Evolution of High-redshift Quasar Hosts and Promotion of Massive Black Hole Seed Formation

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Abstract

High-redshift luminous quasars powered by accreting supermassive black holes (SMBHs) with mass \( \gtrsim 10^9 M_\odot \) constrain their formation pathways. We investigate the formation of heavy seeds of SMBHs through gas collapse in the quasar host progenitors, using merger trees to trace the halo growth in highly biased, overdense regions of the universe. The progenitor halos are likely irradiated by intense H2-photodissociating radiation from nearby star-forming galaxies and heat the internal gas by successive mergers. The kinetic energy of the gas originating from mergers, as well as the baryonic streaming motion, prevents gas collapse and delays prior star formation. With a streaming velocity higher than the rms value, gas clouds in nearly all \( 10^4 \) realizations of merger trees enter the atomic-cooling stage and begin to collapse isothermally with \( T \approx 8000 \) K via \( \text{Ly}\alpha \) cooling. The fraction of trees that host isothermal gas collapse is 14% and increases with streaming velocity, while the rest form H2-cooled cores after short isothermal phases. If the collapsing gas is enriched to \( Z \sim 10^{-3} Z_\odot \), requiring efficient metal mixing, this fraction could be reduced by additional cooling via metal fine-structure lines. In the massive collapsing gas, the accretion rate onto a newly born protostar ranges between 3 \( \times 10^{-3} M_\odot \) yr\(^{-1} \) and 5 \( M_\odot \) yr\(^{-1} \), among which a large fraction exceeds the critical rate suppressing stellar radiative feedback. As a result, we expect a distribution of stellar mass (presumably BH mass) ranging from several hundred to above \( 10^5 M_\odot \), potentially forming massive BH binary mergers and yielding gravitational-wave events.

Unified Astronomy Thesaurus concepts: Supermassive black holes (1663); Quasars (1319); High-redshift galaxies (734)

1. Introduction

Supermassive black holes (SMBHs) with masses of \( 10^6 \)–\( 10^9 M_\odot \) are one of the most fundamental ingredients on the structure formation paradigm and are believed to coevolve with their host galaxies over the cosmic timescale through gas feeding and feedback processes (Kormendy & Ho 2013). The existence of high-redshift quasars at \( z \gtrsim 6 \) suggests that such monster SMBHs form in the first billion years of the cosmic age (Fan et al. 2006; Mortlock et al. 2011; Wu et al. 2015; Jiang et al. 2016; Matsuoka et al. 2018; Onoue et al. 2019; Wang et al. 2021) via rapid assembly processes, such as the formation of heavy BH seeds (initial mass), rapid mass growth via gas accretion, or a combination of the two mechanisms (see a review by Inayoshi et al. 2020).

For massive seed BH formation, a sufficiently high accretion rate of gas onto stellar objects is required. In early protogalaxies where the halo virial temperature is as high as \( T_\text{vir} \approx 10^4 \) K and the temperature of a self-gravitating gas cloud is as warm as that value, the mass accretion rate is expected to be \( M \approx c_s^3/G \approx 0.1 M_\odot \) yr\(^{-1} \) \( (T/10^4 \text{ K})^{3/2} \), where \( c_s \) is the sound speed of the gas and \( G \) is the gravitational constant. To keep the gas warm against efficient cooling via H2 lines, several mechanisms suppressing, delaying, and counteracting H2 formation/cooling have been proposed by many previous studies in literature: photodissociation of H2 by Lyman–Werner (LW) radiation (Omomigai 2001; Oh & Haiman 2002; Shang et al. 2010; Latif et al. 2013; Inayoshi et al. 2014; Regan et al. 2014; Sugimura et al. 2014; Visbal et al. 2014b; Chon et al. 2016), supersonic baryonic streaming motion relative to dark matter (DM; Tanaka & Li 2014; Hirano et al. 2018; Inayoshi et al. 2018; Schauer et al. 2019), and rapid halo mergers that cause heating (Yoshida et al. 2003; Wise et al. 2019; Lupi et al. 2021) and reduce H2 cooling through accretion shocks (Fernandez et al. 2014). All three processes bring the gas cloud into a dense and hot region on the gas-phase diagram, where collisional dissociation from the excited rovibrational levels of H2 reduces the H2 fraction (Inayoshi & Omukai 2012). In the subsequent stage, the gas collapses almost isothermally, keeping itself as warm as \( T \approx 3000–8000 \) K and avoiding vigorous gas fragmentation into smaller clumps (Bromm & Loeb 2003; Latif et al. 2013; Inayoshi et al. 2014; Becerra et al. 2015; Chon et al. 2018). Due to global and monolithic collapse of the warm cloud, the embryonic protostar is fed by rapidly accreting gas at a rate of \( \gtrsim 0.1 M_\odot \) yr\(^{-1} \) through a compact accretion disk where gas clumps could quickly migrate inward and merge with the central protostar (Inayoshi & Haiman 2014; Sakurai et al. 2016). Moreover, since the protostar evolves with an expanding stellar envelope owing to rapid entropy injection from the accreting matter, the surface temperature is limited to \( T_\text{eff} \approx 5000 \) K, which is too low for the protostar to emit ionizing radiation (Hosokawa et al. 2013; Haemmerlé et al. 2018). As a result of inefficient radiative feedback, the protostar would likely reach \( \sim 10^5 \)–\( 10^6 M_\odot \) before the end of its lifetime and collapse into a massive seed BH. However, those formation sites of massive seed BHs are expected to be as rare as the number density of high-\( z \) quasars in a comoving volume \( n_{\text{SMBH}} \sim 10^{-15} \text{ Gpc}^{-3} \) from Willott et al. 2010).

