Cosmic Reionization and the First Nonlinear Structures in the Universe

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Abstract In this Introduction, we outline expectations for when and how the hydrogen and helium atoms in the universe turned from neutral to ionized, focusing on the earliest, least well understood stages, and emphasize the most important open questions. We include a historical summary, and highlight the role of reionization as one of the few milestones in the evolution of the universe since the Big Bang, and its status as a unique probe of the beginning stages of structure formation.

1 Introduction

In the standard cosmological model, dominated by cold dark matter and dark energy, the universe expands and cools dictated by the equations of general relativity and thermodynamics, going through a handful of global milestones. Many of these milestones are well understood, because their physics is within the reach of terrestrial experiments, and observations leave little doubt about their occurrence. These begin with nucleosynthesis, and include the epoch of radiation-matter equality, the recombination of hydrogen and helium, and the decoupling of radiation. In the more recent universe, dark energy has become dominant and begun to accelerate the global expansion.

While the evolution of universe preceding nucleosynthesis is less well understood, a generic prediction of inflation, describing the earliest epochs, is the production of primordial density perturbations. These perturbations obey Gaussian statistics, with a nearly scale-invariant initial power spectrum. The subsequent growth of perturbations over time is again well understood, and leads to remarkable agreement with many observations of the cosmic microwave background (CMB) and large-scale structures (LSS).
The history of the universe is marked by additional milestones, related to the growth of inhomogeneities. The first marks the epoch when the first perturbations – on astrophysically important scales – reach non-linear amplitudes. Ab-initio theoretical predictions become more difficult at later epochs. The first collapsed and gravitationally bound structures form soon afterward, and serve as the natural sites where the first stars and black holes then “light up” the universe. The reionization of the bulk of hydrogen and helium atoms in the universe, several hundred Myr after the big bang, is the most recent of these “global” milestones - resembling a phase transition, and changing the character of the universe as a whole.

In addition to its fundamental place in our cosmic history, there are three practical reasons why reionization is of special interest. First, as will become clear below, and from later chapters in this book, the bulk of reionization is thought to take place between redshifts of $5 < z < 10$. This range does not extend far beyond our present observational horizon, and is within tantalizing reach of experiments with forthcoming and planned instruments. This makes the study of reionization very timely.

Second, while there remains some room for more exotic scenarios, reionization can be attributed to photo-ionizing radiation from two different sources: an early generation of massive stars, or an early generation of black holes powering (mini-)quasars. The ultimate energy source in these two scenarios is very different – nuclear binding energy, in the case of stars, and gravitational binding energy, in the case of black holes. These sources have different efficiencies of producing radiation, and produce different spectra. The details of how reionization unfolded thus depends on the properties of these early stars and quasars (their luminosity and spectral distribution) as well as on their abundance and spatial distribution as a function of redshift.

Finally, the earliest light-sources are quite plausibly too dim to be detected directly, even with next-generation instruments. Studying reionization is therefore one of the very few ways to glean details about these first-generation objects. It is worth emphasizing that current observations only show the “tip of the iceberg”: the luminosity functions in even the deepest surveys show no evidence of a faint-end turn-over, and we expect stars to form inside galaxies orders of magnitude fainter than detectable at current and even forthcoming flux limits.

In this article, we will first present a historical discussion of both observations and modeling of the reionization history (§2). Then, in §3 we discuss two possible ways to directly observe the light of the first generation of ionizing sources. It is important to emphasize that this article contains a biased personal selection of some of the important historical milestones and topics, and is not intended to be a rigorous, complete review of the field.
2 Historical Overview

2.1 The Reionized IGM and its Observational Probes

2.1.1 Early History

The realization that the mass density of neutral hydrogen (HI) in the intergalactic medium (IGM) falls short by many orders of magnitude quickly followed the identification of the first quasars in the early 1960s. Here “falls short” is in comparison to the total mass density expected from cosmology, i.e. comparable to the critical density

\[ \rho_{\text{crit}}(z) = \frac{3 H^2}{8 \pi G}, \]

with \( H = H(z) \) the redshift-dependent Hubble parameter. The quasar 3C 9 was among the first handful of quasars discovered and identified through their spectra. At the time of its discovery, its redshift of \( z = 2.01 \) was an outlier, and held the distance record (with the other several quasars at \( z < 1 \)) \[1\]. Its spectrum lacked any strong absorption on the blue side of the Lyman \( \alpha \) emission line, showing only a modest \( \approx 40\% \) depression of the flux instead \[2\]. This implies that the optical depth to Lyman \( \alpha \) scattering in the foreground IGM is \( \tau_{\alpha} \approx 0.5 \). In their seminal paper, Gunn & Peterson (hereafter GP) in ref. \[2\] compared this to the optical depth,

\[ \tau_{\alpha} \approx \text{few } \times 10^6 \]

expected from Lyman \( \alpha \) scattering by neutral hydrogen spread uniformly over the IGM, with a near-critical mean density \( \rho_{\text{crit}}(z) \approx (1 + z)^3 \), following the expansion of the universe.

