T_1, T_2, T_3$), after removing galaxies with only a single strong emission line (typically Ly$\alpha$, which corresponds to $< 10\%$ of the galaxies in each bin). From these stacks we find no statistically significant difference in the measured $W_{\text{LIS}}$ values. Secondly, we compare our measured $W_{\text{LIS}}$ values with those from the VANDELS spectroscopic measurements catalogue presented in Talia et al. (2023). We find that there is excellent consistency with their two independent measurements (based on a Gaussian fitting method using SLINEFIT and a direct integration technique using PYLICK).

Together, these two tests add further confidence that any deviations between the VANDELS spectroscopic redshift and the systemic redshift do not systematically bias our composite spectra, and thus the inferences of $f_{\text{esc}}^{\text{LyC}}$ from the strength of FUV low-ionization-state absorption lines.
The strength of ISM absorption features

The top panel of Fig. 4.6 is an overlay of four composite spectra. The dark-grey spectrum is a composite of the \( N = 111 \) VANDELS galaxies within the redshift range \( 3.85 \leq z_{\text{spec}} \leq 4.95 \) that display Ly\( \alpha \) in absorption. The other three spectra are composites obtained by splitting our final sample of \( N = 152 \) VANDELS galaxies with Ly\( \alpha \) in emission into three equally occupied bins of \( f_{\text{esc}}^{\text{Ly} \alpha} \) (\( T_1 = f_{\text{esc}}^{\text{Ly} \alpha} < 0.025 \), \( T_2 = 0.025 \leq f_{\text{esc}}^{\text{Ly} \alpha} < 0.1 \) and \( T_3 = f_{\text{esc}}^{\text{Ly} \alpha} \geq 0.1 \)).

Some key features are immediately visible by eye. Compared to the composite spectrum of galaxies displaying Ly\( \alpha \) in absorption, it is clear that the Ly\( \alpha \) emission composites display progressively weaker low-ionization-state ISM absorption lines as a function of increasing \( f_{\text{esc}}^{\text{Ly} \alpha} \). The weak LIS ISM lines are a clear signature of a low covering fraction\(^5\) of neutral H\( \text{I} \) gas, one of the key requirements for an increased escape of Ly\( \alpha \)/LyC photons (Reddy et al., 2016; Saldana-Lopez et al., 2022c).

Although the LIS ISM features in the composite spectra shown in Fig. 4.6 behave as expected, the correlation between \( f_{\text{esc}}^{\text{Ly} \alpha} \) and \( W_A(\text{Ly} \alpha) \) shown in Fig. 4.5 means that it is not clear which of the two parameters is driving the observed trend. To investigate this issue, we also create two composite spectra at fixed \( W_A(\text{Ly} \alpha) \). By selecting all galaxies with \( W_A(\text{Ly} \alpha) \geq 25 \) \( \AA \) and splitting into high-\( f_{\text{esc}}^{\text{Ly} \alpha} \) and low-\( f_{\text{esc}}^{\text{Ly} \alpha} \) sub-sets at a threshold of \( f_{\text{esc}}^{\text{Ly} \alpha} \geq 0.2 \), it was possible to produce two composites with similar \( W_A(\text{Ly} \alpha) \) and sufficiently high signal-to-noise to allow measurements of the LIS absorption features. The high-\( f_{\text{esc}}^{\text{Ly} \alpha} \) and low-\( f_{\text{esc}}^{\text{Ly} \alpha} \) composites are shown in the middle and bottom panel of Fig. 4.6, respectively.

The high-\( f_{\text{esc}}^{\text{Ly} \alpha} \) composite contains \( N = 13 \) galaxies with median (and \( \sigma_{\text{MAD}} \)) values of \( \langle f_{\text{esc}}^{\text{Ly} \alpha} \rangle = 0.41 \pm 0.18 \) and \( \langle W_A(\text{Ly} \alpha) \rangle = 44.1 \pm 21.9 \) \( \AA \). The low-\( f_{\text{esc}}^{\text{Ly} \alpha} \) composite contains \( N = 22 \) galaxies with \( \langle f_{\text{esc}}^{\text{Ly} \alpha} \rangle = 0.11 \pm 0.07 \) and \( \langle W_A(\text{Ly} \alpha) \rangle = 39.7 \pm 19.1 \) \( \AA \).

\(^5\)We highlight that the LIS lines are saturated and therefore act as tracers of the covering fraction, \( C_f \) (see also Section 4.4.2). For the Si\( \text{II} \) line species, we measure \( W_{1260(\text{Si} \text{II})}/W_{1526(\text{Si} \text{II})} \leq 1.6 \pm 0.5 \) for all three \( f_{\text{esc}}^{\text{Ly} \alpha} \)-binned composites (top panel, Fig. 4.6). In the optically-thin regime \( W_{1260(\text{Si} \text{II})}/W_{1526(\text{Si} \text{II})} = 6.0 \) (Shapley et al., 2003; Erb et al., 2010), which is inconsistent with the data.
The top panel shows an overlay of four composite VANDELS spectra. The dark grey composite is a stack of $N = 111$ VANDELS galaxies within the redshift range $3.85 \leq z_{\text{spec}} \leq 4.95$ that display Ly$\alpha$ in absorption (i.e. $W_{\text{Ly} \alpha} < 0$). This composite is shown in all three panels. The purple (light to dark) composites are constructed from three equally-occupied bins of $f_{\text{esc}}^{\text{Ly} \alpha}$ ($T_1: f_{\text{esc}}^{\text{Ly} \alpha} < 0.025$, $T_2: 0.025 \leq f_{\text{esc}}^{\text{Ly} \alpha} < 0.1$ and $T_3: f_{\text{esc}}^{\text{Ly} \alpha} \geq 0.1$). The middle and bottom panels show composites formed from objects with $W_{\text{Ly} \alpha} \geq 25 \, \text{Å}$, that have been split into high- and low-$f_{\text{esc}}^{\text{Ly} \alpha}$ sub-samples at a threshold of $f_{\text{esc}}^{\text{Ly} \alpha} \geq 0.2$. This selection ensures that both composites have approximately the same equivalent width ($\Delta(W_A(\text{Ly} \alpha)) < 5 \, \text{Å}$) but widely different values of $f_{\text{esc}}^{\text{Ly} \alpha}$ (see text for details). The error spectra are shown in light colours and notable absorption features are highlighted with black vertical lines (e.g. Si$\text{II}$ $\lambda 1260$, C$\text{II}$ $\lambda 1334$, O$\text{I}$/Si$\text{II}$ $\lambda 1303$, and Si$\text{II}$ $\lambda 1526$).
LIS equivalent widths

For each spectrum, we measure equivalent widths for the Si\textsc{ii} $\lambda 1260$, C\textsc{ii} $\lambda 1334$, and the O\textsc{i} $\lambda 1303$+Si\textsc{ii} $\lambda 1303$ low-ionization state ISM absorption features (with the final feature blended due to the VANDELS $R \approx 600$ spectral resolution; see Fig. 4.6). The equivalent widths are calculated numerically according to the following equation:

$$W_{\text{LIS}} = \int_{\lambda_0}^{\lambda_0 + \Delta \lambda} \left(1 - \frac{f_{\text{obs}}}{f_{\text{cont}}}\right) d\lambda,$$

where $f_{\text{obs}}$ is the flux density of observed spectrum, $f_{\text{cont}}$ is the underlying stellar continuum flux density, and $\Delta \lambda$ is the width of the region over which the numerical integration is performed, which we set to a default value of $\pm 500 \text{ km s}^{-1}$. The values of $\Delta \lambda$ and $\lambda_0$ are manually adjusted for each line measurement to account for velocity offsets, nearby noise spikes or potential non-resonant fine structure emission\textsuperscript{6}. The stellar continuum component is calculated by fitting a $f_{\lambda} \propto \lambda^{\beta}$ power law to the continuum either side of the line, typically spanning $\pm 4500 \text{ km s}^{-1}$ ($\gtrsim 20$ Å). Uncertainties were calculated using a Monte Carlo procedure.

The connection between $f_{\text{esc}}^{\text{Ly} \alpha}$ and the ISM ionization state

Qualitatively, it can be seen from Fig. 4.6 that the low-ionization ISM lines are somewhat weaker in the high-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite than in the low-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite. In addition, the high-ionization Si\textsc{iv} $\lambda 1393, 1402$ and blended C\textsc{iv} $\lambda 1548, 1550$ absorption lines appear to be more visually prominent in the high-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite. That is, at fixed $W_{\lambda}(\text{Ly} \alpha)$, galaxies with higher $f_{\text{esc}}^{\text{Ly} \alpha}$ appear to show signatures consistent with having a lower covering fraction of neutral gas and a higher covering fraction of ionized gas.

Using the procedure outlined above, we measure equivalent widths for the Si\textsc{iv} $\lambda 1393, 1402$ doublet in the high-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite of $W_{1393}(\text{Si} \text{iv}) = 1.36 \pm 0.33$ Å and $W_{1402}(\text{Si} \text{iv}) = 1.23 \pm 0.34$ Å. Similarly, in the low-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite we measure $W_{1393}(\text{Si} \text{iv}) = 0.74 \pm 0.31$ Å and $W_{1402}(\text{Si} \text{iv}) = 0.51 \pm 0.20$ Å.

\textsuperscript{6}Due to the relatively low resolution of the VANDELS spectra, it is not possible to fully assess the impact of absorption line infilling from non-resonant fine structure emission in the vicinity of the LIS features. However, the close agreement of the observed $W_{\lambda}(\text{Ly} \alpha) - W_{\text{LIS}}$ relation with other literature measurements of SFGs with higher resolution spectra (e.g., Shapley et al., 2003; Du et al., 2018; Pahl et al., 2020), provides confidence that our $W_{\text{LIS}}$ measurements are not significantly influenced by infilling.
The line ratio in the Si\textsuperscript{iv} \(\lambda\lambda 1393, 1402\) doublet can be used to infer whether it originates from optically thin or optically-thick ISM gas. In the optically-thin regime, the doublet ratio will be \(W_{1393}(\text{Si}\text{iv})/W_{1402}(\text{Si}\text{iv}) \approx 2\) (Shapley et al., 2003; Berry et al., 2012), whereas ratios of \(W_{1393}(\text{Si}\text{iv})/W_{1402}(\text{Si}\text{iv}) \approx 1\) are indicative of saturated lines arising from an optically thick, high-ionization-state ISM. For the high- and low-\(f_{\text{esc}}^{\text{Ly}\alpha}\) composites we find doublet ratios of \(W_{1393}(\text{Si}\text{iv})/W_{1402}(\text{Si}\text{iv}) = 1.1 \pm 0.4\) and \(W_{1393}(\text{Si}\text{iv})/W_{1402}(\text{Si}\text{iv}) = 1.45 \pm 0.8\), respectively. For the low-\(f_{\text{esc}}^{\text{Ly}\alpha}\) composite we are clearly unable to conclude anything regarding optical depth, as the doublet ratio is fully consistent with both the optically thin and optically-thick regimes. On the other hand, despite the obvious uncertainty, the high-\(f_{\text{esc}}^{\text{Ly}\alpha}\) doublet ratio is more consistent with saturation, providing evidence of a more-highly ionized ISM environment in the galaxy composite with higher \(f_{\text{esc}}^{\text{Ly}\alpha}\).

This conclusion is further strengthened by comparing the UV spectral slopes of the high- and low-\(f_{\text{esc}}^{\text{Ly}\alpha}\) composites. Fitting a power-law of the form \(f_{\lambda} \propto \lambda^{\beta}\), we find the high-\(f_{\text{esc}}^{\text{Ly}\alpha}\) composite (\(\beta = -1.8 \pm 0.2\)) to be bluer than its low-\(f_{\text{esc}}^{\text{Ly}\alpha}\) counterpart (\(\beta = -1.4 \pm 0.1\)). This spectral slope difference is consistent with recent results (see Gazagnes et al., 2020a; Begley et al., 2022) indicating that galaxies with bluer UV slopes are more likely to display more-highly ionizing environments (and higher \(f_{\text{esc}}^{\text{LyC}}\); Chisholm et al., 2022).

The connection between \(f_{\text{esc}}^{\text{Ly}\alpha}\) and \(f_{\text{esc}}^{\text{LyC}}\)

Recently, Saldana-Lopez et al. (2022b) have identified a strong relationship between \(f_{\text{esc}}^{\text{LyC}}\) and the equivalent width of low-ionization-state absorption lines \((W_{\text{LIS}})^7\), calibrated using the LzLCS dataset (see also Chisholm et al., 2018; Gazagnes et al., 2020a). Using this relationship, we are able to estimate the value of \(f_{\text{esc}}^{\text{LyC}}\) for the composite spectra shown in Fig. 4.6.

We calculate the inverse-variance weighted mean across the Si\textsuperscript{ii} \(\lambda 1260\), C\textsuperscript{ii} \(\lambda 1334\),

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\(^7\)The relation between the strengths of LIS species such as Si\textsuperscript{ii} \(\lambda 1260\) and C\textsuperscript{ii} \(\lambda 1334\) and the covering fraction of neutral Hydrogen gas is likely not 1:1 owing to the differing ionization potentials (e.g., 13.6 eV for Hydrogen and 16.0 eV for Si\textsuperscript{ii} \(\lambda 1260\); see Gazagnes et al., 2020a). As a result, in addition to tracing neutral Hydrogen gas, these metal species can also arise from a ‘partially ionized medium’ (Chisholm et al., 2018). However, as we are using an empirically calibrated relation between \(W_{\text{LIS}}\) and \(f_{\text{esc}}^{\text{LyC}}\), these effects are intrinsically accounted for.
O I λ1303+Si II λ1303 and the Si II λ1526 features. For the three composite spectra shown in the upper panel of Fig. 4.6, we measure values of $W_{\text{LIS}} = 1.84 \pm 0.12$ Å, $1.13 \pm 0.12$ Å and $0.78 \pm 0.17$ Å, in order of increasing $f_{\text{Ly} \alpha}^{\text{esc}}$. Likewise, for the high-$f_{\text{esc}}^{\text{Ly} \alpha}$ and low-$f_{\text{esc}}^{\text{Ly} \alpha}$ composites shown in the middle and bottom panels of Fig. 4.6, we measure $W_{\text{LIS}} = 0.40 \pm 0.17$ Å and $0.80 \pm 0.15$ Å, respectively. We show the corresponding values of $f_{\text{esc}}^{\text{LyC}}$ in the left-hand panel of Fig. 4.7, having employed Eqn. 11 from Saldana-Lopez et al. (2022b) to map between $W_{\text{LIS}}$ and $f_{\text{esc}}^{\text{LyC}}$. For galaxies at $z \approx 4 - 5$, our results indicate that $f_{\text{esc}}^{\text{LyC}}$ and $f_{\text{esc}}^{\text{Ly} \alpha}$ are positively correlated and follow a relationship of the form $f_{\text{esc}}^{\text{LyC}} = 0.15_{-0.04}^{+0.06}f_{\text{esc}}^{\text{Ly} \alpha}$. Crucially, we can be confident that the $f_{\text{esc}}^{\text{LyC}}$–$f_{\text{esc}}^{\text{Ly} \alpha}$ relation is not being driven by $W_{\text{LIS}}(\text{Ly} \alpha)$, given that the $f_{\text{esc}}^{\text{LyC}}$ and $f_{\text{esc}}^{\text{Ly} \alpha}$ values derived for the two equal-$W_{\text{LIS}}(\text{Ly} \alpha)$ composites follow the same relation (red and blue hexagons in Fig. 4.7). We discuss the physical interpretation and implications of this result in Section 5.

Comparing $f_{\text{esc}}^{\text{LyC}}$ inferred from $W_{\text{LIS}}$ to direct $f_{\text{esc}}^{\text{LyC}}$ observations at $z > 3$

Finally, in the right-hand panel of Fig. 4.7 we compare the $f_{\text{esc}}^{\text{LyC}}$–$W_{\text{Ly} \alpha}$ relationship of our $z \approx 4 - 5$ sample, as estimated from LIS absorption-line strength, to more direct measurements at low and high redshift. Our results are consistent with a relation of the form $f_{\text{esc}}^{\text{LyC}} \approx 0.0005W_{\text{Ly} \alpha}$ (black dashed line), which is simply the result of combining the $f_{\text{esc}}^{\text{Ly} \alpha}$–$W_{\text{Ly} \alpha}$ relation shown in Fig. 4.5 with the $W_{\text{LIS}}$–$f_{\text{esc}}^{\text{LyC}}$ calibration from Saldana-Lopez et al. (2022b), our results are consistent with the $f_{\text{esc}}^{\text{LyC}}$–$W_{\text{Ly} \alpha}$ measurements from the low-redshift $Lz$LCS survey at $z = 0.2 - 0.4$ (Flury et al., 2022a), both in terms of normalisation and scatter.

These lines represent a subset of the full suite of LIS features originally employed in Saldana-Lopez et al. (2022b). Specifically, we do not include measurements of the Si II λ989, Si II λ1020, and Si II λ1190, 1193 features and in turn avoid potential systematic biases that may arise from the need to correct for the impact of IGM+CGM absorption blueward of Lyα. We also exclude the Si II λ1526 absorption feature from the high-$f_{\text{esc}}^{\text{Ly} \alpha}$ composite spectra due to a suspected noise spike in the immediate wavelength vicinity affecting the measurement.