Recent cosmological hydrodynamical simulations have suggested that the conditions required to form massive seeds should be more modest than previously considered (e.g., Wise et al. 2019). Even with a moderate level of LW radiation, streaming motion, and merger heating, a high mass accretion rate is sustained at larger radii in a protogalaxy, although the isothermality of gas is not maintained at high densities.
mass accretion rate onto the central protostar is reduced, but the peak rate can exceed the critical rate for bifurcating the protostellar evolution (Latif & Volonteri 2015; Hirano et al. 2017; Regan et al. 2020b). As a result, the central star grows to the intermediate-mass regime at $M_{*} \approx 100-10^{4} M_{\odot}$, which is lower than the expected mass for a supermassive star but still massive enough to form massive seeds that will end up as high-$z$ SMBHs (Sakurai et al. 2020; D. Toyouchi et al., in preparation). Therefore, those environmental effects are potentially important to initiate intermediate-mass BHs (IMBHs) in the high-$z$ universe by $z \sim 6-7$ (Inayoshi et al. 2020) and form gravitational-wave sources for the space-based GW interferometers such as LISA, Taiji, and Tianqin (Sesana et al. 2008; Amaro-Seoane et al. 2017; Bonetti et al. 2019; Dayal et al. 2019; Luo et al. 2016) However, we emphasize that the massive-seed-forming halos in those scenarios do not necessarily merge into high-$z$ quasar host galaxies.

In this paper, we consider a new scenario of the massive seed formation in biased, overdense regions with $\gtrsim 5$ mass variance, where high-$z$ SMBHs are expected to form (Wyithe & Padmanabhan 2006). In such intrinsically rare patches of the universe, stronger halo clustering increases the frequency of halo mergers and boosts the mean intensity of LW radiation background in the regions. Therefore, the modest conditions required to form massive seeds with $100-10^{4} M_{\odot}$ will be naturally satisfied there. We generate merger trees of the progenitor halos that end up a high-$z$ quasar host, based on the extended Press–Schechter formalism, and quantify the expected mean LW intensity irradiating the main progenitors and the merger heating rate along with the trees. By taking into account the environmental input, the thermal and dynamical evolution of a massive gas cloud in the main progenitor halo is calculated in a self-consistent way.

Among previous studies in the literature, Valiante et al. (2016) investigated the origin of SMBHs using semianalytical models and found massive BHs seeded in the quasar progenitor halos, depending on their environmental effects. Recently, Lupi et al. (2021) also proposed a similar idea that massive seed BH formation would be much more efficient in a biased halo merger tree based on DM-only N-body simulation. They found that in an overdense region a large number of atomic-cooling halos experience successive merger heating that counteracts radiative cooling via $H_{2}$ lines and potentially promote massive seed formation. However, most of the halos in their samples do not end up in the most massive DM halo that is supposed to be a high-$z$ quasar host. Instead, we study the statistical properties of the progenitor halos of a high-$z$ quasar host by generating merger trees. Moreover, we explicitly follow the evolution of gas clouds in the main progenitors, taking into account merger heating, radiative cooling, and chemical reaction networks. Thus, the two studies are complementary.

This paper is organized as follows. In Section 2, we summarize our construction of merger histories of a quasar host, the calculation of environmental LW intensity for individual halos, and subsequent gas evolution following the underlying halo mass growth. In Section 3, we discuss the results of LW intensity, the fraction of promising heavy seed formation sites, and the distribution of accretion rate realized. In Section 4, we quantify the critical metallicity that affects thermal evolution of gas and the efficiency of metal enrichment and discuss caveats of our model. In Section 5, we show the mass distribution of seed BHs formed in the high-$z$ quasar progenitors. Finally, in Section 6, we summarize the main conclusions of this paper.

### 2. Methodology

In order to investigate the evolution of luminous quasar progenitors that form in rare, overdense regions in the universe at redshift $z \sim 6$, we construct the merger history of DM halos up to $z = 50$ and model the evolution of the gas properties within the DM halos along each merger tree. The processes we model consist of three parts: (1) We first construct the hierarchical merger history of a quasar host halo using the Monte Carlo merger tree algorithm. For a $10^{5} M_{\odot}$ SMBH powering the luminous quasar at $z \sim 6$, the halo mass is estimated to be $M_{h} \sim 10^{12} M_{\odot}$ by comparing the growth rate of quasar density indicated from observations with that predicted by the Press–Schechter formalism (Wyithe & Padmanabhan 2006). We therefore focus our analysis on halos that grow to $M_{h} = 10^{12} M_{\odot}$ at $z = 6$. (2) For a given merger tree, we calculate the LW radiation background produced by the surrounding star-forming galaxies at each redshift, in order to model the radiative impact on the gas within the halo. (3) The evolution of the gas in the parent halo of each tree is studied by taking into account the injection of thermal and kinetic energy due to violent merger events, as well as LW irradiation calculated in step 2 that dissociates the gas coolants. In the following subsections, we describe in detail the three key ingredients. Throughout the paper, we adopt cosmological parameters estimated by Planck assuming a $\Lambda$CDM universe (Planck Collaboration et al. 2016), i.e., $\Omega_{m} = 0.307$, $\Omega_{\Lambda} = 0.693$, $\Omega_{b} = 0.0486$, $H_{0} = 67.7 \text{ km s}^{-1} \text{ Mpc}^{-1}$.