It is worth quoting the result of this comparison: “We are thus led to the conclusion that either the present cosmological ideas about the density are grossly incorrect, and that space is very nearly empty, or that the matter exists in some other form.” We now know that the mean density of baryons is indeed lower than the critical density, but “only” by a factor of \( \approx 25 \). We also know that space can not be empty – while large voids exist, their densities are at most \( \sim 10\% \) below the mean. The most plausible explanation, by far, is that hydrogen is in ionized form. This was already the favored interpretation at the time; however, interestingly, GP dismissed stars and quasars as the primary ionizing sources. They instead considered free-free emission or collisional ionization in the IGM itself, both requiring that the IGM is hot ( \( \gtrsim 2 \times 10^5 \text{K} \)). Through the study of the Lyman \( \alpha \) forest, we now know that the IGM temperature at \( z \gtrsim 2 \) is \( T_{\text{IGM}} \approx 10^4 \text{K} \), more than an order of magnitude lower than this lower limit.

Interestingly, GP already noted that a fully ionized IGM can produce a large electron scattering optical depth. Taking the electron (or proton) number density from \( \rho_{\text{crit}}(z)/m_p \), this gives a value of \( \tau_e = \text{few } \times 10\% \), which would be relevant for observations of individual sources. This is reduced by a factor of 25 by the low cosmic baryon density, to \( \tau_e = \text{few } \times 1\% \).

Remarkably, the cosmic microwave background (CMB) was discovered in the same year in 1965; precisely 50 years ago \[3\]. This stimulated work on the implications of the ionized IGM on the CMB. With a hot IGM and a large electron scattering optical depth, one would expect large distortions in the spectral shape of the CMB (e.g. ref. \[4,5\]). However, the estimates of the baryon density and temperature were
both soon revised downward significantly. Once again, observations of quasar absorption spectra played important roles in these revisions. First, the discovery of the CMB also stimulated work on big bang nucleosynthesis, making detailed predictions for the abundances of the light elements. The most important of these was the D/H ratio, which placed a tight upper limit ($\Omega_b = \rho_b / \rho_{\text{crit}} \leq 0.1$) on the baryon density. Beginning in the mid 1990s, the relative abundance [D/H] was measured in high-resolution quasar spectra and resulted in the value $\Omega_b \sim 0.04$ (although less robust non-cosmological D/H measurements pre-date these). Second, as many more quasars were discovered, and Lyman $\alpha$ absorption statistics were collected over a large number of sight-lines, the modern view of the Lyman $\alpha$ forest emerged. This revealed that the low-density IGM has a temperature of only $\sim 10^4$K, consistent with being photoionized by the UV radiation of stars and quasars.

2.1.2 Further Development of Observational Diagnostics

In general, the highly ionized IGM can be studied either through measurements of the residual neutral HI, or by detecting the effects of the free electrons (and protons). Beginning in the mid-1990s, both of these possibilities were explored in great detail.

Effect of Free Electrons on the CMB.

On the “electron side”, it was realized that even if the IGM is not dense and hot enough to change the spectrum of the CMB, elastic Thomson scattering by free electrons changes the patterns of both the temperature and polarization power spectra (see reviews by [8] [9] [10]). Scattering a fraction $\tau_e$ of the CMB photons out of each sightline translates into a suppression of the primary CMB anisotropies (both temperature and polarization) by a factor $\exp(-\tau_e)$, below angular scales corresponding to the size of the cosmological horizon at reionization (or $\leq 10'$ for reionization at $z \sim 10$) [11]. This suppression can be difficult to distinguish from a “red” tilt or a reduced normalization of the primordial fluctuation spectrum. However, scattering of the CMB photons in the low-redshift ionized IGM also produces enhanced linear polarization fluctuations on large scales (the so-called “polarization bump”, ref. [12] [13]). This bump, on $\sim 10$ degree scales, is characteristic of reionization and not present otherwise. The precise shape of this feature (polarization power as a function of angular scale) can be used to constrain the ionization history [14] [15]. Finally, if reionization is spatially inhomogeneous (patchy), as generally expected unless the ionizing sources have unusually hard spectra, then this introduces additional power on small ($\sim$ few arcmin) scales. Inhomogeneities in the ionization fraction, rather than in the IGM density, can dominate both the temperature and the polarization power spectra. This was first shown in toy models [16] [17] and was later developed based on CDM structure formation models (e.g. [18]; see ref. [19] for a recent analysis of the kinetic Sunyaev-Zeldovich [kSZ] effect, which gives the largest contribution).