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Figure 4.7 The left-hand panel shows the relationship between $f_{\text{esc}}^\text{LyC}$ and $f_{\text{esc}}^\text{Ly}\alpha$ based on the composite spectra shown in Fig. 4.6, where $f_{\text{esc}}^\text{LyC}$ has been inferred from $W_{\text{LIS}}$ measurements (shown on the secondary y-axis on the right-hand side) using the $W_{\text{LIS}}-f_{\text{esc}}^\text{LyC}$ relation from Saldana-Lopez et al. (2022b). The three composites based on equally-occupied bins of $f_{\text{esc}}^\text{Ly}\alpha$ are shown as purple squares, while the high- and low-$f_{\text{esc}}^\text{Ly}\alpha$ composites at a constant value of $W_{\lambda}(\text{Ly}\alpha)$ are shown as red and blue hexagons. The $f_{\text{esc}}^\text{Ly}\alpha$ and $f_{\text{esc}}^\text{LyC}$ data from the LzLCS sample for strong Lyman continuum emitters (LCEs), weak LCEs and non-emitters are shown as small filled black, filled grey and open grey markers, respectively (typical uncertainties are shown in the lower right, see Flury et al., 2022a,b, for further details). Simulation-derived $f_{\text{esc}}^\text{Ly}\alpha-f_{\text{esc}}^\text{LyC}$ relations are shown as green lines (Dijkstra et al. 2016, dash-dotted; Kimm et al. 2022, dotted; Maji et al. 2022, dashed). The 1:1 relation is shown as thick grey line and $f_{\text{esc}}^\text{LyC} \approx 0.15^{+0.06}_{-0.04} f_{\text{esc}}^\text{Ly}\alpha$ is shown as a dashed black line. The right-hand panel shows the same composite-based $f_{\text{esc}}^\text{LyC}$ constraints as a function of $W_{\lambda}(\text{Ly}\alpha)$, including values for the LzLCS sample. The $W_{\lambda}(\text{Ly}\alpha)-f_{\text{esc}}^\text{LyC}$ relation derived at $z \approx 3$ from the KLCS (Pahl et al., 2021) is shown as the dashed light-blue line, with the light-blue markers indicating constraints for composite KLCS spectra as a function of $W_{\lambda}(\text{Ly}\alpha)$. The dashed black line shows the relationship $f_{\text{esc}}^\text{LyC} \approx 0.0005 f_{\text{esc}}^\text{Ly}\alpha$, derived by combining our best-fitting $f_{\text{esc}}^\text{Ly}\alpha-W_{\lambda}(\text{Ly}\alpha)$ relationship (see Fig. 4.5) with $f_{\text{esc}}^\text{LyC} \approx 0.15^{+0.06}_{-0.04} f_{\text{esc}}^\text{Ly}\alpha$. 
In contrast, our new results are systematically lower than the $f_{\text{esc}}^\text{LyC} - W_\lambda(Ly\alpha)$ relation derived by Pahl et al. (2021). The $W_\lambda(Ly\alpha) - f_{\text{esc}}^\text{LyC}$ constraints from Pahl et al. (2021) are based on direct measurements of $W_\lambda(Ly\alpha)$ and LyC flux from extremely deep spectra of galaxies at $z \approx 3$ (KLCS survey; Steidel et al. 2018) and correspond to $f_{\text{esc}}^\text{LyC} \approx 0.0053 W_\lambda(Ly\alpha)$ (blue dashed line). Although our new results at $z \approx 4 - 5$ follow a $f_{\text{esc}}^\text{LyC} - W_\lambda(Ly\alpha)$ relation with the same functional form, the use of the low-redshift $W_{\text{LIS}} - f_{\text{esc}}^\text{LyC}$ calibration from Saldana-Lopez et al. (2022b) leads to a normalisation that is a factor of $\approx 10$ lower.

To confirm the presence of this normalisation discrepancy, we construct an additional composite VANDELS spectrum from the upper-$W_\lambda(Ly\alpha)$ sub-sample defined in Begley et al. (2022) (with SFGs in the redshift range $3.35 < z_{\text{spec}} < 3.95$ and $W_\lambda(Ly\alpha)$ spanning $-6 \lesssim W_\lambda(Ly\alpha) \lesssim 93$ Å), and infer $f_{\text{esc}}^\text{LyC} \approx 0.005$ (corresponding to $W_{\text{LIS}} \approx 1.2$ Å), following the same method detailed in Section 4.4.2. Comparing with the direct photometry-based constraint of $f_{\text{esc}}^\text{LyC} = 0.12^{+0.06}_{-0.04}$ measured in Begley et al. (2022), we again find independent evidence for a significant (factor $\gtrsim 10 - 20$) normalisation offset at $z \geq 3$ between indirect $f_{\text{esc}}^\text{LyC}$ estimates (using the low-redshift $f_{\text{esc}}^\text{LyC} - W_{\text{LIS}}$ calibration) and direct estimates of $f_{\text{esc}}^\text{LyC}$ from deep $U$-band imaging/spectroscopy.

To achieve consistency, it seems likely that the normalisation of the $W_{\text{LIS}} - f_{\text{esc}}^\text{LyC}$ relation must evolve with redshift to permit significantly higher values of $f_{\text{esc}}^\text{Ly}\alpha$ for a given value of $W_{\text{LIS}}$. The offset in normalisation was previously noted and discussed in detail by Saldana-Lopez et al. (2022b). In Section 4.5 we provide a brief review of the systematics that are likely to be responsible.

### 4.5 Discussion

The results presented in Fig. 4.5 demonstrate that our sample of $z \approx 4 - 5$ galaxies displays a $f_{\text{esc}}^\text{Ly}\alpha - W_\lambda(Ly\alpha)$ relation that is very similar to the relation observed at lower redshifts. We also show in Fig. 4.6 that some of the scatter around this relationship is connected to a genuine range in $f_{\text{esc}}^\text{Ly}\alpha$ at a given value of $W_\lambda(Ly\alpha)$. This figure demonstrates that empirically, composite spectra binned as a function of $f_{\text{esc}}^\text{Ly}\alpha$ display the expected anti-correlation between $f_{\text{esc}}^\text{Ly}\alpha$ and the depth of the LIS absorption features that are believed to be tracers of $f_{\text{esc}}^\text{LyC}$ (and $f_{\text{esc}}^\text{Ly}\alpha$). Based on a low-redshift calibration between $W_{\text{LIS}}$ and $f_{\text{esc}}^\text{LyC}$ from Saldana-Lopez et al. (2022b), the results presented in the left-hand panel of Fig. 4.7 show
that \( f_{\text{LyC}}^{\text{esc}} \) and \( f_{\text{Ly} \alpha}^{\text{esc}} \) are strongly correlated, following a relation consistent with \( f_{\text{esc}}^{\text{LyC}} \approx 0.15^{+0.06}_{-0.04} f_{\text{esc}}^{\text{Ly} \alpha} \). Importantly, the results derived from the composite spectra designed to have the same \( W_A(\text{Ly} \alpha) \) indicate that this correlation is not being driven by a secondary correlation between \( f_{\text{esc}}^{\text{Ly} \alpha} \) and \( W_A(\text{Ly} \alpha) \).

These results are qualitatively consistent with the predictions of so-called ‘picket-fence’ or ‘holes’ models, in which the geometry and physical conditions of the ISM gas and dust in the immediate vicinity of star-forming regions play a decisive role in governing the escape of ionizing and Ly\( \alpha \) photons (Shapley et al., 2003; Chisholm et al., 2018; Gazagnes et al., 2020a). These models suggest \( f_{\text{esc}}^{\text{LyC}} \) is primarily dictated by the covering fraction of optically thick H\( \text{I} \) gas (\( C_{H \text{I}}^{f} \)), with LyC and Ly\( \alpha \) photons escaping through channels of low-column-density and/or high-ionization-state gas. These channels become more abundant with decreasing \( C_{H \text{I}}^{f} \), leading to a \( f_{\text{esc}}^{\text{LyC}} \propto (1 - C_{H \text{I}}^{f}) \) relationship (Verhamme et al., 2017; Steidel et al., 2018; Saldana-Lopez et al., 2022b).

Our results are, to first order, also consistent with the overall trends expected from simulations. In the left-hand panel of Fig. 4.7 we show the predictions of three independent simulations. The dashed green line shows the \( f_{\text{esc}}^{\text{Ly} \alpha} - f_{\text{esc}}^{\text{LyC}} \) relation from Maji et al. (2022), based on the SPHINX suite of cosmological radiation-hydrodynamical simulations (Rosdahl et al., 2018). The dash-dotted green line shows the relation from Dijkstra et al. (2016), derived from a suite of clumpy ISM models covering a wide range of physical conditions. Finally, the dotted green line shows the relation from Kimm et al. (2022) high-resolution simulations of giant molecular clouds, including stellar feedback, that suggest a steeper relationship of the form \( f_{\text{esc}}^{\text{LyC}} \approx (f_{\text{esc}}^{\text{Ly} \alpha})^{3.7} \). All three studies show trends qualitatively consistent with our results, albeit with offsets in absolute \( f_{\text{esc}}^{\text{LyC}} \) values. The Maji et al. (2022) relation appears to imply that a threshold of \( f_{\text{esc}}^{\text{Ly} \alpha} \approx 0.2 \) must be met before LyC leakage can occur, inconsistent with our low-\( f_{\text{esc}}^{\text{Ly} \alpha} \) constraints. However, Maji et al. (2022) also show that a number of their simulated galaxies do occupy this region of \( f_{\text{esc}}^{\text{Ly} \alpha} - f_{\text{esc}}^{\text{LyC}} \) parameter space and that there is generally a large amount of scatter in the relation, consistent with the low-redshift observations.

A final issue that merits discussion is the offset in absolute \( f_{\text{esc}}^{\text{LyC}} \) inferred indirectly from low-ionization FUV absorption lines and direct estimates of \( f_{\text{esc}}^{\text{LyC}} \) at \( z > 3 \) (Steidel et al., 2018; Pahl et al., 2021; Begley et al., 2022). This issue has been explored in detail by Saldana-Lopez et al. (2022b) and we refer the reader to that...
paper for a thorough discussion. However, there are three obvious systematic effects that are worth briefly discussing here.

Firstly, in general, it is worth remembering that the $W_{\text{LIS}} - f_{\text{esc}}^{\text{LyC}}$ relation used here was calibrated using a sample of rare, low-redshift LCE candidates from the LzLCS (Saldana-Lopez et al., 2022b). These galaxies will not be perfect analogues for the $z > 3$ star-forming population in terms of evolutionary stage, star-formation rate, metallicity or dust enrichment. As such, it is not unreasonable to think that the appropriate absolute calibration of the $W_{\text{LIS}} - f_{\text{esc}}^{\text{LyC}}$ at $z > 3$ may well be significantly different from that which is appropriate at low redshifts.

A second potentially important systematic is the choice of model used to describe the ISM gas geometry. In the ‘holes’ geometry adopted by Pahl et al. (2021), the dust and H$\text{I}$ gas reside in pockets around star-forming regions and are optically thick to ionizing radiation. In this geometry, the LyC escape fraction is simply given as $f_{\text{esc}}^{\text{LyC}} = (1 - C_f^{\text{HI}})$, where $C_f^{\text{HI}}$ is the covering fraction of neutral hydrogen gas. Recently, Chisholm et al. (2018) have suggested that this model, by not considering the effects of dust outside the optically thick gas clumps, typically overestimates $f_{\text{esc}}^{\text{LyC}}$ (e.g., see also Gazagnes et al., 2020a; Kakiichi & Gronke, 2021). Accounting for this could potentially lower the $f_{\text{esc}}^{\text{LyC}}$ estimates presented in Pahl et al. (2021). However, we note that the $f_{\text{esc}}^{\text{LyC}} = (1 - C_f^{\text{HI}})$ approximation should be valid at the high $W_{\alpha}(\text{Ly}\alpha)$ values we are considering here, since these galaxies are generally expected to have low dust attenuation. Indeed, Saldana-Lopez et al. (2022b) conclude that this geometric consideration is insufficient to reconcile the $f_{\text{esc}}^{\text{LyC}}$ estimates.

Finally, it is clear that the choice of dust attenuation law can have a strong systematic impact on the derived values of $f_{\text{esc}}^{\text{LyC}}$ (e.g., Begley et al., 2022). Indeed, Saldana-Lopez et al. (2022b) note that their $W_{\text{LIS}} - f_{\text{esc}}^{\text{LyC}}$ calibration would predict $f_{\text{esc}}^{\text{LyC}}$ values that are higher by up to a factor 1.5, if they switch from the Reddy et al. (2016) dust attenuation law to a steeper SMC-like law (e.g., Gordon et al., 2003), which would be closer to the assumptions employed by Pahl et al. (2021) at high $W_{\alpha}(\text{Ly}\alpha)$. However, even in this case, the offset between the two estimates of $f_{\text{esc}}^{\text{LyC}}$ would still be a factor of $\approx 6$.

Ultimately, a combination of all of these different factors is likely to be having an impact. However, it is worth noting that, although the absolute $f_{\text{esc}}^{\text{LyC}}$ values are subject to potentially large systematic uncertainties, the relative values should be much less affected. Consequently, our conclusion that $f_{\text{esc}}^{\text{Ly}\alpha}$ and $f_{\text{esc}}^{\text{LyC}}$ are strongly
correlated, and that the correlation is not driven by varying $W_d(Ly\alpha)$, should still be robust, regardless of the exact normalization of either value.

### 4.6 Summary

We have presented the results of a study exploring the connection between the Ly$\alpha$ escape fraction ($f_{esc}^{Ly\alpha}$) and the Lyman continuum escape fraction ($f_{esc}^{LyC}$) for a sample of $N = 152$ SFGs selected from the ESO VANDELS spectroscopic survey (McLure et al., 2018b; Pentericci et al., 2018a; Garilli et al., 2021) at $3.85 \leq z_{spec} \leq 4.95$.

We combine measurements of $W_d(Ly\alpha)$ from ultra-deep, rest-frame FUV VANDELS spectra with H$\alpha$ equivalent widths derived from IRAC 3.6 $\mu$m flux-excess measurements to estimate individual $f_{esc}^{Ly\alpha}$ values for our full sample. We also employ composites of the VANDELS spectra to investigate the FUV spectral features as a function of $f_{esc}^{Ly\alpha}$, controlling for variations in $W_d(Ly\alpha)$. From these composites, we measure the equivalent width of low-ionization-state ISM absorption features ($W_{LIS}$) to place constraints on $f_{esc}^{LyC}$ using a low-redshift $W_{LIS} - f_{esc}^{LyC}$ calibration presented in Saldana-Lopez et al. (2022b). Our main results can be summarised as follows:

1. We find a positive correlation between $f_{esc}^{Ly\alpha}$ and $W_d(Ly\alpha)$ ($\approx 10\sigma$ significance), in which $f_{esc}^{Ly\alpha}$ monotonically increases from $f_{esc}^{Ly\alpha} \approx 0.04$ at $W_d(Ly\alpha) = 10$ Å to $f_{esc}^{Ly\alpha} \approx 0.1$ at $W_d(Ly\alpha) = 25$ Å. This represents the first measurement of the $f_{esc}^{Ly\alpha} - W_d(Ly\alpha)$ relation at $z > 4$ using individual $f_{esc}^{Ly\alpha}$ estimates.

2. We show that the $f_{esc}^{Ly\alpha} - W_d(Ly\alpha)$ relation does not evolve strongly from $z = 0$ to $z = 5$, and that the correlation holds down to $W_d(Ly\alpha) \approx 0$ Å. Our results imply that the physical processes regulating the production and escape of Ly$\alpha$ photons from low metallicity, high $\xi_{ion}$ Ly$\alpha$ emitters do not change significantly across $\approx 90$ per cent of cosmic history.

3. Using composite spectra, we show that as $f_{esc}^{Ly\alpha}$ increases the strength of low-ionization-state ISM absorption lines decreases, consistent with a decrease in the covering fraction of neutral H$\text{I}$ gas.

4. Using the relationship between the equivalent width of low-ionization
absorption lines \((W_{\text{LIS}})\) and \(f_{\text{esc}}^{\text{LyC}}\) derived from low redshift galaxies in the LzLCS survey (Saldana-Lopez et al., 2022b), we find that \(f_{\text{esc}}^{\text{LyC}} \approx 0.15^{+0.06}_{-0.04} f_{\text{esc}}^{\text{Ly} \alpha}\). Crucially, by constructing high- and low-\(f_{\text{esc}}^{\text{Ly} \alpha}\) composite spectra with the same \(W_L(\text{Ly} \alpha)\), we demonstrate that the \(f_{\text{esc}}^{\text{LyC}} - f_{\text{esc}}^{\text{Ly} \alpha}\) relation is not being driven by a secondary correlation between \(f_{\text{esc}}^{\text{Ly} \alpha}\) and \(W_L(\text{Ly} \alpha)\).