#### 2.1. Merger Histories of Progenitors

We construct DM merger trees based on the extended Press–Schechter formalism (Press & Schechter 1974; Lacey & Cole 1993; Cole et al. 2000) using the GALFORM semianalytic algorithm summarized in Parkinson et al. (2008). Our sample consists of $10^{5}$ merger tree realizations for the DM halos that end up as high-$z$ quasar hosts with $M_{h} = 10^{12} M_{\odot}$ at $z = 6$. For each tree, we adopt a minimum DM halo mass of $M_{h,\text{min}} = 10^{5} M_{\odot}$. Halos smaller than this threshold do not significantly impact the gas evolution, because the critical virial temperature above which gas collapse can be induced by coolant $H_{2}$ is $\sim 10^{3} \text{ K}$ (see Haiman et al. 1996; Tegmark et al. 1997), corresponding to halo mass higher than $M_{h,\text{min}}$ (see also Figure 1). Reflecting the rarity of quasar host galaxies, the progenitor halos form in highly biased regions with $\gtrsim 5$ mass variance (Mo & White 2002). Note that the fraction of all matter in such rare halos is $\lesssim 10^{-7}$.

#### 2.2. Lyman–Werner Background Intensity

Due to the photoionization of $H_{2}$ exposed to LW radiation, we also consider the local LW intensity $I_{LW}$ (at $h\nu = 12.4 \text{ eV}$, hereafter in units of $10^{-21} \text{ erg s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1} \text{ sr}^{-1}$) in order to follow the gas evolution in a given progenitor halo. Along each merger tree, we calculate the cumulative $I_{LW}$ from neighboring star-forming galaxies (hereafter source halos). Based on the model developed by Dijkstra et al. (2014), the basic equations and assumptions we adopt are summarized as below.

We consider a DM halo with mass $M_{h}$ (gas + DM) at redshift $z$, which is supposed to be the main progenitor in a merger tree. The average number of source halos (within mass
where \( \Delta = \frac{\Delta v}{v} \) is the frequency width of the LW band \((11.2 \leq h\nu / eV \leq 13.6)\) are set to \( \langle \nu \rangle = 12.4 \, eV / h \) and \( \Delta \nu = 2.4 \, eV / h \), respectively. The total stellar mass is calculated by \( m_* = f_* (\Omega_b / \Omega_m) m \), assuming the star formation efficiency to be \( f_* = 0.05 \). The escape fraction of LW photons from the halo is assumed to be unity \( (f_{esc, LW} = 1) \). This value tends to be lower for atomic-cooling halos with \( m \gtrsim 10^9 M_\odot \). As a reference, Schauer et al. (2015) calculated the LW escape fraction for a single Population III star in an atomic-cooling halo with 1D simulations and found \( f_{esc, LW} \approx 0.7 \). However, this is considered to be a lower bound because the escape fraction would be higher for 3D calculations through directions with lower optical depths, and besides, a higher star formation rate (SFR) is expected in our case (rather than a single massive star). We estimate the LW luminosity at one freefall time after the burst of star formation:

\[ t_{ff} = \sqrt{\frac{3\pi}{32G}} \Delta v_{vir} \rho_0 \approx 18 \, \text{Myr} \langle (1 + z) / 31 \rangle^{-3/2}, \quad \Delta v_{vir} \approx 18 \, \text{eV}. \]

Using Equations (1)–(3), we obtain the mean LW radiation intensity in the target halo as

\[ J_{LW}(m_*, z) = \int_{m_{\min}}^{m_{\max}} \int_{r_{\min}}^{r_{\max}} \frac{d^2 N(m, r)}{dmdr} \cdot \frac{L_{LW}}{4\pi r^2} \, dr \, dm, \quad (4) \]

where \( r_{\min} \) and \( r_{\max} \) are the minimum and maximum distance, respectively, of the source halo from the target halo. In the absence of metal pollution, \( r_{\min} \) can be safely set by adding the virial radius of the target and source halos. However, metal enrichment of the main progenitor is a main obstacle in the formation scenario of massive seed BHs, because efficient metal-line cooling (and possibly dust thermal emission) will likely lead to gas fragmentation during its gravitational collapse and thus suppress massive star formation. Generically, there are two types of enrichment processes: (1) genetic enrichment due to past star formation episodes in the progenitors, and (2) environmental enrichment owing to metal bubbles created by supernova (SN) explosions in nearby galaxies. In our model, we consider the environmental enrichment process by adopting the minimum distance to source halos as \( r_{\min} = \max \{ r_{\text{vir}} (M_\bullet) + r_{\text{vir}} (m, r) \} \), where \( r_{\text{vir}} \) is the size of the metal-polluted region surrounding the source halo