As will be discussed in a later chapter in this book, the first measurement of $\tau_e$ was made by the WMAP satellite, from the temperature-polarization cross power
spectrum, and yielded the anomalously high value of $\tau_e \approx 0.17$ (translating to a sudden reionization redshift near $z \sim 17$). The increased precision in subsequent WMAP measurements broke degeneracies between $\tau_e$ and the spectral tilt $n_s$, and lowered this value to $\tau_e \approx 0.08$. The most recent determination from Planck’s polarization power spectrum, $\tau_e \approx 0.066 \pm 0.016$ [20], remains consistent with this value, and requires instantaneous reionization to occur around $z \sim 10$. More generally, the measured optical depth is twice the value $\tau_e = 0.04$ of the “guaranteed” contribution from the highly ionized IGM between redshifts $0 < z < 6$. This requires that a tail of ionization extends beyond the current observational horizon. However, such a tail is naturally expected even in the simplest models of reionization, and leaves little room for additional, exotic ionizing sources [21][22].

**Searching for Neutral Hydrogen.**

Going back to history – on the “neutral hydrogen side”, work continued on quasar absorption spectra. An idea that dates back to at least the early 1960s [23] is to detect intergalactic neutral HI through its absorption in the 21cm hyperfine structure line. This “radio analog” of the GP trough, however, is much weaker, due to the low oscillator strength of the 21cm line. As a result, the corresponding upper limits on the neutral IGM density – obtained from the lack of any 21cm absorption in the spectrum of the $z = 0.056$ radio galaxy Cygnus A [23] – were $\sim 10^6$ times weaker than those obtained from the (lack of) Ly$\alpha$ GP troughs. Theoretical work on using the redshifted 21cm line, seen either in absorption or emission (depending on the spin temperature) in the context of an IGM being gradually ionized, and including spatial fluctuations, dates back to ref. [24]. The idea apparently lay dormant for nearly two decades, but received attention again from the mid-1990s, motivated by plans to build the Giant Metrewave Radio Telescope (GMRT), and by the consensus emerging about the modern CDM structure formation paradigm [25, 26, 27]. An excellent review of the many ways of using the statistics of the redshifted 21cm line to study reionization is given in ref. [28].

In parallel with using the 21cm line, work continued on the utility of the Ly$\alpha$ GP trough. On the observational side, as more and more distant quasars were discovered in the late 1990s, it became increasingly puzzling that none of these showed the strong resonant GP trough, expected even from a modestly neutral IGM. This was especially so, since deep optical observations began to show that the abundance of both quasars and galaxies decline beyond their peak at redshifts $\sim 1 – 3$. The question arose whether the observed galaxies and quasars can provide the required ionizing radiation – it became necessary to extrapolate well below the faint end of the observed luminosity functions.

On the theoretical side, progress beyond the simple GP calculation of the resonant optical depth $\tau_\alpha$, from a uniform IGM, was slow to take off. However, beginning in the late 1990s, several studies have begun to explore the expected absorption features in more detail. For example, it was realized that the Ly$\alpha$ absorption from a near-neutral IGM is so strong that the damping wings should be detectable, and the red wings, in particular should offer a useful diagnostic of a neutral IGM [29]. Also, bright quasars would be surrounded by a large (several Mpc) local ionized
bubble [30], blue-shifting the observed location of the GP trough and the damping wings [31]. Another realization was that there should be distinct absorption troughs at Lyα, Lyβ, and possible higher Lyman lines, offering another useful diagnostic [32], at least for the first sources, that would be detected not far beyond the redshift where the IGM turns predominantly neutral. In the context of CDM structure formation models, reionization must be gradual and inhomogeneous, resulting in large line-of-sight variations [33]. All of the above effects had important consequences once the first GP was discovered and had to be interpreted (e.g. [34]).

The discovery [35] of the first GP trough was indeed a watershed event in 2001. The Keck spectrum of a z = 6.28 quasar, one of the first several z > 5 quasars identified in the Sloan Digital Sky Survey (SDSS), showed no detectable flux over a large wavelength range short-ward of ~ (1 + z)1215 Å. This raised the tantalizing possibility that 35 years after the seminal GP paper, we have finally probed the era when the IGM was significantly neutral. This discovery also stimulated a large body of work on the limits that can be placed on reionization, given a “deep” and “long” dark region (or regions) in the spectrum (e.g. [36]). The issue is that “zero flux” can be consistent with resonant absorption from the residual HI in a highly ionized foreground IGM. Placing constraints on reionization therefore necessitated detailed modeling of the fluctuating IGM with a few Mpc of the quasar, including the quasar’s own ionized bubble.

Quasars are of course not unique – a significantly neutral IGM would imprint GP absorption features on any background source at λ_{obs} = (1 + z)λ_{α}. It had long been expected that a strong Lyα emission line would be produced by the first “primeval” galaxies [37]. Numerous searches for high-redshift galaxies using their Lyα emission, however, did not yield any discovery for ~ two decades – the failure was blamed on extinction of this line by dust internal to the galaxies. Immediately after the first high-redshift Lyα emitters were finally discovered in the late 1990s [38], it was realized that they can be used as a probe of reionization: the neutral IGM can strongly suppress these lines, thus also suppressing the observed luminosity function [39]. This field developed rapidly, both observationally, with the discovery of large samples of z > 6 Lyα emitters (now in the hundreds), especially in surveys by the Subaru telescope (e.g. ref. [40]). Theoretical predictions were also refined, including improved estimates of the impact of absorption on the observed line profiles, in the presence of a local ionized bubble around the galaxy, galactic winds causing shifts in the emission line frequency, and a peculiar velocity of the host galaxy [41, 42]. These then begun to be incorporated into more realistic radiative transfer models through the inhomogeneous IGM [43], yielding better estimates of the (more modest) impact of reionization on the observed luminosity function [44].