5. We find that, at a given value of \(W_L(\text{Ly} \alpha)\), the absolute \(f_{\text{esc}}^{\text{LyC}}\) values inferred from the low-redshift \(W_{\text{LIS}} - f_{\text{esc}}^{\text{LyC}}\) calibration are a factor of \(\geq 10\) lower than recent direct measurements of \(f_{\text{esc}}^{\text{LyC}}\) at \(z > 3\) (e.g., Steidel et al., 2018; Pahl et al., 2021; Begley et al., 2022). This is similar to the offset reported in Saldana-Lopez et al. (2022b). A number of systematic considerations may explain the discrepancy, but they remain to be fully understood. We argue that caution must therefore be used in inferring absolute values of \(f_{\text{esc}}^{\text{LyC}}\) from \(W_{\text{LIS}}\) measurements at high-redshift.

In the future, JWST will offer improvements via direct spectroscopic and/or more accurate photometric \(\text{H} \alpha\) measurements, which will lead to better constraints on \(f_{\text{esc}}^{\text{Ly} \alpha}\) for larger numbers of individual galaxies.
Chapter 5

The redshift evolution of the $[\text{O} \text{ III}] + \text{H} \beta$ equivalent width distribution

5.1 Introduction

During the Epoch of Reionization (EOR), Hydrogen ionizing photons (LyC) permeated through the intergalactic medium (IGM), driving its transition from entirely neutral to almost fully ionized (Robertson et al., 2015, 2023). Evidence from the Lyα forest of distant quasars point to this epoch ending at $z \approx 5.5$ (Fan et al., 2006; Goto et al., 2021; Bosman et al., 2021), while Planck Collaboration et al. (2020) measurements of the electron scattering optical depth ($\tau$) suggest an ‘instantaneous’ reionization midpoint of $z_{re} = 7.68 \pm 0.79$. Nonetheless, the exact timeline and topology of the reionization process remains uncertain (Becker et al., 2015; Mason et al., 2018a; Garaldi et al., 2022).

The demographics of the sources of ionizing photons plays a key role in dictating the overall progression of reionization (e.g., Robertson et al., 2015; Mason et al., 2019; Dawoodbhoy et al., 2023). Early quasars likely only played a minor role in sustaining the LyC photon budget required to drive reionization due to their relative scarcity at high redshift (Aird et al., 2015; Kulkarni et al., 2019; Matsuoka et al., 2023; Trebitsch et al., 2023). On the other hand, measurements of the UV
luminosity function at $z > 5$ (Bouwens et al., 2015; Bowler et al., 2020; Harikane et al., 2021; Donnan et al., 2022; McLeod et al., 2023) indicate the presence of a large population of star-forming galaxies (SFGs) during the EOR, particularly at faint $M_{UV} \gtrsim -18$ luminosities as a result of relatively steep faint-end slopes (e.g., $\alpha \lesssim -2$ Finkelstein et al., 2015). Although a consensus has been reached regarding the dominant role of early SFGs in producing the bulk of the ionizing photon budget (Chary et al., 2016; Robertson et al., 2023), with only a minor contribution from AGN suggested by recent JWST results (Maiolino et al., 2023), questions about the properties of these galaxies remain.

Two of the key galaxy properties interlinked with the EOR timeline and topology are the ionizing photon production rate, often quantified as the ionizing photon production efficiency $\xi_{\text{ion}}$, the number of LyC photons produced per unit UV luminosity ($\xi_{\text{ion}} \equiv N(H^0)/L_{UV}$) and the fraction of these photons that then escape into the surrounding IGM ($f_{\text{esc}}^{\text{LyC}}$, e.g., Robertson et al., 2015; Finkelstein et al., 2019; Mason et al., 2019). A number of state-of-the-art radiative hydrodynamical simulations provide supporting evidence for a ‘democratic’ reionization process, whereby the faint but numerous population of $M_{UV} \gtrsim -18$ galaxies dominate the overall LyC photon budget (Lewis et al., 2022; Rosdahl et al., 2022). This scenario is in contrast to alternative models suggesting reionization is driven by the rarer, UV-luminous ‘oligarchs’ (e.g., Naidu et al., 2020), or alternatively by a small subset of the brightest Ly$\alpha$ emitters with high $\xi_{\text{ion}}$ and $f_{\text{esc}}^{\text{LyC}}$ (e.g., Matthee et al., 2022; Naidu et al., 2022).

Each of these models are broadly consistent with the late, rapid reionization inferred from constraints of the evolution in the global neutral Hydrogen fraction (e.g., McGreer et al., 2015; Hoag et al., 2019; Mason et al., 2019). It is therefore clear that deciphering the relative contributions of different galaxy sub-populations remains an open debate, and that a better understanding of $\xi_{\text{ion}}$ and $f_{\text{esc}}^{\text{LyC}}$ across these populations is demanded.

Direct measurements of $f_{\text{esc}}^{\text{LyC}}$ are restricted to $z \lesssim 4$ on account of the increasing opacity of the IGM to LyC photons at higher redshifts (Madau, 1995; Inoue et al., 2014). Studies based on deep $U$-band imaging and spectroscopy have shown SFGs at $z = 3–4$ have $f_{\text{esc}}^{\text{LyC}} \approx 5–10$ per cent (Steidel et al., 2018; Pahl et al., 2021; Begley et al., 2022), and provide clear evidence that higher Ly$\alpha$ equivalent widths, lower
stellar-masses and dust content, and fainter UV magnitudes all likely indicate higher $f_{\text{esc}}^{\text{LyC}}$ (Marchi et al., 2018; Fletcher et al., 2019; Begley et al., 2023; Pahl et al., 2023). Moreover, results from low-redshift analogues are finding success in uncovering which galaxy properties or spectral features can be used as robust indicators of non-negligible $f_{\text{esc}}^{\text{LyC}}$ (e.g., the UV spectral slope $\beta$ or properties sensitive to the neutral Hydrogen geometry, see; Chisholm et al., 2018; Gazagnes et al., 2020a; Flury et al., 2022a,b; Saldana-Lopez et al., 2022a,b).

Complimentary to studies of $f_{\text{esc}}^{\text{LyC}}$, significant progress has also been made establishing the ionizing photon production efficiencies of star-forming galaxies. Analytic models typically require $\log_{10}(\xi_{\text{ion}} / \text{erg s}^{-1} \text{Hz}) \gtrsim 25.2 - 25.3$ for reionization to be complete by $z \sim 5 - 6$, which is generally in agreement with inferences of $\xi_{\text{ion}}$ based the UV spectral slope ($\beta$; Duncan & Conselice, 2015; Castellano et al., 2023). However, these inferences rely heavily on assumptions about the stellar population models (e.g., see Robertson et al., 2013, 2015). As highlighted in Eldridge et al. (2017) and Stanway & Eldridge (2018), $\xi_{\text{ion}}$ can vary by factors of $\approx 2 - 3$ depending on the metallicity, assumed IMF, and whether or not binary stellar evolution is factored into the models, adding significant uncertainty to measurements of $\xi_{\text{ion}}$.

Alternatively, probing the ionization conditions of galaxies can be achieved through measuring the strong nebular emission lines powered by the intense ionizing radiation from young stellar populations (Tang et al., 2019, 2021b; Endsley et al., 2021, 2023). For example, the $\text{H}\alpha$ emission, when combined with measurements of the UV continuum has successfully allowed $\xi_{\text{ion}}$ to be measured across a range of redshifts (Bouwens et al., 2016; Matthee et al., 2017; Shivaei et al., 2018; Maseda et al., 2020).

Extreme $[\text{O} \text{III}] + \text{H} \beta$ emission has also been a considerable focus in recent years after a number of studies highlighted that a high proportion of confirmed LyC leaking galaxies have strong $[\text{O} \text{III}]$ emission. Moreover, many display high $O32(=\log([\text{O} \text{III}]\lambda4959, 5007/\text{[O II]}\lambda\lambda3726, 3729))$ values (Vanzella et al., 2016b; Rivera-Thorsen et al., 2017; Izotov et al., 2018c; Fletcher et al., 2019), which has been suggested as a necessary requirement for high $f_{\text{esc}}^{\text{LyC}}$ (Nakajima et al., 2020). Coupled with the high $\xi_{\text{ion}}$ found in galaxies with the most extreme $[\text{O} \text{III}]$ emission (Chevallard et al., 2018; Tang et al., 2019; Onodera et al., 2020), this provides significant motivation to investigate $[\text{O} \text{III}] + \text{H} \beta$ emission across cosmic time.
In this work we aim to piece together the evolution of the \([\text{O} \, \text{iii}] + \text{H} \beta\) equivalent width \(W_\lambda([\text{O} \, \text{iii}] + \text{H} \beta)\) distribution across the redshift range \(3 \leq z \leq 8\) using a sample of galaxies selected from VANDELS and CEERS. Studying the evolution in the \([\text{O} \, \text{iii}] + \text{H} \beta\) emission of galaxies will provide a crucial insight into the evolution of \(\xi_{\text{ion}}\) directly into the the reionization epoch.

5.2 Data and sample selection

To assess the redshift evolution of \(W_\lambda([\text{O} \, \text{iii}] + \text{H} \beta)\), we assemble two samples of star-forming galaxies, one at \(z = 3.2 - 3.6\) from the VANDELS survey (McLure et al., 2018b; Garilli et al., 2021) and another at \(z \approx 7.0 - 7.6\) from CEERS (Finkelstein et al., 2017), described below in Sections 5.2.1 and 5.2.2, respectively. Literature results for the \(W_\lambda([\text{O} \, \text{iii}] + \text{H} \beta)\) distribution at \(z \approx 2\), assembled to provide a wider dynamic range in redshift, are outlined in Section 5.2.4.

5.2.1 The VANDELS sample at \(3.2 \leq z_{\text{spec}} \leq 3.6\)

The VANDELS survey

The VANDELS spectroscopic survey is a large ESO public program (McLure et al., 2018b; Pentericci et al., 2018a) using the VLT/VIMOS spectrograph. In total, \(N = 2087\) spectroscopic redshifts for galaxies in the range \(1.0 \leq z_{\text{spec}} \leq 7.0\) were measured using \(R \approx 600\), ultra-deep optical spectroscopy spanning \(0.48 \mu\text{m} \leq \lambda_{\text{obs}} \leq 1.0 \mu\text{m}\) wavelengths.

Approximately half the VANDELS target galaxies were selected from the *Hubble Space Telescope* (HST) based CANDELS program, covering the central regions of the Chandra Deep Field South (CDFS) and UKIDSS Ultra Deep Survey (UDS) fields (Grogin et al., 2011; Koekemoer et al., 2011). For the sample galaxies within the CANDELS footprints, we use the available deep multi-wavelength photometry catalogues from Guo et al. (2013) and Galametz et al. (2013), respectively.

The VANDELS target list was also supplemented by galaxies selected from ground-based optical and NIR imaging spanning a wider area than the central HST CANDELS region (McLure et al., 2018b). The photometric catalogues
constructed for the final VANDELS public data release (DR4, described in; Garilli et al., 2021) are used for these VANDELS galaxies selected from ground-based imaging.

Overall, after the inclusion of Spitzer/IRAC imaging at 3.6 \( \mu \text{m} \) and 4.5 \( \mu \text{m} \) taken as part of the Spitzer Extended Deep Survey (Ashby et al., 2013), all VANDELS galaxies benefit from deep multi-wavelength photometry spanning 0.35 \( \mu \text{m} \) \( \lesssim \lambda_{\text{obs}} \lesssim 4.5 \mu \text{m} \).

For this work, we select star-forming galaxies at redshifts 3.2 \( \leq z_{\text{spec}} \leq 3.6 \), with the additional requirement of having a \( z_{\text{flag}} = 3, 4 \) or 9, redshift quality flag to ensure only galaxies with robust spectroscopic redshifts having a \( \gtrsim 95 \) per cent probability of being correct are included in our final sample (e.g., see Garilli et al., 2021).

In this redshift range the \([\text{O III}]+\text{H} \beta\) emission lines are present in the \(K\)-band, enabling the equivalent width of these emission lines (\(W_{\lambda}(\text{[O III]}+\text{H} \beta)\)) to be measured using the photometric excess method (see Section 5.3) commonly employed to infer nebular emission line strengths (e.g., Stark et al., 2013; Smit et al., 2014; Mármol-Queraltó et al., 2016; Smit et al., 2016; Bollo et al., 2023; Simmonds et al., 2023). Specifically, due to the multiple \(K\)-band filters used across the four VANDELS photometric catalogues (see Table 5.1), the restricted redshift range ensures the \([\text{O III}]+\text{H} \beta\) lines are contained within the \(\geq 80\) per cent transmission regions of their respective ‘measurement’ \(K\)-band filter profiles. We further exclude a small number (\(\approx 4\) per cent) of galaxies due to bad/contaminated \(K\)-band photometry. Using the selection criteria outlined, we obtain a final sample of \(N = 326\) star-forming galaxies with robust spectroscopic redshifts and photometry.

The NIRVANDELS sample

A subset of the full VANDELS spectroscopic sample also benefit from near-IR spectroscopy from NIRVANDELS - a near-IR follow-up program using the Multi-object Spectrometer for Infrared Exploration (MOSFIRE McLean et al., 2012) instrument on Keck I in the \(H\)- (1.5 \( \mu \text{m} \) \( \leq \lambda_{\text{obs}} \leq 1.8 \mu \text{m} \)) and \(K\)-bands.
Table 5.1  Table of the available $K$–band filters in the VANDELS photometric catalogues that are contaminated by potential $[\text{O} \text{III}] + H\beta$ emission at redshifts $3.2 \leq z \leq 3.6$. The $K$–band filter used in the photometric excess method to measure $W_d([\text{O} \text{III}] + H\beta)$ (see Section 5.3) is in centre column.

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<tr>
<th>VANDELS Catalogue</th>
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<th>Other $K$–bands</th>
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<td>Hawk–I/Ks</td>
<td>ISAAC/Ks</td>
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<td>VISTA/Ks</td>
<td>WIRCam/Ks</td>
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$(2.0 \mu m \leq \lambda_{\text{obs}} \leq 2.4 \mu m)$. The reader is directed to Cullen et al. (2021) for a full description of the target selection and data reduction procedures of the NIRVANDELS program.

The additional NIR observations allow direct spectroscopic measurements of both the $[\text{O} \text{III}]$ and $H\beta$ lines for $N = 21$ galaxies in the $3.0 < z_{\text{spec}} < 3.8$ redshift range, of which $N = 13$ are also selected in the $3.2 \leq z_{\text{spec}} \leq 3.6$ spectroscopic sample defined above.

The overlap between two samples of galaxies, one with photometrically inferred $W_d([\text{O} \text{III}] + H\beta)$ values and another with direct spectroscopic measurements, enables a direct assessment of the accuracy of the photometric excess method outlined in Section 5.3. The spectroscopic calibration with NIRVANDELS, together with the $W_d([\text{O} \text{III}] + H\beta)$ recovery simulations detailed in Section 5.3.3, are used to ensure accurate constraints on the $W_d([\text{O} \text{III}] + H\beta)$ distribution of our sample.

5.2.2  The CEERS sample at $7.0 \leq z \leq 7.6$

To investigate the evolution of the $W_d([\text{O} \text{III}] + H\beta)$ distribution into the EOR, we assemble a sample of galaxies at $7.0 \leq z \leq 7.6$ from the Cosmic Evolution Early Release Science survey (CEERS ERS 1345; PI Finkelstein). Within this redshift range, the $[\text{O} \text{III}] + H\beta$ emission lines lie within the F410M and F444W filters. The construction of our high-redshift CEERS photometric catalogues are discussed below in Section 5.2.2, while Section 5.2.3 reviews our photometric redshift determinations and sample selection. In Sections 5.3.3 and 5.3.2, we outline the adjusted photometric excess, and colour measurement methods used to
Figure 5.1  Illustration of the CEERS (Finkelstein et al., 2023) Epoch 1 north-east footprints used to ensure all galaxies in the initial sample had high-quality $N = 10$ band photometry. **Left:** HST/ACS band footprints for F435W from UVCANDELS and F606W+F814W from the CEERS HDR1 release of CANDELS imaging (e.g., see Koekemoer et al., 2011). **Centre:** Footprint layout for the JWST/NIRCam short wavelength channel F115W+F150W+F200W filters, with the intra-module detector gaps clearly shown. **Right:** Same as the centre panel, but for the long wavelength channel F277W+F356W+F410M+F444W filters.

measure the $[\text{O III}] + \text{H} \beta$ equivalent widths for the CEERS galaxies in our sample.

### CEERS Photometric Catalogues

In this work we use CEERS Epoch 1 observations (Finkelstein et al., 2023) consisting of $\approx 40$ arcmin$^2$ of NIRCam imaging of the EGS field in each of the F115W, F150W, F200W, F356W, F410M and F444W bands. The raw imaging ‘rate’ files were processed using PENCIL (Primer Enhanced NIRCam Image Processing Library; Magee et al. in prep), a custom reduction pipeline based on the JWST NIRCam pipeline (version 1.6.2, pmap 0989 including the most recent zero-point corrections). The updated pipeline includes routines to remove the ‘snowball’ and ‘wisp’ artifacts commonly seen in NIRCam imaging (see also Bagley et al., 2023). In addition, PENCIL corrects the $1/f$ noise striping and performs a robust background subtraction procedure. The reductions split the 4 NIRCam pointings of Epoch 1 CEERS into separate north-east and south-west regions.