\[ r_{\text{vir}}(m, t) = \left( \frac{E_{SN} m_*}{m_0 \rho_0} \right)^{1/5} t^{2/5}, \quad (5) \]

where \( m_0 = 100 M_\odot \) is the stellar mass budget required to form an SN progenitor and \( E_{SN} = 10^{51} \, \text{erg} \) is the explosion energy of an SN. The density \( \rho_0 \) of gas surrounding the wind is considered to be \( \Delta \rho_{\text{vir}} \), where \( \rho_{\text{vir}} \) is the intergalactic medium (IGM) baryon density, and \( \Delta = 60 \) corresponding to the typical baryonic overdensity of halos at their virial radius for an NFW profile (Dijkstra et al. 2014). Similar to the production of LW radiation, we estimate the size of metal-enriched bubbles at \( t_{\text{ff}} \).

We note that metal enrichment through in situ star formation should be subdominant because intense LW radiation suppresses star formation in low-mass progenitors (see Section 4).

On the other hand, the maximum distance in the integration is given by \( r_{\max} = (\Delta \lambda_{W,1} - \lambda_\text{min}) c / [\lambda_\text{min} H(z)] \), where the \( \lambda_{W,1} = 1110 \, \text{Å} \) and \( \lambda_\text{min} \) are wavelengths of the lowest LW energy and Lyα line, respectively (see Haiman et al. 1997). We consider the redshift effect by cosmic expansion, where \( H(z) = H_0 (1 + z)^3 + \Omega_\Lambda^{1/2} \) is the Hubble constant at
redshift $z$ and $c$ is the light speed. LW photons emitted at $r > r_{\text{max}}$ are redshifted into one of the Lyman series resonances and are converted into low-energy photons before reaching the target halo. The $r_{\text{max}}$ is thus set as an absorbing screen, i.e., we exclude the contribution of $J_{\text{LW}}$ from halos located at $r > r_{\text{max}}$.

2.3. Energy Injection through Halo Mergers

The main progenitor halo experiences vigorous halo mergers in the high-$z$ universe. Successive merger events, in particular major mergers, inject energy into the gas in the parent halo. At early phase, energy loss through radiative cooling is inefficient, i.e., the cooling timescale is comparable to or longer than the Hubble timescale. Gas is heated through shock formation at the halo virial radius in an adiabatic manner. Subsequently, the energy is transported into the halo interior, leading to gas virialization with a nearly constant temperature profile ($T_{\text{gas}} \sim T_{\text{vir}}$) across all radii (Wise & Abel 2007). Assuming that the virial equilibrium state is reached after a merger event, the virial theorem applies to the gas in the post-merger halo, where the internal and kinetic (turbulence) energy is balanced with the gravitational energy as

$$e_{\text{tot}} = e_{\text{th}} + e_{k} + \Phi_{R_{\text{vir}}} = \frac{1}{2} \Phi_{R_{\text{vir}}},$$

where $e_{\text{tot}}$, $e_{\text{th}}$, and $e_{k}$ are the total, thermal, and kinetic energy per unit mass, respectively, and $\Phi_{R_{\text{vir}}}$ is the gravitational energy at the virial radius. In this work, we adopt the NFW potential for DM halos given by

$$\Phi_{R_{\text{vir}}} = -\frac{2 \kappa_{\text{B}} T_{\text{vir}}}{\mu m_{\text{p}}} \ln \left( \frac{1 + c_{\text{vir}}}{1 + c_{\text{vir}} (1 + z) / (1 + c_{\text{vir}})} \right),$$

where $T_{\text{vir}}$ is the halo virial temperature, the concentration parameter of the DM density profile $c_{\text{vir}} = 1.9 \left(M_{\odot} / 10^{12} M_{\odot}\right)^{-0.13}$ [(1 + $z$)/3]$^{-1}$ (Bullock et al. 2001), $k_{\text{B}}$ is the Boltzmann constant, $\mu = 1.22$ is the mean molecular weight, and $m_{\text{p}}$ is the proton mass. Therefore, the total energy change owing to the halo evolution is given by

$$\Gamma_{\text{merg}} = -\frac{1}{2} \Phi_{R_{\text{vir}}} \left( \frac{2 \kappa_{B} T_{\text{vir}}}{3 M_{\text{h}}} = \frac{1}{1 + z} \frac{dz}{dt} \right),$$

where the first term on the right-hand side denotes the energy change associated with mass growth and the second term represents the cosmic expansion effect. In the generally turbulent virialized gas, the kinetic-to-thermal energy ratio is equal to 1 around the virial radius and decreases to 1/3 at the center (see Wise & Abel 2007). Adopting this branching ratio of the total injected energy, the thermal and kinetic heating rates associated with mergers are given by $\Gamma_{\text{merg,th}} = 3 \Gamma_{\text{merg}} / 4$ and $\Gamma_{\text{merg,kin}} = \Gamma_{\text{merg}} / 4$, respectively. Combining Equations (6)-(8), the gas temperature follows the halo virial temperature as

$$\frac{T_{\text{gas}}}{T_{\text{vir}}} = \frac{1}{2} \frac{\ln (1 + c_{\text{vir}})}{\ln (1 + c_{\text{vir}}) - c_{\text{vir}} / (1 + c_{\text{vir}})}.$$