Finally, as the epoch of reionization receded farther and farther in redshift, it became increasingly clear that observed galaxies do not provide sufficient UV radiation to account for this ionization. The general search for high-redshift galaxies is therefore an important part of the history of reionization. Summarizing this history is beyond the scope of this article. However, it was not until deep fields with the Hubble Space Telescope discovered a sizable population of galaxies that the integrated emission of the observed objects even came close to providing enough
ionizing radiation. At the present time, the observed galaxy population at redshift $z \geq 6$ still fails to reionize the IGM by a factor of a "few", unless extreme assumptions are made about the UV spectrum, and the escape fraction of ionizing radiation from these galaxies (see, e.g. [45]).

### 2.2 Reionization in Hierarchical Structure Formation Models

In parallel with developing observational probes of reionization, over the past several decades, we have gained an understanding of how reionization was likely driven by an early generation of stars and quasars. As mentioned above, at the current horizon of observations at $z \sim 7$, the observed population of galaxies fails by only a factor of $\sim$ few to reionize the IGM. It is quite natural to attribute the missing ionizing emissivity to fainter galaxies, just below the current detection threshold. In support of such an extrapolation, there is a firm upper limit on the contribution from faint (individually undetectable) quasars to reionization at $z \sim 6 - 7$.

A population of black holes at these redshifts ($z \approx 6 - 7$) would be accompanied by the copious production of hard ($\gtrsim 10$ keV) X-ray photons. The resulting hard X-ray background would redshift and would be observed as a present-day soft X-ray background (SXB). This severely limits the abundance of accreting quasar BHs at $z \sim 6 - 7$: in order to avoid over-producing the unresolved component of the observed SXB in the 0.5-2 keV range, these BHs can not significantly contribute to reionization [46, 47, 48], or make up more than a few percent of the present-day total BH mass density [49, 50]. It is important to emphasize, however, that these constraints still allow accreting BHs to be dominant over stellar UV radiation at the earliest stages of reionization $z \sim 15$, partially “pre-ionizing” the IGM (see below).

Because reionization at $z \sim 6 - 7$ is an (almost) solved problem, the most interesting open questions concern the earlier stages of reionization. **When did the first light sources turn on? When did the IGM first get significantly ionized (and heated)? What was the relative contribution of the first stars, of their accreting BH remnants, or of possibly more exotic sources of ionization, such as “direct collapse” supermassive stars or BHs, or decaying dark matter particles?**

#### 2.2.1 The Astro-chemistry of H$_2$ and The First Stars

It has long been recognized that the key physics governing the formation of the first stars (or black holes) is the abundance of H$_2$ molecules, which form via gas-phase reactions in the early universe (in 1967, ref. [51]). It is impossible to form an astrophysical object if gas contracts adiabatically, because even with the help of cold dark matter, it is not possible to reach high gas densities. The numerical upper limits on the gas density in halo cores are extremely tight, especially when including the entropy generated during adiabatic collapse (see the recent work in ref. [52]). In the primordial gas, H$_2$ is the only possible coolant, and determines whether gas can
collapse to high densities. Following the pioneering paper in 1967 by Saslaw & Zipoy \cite{Saslaw1967}, several groups constructed complete gas–phase reaction networks, and identified the two possible ways of forming $\text{H}_2$ in primordial gas: via the $\text{H}_2^+$ or $\text{H}^-$ channels. These were applied to derive the $\text{H}_2$ abundance in the smooth background gas in the post–recombination universe \cite{Saslaw1967}, and also at the higher densities and temperatures expected in collapsing high–redshift objects \cite{Saslaw1967, Saslaw1969}.

The basic picture that emerged from these early papers is as follows. The $\text{H}_2$ fraction after recombination in the background universe is small $(x_{\text{H}_2} = n_{\text{H}_2}/n_{\text{H}} \sim 10^{-6})$. At high redshifts ($z \gtrsim 100$), $\text{H}_2$ formation is inhibited even in overdense regions because the required intermediaries $\text{H}_2^+$ and $\text{H}^-$ are dissociated by the CMB photons. However, at lower redshifts, when the CMB temperature drops, a sufficiently large $\text{H}_2$ abundance builds up inside collapsed clouds $(x_{\text{H}_2} \sim 10^{-3})$ at redshifts $z \lesssim 100$ to cause cooling on a timescale shorter than the dynamical time – leading to a runaway thermal instability and eventual star-formation \cite{Saslaw1969, Saslaw1970, Saslaw1971}. In summary, these early papers identified the most important reactions for $\text{H}_2$ chemistry, and established the key role of $\text{H}_2$ molecules in cooling the first, relatively metal–free clouds, and thus in the formation of population III stars.