The NIRCam imaging was supplemented with CANDELS HST/ACS F606W and F814W imaging reprocessed by the CEERS team (HDR1; see Koekemoer et al.,
2011), as well as F435W imaging from the UVCANDELS survey (GO 15647, PI Teplitz; DOI: 10.17909/8s31-f778) that was aligned to the JWST imaging using SWARP (e.g., Donnan et al., 2022; McLeod et al., 2023).

To remove potential biases in our aperture photometry arising from the wavelength-dependent point spread function (PSF), we first PSF-homogenise each of the HST/ACS and JWST/NIRCam images by convolving to match the F444W PSF. The PSF kernels were produced from empirical PSF models based on stacks of isolated, bright stars in each image.

To create the initial photometric catalogues we run SOURCE EXTRACTOR (Bertin & Arnouts, 1996) in dual-image mode on each PSF-homogenised image with the F200W image as the detection image. For the aperture photometry we employ 0.33 arcsec diameter apertures (i.e., 11 pixel diameter for the 0.03 arcsec/pixel imaging), corresponding to ≈ 71 – 72 per cent enclosed flux from the convolved image curves-of-growth. To ensure robust photometric redshift (and physical property) estimates, we restrict our catalogue to objects with a full set of $N = 10$ band photometry using the common footprint area as shown in Fig. 5.1, and apply a $> 5\sigma$ cut in the F200W detection image. We also ensure that objects in the catalogue have $\leq 2\sigma$ detections in the two bluest filters (F435W and F606W).

Photometric uncertainties are assigned as the local depth for each object, calculated as the scaled median absolute deviation ($\sigma_{\text{local}} = 1.4826\sigma_{\text{MAD}}$) of the flux distribution from the nearest 200 empty-sky apertures. The empty sky apertures were selected using the dilated SOURCE EXTRACTOR segmentation map from the detection image. The resulting local-depth map using the entire empty-sky aperture grid is shown in Fig. 5.2.

### 5.2.3 CEERS photometric redshifts and target selection

To find the best photometric redshift for each object in our initial sample, we perform three independent photometric-redshift runs, using two separate SED-fitting codes, on the entire sample. Firstly, we perform SED-fitting using LePHARE (Arnouts et al., 1999; Ilbert et al., 2006), with a BC03 template set (Bruzual & Charlot, 2003) and a Chabrier (2003) IMF. The templates are constructed using a declining star-formation history with $\tau$ varying between 0.1 – 15 Gyr, and metallicities in the 0.2$Z_\odot$ to $Z_\odot$ range. A Calzetti et al. (2000) dust attenuation law is adopted, with $A_V = 0 – 4$, and emission lines are included.
Figure 5.2  Local depth map in magnitudes for the PSF-homogenised F200W detection image in the CEERS Epoch 1 north-east region, with the deepest (shallowest) regions shown in black (white). Depths are shown at the 1σ level, in 0.33 arcsec diameter apertures enclosing ≃ 71 per cent of the total flux, assuming point sources. The local depths used to assign photometric uncertainties in our CEERS photometry catalogues are described in Section 5.2.2. The global 1σ depth is $m_{1\sigma} \approx 30.5$ but can vary at the $\Delta(m_{1\sigma}) \approx 0.5$ level across the field, particularly in the vicinity of bright foreground stars.

We then do two separate runs using the eazy photometric redshift code (Brammer et al., 2008) in PCA mode and single template mode, respectively. For the PCA run, we use the default eazy template set defined in Brammer et al. (2008), with an additional high equivalent width emission line model to better account for the stronger emission lines found in high-redshift galaxies. In the single template mode, we use the PEGASE model templates (Fioc & Rocca-Volmerange, 1997, 2019), which include self-consistently calculated emission lines by default.

Hierarchical Bayesian Combination

The best photometric redshift is then found using the consensus $P(z)$, calculated from the three independent photometric-redshift runs described above using the hierarchical Bayesian combination method (e.g., Dahlen et al., 2013, see also Duncan et al. 2018; Hatfield et al. 2022). Briefly, for each object and for a given SED-fit based redshift estimate $i$ we define $P(z, f_{bad})$, the joint probability of the redshift $z$ and the nuisance parameter $f_{bad}$ that encodes the possibility that an
individual $P(z)$ is incorrect;

$$
P(z, f_{\text{bad}})_i = P(z | \text{bad})_i \cdot f_{\text{bad}} + P(z | \text{good})_i \cdot (1 - f_{\text{bad}})
$$

(5.1)

where $P(z|\text{bad})$ is the redshift PDF assumed in the case where the SED-fitting derived $P(z)_i$ is incorrect, and $P(z|\text{good})$ is the redshift PDF assuming the measured PDF is correct (i.e., $P(z|\text{good}) \equiv P(z)_i$).

Under the assumption that there is no information on the redshift, $P(z|\text{bad})$ could simply be set as a uniform prior (e.g., $P(z|\text{bad}) = 1/z_{\text{max}}$). Alternatively, in this work we use a redshift–volume prior assigning $P(z|\text{bad}) = dV(z)/dz$, which is the normalised differential comoving volume. For a comparison of the various options of the bad measurement redshift prior, the reader is referred to Duncan et al. (2018), however we note that the choice of this prior is inconsequential in almost all cases, except those in which an extremely poor fit is found across all three photometric-redshift runs.

Given the choice of $P(z|\text{bad})$, the combined $P(z, f_{\text{bad}})$ for all $n$ (SED-fitting derived $P(z)$) measurements is then given as;

$$
P(z, f_{\text{bad}}) = \prod_{i=1}^{n} P(z, f_{\text{bad}})_i^{1/\beta_i}
$$

(5.2)

where $\beta_i$ characterises the level of covariance and weighting between the different $P(z)$ estimates. Given that some level covariance is inevitable as each SED-fitting run uses the same photometry, we follow the approach described in Hatfield et al. (2022) and set $\beta_i$ based on the relative quality of the best-fitting solutions (i.e., a weighted geometric mean);

$$
\frac{1}{\hat{\beta}_i} = \frac{e^{-\chi_i^2/2}}{\sum_{j=1}^{n} e^{-\chi_j^2/2}}
$$

(5.3)

where $\chi_i^2$ is from the best fit of an individual run. It is worth highlighting that, in the case of a equally-well-fitted solution from each SED code, $\beta_i = 1/n$ corresponds to the geometric mean. Similarly, if a solution is strongly favoured (disfavoured) then its weighting tends to $1/\beta_i \rightarrow 1$ (0).
Lastly, the final consensus $P(z)$ of each object is produced by marginalising over $f_{\text{bad}}$:

$$P(z) = \int_{f_{\text{bad}}^{\text{min}}}^{f_{\text{bad}}^{\text{max}}} P(z, f_{\text{bad}}) df_{\text{bad}}$$  \hspace{1cm} (5.4)

As discussed in Duncan et al. 2018 (see also Hatfield et al., 2022), the $f_{\text{bad}}$ range should be chosen to represent the expected (and measured) outlier fraction in the photometric redshift measurements. Using $P(z)$ from individual SED-fits, the outlier fraction is relatively high at $\approx 17 - 20$ per cent, so we conservatively set the range from $f_{\text{bad}}^{\text{min}} = 0.1$ to $f_{\text{bad}}^{\text{max}} = 0.2$. As with the influence of the $P(z | \text{bad})$ prior choice, we find that the choice of this range does significantly impact our photometric redshift quality (a comparable finding to Duncan et al., 2018; Hatfield et al., 2022).

The best-estimate photometric redshift can then be given as the peak redshift $z_{\text{peak}}$, or as the median from CDF of the ‘consensus’ $P(z)$, designated $z_{\text{HBC}}$ (where $C(z_{\text{phot}}) = 0.5$), which we adopt here. An example of this method applied to a galaxy with measured $z_{\text{phot}} \approx 7.4$ and confirmed $z_{\text{spec}} = 7.45077$ (A. E. Shapley, private communication) from our CEERS photometric catalogue is shown in Fig. 5.3.

**Spectroscopic redshifts in the EGS field**

To test the accuracy of our photometric redshifts we compare with an ensemble of spectroscopically confirmed redshifts, as shown in Fig. 5.4. The spectroscopic redshift sample comprises $N = 284$ galaxies in the EGS field primarily at $z_{\text{spec}} < 1.5$ with robust redshift flags from a variety of pre-JWST ($HST$- and ground-based) spectroscopic surveys, and $N = 68$ galaxies spanning the redshift range $0.2 \lesssim z_{\text{spec}} \lesssim 12$ from CEERS (and DDT; ID 2750, PI P. Arrabal Haro) spectroscopy (Fujimoto et al., 2023; Arrabal Haro et al., 2023b,d; Kocevski et al., 2023; Nakajima et al., 2023, and A. E. Shapley, private communications). To assess the performance of our photometric redshifts we use $\sigma_{d^z} = 1.4826 \times \sigma_{\text{MAD}}(d^z)$, where $d^z = (z_{\text{phot}} - z_{\text{spec}})/(1+z_{\text{spec}})$. We also consider the catastrophic outlier rate $f_{\text{outlier}}$, defined as the fraction of galaxies with $|d^z| > 0.15$

Generally, the individual redshift estimates from the three photometric-redshift runs achieve $\sigma_{d^z} \gtrsim 0.05$ and outlier fractions of $f_{\text{outlier}} \gtrsim 10 - 20$ per cent, which is generally worse than robust literature photometric redshift catalogues in the
Figure 5.3 Example of a CEERS photometrically selected galaxy, with $z_{\text{phot}} = 7.38^{+0.10}_{-0.09}$ measured through the hierarchical Bayesian combination method applied to three independent photometric-redshift runs (see Section 5.2.3). The photometric redshift estimate of this galaxy is in good agreement with the confirmed spectroscopic redshift ($z_{\text{spec}} = 7.45^{+0.07}_{-0.02}$; A. E. Shapley, private communication). The individual $P(z)$ estimates from LePhare and from eazy in PCA and single template modes are shown in green, blue, and red, respectively. The ‘consensus’ $P(z)$ is shown in black, and in the inset shows the CDF for each $P(z)$.

literature without JWST photometry (e.g., Brammer et al., 2008; McLure et al., 2018b; Garilli et al., 2021). One possible option to improve the photometric redshift accuracy is to take the median of the multiple redshift estimates (e.g., McLeod et al., 2021). Here, taking the median of the best estimate $z_{\text{phot}}$ from the three SED fits achieves $\sigma_{dz} = 0.032$ and $f_{\text{outlier}} = 8.2$ per cent, improving on the individual estimates, albeit still slightly higher than typical.

Lastly, using the hierarchical Bayesian combination method, the catastrophic outlier rate drops further to $f_{\text{outlier}} = 6.3$ per cent with $\sigma_{dz} = 0.032$. This is comparable to the photometric redshift accuracy achieved from a number of independent CANDELS photometric redshift catalogues (e.g., see Kodra et al., 2023, for a comprehensive comparison).
Figure 5.4 Comparison of the spectroscopic redshifts and the Hierarchical Bayesian Combination-based photometric redshifts for \( N \approx 350 \) galaxies detected in the CEERS Epoch 1 imaging. The best-redshift for each galaxy is quoted as the median of the HBC \( P(z) \), with the error bars shown as the ±1σ (68 per cent) confidence intervals (green markers). We find \( \sigma_{dz} = 0.032 \) and an outlier fraction of \( f_{\text{outlier}} = 6.5 \) per cent (e.g., as described in Section 5.2.3), which is a comparable accuracy to that found from large CANDELS photometric catalogues (e.g., see Damen et al., 2009; Kodra et al., 2023). The 1:1 relation is shown as a black dashed line. The grey-shaded regions represent the threshold (\(| dz | \geq 0.15 \)), outside of which galaxies are classed as catastrophic outliers (non-solid markers). The green-shaded regions denotes galaxies with \( 7.0 \leq z \leq 7.6 \) that have \( F410M \) (and \( F444W \)) photometry contaminated by \( [OIII]+H\beta \) emission and are selected as our high-redshift CEERS sample. The top panel shows \( dz \) as a function of \( z_{\text{spec}} \).
For our final sample, we initially select galaxies with $z_{\text{phot}}$ in the range $7.0 \leq z_{\text{HBC}} \leq 7.6$, within which the F410M filter fully encloses any potential emission from the $[\text{O\,iii}]+\text{H}\beta$ lines. We then carry out a robust visual inspection of each object using image cutouts across the entirety of the available imaging, with the aim of removing objects too close to the image edges, objects contaminated by bright foreground sources and image artifacts (e.g., diffraction spikes) that masquerade as genuine high-redshift candidates. The final photometrically-selected CEERS sample consists of $N = 93$ galaxies with robust 10-band photometry and photometric redshift estimates. This sample includes 7 spectroscopically confirmed galaxies from the EGS field in the $7.0 \leq z \leq 7.6$ redshift range (e.g., see Section 5.2.3).

5.2.4 Literature results at $z \simeq 2$

To assess the evolution of the $W_A([\text{O\,iii}]+\text{H}\beta)$ distribution across a broader redshift dynamic range, we compare the results presented in this work with the $z \simeq 2$ $[\text{O\,iii}]\lambda5007$ equivalent width distribution reported by Boyett et al. (2022). This $W_A([\text{O\,iii}])$ distribution is measured from a sample of $N = 672$ galaxies in the redshift range $1.7 \leq z \leq 2.3$, photometrically selected from the HDUV legacy survey (e.g., see Oesch et al., 2018a). The sample also has a UV magnitude cut, restricting the sample to galaxies with $M_{\text{UV}} \leq -19.0$. This dataset overlaps with the 3D-HST program (Brammer et al., 2012) providing HST/WFC3 G141 grism slitless spectroscopy, enabling direct spectroscopic $[\text{O\,iii}]$ measurements for their galaxy sample. Fitting a log-normal functional form to the observed $W_A([\text{O\,iii}])$ distribution, Boyett et al. (2022) find best-fitting parameters of $\mu_{\text{LN}} = 1.84 \pm 0.03$ and $\sigma_{\text{LN}} = 0.58 \pm 0.03$ (quoted in base 10 log-space).

To directly compare the Boyett et al. (2022) results with our VANDELS and CEERS measurements, we need to first convert their $W_A([\text{O\,iii}])$ distribution to a $W_A([\text{O\,iii}]+\text{H}\beta)$ distribution. In this conversion, the additional flux from the $[\text{O\,iii}]\lambda4960$ and $\text{H}\beta$ emission lines needs to be accounted for. To correct for the $[\text{O\,iii}]\lambda4960$ line flux, we adopt the theoretical line ratio $[\text{O\,iii}]\lambda5007 / [\text{O\,iii}]\lambda4960 \simeq 2.98$ (e.g., Storey & Zeippen, 2000). Establishing the contribution from the $\text{H}\beta$ emission line is less straightforward due to
observational evidence suggesting the [O III]λ5007 / H β ratio, and therefore the $W_A([\text{O III}]\lambda5007) \rightarrow W_A([\text{O III}]+H \beta)$ conversion factor, evolves with redshift and stellar-mass (Kewley et al., 2015; Cullen et al., 2016; Dickey et al., 2016). In this regard, Reddy et al. (2018b) find a conversion factor of $f_{\text{conv}} \approx 1.44 - 1.76$ over log($M_*/M_\odot$) ≈ 9.0 – 11.0 at $z \sim 2.3$ (with $df_{\text{conv}}/dz \simeq 0.1$), based on galaxies in the MOSDEF survey.

For a more direct empirical conversion, we opt to use the $W_A(H \beta) \approx 0.115 \times W_A([\text{O III}]\lambda5007)^{1.065}$ relation presented in Boyett et al. (2022) (based on the results by Tang et al. 2019), resulting a in conversion factor $f_{\text{conv}} \approx 1.48$. This shifts the location parameter in the best-fitting log-normal distribution by $\Delta(\mu_{LN}) \approx 0.17$ dex to $\mu_{LN} \approx 2.01$.

We note that any residual mass dependence not intrinsically included in the correction inferred from the $W_A(H \beta) - W_A([\text{O III}]\lambda5007)$ correlation contributes by at most $\sigma_{\Delta\mu_{LN}} \sim 0.05$ in our conversion. Moreover, by scaling individual values drawn from the log-normal distribution presented in Boyett et al. (2022), we confirm the shape of the distribution is consistent with a simple shift in the location parameter $\mu_{LN}$. In summary, the corresponding mean (median) $[\text{O III}]+H \beta$ equivalent width from the Boyett et al. (2022) galaxy sample is $W_A([\text{O III}]+H \beta) \approx 100$ Å.