This ratio is close to unity for a wide range of $(M_{\odot}, z)$ halos of interest, e.g., $T_{\text{gas}} / T_{\text{vir}} \simeq 1.3$ and 0.81 for $c_{\text{vir}} = 2$ and 10. Note that our method is different from that adopted in previous papers (e.g., Yoshida et al. 2003; Lupi et al. 2021), where $T_{\text{gas}} = T_{\text{vir}}$ is imposed. The treatment allows us to precisely calculate the radiative cooling rates and chemical reaction coefficients, which sensitively depend on the gas temperature.

2.4. Turbulence and Baryonic Streaming Motion

The kinetic energy injected through mergers is stored in the halo as turbulence. During the virialization process, turbulence plays an important role in massive star formation (e.g., McKee & Tan 2002). Namely, turbulence acts as a source of pressure, which stabilizes the gas against self-gravity and delays the collapse until the cloud becomes massive enough to overcome the turbulent pressure. In addition to turbulence, the baryonic streaming motion relative to the DM produced in the epoch of cosmic recombination at $z_{\text{rec}} \approx 1100$ also significantly delays gas collapse and star formation in protogalaxies. The streaming velocity is found to follow a Maxwell–Boltzmann distribution with the rms speed of $\sigma = 30$ km s$^{-1}$ at $z = z_{\text{rec}}$ and decays as $v_{\text{bhm}} = v_{\text{bhm}}(1 + z)/(1 + z_{\text{rec}})$ (Tseliakhovich & Hirata 2010). We note that the volume fraction of the universe with streaming velocities of $v_{\text{bhm}} \geq A \sigma$ is estimated as $0.4, 8 \times 10^{-3}$, and $5.9 \times 10^{-6}$ for $A = 1, 2$, and 3, respectively.

Considering both the three-dimensional turbulence and coherent baryonic streaming motion, we approximate the effective pressure by kinetic motion of gas as

$$P_{\text{tur}} \approx \frac{1}{3} \rho v_{\text{tur}}^2 + \rho \left( \alpha_{0} v_{\text{bhm}}(z) \right)^2,$$

where $v_{\text{tur}}^2 = 2 \int \Gamma_{\text{merg,kin}} dt$ is the kinetic specific energy accumulated through successive mergers and the coefficient of 1/3 is required to estimate the pressure due to isotropic turbulence (Chandrasekhar 1951a, 1951b). With pressure support from turbulence, gas collapse is delayed to different extents, with varying strengths of the streaming motion. In this work, we adopt $\alpha_{0} = 4.7$ in our fiducial model, in order to match the delay of collapse obtained from cosmological simulations (Hirano et al. 2018). The total gas pressure is therefore defined by $P_{\text{tot}} = P_{\text{gas}} + P_{\text{tur}}$.

2.5. Density Evolution

With the energy injection processes defined above, in this section we describe our model for calculating the density evolution of a gas cloud concentrated in a DM halo that grows through successive merger episodes. There are three characteristic stages of the evolution: (1) initial adiabatic phase, (2) transition to isothermal gas due to radiative cooling, and (3) gravitationally collapsing phase in a runaway fashion. We model the gas dynamics in these stages based on a one-zone model (e.g., Omukai 2001), which is often used to follow the physical quantities at the center of a gravitationally collapsing cloud with a self-similar density profile $\rho_{\text{gas}} \propto r^{-2}$. However, this profile does not apply to gas in hydrostatic equilibrium before the onset of gravitational collapse. Therefore, we construct a new method to model the three characteristic stages in a physically motivated way.

2.5.1. Adiabatic Stage

In the early stage, since the gas density is not high enough for radiative cooling to operate through collisionally excited transitions, the gas is adiabatically compressed in the DM halo as the underlying DM gravitational potential evolves. In the DM assembly history through mass accretion, the entropy
profile $K(r)$ of the adiabatic gas is characterized by a power-law outer profile of $K(r) = K_{\text{vir}}(r/R_{\text{vir}})^{1.1}$ and a constant core with $K_0 \approx 0.1 K_{\text{vir}}$, where $K_{\text{vir}} = \rho_b R_{\text{vir}}/(\mu m_p)^2/3$ is the gas entropy at the virial radius (Voit et al. 2003, 2005). This self-similar entropy profile is also found to be established inside high-$z$ protogalaxies formed in DM halos more massive than $3 \times 10^9 M_\odot$ at $z = 10$, while the core entropy for less massive halos is maintained at the IGM entropy when gas decouples from the cosmic microwave background (CMB; see more details in Visbal et al. 2014a). Motivated by both numerical simulations and galaxy cluster observations, we approximate the entropy profile as

$$K(r) \approx K_{\text{vir}} \left( \frac{r}{R_{\text{vir}}} \right) + K_0,$$  

where $K_0 = \max(0.1 K_{\text{vir}}, K_{\text{IGM}})$. Using the entropy profile and the equation of state given by $P_{\text{gas}} = K(r) \rho_{\text{gas}}^\gamma$, where $\gamma = 5/3$, we calculate the density profile by solving the hydrostatic equation (the so-called Lane–Emden equation) for the cloud embedded in the DM potential:

$$\frac{1}{r^2} \frac{d}{dr} \left[ r^2 \frac{d(K_{\text{gas}} \rho_{\text{gas}} + P_{\text{gas}})}{dr} \right] = -4\pi G (\rho_{\text{gas}} + \rho_{\text{DM}}).$$