### 2.2.2 The First Stars in Cosmological Structure Formation Models

The work on $\text{H}_2$ chemistry was soon connected with cosmological models for structure formation. Peebles & Dicke \cite{Peebles1968} speculated already in 1968 that globular clusters, with masses of $\sim 10^{5-6} \, M_\odot$ (somewhat above the cosmological Jeans mass, set by Compton-heating of the protogalactic gas by the CMB \cite{Dicke1968}) forming via $\text{H}_2$ cooling, constitute the first building blocks of subsequent larger structures. Early discussions of the formation of galaxies and clusters have argued that the behavior of gas in a collapsed and virialized object is determined by its ability to cool radiatively on a dynamical time \cite{Peebles1968, Peebles1969, Peebles1970}. The same ideas apply on the smaller scales expected for the very first collapsed clouds \cite{Peebles1968, Peebles1969}. Objects that are unable to cool and radiate away their thermal energy maintain their pressure support and identity, until they become part of a larger object via accretion or mergers. On the other hand, objects that can radiate efficiently will cool and continue collapsing.

In the late 1990s, these ideas were developed further, in the context of modern “bottom-up” hierarchical structure formation in a ($\Lambda$)CDM cosmology. In particular, the first DM halos in which gas can cool efficiently via $\text{H}_2$ molecules, and condense at the center, are “minihalos” with virial temperatures of $T_{\text{vir}} \sim \text{few} \times 100 \, \text{K}$ \cite{Blumenthal1985, Blumenthal1986, Blumenthal1988}. This is essentially a gas temperature threshold, above which roto-vibrational levels of $\text{H}_2$ are collisionally excited, allowing efficient cooling. Because of the emergence of a concordance ($\Lambda$CDM) cosmology \cite{Planck2018}, we can securely predict the

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1. This topic was recently revisited \cite{Barkana2020} in a more rigorous analysis, following the time-dependent, non-equilibrium $\text{H}_2$ population levels. This yielded the same conclusion, i.e. that the post-recombination “intergalactic” $\text{H}_2$ abundance is negligibly low.
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The collapse redshifts of these minihalos: $2 - 3\sigma$ peaks of the primordial density field on the corresponding mass scales of $10^{5-6} \textup{ M}_\odot$ collapse at redshifts $z = 15 - 20$.\(^2\)

The Abundance of Low-Mass Minihalos at High Redshift.
The halo mass functions are now robustly determined, since three–dimensional cosmological simulations reached the required dynamical range to directly resolve the low–mass end of the high–$z$ halo mass function [71, 72]. The predictions for the halo mass functions are now therefore limited mainly by the few % uncertainty in the normalization ($\sigma_8 = 0.82 \pm 0.02$) and the power-law index ($n_s = 0.972 \pm 0.013$) of the primordial power spectrum [69]. A possibly (much) larger source of uncertainty is that the primordial power spectrum on the relevant scales is not directly measured - it is extrapolated using the shape of the processed CDM power spectrum ($P(k) \propto k^\alpha$ with $\alpha \approx -3$ on the relevant small scales). In principle, the small-scale power could deviate from this prediction significantly, reducing the minihalo abundance by a large factor. This could be caused by a generic “running” ($d\alpha / dk \neq 0$) of the primordial scalar index [25], or by free-streaming due to the finite temperature of a low–mass ($< \sim 1 \textup{ keV}$) warm dark matter (WDM) particle [74, 71]. While these could have large effects on the expected halo abundance at $z = 15 - 20$, in practice, there is no evidence of “running” on $> \sim \textup{ Mpc}$ scales, and the mass of a putative WDM particle is limited to $> \sim 1 \textup{ keV}$ by the detections of lensed $z > 8$ galaxies [75] and gamma-ray bursts [76].

Cosmological Simulations of the Formation of First Stars.
In addition to robustly predicting DM halo formation, high-resolution 3D numerical simulations, including hydrodynamics and H\(_2\) chemistry, have become possible, with several groups simulating the cooling and collapse of gas into the first minihalos, located at the intersections of a “protogalactic” cosmic web [77, 78, 79]. These simulations showed convergence toward a gas temperature $T \sim 300 \textup{ K}$ and density $n \sim 10^4 \textup{ cm}^{-3}$, dictated by the thermodynamic properties of H\(_2\), which allows the collapse of a clump of mass $10^2 - 10^3 \textup{ M}_\odot$ at the center of the high-redshift minihalos. These early works suggested that the first stars may have been unusually massive, a conclusion based on the low mass accretion rate in the cores of these halos. In a self-gravitating gas, the mass accretion rate depends only on the sound speed $c_s$, and is of order $\sim c_s^3 / G \propto T^{3/2} / G$ (e.g. [80]). Three-dimensional simulations have confirmed this scaling (e.g. [81, 82, 83]), and in minihalos, the corresponding mass accretion rates are $\sim 10^{-3} \textup{ M}_\odot \textup{ yr}^{-1}$. At this accretion rate, the mass that will accumulate in the halo nucleus within a Kelvin-Helmholtz time ($\sim 10^5 \textup{ years};$ only weakly dependent on mass for massive protostars) is of order $10^2 \textup{ M}_\odot$.