### 5.3 Inferring [O III]+H β equivalent widths

#### 5.3.1 The VANDELS sample

**Stellar population fitting with fast++**

We use the photometric excess method based on the difference between the observed $K$–band flux and predicted stellar continuum probed by the $K$–band, to measure the the $[\text{O III}]+H \beta$ emission line equivalent widths for our VANDELS 3.2 ≤ $z_{\text{spec}}$ ≤ 3.6 sample. The predicted stellar continuum for each galaxy is estimated from the best-fitting SED determined using the fast++ code (Kriek et al., 2009; Schreiber et al., 2018). In the fast++ fits we use the Bruzual & Charlot (2003) (BC03) stellar population synthesis models, assuming a Chabrier
(2003) IMF and with 0.2 - 0.4\( Z_\odot \) metallicity. The star-formation history is assumed to be constant, with ages permitted in the range 6.7 \( \leq \log(t/\text{yr}) \leq 10.0 \) and incremented in steps of \( \Delta(\log(t/\text{yr})) = 0.2 \). We adopt a Calzetti et al. (2000) dust attenuation law, with the V-band attenuation varying between 0.0 \( \leq A_V \leq 4.0 \). Throughout the fast++ SED fits, the redshift of each galaxy is fixed at the spectroscopic redshift measured from the VANDELS spectra.

As a result of potentially strong contamination by \([\text{O III}]+\text{H}\beta\) and \([\text{O II}]\) emission, the \( K^- \) and \( H^- \) band photometry are excluded from the SED fits. As outlined in Cullen et al. (2021), the rest-frame FUV-to-NIR wavelength coverage offered by the remaining \( U^- \) to \( J^- \) band photometry, as well as the IRAC 3.6\( \mu m \) and 4.5\( \mu m \) photometry, allows robust estimates of the galaxy SED and relevant physical parameters even if the \( H^- \) and \( K^- \) bands are not included.

The physical parameters including the stellar-mass \( \log(M_*/M_\odot) \), the absolute \( V^- \) band dust attenuation \( A_V \) and the rest-frame UV magnitude \( M_{1500} \) are taken from the best-fitting SED template of each object, with the latter calculated using a \( \Delta \lambda = 100 \AA \) wide top-hat filter placed at \( \lambda_{\text{rest}} = 1500 \AA \). For our final galaxy sample, we infer stellar-masses in the range \( \log(M_*/M_\odot) \approx 7.6 - 10.6 \), with a median of \( \langle \log(M_*/M_\odot) \rangle = 9.3 \), and absolute UV magnitudes spanning \( M_{1500} \approx -18.00 \) to \( M_{1500} \approx -22.00 \), with a median \( \langle M_{1500} \rangle \approx -20.23 \).

**The Photometric Excess Method**

The ‘excess’ observed \( K^- \) band flux \( f_{K,\text{obs}} \) relative to that predicted from the best-fitting SED template (\( f_{K,\text{mod}} \), excluding bands potentially contaminated by strong nebular emission) can be used to estimate the rest-frame \( W_A([\text{O III}]+\text{H}\beta) \) (e.g., see Chapter 4 and examples in Stark et al., 2015; Mármol-Queraltó et al., 2016; Smit et al., 2016; Begley et al., 2023) via the following equation:

\[
W_A([\text{O III}]+\text{H}\beta) = \frac{W_{K}^{\text{eff}}}{1+z_{\text{spec}}} \times \left( \frac{f_{K,\text{obs}}}{f_{K,\text{mod}}} - 1 \right)
\]

(5.5)

where \( W_{K}^{\text{eff}} \) is the effective width of the \( K^- \) band filter (\( \approx 2795 - 3175 \AA \) depending on the relevant VANDELS \( K^- \) band filter), and \( z_{\text{spec}} \) is the spectroscopic redshift.

To demonstrate that the photometric excess does indeed indicate the presence of
[OIII]+Hβ emission lines, we measure the photometric excess of a control sample of VANDELS SFGs selected in the redshift range 2.6 ≤ zspec ≤ 2.9 (with the same redshift quality criteria used in the main 3.2 ≤ zspec ≤ 3.6 sample). In this redshift range, the K–band photometry is not ‘contaminated’ by the presence of any strong emission lines, and only probes the stellar continuum flux.

We show the Wd([OIII]+Hβ) distribution for this ‘null’ sample of galaxies measured using the photometric excess in Fig. 5.5 (green) alongside the Wd([OIII]+Hβ) distribution measured for the main 3.2 ≤ zspec ≤ 3.6 VANDELS sample (grey hatched). As expected the Wd([OIII]+Hβ) distribution for the control sample is comfortably centred on zero in contrast the distribution seen in the 3.2 ≤ zspec ≤ 3.6 sample. Fitting a normal distribution to the control sample gives best-fitting parameters μEW = −2^{+14}_{−13} and σEW = −84^{+15}_{−14}. The consistency of the control sample with Wd([OIII]+Hβ) ≃ 0 Å provides reassurance that the observed K–band photometric excess is a reliable tracer of [OIII]+Hβ line emission in our 3.2 ≤ zspec ≤ 3.6 VANDELS sample (see also Sections 5.3.4 and 5.3.3).

5.3.2 Inferring Wd([OIII]+Hβ) from CEERS photometric colours

When applying the photometric excess method to the CEERS sample using the F410M band that is contaminated by [OIII]+Hβ emission, there is added uncertainty (compared with the VANDELS K–band measurements) as a result of the need to further exclude the F444W band from the fitted photometry because it is also contaminated by the [OIII]+Hβ emission lines. To confirm this added error does not add significant systematic bias and that the correction factor applied from our recovery simulations described in Section 5.3.3 are robust, we further estimate Wd([OIII]+Hβ) using a colour-based methodology (e.g., Smit et al., 2014, 2015; Labbè et al., 2013; Rasappu et al., 2016; Roberts-Borsani et al., 2016; Endsley et al., 2021).

To infer the [OIII]+Hβ equivalent width from the observed F356W–F410M colour, we first produce a reference translation using mock SED models created using BAGPIPES. Similar to the method employed for the emission line recovery simulations (see Section 5.3.3), we construct models with properties spanning the range of typical physical parameters inferred from the CEERS sample SED
fitting and add artificial [O III]+H β emission lines to the model SED. The relation between the F356W–F410M colour and $W_A([\text{O III}]+H\beta)$ and how this varies as a function of physical properties is illustrated in Fig. 5.6. In Fig. 5.6, models with ages spanning $t_{\text{age}} = 10 - 100$ Myr (assuming constant SFH) and absolute dust attenuation values in the range $A_V = 0.0 - 0.5$ (using a Calzetti et al. (2000) attenuation law) are shown in blue solid and green dashed lines respectively (age varying models have $A_V = 0.0$, whilst attenuation varying models have $t_{\text{age}} = 50$ Myr). Variations up to $\Delta(W_A([\text{O III}]+H\beta)) = 50 - 200$ Å are seen across the mock colour-$W_A([\text{O III}]+H\beta)$ relations at fixed colour.

The reference model is then defined as the median of the colour–$W_A([\text{O III}]+H\beta)$
relations, with its errors computed from the standard deviation of $W_A([\text{O} \text{ III}]+\text{H} \beta)$ values spanned by the models at a fixed F356W$-$F410M colour. We emphasise that the models span a narrow range of $W_A([\text{O} \text{ III}]+\text{H} \beta)$ values at a given F356W$-$F410M colour, thus enabling relatively accurate $W_A([\text{O} \text{ III}]+\text{H} \beta)$ measurements without the potential for large systematic biases. To calculate the $W_A([\text{O} \text{ III}]+\text{H} \beta)$ values for the CEERS galaxy sample, a Monte Carlo approach is taken. First, the observed F410M and F356W flux is perturbed by its associated photometric error. The associated colour measurement is then translated into a $W_A([\text{O} \text{ III}]+\text{H} \beta)$ value using the reference colour$-W_A([\text{O} \text{ III}]+\text{H} \beta)$ relation (scattered by its typical error at a fixed colour). This process is repeated $N = 1000$ times for each object to produce a $W_A([\text{O} \text{ III}]+\text{H} \beta)$ distribution for each galaxy, with the median and $\pm 1\sigma$ (68 per cent) percentiles adopted as the best $W_A([\text{O} \text{ III}]+\text{H} \beta)$ measurement and its uncertainty, respectively. The resulting constraints for an example ($N = 10$) subset of our CEERS galaxy sample are shown in Fig. 5.6 (open grey hexagons).

### 5.3.3 Photometric excess simulations: assessing the $W_A([\text{O} \text{ III}]+\text{H} \beta)$ recovery

To assess our $[\text{O} \text{ III}]+\text{H} \beta$ emission line equivalent width measurements, we test the photometric excess method on an ensemble of model galaxies, constructed using BAGPIPES (Carnall et al., 2018, 2019) with a variety of physical properties and $W_A([\text{O} \text{ III}]+\text{H} \beta)$ values.

We initially construct the model galaxies using the Bruzual & Charlot (2003) BC03 stellar population models with a constant star-formation history and a permitted range of physical properties comparable to those recovered by the SED-fitting described in Section 5.3.1. To best mimic the VANDELS $W_A([\text{O} \text{ III}]+\text{H} \beta)$ measurements, we also restrict redshifts in the same $3.2 \leq z \leq 3.6$ range as our spectroscopic sample, and randomly allocate absolute dust attenuation and stellar-mass values uniformly in the range $0.0 \leq A_V \leq 1.2$ and $7.8 \leq \log(M_*/M_\odot) \leq 10.5$. Similarly, ages ranging from $\approx 50$ Myr to the age of the Universe at $z = 3.2 - 3.6$ ($\approx 1.6$ Gyr) are sampled.

We artificially add an emission line at $\lambda_{\text{rest}} \approx 5000$ Å to each model with an specified equivalent width value and the model galaxy photometry is measured from the resulting simulated SED in the same filter set as the VANDELS sample.
Figure 5.6 Demonstration of the photometric $F_{356W}-F_{410M}$ colour-based $W_A([\text{OIII}]+H\beta)$ measurements using the colour models described in Section 5.3.2. Example $F_{356W}-F_{410M}$ versus $[\text{OIII}]+H\beta$ equivalent width relations for a number of mock SED-models are shown as a function of age with $t=10, 50, 100 \text{ Myr}$ (blue solid line, with $Z_*=0.2Z_\odot$, $A_V=0$), and as a function of absolute dust attenuation with $A_V=0.0, 0.2, 0.5$ (green dashed line, with $Z_*=0.2Z_\odot$, $t=50 \text{ Myr}$). An example subset of the corresponding CEERS sample $W_A([\text{OIII}]+H\beta)$ measurements are over-plotted (open grey hexagons), where the measured colour and its error has been propagated through to an associated error in $W_A([\text{OIII}]+H\beta)$ using a Monte Carlo procedure (including scatter in the colour-equivalent width relation).

To assign realistic noise properties to each simulated galaxy, the photometric errors are calculated randomly using the depth of a galaxy in the real sample and the model galaxy photometry in each band is perturbed according to its assigned errors.

We input emission lines into the simulated galaxies with equivalent widths spanning the range $10 \text{ Å} \leq W_A([\text{OIII}]+H\beta) \leq 4000 \text{ Å}$, with $\Delta(W_A([\text{OIII}]+H\beta)) = 100 \text{ Å}$, generating $N=1000$ simulated models at each input $W_A([\text{OIII}]+H\beta)$ value to ensure the full parameter space is well-sampled across the range of equivalent widths. The equivalent width is then measured for each of the simulated galaxies using the same SED-fitting and photometric excess methods described in Section 5.3.1. We repeat this entire process using a delayed declining exponential SFH,
in addition to runs using the BPASS (v.2.2; Eldridge et al., 2017; Stanway & Eldridge, 2018) stellar population synthesis models (with both a constant and delayed declining exponential SFH), to ensure any potential biases that may be introduced by our particular SED-fitting configuration are explored.

We show the results of the $W_\lambda([\text{O\,iii}] + \text{H}\beta)$ recovery simulations in Fig. 5.7, averaged across the multiple runs of SFH and stellar population models. Overall, we find that the $K$-band photometric excess method performs well in recovering the input equivalent width across the entire range of values, with a small downwards bias that increases slightly with increasing $W_\lambda([\text{O\,iii}] + \text{H}\beta)$. Using emcee, we fit a linear relation between the measured and input $W_\lambda([\text{O\,iii}] + \text{H}\beta)$ values given by $W_\lambda(\text{Input}) = (1.05^{+0.08}_{-0.08}) \times W_\lambda(\text{Measured}) + (47.0^{+64.1}_{-63.8})$, which we use to correct our VANDELS measurements.

We note that the slight bias is primarily driven by the recovery results for models constructed using the BPASS stellar population models. With limited a-priori knowledge about the true underlying stellar populations of the observed galaxies, in Section 5.3.1 we have opted to use BC03 templates. Fitting the BPASS-based mock galaxies with BC03 templates produces a slight over-estimation of the stellar continuum flux at $\lambda_{\text{rest}} \approx 5000$ Å resulting in a slight under-prediction of the recovered $W_\lambda([\text{O\,iii}] + \text{H}\beta)$.

For the CEERS sample, we make two independent measurements of $W_\lambda([\text{O\,iii}] + \text{H}\beta)$, using the photometric excess method and the colour-based method described in Section 5.3.2. With two separate $W_\lambda([\text{O\,iii}] + \text{H}\beta)$ measurements, we can test for any potential systematic bias introduced by the [O iii]+H\beta contamination of both the F410M and F444W filters.

Firstly, we perform SED-fitting excluding both the contaminated NIRCam filters using fast++ with the same set-up as outlined in Section 5.3.1. The excess observed in the F410M photometry can then be used to calculate $W_\lambda([\text{O\,iii}] + \text{H}\beta)$ (i.e., adjusting Eq. 5.5 for the CEERS F410M filter).

We repeat the emission line recovery simulations using the photometric errors from the CEERS sample at $7.0 \leq z \leq 7.6$ described in Section 5.2.2, and find a relation $W_\lambda(\text{Input}) = (1.13^{+0.12}_{-0.12}) \times W_\lambda(\text{Measured}) + (67.9^{+97.1}_{-96.8})$.

After applying the correction, we find that the photometric excess-based
Figure 5.7 The input $W_A([\text{O}\text{iii}]+H\beta)$ against the measured $W_A([\text{O}\text{iii}]+H\beta)$ from the emission line recovery simulations outlined in Section 5.3.3. The simulations employed for assessing the VANDELS sample $W_A([\text{O}\text{iii}]+H\beta)$ measurements, binned in the measured equivalent width with $\Delta(W_A([\text{O}\text{iii}]+H\beta)) = 100\,\text{Å}$, are shown as blue diamonds. We perform a linear fit using emcee, finding a relation given as $W_A(\text{Input}) = (1.05^{+0.08}_{-0.08}) \times W_A(\text{Measured}) + (47.0^{+64.1}_{-63.8})$, which we use to correct the raw VANDELS photometrically-based $W_A([\text{O}\text{iii}]+H\beta)$ estimates. The posterior probability distribution (and single-parameter marginalised probability distributions) are shown in the top-left inset, with the $(m=1,c=0)$ point marked with a black cross. The dashed black line is the 1:1 relation.

$W_A([\text{O}\text{iii}]+H\beta)$ measurements and those from the colour-based method are in excellent agreement, with the mean $W_A([\text{O}\text{iii}]+H\beta)$ consistent within $\Delta(\log(W_A([\text{O}\text{iii}]+H\beta))) \lesssim 0.04$ dex. In the remainder of this analysis, we adopt the colour-based CEERS galaxy $W_A([\text{O}\text{iii}]+H\beta)$ measurements as the fiducial values to avoid the need to apply a correction (adding uncertainty).

5.3.4 The NIRVANDELS sample

The line fluxes of the $\text{[O}\text{iii}]\lambda \lambda 4960, 5007$ and $H\beta$ lines were measured directly from the MOSFIRE spectra in the NIRVANDELS sample. The measurements and the correction applied to account for the impact of stellar absorption on $H\beta$ are described in Cullen et al. (2021). The equivalent width $W_A([\text{O}\text{iii}]+H\beta)$ can then
be calculated by dividing the combined measured line fluxes by the continuum flux at $4850 \, \text{Å} \leq \lambda \leq 5020 \, \text{Å}$ estimated from the best-fitting SED using FAST++. This process is repeated 1000 times to produce a $W_\lambda([\text{O} \text{III}] + \text{H} \beta)$ distribution for each galaxy, every time perturbing both the line flux and the galaxy photometry by their respective errors, with the continuum flux re-computed from the resultant best-fitting FAST++ SED (e.g., see Cullen et al. 2021). The median and scaled median absolute deviation of the distribution are then taken as the fiducial $W_\lambda([\text{O} \text{III}] + \text{H} \beta)$ measurement and its uncertainty $\sigma_{W_\lambda([\text{O} \text{III}] + \text{H} \beta)}$, respectively.