Throughout this paper, we adopt the NFW density profile of DM halos of all masses characterized by a simple analytical form of

$$\rho_{\text{DM}}(r) = \rho_m(z) \frac{\delta_0}{(c_{\text{vir}} r/R_{\text{vir}})(1 + c_{\text{vir}} r/R_{\text{vir}})^2},$$

where $\rho_m(z)$ is the mean matter density and

$$\delta_0 = \frac{200}{3} \frac{c_{\text{vir}}^3}{\ln(1 + c_{\text{vir}}) - c_{\text{vir}}/(1 + c_{\text{vir}})}$$

is the characteristic overdensity within the halo virial radius (Navarro et al. 1997).

We integrate this hydrostatic equation with respect to $\rho_{\text{gas}}(r)$, imposing the regularity conditions at the center, i.e., $\rho_{\text{gas}} = \rho_0$ and $d\rho_{\text{gas}}/dr = 0$ at $r = 0$. Since the solution for adiabatic gas generally has the radius $r_0$ where $\rho_{\text{gas}}(r_0) = 0$, we determine the central density $\rho_0$ so that the enclosed gas mass at $r \leq r_0$ satisfies $M_{\text{gas}} = f_b M_{\text{baryons}}$, where $f_b = \Omega_b/\Omega_m$ is the baryonic fraction.

### 2.5.2. Isothermal Stage

As the gas temperature increases owing to gravitational compression and merger heating, radiative cooling processes begin to operate in the cloud and the adiabatic assumption no longer applies. When the radiative cooling timescale is shorter than the heating timescale, we solve the hydrostatic equation for the density profile assuming an isothermal equation of state:

$$\frac{1}{r^2} \frac{d}{dr} \left[ r^2 \rho_{\text{gas}}^\gamma \frac{d \ln \rho_{\text{gas}}}{dr} \right] = -4\pi G (\rho_{\text{gas}} + \rho_{\text{DM}}).$$

where $c_{\text{eff}} \equiv \left( c_l^2 + v_{\text{vir}}^2 / 3 + (\alpha_0 \tilde{v}_{\text{rms}})^2 \right)^{1/2}$ is the effective sound speed developed from the isothermal sound speed $c_l \equiv \sqrt{k_b T_{\text{gas}}/(\mu m_p)}$. The solution of the isothermal Lane–Emden equation with the regularity condition does not have the radius where the density becomes zero but connects to the external medium with a density of $\rho_{\text{ext}} = f_b \rho_{DM}$. The central density is determined so that $\rho_{\text{gas}} = \rho_{\text{ext}}$ at the virial radius.

From the analogy of the Bonnor–Ebert sphere, the isothermal gas cloud embedded in a DM halo potential has a critical mass for the onset of its gravitational collapse. Practically, for a given $T_{\text{gas}}$ and $\rho_{DM}(r)$, we construct the density profile with different values of the gas central density $\rho_0$ and thus obtain $\rho_{\text{gas}}(R_{\text{vir}})$ as a function of $\rho_0$. Since this function has a local maximum value and the value decreases with increasing halo mass, a hydrostatic equilibrium solution where $\rho_{\text{gas}}(R_{\text{vir}}) = \rho_{\text{ext}}$ no longer exists for $M_h \geq M_{\text{baryons}}$ (see the Appendix). In this case, the gas evolution is described by the freefall stage below.

#### 2.5.3. Freefall Stage

Once the gas cloud becomes gravitationally unstable, the evolution of the gas density profile is well described by the Penston–Larson self-similar solution (Penston 1969; Penston 1969), which has a density profile with a flat core of the Jeans scale and an envelope with a power-law density distribution $\rho_{\text{gas}}(r) \propto r^{-2}$. The central density increases over the freefall timescale as

$$\frac{d \rho_{\text{gas}}}{dt} = \frac{\rho_{\text{gas}}}{t_{\text{ff}}},$$

where the freefall timescale is calculated with

$$t_{\text{ff}} \equiv \sqrt{\frac{3\pi}{32 G (\rho_{\text{gas}} + \langle \rho_{\text{DM}} \rangle)}}.$$

where $\langle \rho_{\text{DM}} \rangle = \rho_m(z) \delta_0$ represents the averaged DM density.1

In the collapsing stage, compressional heating by the self-gravitating gas is taken into account and the rate is given by

$$\Gamma_{\text{comp}} \equiv \frac{P_{\text{gas}} + P_{\text{turb}}}{\rho_{\text{gas}}^2} \frac{d \rho_{\text{gas}}}{dt} = \frac{c_{\text{eff}}^2}{t_{\text{ff}}}.$$  

We note that the compressional heating rate is enhanced by turbulent pressure through the effective sound speed.