Simulations in the past few years have been pushed to higher spatial resolution, and, in some cases with the help of sink particles, were able to continue their runs beyond the point at which the first ultra-dense clump developed. The gas in the central regions of at least some of the early minihalos were found to fragment into two or more distinct clumps [84, 85, 86, 87, 88]. This raises the possibility that

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\(^2\) As an amusing aside: the highest redshift in our Hubble volume where we may find a star in a collapsed minihalo is $z = 65$, corresponding to an $\approx 8\sigma$ fluctuation on the mass scale $10^5 \textup{ M}_\odot$. [70].
the first stars formed in multiple systems, and that some of these stars had masses \( \lesssim 100 \, M_\odot \), lower than previously thought (but see [89] for still higher resolution simulations that suggest less efficient fragmentation).

**The First Stars and the Beginning of Reionization.**

Even if star–formation in minihalos was inefficient, these early minihalos should have begun ionizing the universe. With a usual Salpeter IMF, each proton in a population of stars would create \( \approx 4,000 \) ionizing photons (e.g. [90]). A population of massive, metal–free stars would increase the efficiency of ionizing photon production per unit mass by a factor of \( \sim 20 \) to \( \sim 10^5 \) [91, 92, 93]. Each proton accreted onto a BH could release \( \sim 0.1 m_p c^2 = 0.1 \text{GeV} \) of energy, most of it in ionizing radiation, implying enough energy to cause up to \( 10^7 \) ionizations. These numbers suggest that once a small fraction ( \( \lesssim 10^{-5} \)) of the gas in the universe is converted into massive stars or black holes, a significant ionization of the rest of the IGM can occur.

The simple argument above ignores recombinations (in a fully ionized IGM, each hydrogen atom would recombine several times at \( z > \sim 10 \)) and the details of the ionizing spectrum and the photoionization process (which, in the case of hard-spectrum sources, needs to account for secondary ionizations by photoelectrons). Nevertheless, the main conclusion, namely that early stars or black holes should have “kick-started” reionization, is hard to avoid. In particular, if each minihalo is allowed to form PopIII stars, it would result in a significant \( \tau_e \), in tension with the electron scattering optical depth measured by WMAP and Planck [21, 22]. Indeed, in the wake of the “false alarm” from WMAP’s first measurement of a large \( \tau_e \), several authors investigated the even more efficient “pre-ionization” of the IGM at \( z \sim 20 \) by accreting BHs [94, 95]. While those models with a large X-ray emissivity are now ruled out, a contribution from early accreting BHs still remains a natural possibility, especially if fragmentation in early halos (mentioned above) leads to the frequent formation of high-mass X-ray binaries [96, 97, 98].

### 2.2.3 Global Reionization Models in a Hierarchical Cosmology

Beginning in the late 1990s, detailed models were put together, in which the well-understood cosmological dark matter halos were populated by stars or black holes (early examples include [99, 90, 100]). These models allowed physically motivated calculations of the entire reionization history, between \( 6 < z < 30 \), to be confronted with data.

An important physical ingredient in reionization models, especially at the earliest stages, is global radiative feedback. Soon after the first stars appear, early radiation backgrounds begin to build up, resulting in feedback on subsequent star–formation. In particular, the UV radiation in the Lyman–Werner (LW) bands of \( \text{H}_2 \) can photodissociate these molecules and suppress gas cooling, slowing down the global star-formation rate [101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115].
If the metal–free stars forming in the early minihalos were indeed very massive (\(\sim 100 \, M_\odot\)), then these stars would leave behind remnant BHs with similar masses \([116]\), and could produce significant X-rays, either by direct accretion or by forming high-mass X-ray binaries. A soft X-ray background at photon energies of \(\gtrsim 1\, \text{keV}\), at which the early intergalactic medium (IGM) is optically thin, then provides further global feedback: both by heating the IGM, and by catalyzing H\(_2\) formation in collapsing halos \([117, 118, 119, 120, 94, 121, 122, 123]\).

On the other hand, if fragmentation was very efficient, and the typical PopIII stars had low masses, they would not leave BH remnants and they would have softer spectra, with copious infrared (IR) radiation at photon energies \(\sim 1\, \text{eV}\). Similar to LW and X-ray photons, these photons have a mean–free path comparable to the Hubble distance, building up an early IR background. If soft–spectrum stars, with masses of a few \(M_\odot\), contributed \(\gtrsim 0.3\%\) of the UV background (or their mass fraction exceeded \(\sim 80\%\)), then their IR radiation would have dominated the global (negative) radiative feedback in the early Universe \([124]\). This feedback is different from the LW feedback from high-mass stars, and occurs through the photo-detachment of H\(^-\) ions, necessary for efficient H\(_2\) formation. Nevertheless, the baryon fraction which must be incorporated into low–mass stars in order to suppress H\(_2\)–cooling is comparable to the case of high-mass stars.