![Figure 5.8](image)

**Figure 5.8** Comparison of the photometrically inferred $[\text{O} \text{III}] + \text{H} \beta$ equivalent widths (e.g., Section 5.3.1), with the equivalent spectroscopic-based measurements for the sample of $N=13$ observed in NIRVANDELS (see Sections 5.2.1 and 5.3.4). The ‘photometric excess’ $W_\lambda([\text{O} \text{III}] + \text{H} \beta)$ measurements have been corrected according to the emission line recovery simulations discussed in Section 5.3.3. The dashed black line shows the 1:1 line. No large systematic offsets between the independent photometry- and spectroscopy-based measurements are seen across a large dynamic range of $W_\lambda([\text{O} \text{III}] + \text{H} \beta) \approx 50 - 1500 \, \text{Å}$. Although somewhat limited by a small-sample size, this comparison strengthens our confidence that the photometric excess method recovers reliable $W_\lambda([\text{O} \text{III}] + \text{H} \beta)$ measurements. In particular, it is clear that the method can be used to isolate the population of ‘extreme’ emission line galaxies with $W_\lambda([\text{O} \text{III}] + \text{H} \beta)$ in excess of $> 1000 \, \text{Å}$.
In Fig. 5.8, we compare the spectroscopic \( W_\lambda([\text{O} \text{III}]+H\beta) \) measurements with the photometric-excess measurements derived from the associated VANDELS photometry for the NIRVANDELS sample. The photometric-\( W_\lambda([\text{O} \text{III}]+H\beta) \) measurements have been corrected using the simulations described in Section 5.3.3. Within the small-sample size of \( N = 14 \) NIRVANDELS galaxies at \( 3.2 \leq z_{\text{spec}} \leq 3.6 \), there is good agreement between the spectroscopic and photometric \( W_\lambda([\text{O} \text{III}]+H\beta) \) measurements and the extreme \([\text{O} \text{III}]+H\beta \) emitters (\( W_\lambda([\text{O} \text{III}]+H\beta) \gtrsim 1000 \) Å) are clearly identified. The independent NIRVANDELS \( W_\lambda([\text{O} \text{III}]+H\beta) \) measurement comparison in Fig. 5.8, together with the simulations outlined in Section 5.3.3 demonstrate that the photometric excess method provides accurate \( W_\lambda([\text{O} \text{III}]+H\beta) \) measurements for our VANDELS sample.

### 5.4 The \( W_\lambda([\text{O} \text{III}]+H\beta) \) distribution

#### 5.4.1 VANDELS

The \([\text{O} \text{III}]+H\beta \) equivalent width distribution for the VANDELS sample of galaxies with \( W_\lambda([\text{O} \text{III}]+H\beta) > 0 \) Å (\( N = 283; \approx 87 \) per cent of the final sample) is shown in Figure 5.9. To allow us to robustly characterise the redshift evolution of the equivalent width distribution, and to compare with the existing literature (e.g., see Schenker et al., 2014b; Endsley et al., 2021; Boyett et al., 2022; Endsley et al., 2023), we fit our observed \( W_\lambda([\text{O} \text{III}]+H\beta) \) distribution with a Gaussian distribution in \( W_\lambda([\text{O} \text{III}]+H\beta) \) log-space (equivalent to a log-normal distribution in linear space).

To determine the best-fitting parameters of the distribution, \( \mu_{\text{EW}} \) and \( \sigma_{\text{EW}} \), we follow the Bayesian method outlined in Endsley et al. (2023) (see also; Schenker et al., 2014b; Boyett et al., 2022), where the full probability posterior for a given set of parameters \( \theta \equiv [\mu_{\text{EW}}, \sigma_{\text{EW}}] \) is given as;

\[
P(\theta) \propto \prod_i \int P_i(\text{EW}) \cdot P(\text{EW}|\theta) \, d\text{EW} \tag{5.6}
\]

where the product is over the posterior probabilities for individual galaxies \( i \), and \( P(\text{EW}|\theta) \) is the log-normal probability distribution for a given set of parameters \( \theta \) (or equivalently \( \theta = [\log(\mu_{\text{EW}}), \log(\sigma_{\text{EW}})] \) for a Gaussian in log-space). In Eq. 5.6, \( P_i(\text{EW}) \) denotes the \( W_\lambda([\text{O} \text{III}]+H\beta) \) measurement for each galaxy, and is
The $W_\lambda([\text{OIII}]+H\beta)$ distribution (black hatched histogram) for the VANDELS spectroscopic galaxy sample at $3.2 \leq z_{\text{spec}} \leq 3.6$, measured using the $K$-band photometric excess method outlined in Section 5.3.1. The raw $W_\lambda([\text{OIII}]+H\beta)$ measurements are corrected using the relation fit to the recovery simulation results presented in Section 5.3.3 (see also Fig. 5.7). We fit a Log-Normal functional form to our measured $W_\lambda([\text{OIII}]+H\beta)$ distribution finding best-fitting parameters of $\log(\mu_{\text{EW}}) = 2.60^{+0.02}_{-0.02}$ and $\log(\sigma_{\text{EW}}) = 0.31^{+0.02}_{-0.02}$, denoted by the blue dashed line and shading (1σ and 2σ confidence intervals). The posterior (and marginalised) probability distribution for the fit parameters are shown in the inset.
characterised by a Gaussian with the inferred $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ and its associated uncertainty.

To best-cover the full parameter space and generate accurate parameter uncertainties we use **emcee** (Foreman-Mackey et al., 2013) to sample the posterior probability distribution, using a flat prior for the parameters $\theta$, and adopting individual uncertainties ($\sigma_{\log(W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta))}$) for each object based on the observed $K$-photometric error. We also apply a 20 per cent error floor on the $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ measurements. The best-fitting parameters and associated uncertainties we quote are the median and $\pm 1\sigma$ ($\approx 68$ per cent) confidence levels taken directly from the marginalised posterior distributions.

In practice, we carried out the Markov Chain Monte Carlo (MCMC) sampling on the discretised posterior probability distribution (e.g., see Eq. 2 in Endsley et al., 2023), using $\Delta(\log(W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)/\text{Å}) \approx 0.2$ sized bins over the full $\log(W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)/\text{Å}) = 0.0 - 4.0$ range.

As shown in Fig. 5.9, we find best-fitting parameters of $\log(\mu_{\text{EW}}) = 2.60 \pm 0.02$ and $\log(\sigma_{\text{EW}}) = 0.31 \pm 0.02$ for the Log-Normal distribution fit. The VANDELS sample displays, on average, $[\text{O} \text{\textsc{iii}}]+\text{H} \beta$ emission with $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta) \approx 400 \pm 20$ Å (quoted as the median and standard deviation).

We note the presence of a small excess of galaxies in the low-$W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ tail of the $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ distribution at $\log(W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)/\text{Å}) \approx 1.7$. Excluding this tail from the $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ distribution fit only has a minor impact, shifting the best-fitting parameters to $\log(\mu_{\text{EW}}) = 2.61$ and $\log(\sigma_{\text{EW}}) = 0.30$. We also highlight that the best-fitting parameters are insensitive to reasonable choices of the bin size (e.g., $\Delta(\log(W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)/\text{Å})) \approx 0.1 - 0.4$).

To investigate the $[\text{O} \text{\textsc{iii}}]+\text{H} \beta$ emission line strength as a function of galaxy properties, we construct VANDELS $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ distributions for two sub-samples, split at the median UV luminosity and stellar-mass values of $\langle M_{\text{UV}} \rangle = -20.2$ and $\langle \log(M_*/M_\odot) \rangle = 9.3$, respectively. The sub-sample distributions are fit using the same method employed on the full sample, with the resulting best-fitting Log-Normal distributions displayed in Fig. 5.10. The $W_A([\text{O} \text{\textsc{iii}}]+\text{H} \beta)$ distribution shows a significant dependence on stellar-mass (bottom panel Fig. 5.10), with the lower stellar-mass sub-sample ($\langle \log(M_*/M_\odot) \rangle = 8.92$) having best-
Figure 5.10  The $W_A([\text{O III}]+H\beta)$ distribution for the VANDELS sample split into two sub-samples based on the UV magnitude (top panel) and stellar-mass (bottom panel), with the same figure layout as Fig. 5.9. To form the two sub-sample distributions, the sample is split at the median UV magnitude and stellar-mass, with values $\langle M_{\text{UV}} \rangle = -20.2$ and $\langle \log(M_*/M_\odot) \rangle = 9.3$ respectively. Following the same fitting routine as for the full VANDELS $W_A([\text{O III}]+H\beta)$ distribution (e.g., see Section 5.4.1 and Fig. 5.9), we find the higher-mass (bottom, purple) and brighter-$M_{\text{UV}}$ (top, red) sub-samples have Log-Normal parameters of $\log(\mu_{\text{EW}}) = 2.45 \pm 0.02$ and $\log(\sigma_{\text{EW}}) = 0.24 \pm 0.02$, and $\log(\mu_{\text{EW}}) = 2.55 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.28 \pm 0.02$, respectively. In contrast, we find evidence that fainter luminosity (top, green) and lower-mass (bottom, yellow) galaxies have stronger $[\text{O III}]+H\beta$ emission, with best-fitting parameters of $\log(\mu_{\text{EW}}) = 2.65 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.34 \pm 0.02$, and $\log(\mu_{\text{EW}}) = 2.76 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.29 \pm 0.02$, respectively.
fitting parameters \( \log(\mu_{\text{EW}}) = 2.76 \pm 0.03 \) and \( \log(\sigma_{\text{EW}}) = 0.29 \pm 0.02 \), while the higher stellar-mass sub-sample \( \langle \log(M_*/M_\odot) \rangle = 9.55 \) has \( \log(\mu_{\text{EW}}) = 2.45 \pm 0.02 \) and \( \log(\sigma_{\text{EW}}) = 0.24 \pm 0.02 \).

We also find a less significant \( M_{UV} \) dependence, finding best-fitting parameters of \( \log(\mu_{\text{EW}}) = 2.65 \pm 0.03 \) and \( \log(\sigma_{\text{EW}}) = 0.34 \pm 0.02 \) for the fainter-\( M_{UV} \) sub-sample \( \langle M_{UV} \rangle = -19.88 \), and \( \log(\mu_{\text{EW}}) = 2.55 \pm 0.03 \) and \( \log(\sigma_{\text{EW}}) = 0.28 \pm 0.02 \) for the brighter-\( M_{UV} \) sub-sample \( \langle M_{UV} \rangle = -20.62 \).

Taken together, these results show a clear statistical difference in the \([\text{OIII}]+\text{H}\beta\) properties within the our \( 3.2 \leq z_{\text{spec}} \leq 3.6 \) VANDELS sample, with fainter, low-mass galaxies displaying higher \( W_A([\text{OIII}]+\text{H}\beta) \). This finding is consistent with the faint, low-mass population of galaxies being on average lower metallicity and younger \((\text{Izotov et al., 2015}; \text{Cullen et al., 2019})\), with higher ionizing photon production efficiencies \((\text{e.g., Tang et al., 2019}; \text{Saldana-Lopez et al., 2022b, see also Section 5.4.4})\).

### 5.4.2 CEERS

The best-fitting parameters for the \( 7.0 \leq z \leq 7.6 \) CEERS sample are determined using the same method employed for the VANDELS sample outlined in Section 5.4.1. When performing the fit we limit the \( W_A([\text{OIII}]+\text{H}\beta) \) range to \( \log(W_A([\text{OIII}]+\text{H}\beta)/\text{Å}) = 2.1 - 4.0 \), with the adjusted lower limit of \( W_A([\text{OIII}]+\text{H}\beta) \) chosen to exclude an excess tail of galaxies in the low-\( W_A([\text{OIII}]+\text{H}\beta) \) tail of the sample \((\text{see Section 5.4.4})\). This tail excludes \( \approx 12 \) per cent of the galaxies from our CEERS sample, compared with the \( \approx 3 \) per cent expected given the median and \( \sigma_{\text{MAD}} \) of the \( \log(W_A([\text{OIII}]+\text{H}\beta)) \) distribution.

We show the best-fitting Log-normal distribution for our CEERS sample in Fig. 5.11, finding best-fit parameters for the full \( W_A([\text{OIII}]+\text{H}\beta) \) distribution of \( \log(\mu_{\text{EW}}) = 2.81 \pm 0.03 \) and \( \log(\sigma_{\text{EW}}) = 0.41 \pm 0.06 \). Comparing with the VANDELS sample \( W_A([\text{OIII}]+\text{H}\beta) \) results, we find significant evolution in the average \( W_A([\text{OIII}]+\text{H}\beta) \), increasing by \( \gtrsim 60 \) per cent from \( W_A([\text{OIII}]+\text{H}\beta) \approx 400 \pm 20 \) Å at \( z \approx 3.2 - 3.6 \) to \( W_A([\text{OIII}]+\text{H}\beta) \approx 650 \pm 45 \) Å for the \( z \approx 7.0 = 7.6 \) CEERS sample. This evolution in the average \( W_A([\text{OIII}]+\text{H}\beta) \) with redshift is generally expected as galaxies are increasingly young and metal-poor towards high-redshift \((\text{Cullen et al., 2019}; \text{Langeroodi et al., 2022})\).
Figure 5.11 **Top Panel:** The $W_\lambda([\text{OIII}]+H\beta)$ distribution for the full CEERS sample at $7.0 \leq z_{\text{phot}} \leq 7.6$, using $W_\lambda([\text{OIII}]+H\beta)$ derived from the colour-modelling method (e.g., Section 5.3.2). Fitting a log-normal distribution, we find best-fitting parameters of $\log(\mu_{\text{EW}}) = 2.81^{+0.03}_{-0.03}$ and $\log(\sigma_{\text{EW}}) = 0.41^{+0.06}_{-0.06}$ (black dashed line with grey shaded $\pm 1\sigma$ regions). The $W_\lambda([\text{OIII}]+H\beta)$ distributions after splitting the CEERS sample into ‘faint’ and ‘bright’ subsets at $\langle M_{\text{UV}} \rangle = -18.6$ are shown in blue and red, respectively. The ‘faint’ and ‘bright’ subsamples have parameters of $\log(\mu_{\text{EW}}) = 2.70^{+0.08}_{-0.08}$ and $\log(\sigma_{\text{EW}}) = 0.44^{+0.13}_{-0.13}$, and $\log(\mu_{\text{EW}}) = 2.84^{+0.04}_{-0.04}$ and $\log(\sigma_{\text{EW}}) = 0.40^{+0.06}_{-0.06}$, respectively. **Bottom Panel:** Comparison of our full sample $W_\lambda([\text{OIII}]+H\beta)$ distribution with the $W_\lambda([\text{OIII}]+H\beta)$ derived by Endsley et al. (2023) for the JADES survey, which are in excellent agreement. We also recover the trend seen in the high-redshift JADES sample ($6.5 \leq z \leq 8.0$, $\langle z \rangle \approx 7.3$) in which the fainter galaxy population have a slightly broader $W_\lambda([\text{OIII}]+H\beta)$ distribution shifted to lower $W_\lambda([\text{OIII}]+H\beta)$ values.
As with the VANDELS sample, we construct two CEERS sub-sample, split into fainter and brighter subsets based on the median UV magnitude ($\langle M_{UV} \rangle = -18.6$). For the ‘faint’ CEERS sub-sample ($\langle M_{UV} \rangle = -18.26$), we recover best-fitting parameters of $\log(\mu_{EW}) = 2.70 \pm 0.08$ and $\log(\sigma_{EW}) = 0.44 \pm 0.13$, whilst for the ‘bright’ sub-sample ($\langle M_{UV} \rangle = -19.09$) we infer $\log(\mu_{EW}) = 2.84 \pm 0.03$ and $\log(\sigma_{EW}) = 0.40 \pm 0.06$ (shown in Fig. 5.11). We note that these best-fitting parameters are approximately mirrored when splitting the CEERS sample based on stellar-mass ($\langle \log(M_*/M_\odot) \rangle = 7.88$). The best-fitting parameters in the lower-mass ($\langle \log(M_*/M_\odot) \rangle = 7.62$) CEERS sub-sample are $\log(\mu_{EW}) = 2.71 \pm 0.07$ and $\log(\sigma_{EW}) = 0.40 \pm 0.13$, and $\log(\mu_{EW}) = 2.85 \pm 0.04$ and $\log(\sigma_{EW}) = 0.41 \pm 0.07$ in the higher-mass ($\langle \log(M_*/M_\odot) \rangle = 8.2$) CEERS sub-sample.

Intriguingly, the $W_A([\text{O} \text{III}]+\text{H} \beta)-M_{UV}$ (and $W_A([\text{O} \text{III}]+\text{H} \beta)-\log(M_*/M_\odot)$) dependence between the two CEERS sub-samples is reverse to that found in the lower-redshift VANDELS sample. A similar $W_A([\text{O} \text{III}]+\text{H} \beta)-M_{UV}$ trend is found by Endsley et al. (2023) using JADES (see Fig. 5.11, lower panel). For sub-samples in decreasing UV magnitude at $\langle M_{UV} \rangle \approx -20.1, -18.6, -17.5$, Endsley et al. (2023) find $\mu_{EW}$ decreases to $\mu_{EW} \approx 780, 590, 340$ Å, respectively. In our ‘bright’ and ‘faint’ CEERS sub-samples with $\langle M_{UV} \rangle \approx -19.01$ and $\langle M_{UV} \rangle \approx -18.26$, the average $W_A([\text{O} \text{III}]+\text{H} \beta)$ implied by the best-fitting parameters are $\mu_{EW} \approx 690$ Å and $\mu_{EW} \approx 500$ Å, respectively. The observed $M_{UV}$ dependence between the two samples are in remarkable agreement, showing an approximate $dW_A([\text{O} \text{III}]+\text{H} \beta)/dM_{UV} \approx 200$ Å trend across $\geq 2$ magnitudes in $M_{UV}$.