#### 2.6. Temperature and Chemical Evolution

We consider the evolution of thermal and kinetic energy of the gas by solving the two energy equations:

$$\frac{d e_{\text{th}}}{dt} = \Gamma_{\text{norm}, \text{th}} + \Gamma_{\text{comp}} - \mathcal{L}_{\text{chem}} - \mathcal{L}_{\text{rad}},$$

where $\mathcal{L}_{\text{chem}}$ is the cooling/heating rate associated with chemical reactions and $\mathcal{L}_{\text{rad}}$ is the radiative cooling rate (note that all the rates are in units of erg s$^{-1}$ g$^{-1}$). While the compressional heating rate is included only in the collapse stage, the other effects are taken into account to calculate the gas temperature over the three evolutionary stages. The cooling term includes radiative cooling by H, He, He$^+$, and He$^{++}$ (Glover & Jappsen 2007); H$_2$ (Glover & Abel 2008; Glover 2015a, 2015b); and cooling/heating associated with chemical reactions.

We solve the chemical reactions of primordial gas among the following nine species: H, H$_2$, e$^-$, H$^+$, H$^2$, H, He, He$^+$, and

---

1 The squared density of an NFW profile averaged within the characteristic radius of $R_{\text{vir}}/c_{\text{vir}}$ is given by $\langle \rho^2 \rangle = \frac{\pi^2}{4} \rho_m(z) b_h^3$, independent of the concentration factor $c_{\text{vir}}$. This is true for $b_h \gg 1$, but not for $b_h \approx 1$. Anticipating this, one may apply this result only for $b_h \gg 1$. This is not an issue for very massive halos, such as those which dominate the IGM entropy, since their critical overdensity is high (e.g., $\delta_0 \approx 500$). The critical overdensity, however, is less than 50 for the least massive halos of interest in the IGM, and the square of the density is therefore strongly dependent on the concentration factor. The results for two typical halos are shown in Table 1.


Table 1

| Number | Reaction | Reference |
|--------|----------|-----------|
|        | **H Collisional Reactions** |           |
| 1      | $H + e^- \rightarrow H^+ + 2e^-$ | 1         |
| 2      | $H^+ + e^- \rightarrow H + \gamma$ | 2         |
| 3      | $H + e^- \rightarrow H^- + \gamma$ | 3         |
| 4      | $H^- + H \rightarrow H_2 + e$ | 4         |
| 5      | $H + H \rightarrow H_2 + e$ | 5         |
| 6      | $H_2^+ + H \rightarrow H_2 + H^+$ | 6         |
| 7      | $H_2 + H \rightarrow 3H$ | 7         |
| 8      | $H_2 + H^- \rightarrow H_2^- + H$ | 8         |
| 9      | $H + e^- \rightarrow 2H + e^-$ | 9         |
| 10     | $H^- + e^- \rightarrow H + 2e^-$ | 10        |
| 11     | $H^- + H \rightarrow 2H$ | 11        |
| 12     | $H^- + H_2 \rightarrow H_2^- + e^-$ | 12        |
| 13     | $H_2 + e^- \rightarrow 2H$ | 13        |
| 14     | $H_2 + H^- \rightarrow H_2^- + H$ | 14        |
| 15     | $3H \rightarrow H_2 + H$ | 15        |
| 16     | $2H + H_2 \rightarrow 2H_2$ | 16        |
| 17     | $2H \rightarrow 2H + H_2$ | 17        |
| 18     | $H^- + H \rightarrow 2H + e^-$ | 18        |
| 19     | $H^- + H_2 \rightarrow 3H$ | 19        |
| 20     | $H_2 + e^- \rightarrow H + H^+$ | 20        |
|        | **Photodissociation and Detachment Reactions** |           |
| 21     | $H_2 + \gamma \rightarrow 2H$ | 21        |
| 22     | $H^- + \gamma \rightarrow H + e^-$ | 22        |
| 23     | $H_2^+ + \gamma \rightarrow H + H^+$ | 23        |
|        | **He Reactions** |           |
| 24     | $He + e^- \rightarrow He^+ + 2e^-$ | 24        |
| 25     | $He^+ + e^- \rightarrow He + \gamma$ | 25        |
| 26     | $He^+ + e^- \rightarrow He^+ + 2e^-$ | 26        |
| 27     | $He^{++} + e^- \rightarrow He^+ + H^+ + \gamma$ | 27        |
| 28     | $H_2 + He \rightarrow 2H + He$ | 28        |
| 29     | $H_2 + He^+ \rightarrow He + H + H^+$ | 29        |
| 30     | $H_2 + He^+ \rightarrow H_2^+ + He$ | 30        |
| 31     | $He^+ + H \rightarrow He + H^+$ | 31        |
| 32     | $He + H^- \rightarrow He^- + H$ | 32        |
| 33     | $He^+ + H^- \rightarrow He + H$ | 33        |
| 34     | $He + H^- \rightarrow He + H + e^-$ | 34        |
| 35     | $2H + He \rightarrow H_2 + He$ | 35        |

Figure 2. Time evolution of LW radiation intensity $J_{LW}$ (in units of $10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ s$^{-1}$) irradiating the quasar progenitors for the four cases shown in Figure 1. For the median tree, we show two cases where the metal-bubble size $r_s$ is calculated as described in Section 2.2 (solid) and a value twice the fiducial value is adopted (dashed).