The net effect of the above long-range “global” feedback effects remains poorly understood. This is a significant outstanding question, as these feedback effects likely determined the earliest stages of the global reionization history. The difficulties with a self-consistent reionization model are two-fold. First, one needs a detailed ab-initio understanding of the feedback on individual protogalaxies with different masses and redshifts. Second, the feedback processes (such as photo–ionization heating, H\(_2\)–dissociation \([125, 126]\), and also metal–enrichment), are all affected by the strong clustering of the earliest sources. Semi-analytical models have included either various feedback effects (e.g. \([100, 127, 128, 129, 130, 131]\)) or the effect of source clustering on the HII bubble–size distribution (e.g. \([132]\)), but not yet both self-consistently. Only the first steps were taken towards such a self-consistent treatment, incorporating photo-ionization feedback, in a simplified way, into a model that partially captures the source clustering (only in the radial direction away from sources) \([133]\).

Numerical simulations do not have the dynamical range for an ab-initio treatment of this issue. The minihalos hosting the first stars arise from primordial perturbations on the scale of \(\sim 10\) (comoving) kpc. On the other hand, the global feedback effects operate over a distance comparable to the Hubble length, \(\sim 1\) Gpc. Even if one were to resolve a minihalo with only \(10^3\) particles, 3D simulations would need to cover a factor of \(\sim 10^6\) in spatial scales (or contain \(10^{18}\) particles). Clearly, this can not be achieved by N-body simulations - let alone hydrodynamical simulations that include the basic physics, such as cooling, chemistry, and radiative transfer.\(^3\) Semi-numerical treatments \([134]\) can offer an order of magnitude higher dynamical range, and have incorporated radiative feedback \([135]\), but are still short of covering

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\(^3\) For reference, the largest existing N-body simulation is the Millennium-XXL project with \(3 \times 10^{11}\) particles.
the required range of scales (i.e. still to need to prescribe small-scale non-linear processes with sub-grid prescriptions).

### 2.2.4 Stars vs. Black Holes as Sources of Reionization

As is clear from above, whether the first stars were formed as single stars, or in binaries, matters for the early stages of reionization. If the majority of the first stars formed high-mass X-ray binaries, they could have produced sufficient X-rays to significantly change the expected “Swiss-cheese” morphology of reionization [118, 119, 120, 121]. The thickness of the edges of the cosmological ionized regions would be of order the mean free path of the typical ionizing photon. For the UV photons from stars, this mean free path is small, resulting in sharply defined ionization fronts. But for the hard spectra of X-ray binaries (or more generally, accreting black holes), the mean free path can be long, comparable to the Hubble distance for photon energies above $E > \left(\frac{(1+z)}{11}\right)^{1/2} \times_{\text{HI}}^{1/3} \text{keV}$ (where $x_{\text{HI}}$ is the mean neutral H fraction in the IGM). The diffuse nature of the boundaries of individual ionized regions could be detectable, in principle, through 21cm or $\text{Ly}_{\alpha}$ observations [136, 137].

Since X-rays in the early Universe can travel across the Hubble distances, they can also change the global reionization topology. The X-rays would ionize and heat the plasma much more uniformly than stars (although they could increase the ionized fraction only to $\sim 20\%$: nearly all of the energy of the fast photo-electron from the first ionization will subsequently go into heating the IGM). If X-rays are sufficiently prevalent, a range of other interesting effects will occur: the extra heating will raise the pressure of the plasma everywhere, making it resistant to clumping, and more difficult to compress to form new galaxies [118, 49]. On the other hand, X-rays can penetrate the successfully collapsing protogalaxies and can ionize hydrogen and helium atoms in their interior. This will catalyze the formation of molecular hydrogen, and help the gas to cool and form new stars [103]. These effects will leave behind their signatures in the spatial distribution of neutral and ionized hydrogen and helium in the Universe. Distinguishing these different global morphologies could be possible in 21cm experiments [138], or in the CMB through the kSZ effect [19].

There are other possible sources of X-rays, in addition to binaries, connected to the formation of the first stars. One example is gas accretion onto the black–hole remnants left behind by the collapse of single (super)massive stars [116, 94, 95]. Another possible source is supernovae (SNe): if the first stars exploded as SNe, then similar X-rays would be produced by thermal emission from the gas heated by these SNe, and by the collisions between the energetic electrons produced in the SN explosion and the CMB photons [118]. Thermal emission from a hot ISM has indeed been found to dominate the soft X-ray emission in a sample of local star-forming galaxies [139].