The $W_A([\text{O} \text{III}]+\text{H} \beta)-M_{UV}$ trend may be symptomatic of the faint galaxy population at high-redshift entering an extremely low metallicity ($\leq 0.05 Z_\odot$) regime in which [O III] emission becomes suppressed (e.g., Endsley et al., 2023). We note however that the trends with luminosity in the CEERS sample are only considered tentative ($\approx 2\sigma$ in $\mu_{EW}$) and not as statistically robust as the trends seen in VANDELS. This may part may be due to the smaller CEERS sample size ($\approx 30$ per cent that of VANDELS) leading to larger uncertainties in our best-fit parameters. Despite these uncertainties, we discuss the possible $M_{UV}$ and $\log(M_*/M_\odot)$ trends further in Section 5.4.4 as well as observed excess tail of low–$W_A([\text{O} \text{III}]+\text{H} \beta)$ galaxies observed in CEERS.
5.4.3 Evolution of the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution

Redshift evolution of the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution

The evolution of the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution over the redshift range $2 \leq z \leq 8$ is shown in Fig. 5.12. To complement the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distributions derived in this work at $3.2 \leq z \leq 3.6$ and $7.0 \leq z \leq 7.6$ from VANDELS (blue) and CEERS (red), respectively, we also plot the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution from Boyett et al. (2022) (converted from their $[\text{O} \text{ iii}]_\lambda5007$ distribution; see Section 5.2.4). From Boyett et al. (2022), the average $[\text{O} \text{ iii}]+\text{H} \beta$ equivalent width is $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta) \approx 100 \pm 10$ Å, which we find increases to $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta) \approx 400 \pm 20$ Å at $z \approx 3.2-3.6$ and then to $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta) \approx 650 \pm 45$ Å at $7.0 \leq z \leq 7.6$.

The dependence on UV luminosity and stellar mass

At face-value, the redshift evolution could be explained solely as an evolution in the average global properties of the galaxy population towards high-redshift, with younger, metal poor galaxies becoming more common. However, as seen in both the VANDELS and CEERS samples (see also Endsley et al., 2023), there is an underlying $M_{\text{UV}}$ dependence that is not accounted for. In general, the regions of $M_{\text{UV}}$ (and log($M_*/M_\odot$)) parameter space occupied by the two galaxies samples are quite distinct (e.g., see Fig. 5.14) which would likely influence the $[\text{O} \text{ iii}]+\text{H} \beta$ emission properties. As a consequence, some of the observed evolution between the VANDELS and CEERS samples may be attributed to differences in the underlying $M_{\text{UV}}$ regime probed, as well as an intrinsic redshift evolution. Ultimately, the exact contribution from these two factors to the $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ evolution would require samples including comparably faint galaxies at intermediate redshifts ($z \approx 3$), and improved number statistics at high redshift ($z \approx 7$, e.g., from surveys such as PRIMER Dunlop et al., 2021). In Fig. 5.13, we investigate the redshift evolution of $[\text{O} \text{ iii}]+\text{H} \beta$ emission properties by calculating the fraction of galaxies classified as extreme emission line galaxies (EELGs), with $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta) \geq 1000$ Å from the best-fitting $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution, shown in the left panel. From the VANDELS $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ distribution $9.7^{+1.7}_{-1.6}$ per cent of the galaxies have $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta) \geq 1000$ Å, with this increasing (decreasing) to $15.1^{+3.0}_{-2.7}$ ($5.4^{+1.7}_{-1.5}$) per cent in the fainter (brighter) sub-set. The VANDELS results presented in this work play a crucial role filling in the redshift parameter space between $z \approx 2$ and $z \approx 7$, and strengthens evidence for a strong increase in the prevalence of strong $W_\lambda([\text{O} \text{ iii}]+\text{H} \beta)$ emitters from
Evolution in the $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ properties of star-forming galaxies from $2 \leq z \leq 8$. The $\text{[OIII]}+\text{H}\beta$ equivalent width distribution as a function of redshift, with the derived $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ distribution at $z \approx 2$ from Boyett et al. (2022) (green, see Section 5.2.4) shown alongside the best-fitting Log-normal distributions found in this work for the $3.2 \leq z_{\text{spec}} \leq 3.6$ VANDELS (blue) and $7.0 \leq z_{\text{spec}} \leq 7.6$ CEERS (red) samples.

At $7.2 \leq z \leq 7.6$, we measure the fraction of galaxies with $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ emission in excess of $W_{\lambda}(\text{[OIII]}+\text{H}\beta) \geq 1000$ Å to be $31.6^{+2.9}_{-3.0}$ per cent from our CEERS sample. We also display measurements inferred from other studies at $z \approx 5$ (Endsley et al., 2021, 2022, 2023), highlighting the consistent increase in the fraction of galaxies displaying extreme $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ across high-redshift galaxy samples. It is evident from Fig. 5.13 (see also bottom panel Fig. 5.11) that there is a large scatter in the $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ values of star-forming galaxies, which is likely in part due to the underlying $W_{\lambda}(\text{[OIII]}+\text{H}\beta) - M_{\text{UV}}$ dependence discussed in Section 5.4.2. This is particularly visible at higher-redshift, possibly reflective of the bursty star-formation histories increasing the intrinsic scatter of the observed $W_{\lambda}(\text{[OIII]}+\text{H}\beta)$ properties (see also Cullen et al., 2016; Reddy et al., 2018b).

At lower-redshifts, the rarity of strong $\text{[OIII]}+\text{H}\beta$ emitters results in a very low or negligible contribution to the total ionizing emissivity (Boyett et al., 2022), regardless of their elevated ionizing photon production rates (e.g., Tang et al., 2019, 2021b). In contrast at $z \geq 6$, EELGs appear to form a significant proportion...
**Figure 5.13**  Redshift evolution of the fraction of galaxies displaying extreme [OIII]+Hβ emission ($W_A([\text{OIII}]+H\beta) \geq 1000$ Å). The $z \approx 2$ Boyett et al. (2022) value, as well as the VANDELS and CEERS extreme [OIII]+Hβ emitter fractions derived from the associated $W_A([\text{OIII}]+H\beta)$ distributions, are shown as hexagons (same colours as left panel). We also plot the $W_A([\text{OIII}]+H\beta) \geq 1000$ Å fraction for the VANDELS (pale blue) and CEERS (pale red) samples split into fainter (down triangle), and brighter (up triangle) sub-samples at the median parameter value (see Fig. 5.10 and Fig. 5.11). Additional high-redshift ($z > 5$) constraints assembled from Endsley et al. (2021), Endsley et al. (2022) and Endsley et al. (2023) in CEERS ($z \approx 7.0$, square), COSMOS ($z \approx 6.8$, diamond), and JADES ($z \approx 5.5 - 6.5$, pentagons; $z \approx 6.5 - 8.0$, circles), respectively (grey markers) are also shown. The growing prevalence of galaxies with extremely strong [OIII]+Hβ emission highlights the increasing $\xi_{\text{ion}}$ with redshift (e.g., see Fig. 5.14), which is likely as a result of a combination of lower metallicities and younger ages (e.g., Endsley et al., 2023).

of the galaxy population (although we again highlight the different $M_{\text{UV}}$ ranges occupied by the two samples) and therefore likely play a vital role imparting large quantities of the ionizing photons required to power reionization.
The influence of AGN

Active galactic nuclei (AGN) within galaxies can also drive strong \([\text{O}\,\text{iii}] + \text{H}\beta\) emission (e.g., see Kewley et al., 2013; Coil et al., 2015). Here, we consider the possible impact of AGN driven \([\text{O}\,\text{iii}] + \text{H}\beta\) emission, and the underlying evolution in the AGN population on the observed evolution of the \(W_d([\text{O}\,\text{iii}]+\text{H}\beta)\) distribution between our samples. For the sample of galaxies at \(z = 3.2 - 3.6\), we specifically select SFGs (and LBGs) from the VANDELS survey, ensuring to remove sources that have been flagged as AGN within VANDELS DR4. For the higher-redshift photometrically-selected CEERS sample at \(z = 7.0 - 7.6\), the potential contribution of AGN is expected to be minimal as result of the rapid falloff in number density of AGN at \(z \gtrsim 5\) (e.g., Aird et al., 2015; Parsa et al., 2018; McGreer et al., 2018; Kulkarni et al., 2019; Faisst et al., 2021). It is worth noting that recent evidence has suggested the decline in the AGN population is not quite as rapid as previously thought, with recent discoveries driven by JWST uncovering samples of galaxies with low-mass AGN at \(z \approx 5 - 7\) (Labbe et al., 2023). Nonetheless, these types of galaxies tend to be rare, heavily dust-obscured (‘little red dots’) and with a low ionizing output (Matthee et al., 2023), and are not expected to contribute significantly to the population of high-redshift \([\text{O}\,\text{iii}] + \text{H}\beta\) emitters. As a result, the underlying population of AGN, and its evolution over \(z \approx 3 - 7\) are unlikely to significantly influence the \(W_d([\text{O}\,\text{iii}]+\text{H}\beta)\) evolution presented in this work.

5.4.4 The ionizing photon production efficiency \(\xi_{\text{ion}}\)

Motivated by the potential contribution of strong \([\text{O}\,\text{iii}] + \text{H}\beta\) emitters to the ionizing photon budget, we investigate the ionizing photon production efficiency (\(\xi_{\text{ion}}\)) across our samples. To infer \(\xi_{\text{ion}}\), we adopt the \(\xi_{\text{ion}}-W_d([\text{O}\,\text{iii}],\lambda 5007)\) relation presented in Tang et al. (2019): \(\log(\xi_{\text{ion}}) = 0.76 \times \log(W_d([\text{O}\,\text{iii}],\lambda 5007)) + 23.27\). We convert our \(W_d([\text{O}\,\text{iii}]+\text{H}\beta)\) measurements into \(W_d([\text{O}\,\text{iii}],\lambda 5007)\) estimates using the correction factor \(\approx 0.67\) (see Section 5.2.4) before applying the Tang et al. (2019) relation. The inferred \(\xi_{\text{ion}}\) values for our VANDELS (blue) and CEERS (red) samples are shown in Fig. 5.14 as a function of stellar mass (left panel) and UV magnitude (right panel). Reflecting the evolution in \(W_d([\text{O}\,\text{iii}]+\text{H}\beta)\) with redshift between our sample, we find that the higher-redshift CEERS galaxies have \(\Delta(\log(\xi_{\text{ion}})) \approx 0.2 - 0.3\) dex higher \(\xi_{\text{ion}}\) compared to the VANDELS galaxies at \(z \approx 3.4\). The high-redshift \(\xi_{\text{ion}}\) values are in excellent agreement with those
found by Simmonds et al. (2023) and Stefanon et al. (2022).

Considering the trends with $\log(M_*/M_\odot)$ and $M_{UV}$ together, there is a clear relation whereby $\xi_{\text{ion}}$ increases towards lower stellar-masses and fainter UV luminosities. The highest inferred $\xi_{\text{ion}}$ values are $\log(\xi_{\text{ion}}) \approx 25.8$, in good agreement with constraints from ultra-faint $z = 6 - 7$ lensed galaxies spectroscopically confirmed by the UNCOVER survey (Atek et al., 2023).

There is also tentative evidence for a drop in $\xi_{\text{ion}}$ towards the lowest masses and faintest UV magnitudes, with a number of galaxies displaying low $W_\lambda([\text{O III}]+H\beta)$ (i.e., those excluded from the CEERS distribution fit in Section 5.4.2). As discussed by Endsley et al. (2023), these galaxies with low $W_\lambda([\text{O III}]+H\beta)$ ($/\xi_{\text{ion}}$) are consistent with being objects with low metallicity and / or systems with a recent downturn in their SFH (e.g., Looser et al., 2023). Alternatively, and potentially with significant implications for reionization, these galaxies could have high ionizing photon escape fractions ($f_{\text{LyC}}$). Indeed, the CEERS galaxies with low inferred $\xi_{\text{ion}}$ of $\log(\xi_{\text{ion}}) \approx 25.1$, would be consistent with an intrinsic $\xi_{\text{ion}}$ more similar to the rest of the $z \approx 7.0 - 7.6$ sample ($\log(\xi_{\text{ion}}) \approx 25.5$) if they have LyC escape fractions approaching $f_{\text{esc}}^{\text{LyC}} \approx 0.5$. A final alternative explanation is that a subset of the sources with extremely low measured $W_\lambda([\text{O III}]+H\beta)$ values may in fact be lower-redshift contaminants in our sample. The photometric redshift failure rate typically increases towards fainter magnitudes as a result of less secure photometry; in the case where galaxies are incorrectly assigned $z_{\text{phot}} = 7.0 - 7.6$, $[\text{O III}]+H\beta$ emission would not fall within the F410M bandpass. However, as the extreme tail of $W_\lambda([\text{O III}]+H\beta)$ values ($\lesssim 100 \text{ Å}$) was not included in the fit to the overall distribution (see Section 5.4.2), this factor is not expected to impact the observed $W_\lambda([\text{O III}]+H\beta)-M_{UV}$ trend in the CEERS sample.

Overall, from the results presented in Fig 5.14 we find that a significant fraction of the faint, low-mass galaxy population detected in our CEERS sample ($\log(M_*/M_\odot) \approx 7.5 - 8.5$) and $M_{UV}$ between $\approx -19.5$ and $\approx -18.0$ have $\xi_{\text{ion}}$ values elevated above the values $\log(\xi_{\text{ion}})=25.2 - 25.3$ canonically required in analytical models for reionization to be completed by $z \sim 5.5$ (e.g., Robertson et al., 2013, 2015; Mason et al., 2019). Combined with outcomes from intermediate redshift studies suggesting moderate LyC escape fractions in the range $f_{\text{esc}}^{\text{LyC}} = 5 - 10$ per cent for SFGs (e.g., $f_{\text{esc}}^{\text{LyC}} = 7$ per cent; Begley et al., 2022, see also Pahl et al. 2021), we find strong evidence in favour of a scenario in which the faint, low-mass galaxy population supply the necessary quantities of ionizing photons needed to maintain reionization.
Figure 5.14 The ionizing photon production efficiency $\xi_{\text{ion}}$ as a function of stellar-mass ($\log(M_*/M_\odot)$) and the rest-frame UV magnitude ($M_{1500}$) for our $3.2 \leq z_{\text{spec}} \leq 3.6$ VANDELS and $7.0 \leq z_{\text{phot}} \leq 7.6$ CEERS galaxy samples. The values of $\xi_{\text{ion}}$ are derived from our $W_A([\text{OIII}]+\text{H}\beta)$ measurements (e.g., Sections 5.3.1 and 5.3.2) assuming the $W_A([\text{OIII}]+\text{H}\beta)-\xi_{\text{ion}}$ relation presented in Tang et al. (2019), and the $\log(M_*/M_\odot)$ and $M_{1500}$ values are derived from the best-fitting SED models derived in Section 5.3.1. To more easily discern any trends present, we also shown the results in $\Delta(\log(M_*/M_\odot)) \approx 0.5$ mass bins and $\Delta(M_{1500}) \approx 0.5$ luminosity bins, with the $\xi_{\text{ion}}$ bin values shown as the bin median and $\pm1\sigma$ (68 per cent) ranges. The dashed black line equates to $\xi_{\text{ion}} = 10^{25.2}$ erg s$^{-1}$ Hz, the commonly used fiducial value in reionization models (e.g., Robertson et al., 2013, 2015).
5.5 Conclusions

In this work we have presented the results of an investigation into the evolution of the [O\textsc{iii}]+H\textbeta\ equivalent distribution across the redshift range $2 \leq z \leq 8$. With a sample of spectroscopically confirmed VANDELS star-forming galaxies at $3.2 \leq z_{\text{spec}} \leq 3.6$, we measure $W_d([\text{O\textsc{iii}}]+\text{H\textbeta})$ on an individual galaxy basis using the observed $K$-band photometric excess.

We compliment these measurements with a sample of galaxies during the Epoch of Reionization photometrically selected from the JWST Cosmic Evolution Early Release Science (CEERS) survey at $7.0 \leq z_{\text{phot}} \leq 7.6$. The [O\textsc{iii}]+H\textbeta\ equivalent widths of the CEERS high-redshift sample are inferred based on the observed F356W–F410M photometric colour combined with an empirically motivated model. The main findings of this study are summarised as follows:

1. Fitting the observed $W_d([\text{O\textsc{iii}}]+\text{H\textbeta})$ distributions measured in this analysis with Log-Normal functional forms, we infer best-fitting parameters of $\log(\mu_{\text{EW}}) = 2.60 \pm 0.02$ and $\log(\sigma_{\text{EW}}) = 0.31 \pm 0.02$ for the VANDELS spectroscopic sample at $z \approx 3.4$ (see Fig. 5.9), and $\log(\mu_{\text{EW}}) = 2.80 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.41 \pm 0.06$ for the CEERS photometric sample at $z \approx 7.3$ (see Fig. 5.11). Combining these measurements with the results of Boyett et al. (2022), we find that the typical [O\textsc{iii}]+H\textbeta\ emission line strength increases with redshift, evolving from $W_d([\text{O\textsc{iii}}]+\text{H\textbeta}) \approx 100 \pm 10$ $\text{\AA}$ at $z \approx 2$, to $W_d([\text{O\textsc{iii}}]+\text{H\textbeta}) \approx 400 \pm 20$ $\text{\AA}$ at $z \approx 3.4$ and then to $W_d([\text{O\textsc{iii}}]+\text{H\textbeta}) \approx 650 \pm 45$ $\text{\AA}$ at $z \approx 7.3$ during the EOR.