We emphasize that X-ray sources can not contribute significantly to reionization at lower redshifts, as they would then have overproduced the unresolved X-ray background [46, 47, 48], nor could they have elevated the ionized fraction to $\gtrsim 20\%$ at
early times. However, a smooth partial “pre”ionization by sources whose spectrum peaks near $\sim 1\text{keV}$ remains a plausible an interesting scenario.

In summary – the simplest possibility is that the first stars and black holes started reionizing the universe by redshift $z \approx 15 - 25$; the process then was completed predominantly by small galaxies, in the redshift range $6 \lesssim z \lesssim 10$. The relative contribution of these two types of sources is yet to be understood, especially at the earliest epochs; as is the net effect of the global radiation backgrounds that should build up early on. These are fundamental outstanding questions. The relative abundance of the two types of sources determined the global ionization topology, and their feedback processes likely drove global time-evolution of reionization.

Finally, for completeness, it is useful to note that there are several other, more exotic sources that may have contributed to reionization in principle. These include decay products of various different dark matter particles [141, 142, 143, 144, 145], high energy cosmic rays [118, 146, 147], or excess small-scale structure formation arising from primordial non-Gaussianities [148], a running of the spectral index [73], or a red spectral tilt [149, 15]. Many of these alternatives were proposed in the wake of the anomalously high $\tau_e$ in the WMAP3 data, and, at the present time, there is no longer a need for these additional contributions.

3 Can We Detect the First Stars Directly?

As mentioned in the Introduction, reionization is a probe of the earliest light sources. The redshift and duration of reionization of reionization, inferred from quasar absorption spectra, 21cm signatures, and the CMB, will place a constraint on the host halos and the ionizing efficiencies. The observed level of “patchiness” will constrain the spectral hardness of the typical source, constrain the relative contribution of stars and black holes, and shed light on the birth and death of the first galaxies.

One may, however, ask: is this the best we can do, or is there a hope to directly detect the light from the first stars or black holes? It is simple to obtain a rough estimate for the stellar mass of in a proto-galaxy, or the mass of a bright (near-Eddington) black hole, which could be detected at the $\sim 1\text{Jy}$ detection threshold in a deep exposure with the James Webb Space Telescope. At $z = 10$, this requires a mass of about $10^5 \text{M}_\odot$, either in stars [90] or in a BH [100]. (The former is consistent with a recent detailed estimate [150].) It is quite plausible (or even likely) that the very first galaxies and quasars were below this threshold.

So what hopes do we have of directly seeing the light of these first sources? I believe there are three possibilities.

First, observations can be about an order of magnitude more sensitive, using a foreground cluster to gravitationally lens and magnify the $z \sim 10$ background sources. Indeed, there are two examples of detecting $z = 8 - 10$ galaxies [151, 152].

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4 Reionization must end by $z \sim 6$, as shown recently using the fraction of dark Ly$\alpha$ and Ly$\beta$ pixels in a sample of 22 quasars [140]
using this technique on 28 foreground clusters the CLASH survey [153]. The ongoing Hubble Frontier Fields, going an order of magnitude deeper using 4-6 clusters. This technique gives a chance of discovering $10^4 M_\odot$ mini-galaxies or miniquasars at $z \sim 10$.

Second, and most promising, would be to detect the individual supernovae (SNe) from the first stellar populations. Even “normal” core collapse SNe are bright enough to be visible well beyond $z = 10$, and the pair instability SNe expected from massive PopIII stars with $\sim 130 - 250 M_\odot$ would be even brighter. It has been shown that JWST could detect many hundreds of these SNe; the challenge will be that repeated observations will be required on many JWST fields, separated by years, to identify the slowly evolving light-curves of these ultra-distant SNe [154].

Third, even if we cannot directly detect individual stars, black holes, or SNe, we can still directly detect their cumulative faint emission, through the technique known as “intensity mapping”. In general this technique consists of “tomographic” observations of the fluctuating intensity in the emission lines from faint, individually undetectable sources [155, 156]. In practice, at least two emission lines are required, so that their spatial fluctuations (in sky position and in redshift space) can be cross–correlated, eliminating contaminating signals from a foreground line. The same technique can be applied, in principle, to the strong HeII 1640Å emission lines expected from the first generation PopIII stars, cross–correlated with CO emission from the same galaxies, or with 21cm emission from the IGM [157]. This would require a next-generation UV instrument (the example considered in [157] is a space-borne 2m dish, with 100 individual detector pixels with spectral resolution $R=1000$).

4 The Future

As the rest of this book will make clear, the future is bright, with JWST, ALMA, and several new 21cm experiments coming on line, allowing us to peer farther back in redshift. The main challenge will likely become to constrain parametric models, since it is unlikely that we will have full, ab-initio calculations of the reionization process incorporating all the relevant physics, on scales ranging from star-formation inside minihalos, to the global radiative feedback processes operating on the Hubble scale. With a combination of multiple observational probes, this will nevertheless give us a chance to understand the cosmic history of structure formation from its very beginning.

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