2. Splitting the VANDELS sample into subsets based on stellar-mass and UV luminosity, both inferred from robust SED-fitting to the available multi-wavelength photometry, we find a statistically significant evolution with both properties. For the $W_d([\text{O\textsc{iii}}]+\text{H\textbeta})$ distribution of the lower-mass ($\langle \log(M_*/M_\odot) \rangle = 8.92$) sample, we infer $\log(\mu_{\text{EW}}) = 2.76 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.29 \pm 0.02$, whilst for the higher-mass ($\langle \log(M_*/M_\odot) \rangle = 9.55$) sample we measure $\log(\mu_{\text{EW}}) = 2.45 \pm 0.03$ and $\log(\sigma_{\text{EW}}) = 0.24 \pm 0.02$. This finding is consistent with the scenario in which faint, low-mass galaxies on average have lower-metallicities and have higher ionizing photon production efficiencies.

3. We also find trends, although evidently weaker, with stellar-mass and UV
luminosity within the CEERS sample. Intriguingly, the parameter dependence is reversed compared to that seen at lower-redshifts in VANDELS. The relative weakness of [O III]+Hβ emission in fainter, low-mass galaxies during the EOR is possibly indicative of an emerging low-metallicity population with younger ages. Additionally, the observed $W_A([\text{O III}]+\text{H} \beta)$ of these galaxies could be indicative of elevated Lyman-continuum escape fractions. This evolution at higher-redshifts is in excellent agreement with Endsley et al. (2023) (see Fig. 5.11), and are consistent with a $dW_A([\text{O III}]+\text{H} \beta)/dM_{\text{UV}} \approx 200 \text{ Å}$ trend across $\gtrsim 2$ magnitudes in $M_{\text{UV}}$.

4. We show the fraction of galaxies with extreme ($W_A([\text{O III}]+\text{H} \beta) \gtrsim 1000 \text{ Å}$) [O III]+Hβ emission grows steadily with redshift (see Fig. 5.13) from $\approx 4.35$ per cent at $z \approx 2$ to $\approx 9.7$ per cent and $\approx 31.6$ per cent in the VANDELS ($z \approx 3.4$) and CEERS ($z \approx 7.3$) samples, respectively. However, we also highlight the strong apparent $M_{\text{UV}}$ dependence on the EELG fraction.

5. Using the analysis presented by Tang et al. (2019), we estimate the ionizing photon production efficiency $\xi_{\text{ion}}$ of the galaxies in our sample from their measured $W_A([\text{O III}]+\text{H} \beta)$, as shown in Fig. 5.14. From these results, we find that a significant fraction of the faint, low-mass galaxy population detected in our CEERS sample have $\xi_{\text{ion}}$ values of $\log(\xi_{\text{ion}} \text{ erg s}^{-1} \text{ Hz}) \approx 25.4 \pm 0.3$, and are therefore elevated above the values assumed to be required in analytical models for reionization to be completed by $z \approx 5$. Combined with recent literature estimates of $f_{\text{esc}^{\text{LyC}}}$ (e.g., $\approx 7$ per cent; Begley et al., 2022, see Chapter 3), we find strong evidence in support of the picture in which faint, low-mass galaxies can supply the bulk of the required ionizing photons to power reionization.
Chapter 6

Conclusions and future work

6.1 Thesis conclusions

The investigation of the Epoch of Reionization (EOR) faces significant challenges due to our limited understanding of the ionizing properties of young star-forming galaxies (SFGs) responsible for the Universe’s phase transition. The central uncertainty is the escape fraction of hydrogen ionizing (Lyman continuum) photons ($f_{\text{esc} \text{LyC}}$) from galaxies into the surrounding IGM.

This thesis addresses some of these challenges by offering measurements of $f_{\text{esc} \text{LyC}}$ and its interplay with crucial galaxy attributes like the Lyα escape fraction ($f_{\text{esc} \text{Lyα}}$), UV luminosity and stellar mass. Another essential component need to construct an accurate reionization timeline is the ionizing photon production rate of galaxies at high redshifts. In conjunction with exploring LyC escape fractions, this thesis examined the redshift-dependent evolution of the average ionizing photon production rate using [O III]+H β nebular emission from galaxies spanning the range $2 \leq z \leq 8$.

A detailed overview of the scientific results presented in this thesis can be found in each the final sections of Chapters 3, 4 and 5. Below, I briefly summarise the most important results and conclusions within the work.

Considering the opacity of the intergalactic medium at higher redshifts, it was imperative to directly measure $f_{\text{esc} \text{LyC}}$ at $z \leq 4$. Employing a spectroscopically confirmed sample of SFGs from the VANDELS survey with complementary ultra-
deep $U$-band imaging, the work presented in Chapter 3 (e.g., Begley et al. 2022) provides significant constraints ($\gtrsim 3.5\sigma$) on $f_\text{esc}^{\text{LyC}}$ at $3.35 \leq z_{\text{spec}} \leq 3.95$. The measured average of $\langle f_\text{esc}^{\text{LyC}} \rangle \approx 0.07 \pm 0.02$ across the sample supports the scenario in which the population of low-dust, low-metallicity galaxies at $z > 6$ likely dominate the photon budget need to drive reionization and fulfill its completion by $z \approx 5 - 6$. Additionally, I confirm strong correlations between $\langle f_\text{esc}^{\text{LyC}} \rangle$ and the Ly$\alpha$ equivalent width ($W_\lambda(\text{Ly}\alpha)$), while finding anti-correlations with the intrinsic UV luminosity and UV dust attenuation.

In Chapter 4, building upon the connection between LyC and Ly$\alpha$ escape, the Ly$\alpha$ emission properties of galaxies in the VANDELS survey at $z \approx 4 - 5$ were explored. The non-evolving correlation between $W_\lambda(\text{Ly}\alpha)$ and Ly$\alpha$ escape fraction ($f_\text{esc}^{\text{Ly}\alpha}$) suggests that the physical processes governing Ly$\alpha$ photon production and escape are consistent over a large majority of the Universe’s history.

Moreover, from investigations into the relationship between $f_\text{esc}^{\text{Ly}\alpha}$ and the escape fraction of ionizing photons inferred from measurements of the rest-frame FUV ISM absorption lines using ultra-deep VANDELS spectroscopy, I demonstrated a monotonic rise of $f_\text{esc}^{\text{LyC}}$ with $f_\text{esc}^{\text{Ly}\alpha}$, reinforcing the use of proxies tracing neutral gas geometry and dust attenuation to infer $f_\text{esc}^{\text{LyC}}$.

Finally, in Chapter 5, by amalgamating data from VANDELS and the JWST/CEERS program, I presented results of the evolution of [OIII]+H$\beta$ equivalent width ($W_\lambda([\text{OIII}]+H\beta)$) distribution across the redshift range $z \approx 2 - 8$. The evolution of the $W_\lambda([\text{OIII}]+H\beta)$ distribution and growing prevalence of strong [OIII]+H$\beta$ emitters towards higher redshifts suggests that these galaxies at $z \gtrsim 6$ exhibit higher ionizing photon production efficiencies than canonically assumed in analytic models of reionization.

In summary, this thesis attempted to improve our understanding of Lyman continuum escape fractions, ionizing photon production rates and their connection with the broader physical properties of high-redshift galaxies. The evidence presented strongly supports the scenario that faint, low-mass galaxies during the EOR can comfortably provide the ionizing photon budget required for reionization.
6.2 Future work

As emphasised throughout this thesis, the Epoch of Reionization is governed by a range of complex and intertwined processes, primarily driven by the young star-forming galaxy population emerging in the high-redshift Universe. Gaining a deeper, more nuanced understanding of the ionizing properties of these galaxies is a key goal in astronomy - what is typical escape fraction of ionizing photons from high-redshift galaxies and how does this evolve across the galaxy population? Which galaxies dominate the budget of photons necessary to maintain reionization, and what is the topology and timeline of the reionization process?

In Chapters 3, 4 and 5, I have presented work that aims to make progress in answering some of these challenging questions, including: outlining novel photometric-based measurements of the Lyman-continuum escape fraction, investigating its connection with Lyα emission at the highest redshift to-date and exploring the $W_4([\text{O III}]+\text{H}\beta)$ distribution, which offers insight into the ionizing photon production rate of galaxies, across a range of redshifts ($2 \leq z \leq 8$) and galaxy physical properties.

In this section I discuss a number of possible avenues of further scientific exploration, building on the work presented in this thesis, to push forward our knowledge of the relationship between galaxy evolution and the reionization of the Universe.

6.2.1 The ionizing photon production efficiency of SFGs

The ionizing photon production efficiency from Hα

The ionizing photon production efficiency can be constrained empirically through the dust-corrected Hα luminosity ($L_{\text{H}\alpha}$) as:

$$1.36 \times 10^{-12} \cdot (1 - f_{\text{esc}}^{\text{LyC}}) \cdot \xi_{\text{ion}} = \frac{L_{\text{H}\alpha}}{L_{\text{UV}}}$$

(6.1)

where $L_{\text{UV}}$ is the intrinsic UV luminosity, and the Case-B recombination coefficient has been assumed. Importantly, this method is independent of assumptions about the underlying stellar populations, unlike techniques based
I will investigate the ionizing properties using H\(\alpha\) emission in two ways. Firstly, with multi-wavelength imaging from the PRIMER survey, I will robustly identify (potentially 100’s of) H\(\alpha\) emitters at \(z \approx 5\) from the strong H\(\alpha\) signature imprinted on the observed F410M medium-band photometry. Then using the techniques to infer the nebular line emission properties established in Chapters 4 and 5, I will constrain \(\xi_{\text{ion}}\) for a large sample of galaxies leading up to the EOR.

The exploration of \(\xi_{\text{ion}}\) enabled from these large photometric sample sizes will be amplified by complimentary spectroscopic analyses made possible by ultra-deep JWST/NIRSpec observing campaigns. As one of the Co-Investigators of a recently awarded JWST cycle-2 NIRSpec program, I will have access to \(\gtrsim 50\) hr, \(R \approx 1000\) rest-frame optical spectra for \(N \approx 60\) galaxies at \(3.0 \leq z \leq 6\) over the UDS-VANDELS footprint of PRIMER (see Fig. 6.2). This data will allow direct spectroscopic measurements of the H\(\alpha\) nebular line, as well as the ability to robustly correct for nebular attenuation using the Balmer decrement.

Moreover, the spectroscopic samples used will be expanded further using the publicly available CEERS NIRSpec spectroscopy (see Fig. 6.1), in addition to data from the Cycle-1 AURORA programme.
The \([\text{O} \text{\,III}] + \text{H}\,\beta\) equivalent width during the Epoch of Reionization

The final science chapter of this thesis (see Chapter 5) reinforced strong evidence that the ionizing properties of galaxies, traced through their \([\text{O} \text{\,III}] + \text{H}\,\beta\) emission lines, were strongly evolving from cosmic noon \((z \approx 2)\) up to the EOR \((z \approx 7)\). Moreover, in this analysis I uncovered a relatively strong reversal in the stellar-mass and UV magnitude dependence of the ionizing photon production efficiency of SFGs (inferred from their \(W_{\lambda}([\text{O} \text{\,III}] + \text{H}\,\beta)\)). This signature is possibly indicative of an emerging population of faint, low-mass galaxies with very low-metallicities, bursty SFHs or elevated \(f_{\text{LyC}}^{\text{esc}}\).

To further explore this interesting population of galaxies, which may make a significant contribution to the ionizing photon budget, I will expand the analysis outlined in Chapter 5 using additional JWST datasets (e.g., PRIMER). The second epoch of the CEERS survey alone could serve to double the sample size of galaxies currently used in this work, whilst imaging from the publicly available JADES survey would enable the analysis to be extended to magnitudes as faint as \(M_{\text{UV}} \approx -17\).

6.2.2 What regulates the escape of Lyman-continuum photons

Understanding Lyman-continuum escape across the galaxy population

The importance of the Lyman-continuum escape fraction as a cornerstone needed to understand galaxy evolution during the reionization epoch cannot be overstated. Significant effort has been invested in establishing accurate, well-calibrated observational indicators of \(f_{\text{esc}}^{\text{LyC}}\), yet such a reliable tracer remains elusive.

As noted in this thesis, proxies based on Ly\(\alpha\) and \([\text{O} \text{\,III}]\) emission properties, or the observed UV spectral slope \((\beta)\), have returned mixed results. In Chapter 3, I confirmed the promising correlation between \(f_{\text{esc}}^{\text{LyC}}\) and \(W_{\lambda}(\text{Ly}\alpha)\), and further explored the connection between the escape of Ly\(\alpha\) photons and LyC emission in Chapter 4. However, these studies have generally been limited to small sample sizes, and find that galaxies with strong Ly\(\alpha\) emission display a wide range of \(f_{\text{esc}}^{\text{LyC}}\) values.
To help shed further light on these potential $f_{\text{esc}}^{\text{LyC}}$ tracers, the deep publicly available MUSUBI/CLAUDS $U$-band imaging can be used to directly measure $f_{\text{esc}}^{\text{LyC}}$ for VANDELS galaxies in UDS survey area. Moreover, by including galaxies selected from the MUSE-WIDE (Urrutia et al., 2019) and MUSE-DEEP-DR2 (Bacon et al., 2023) surveys, it will be possible to triple the size of the sample used in Begley et al. (2022) (see Chapter 3) providing significantly increased statistical power. The latest JWST imaging of both the UDS and CDFS (e.g., JADES, NGDEEP), will also provide the high-resolution imaging required to accurately measure the star-formation rate surface density ($\Sigma_{\text{SFR}}$), hence allowing robust tests of any potential $\Sigma_{\text{SFR}} - f_{\text{esc}}^{\text{LyC}}$ correlations.

Leading on from this, the NIRCAM F277W imaging from PRIMER targeting the H$\alpha$ emission of VANDELS galaxies at $z \simeq 3$ will enable the Ly$\alpha$ escape fraction to be measured for galaxies with direct LyC emission constraints. As such, a direct study at $z \simeq 3$ of the connection between Ly$\alpha$ escape and LyC escape will be uniquely possible. This specific analysis will also strongly benefit from the recently awarded JWST cycle-2 NIRSpec programme discussed in Section 6.2.1 (see Fig. 6.2).

Building a larger sample of Lyman-continuum leakers

Lastly, in addition to the population-based statistical constraints of large samples of galaxies outlined above, more targeted studies based on individual Lyman-continuum leaking galaxies are essential for a nuanced investigation into the escape of ionizing radiation. In an attempt to alleviate the current dearth of known LCEs at $z \simeq 3$, adopting a ‘bottom-up’ approach in a large-scale search within the available HST/JWST footprints (PRIMER, CDFS, COSMOS-Web), that have ultra-deep $U$-band, imaging will be carried out. This novel approach outlined in Rivera-Thorsen et al. (2022), helps address the biased sample selection process commonly used in LyC leaker searches, and has already proven successful in uncovering previously unknown LyC-emitting galaxies.

Star-forming galaxies that leak Lyman-continuum during the EOR

To compliment the essential, direct studies of Lyman-continuum escape in lower-redshift reionization epoch analogues and LCEs, the PRIMER dataset offers the ideal opportunity to measure the number densities and physical properties of
Demonstration of the spectroscopy datasets available for targeted VANDELS galaxies at \( z \approx 3.5 \), upon completion of the recently awarded JWST cycle-2 NIRSpec programme (EXCELS, PI A. C. Carnall). The key nebular emission lines provided by the G235M+G395M observations are highlighted in the lower panels.

6.2.3 The dust attenuation in high-redshift galaxies

As alluded to in Chapter 3 and 4, the exact form of the dust attenuation law in high-redshift galaxies provides a significant systematic uncertainty (by up to a factor of \( \approx 2 \)) in measurements of \( f_{\text{esc}}^{\text{LyC}} \). Investigations by McLure et al. (2018a) and Cullen et al. (2018) indicate that higher-mass (log(\( M_*/M_\odot \)) \( \gtrsim \) 10) star-forming galaxies have a relatively flat dust attenuation curves consistent with the Calzetti et al. (2000) dust law. In contrast, there is tentative evidence that
lower-mass and lower-metallicity galaxies may have steeper dust attenuation laws (e.g., Reddy et al., 2015).

Here, the PRIMER 7.7 μm MIRI imaging, when combined with a large sample of spectroscopically confirmed 3.0 ≤ z ≤ 5.0 galaxies from VANDELS, offers the ideal opportunity to address this systematic dust attenuation uncertainty. Specifically, the MIRI imaging allows a vital ‘anchor’ of the SEDs at longer wavelengths were the dust attenuation is minimal. Importantly, two independent approaches; the intrinsic SED model-based method (e.g., Cullen et al., 2018), and the more empirical galaxy-pair method (e.g., Wild et al., 2011), can be used to infer the dust attenuation law in a large statistical sample of high-redshifts galaxies.
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