The cross sections we adopt are from references listed in Table 1.

3.3. Merger History and Evolution of LW Radiation Background

In Figure 1, we show the evolution of the main progenitors, i.e., the most massive halos at each epoch, for all the 10$^4$ merger trees that grow to $M_h \approx 10^{12} M_\odot$ at $z = 6$. In such overdense regions of the universe, the DM halo mass increases via rapid mergers. The median halo mass (dashed curve) reaches $M_h \approx 8 \times 10^{10} M_\odot$, $6 \times 10^{10} M_\odot$, $2 \times 10^{10} M_\odot$, and $8 \times 10^9 M_\odot$ at $z = 10, 20, 30$, and 40, respectively, and the virial temperature exceeds the atomic-cooling threshold of $T_{cool} \approx 10^4 K$ at $z \approx 34$. Therefore, the gas cloud concentrated in the massive halo collapses at an epoch earlier than when typical first galaxies would form in atomic-cooling halos ($M_h \approx 10^7 M_\odot$ at $z \approx 10$; see Bromm & Yoshida 2011), which are usually considered to be massive-seed-forming sites in most previous studies (e.g., Dijkstra et al. 2014). For illustration purposes, we highlight three merger trees: the blue (id 1, a less massive tree), orange (id 2, a tree comparable to the median evolution), and green curves (id 3, a more massive tree). In the following sections, we focus our analysis on these three representative cases.

Following the method laid out in Section 2, in Figure 2 we present the redshift evolution of $J_{LW}$ for the three representative trees and the median track. For all the cases, the LW background intensity gradually increases from higher redshifts, peaks at the intermediate redshifts, and decreases toward lower redshifts. This redshift dependence reflects the nature of the nonlinear bias function that boosts the abundance of halo pairs with comparable masses (Scannapieco & Barkana 2002).
Namely, when the mass of the main progenitor is close to the atomic-cooling halo mass ($m_{ac,z} \sim 10^7 M_{\odot}$), a large number of source halos form nearby owing to the halo clustering effect, and thus the LW intensity is maximized. As the main progenitor grows, its mass difference from $m_{ac,z}$ is larger, and thus the clustering effect of atomic-cooling sources becomes weaker so that their spatial distribution is approximated to be uniform (i.e., $\xi \ll 1$). As a result, the LW intensity is dominated by the contribution from a large number of atomic-cooling source halos within the absorbing screen ($r \lesssim r_{\text{max}}$) and begins to decline owing to the cosmic dilution effect at lower redshifts. For rapidly growing progenitor halos exceeding $m_{ac,z}$ earlier, the LW intensity quickly rises at higher redshifts and the peak values become higher owing to stronger clustering at earlier epochs. Namely, the peak values of LW intensity in the overdense regions are $J_{\text{LW}} \approx 60$ (id 1), $J_{\text{LW}} \approx 400$ (id 2), $J_{\text{LW}} \approx 600$ (median), and $J_{\text{LW}} \approx 6 \times 10^3$ (id 3), which are significantly higher than the level of LW intensity irradiating typical atomic-cooling halos that are expected to form massive BH seeds (see Dijkstra et al. 2008; Agarwal et al. 2012; Johnson et al. 2013).

In our semianalytical approach, we model metal pollution of the progenitor halos due to SN explosions that occur in source halos. Although we treat this effect by replacing the minimum distance between the target and source halos with $r_s$, there is no information on the time-dependent spatial distributions of DM halos in our framework. To examine the impact of the model assumptions, in Figure 2 we also show the case where the size of the metal-polluted bubbles ($r_s$) is doubled and the corresponding $t_{sf}$ is comparable to the Hubble time at the redshift, or equivalent to setting $\Delta = 1$ with the fiducial value of $t_{sf}$. In this case, the LW intensity is overall reduced at higher redshifts, indicating a significant contribution from nearby source halos with $m_{ac,z}$ to the LW radiation background. We note that our treatment simply removes the contribution from source halos within distances of $r_s$, but does not address how likely it is for the main progenitor to be affected by environmental metal enrichment. Our argument nevertheless provides a conservative estimate of $J_{\text{LW}}$ if the efficiency of environmental metal enrichment is low. As discussed in Section 4, the efficiency should be negligibly low because metal-polluted bubbles rarely penetrate the interior of the target halo (Chiaki et al. 2018).

In Figure 3, we present the histograms of the LW background intensity that irradiates the main progenitor halos for the $10^4$ trees at different redshifts. For the whole sample of the target halos in highly biased regions, the histogram resembles a probability distribution function (pdf) of $J_{\text{LW}}$, with the bar height in each bin ($\Delta \log J_{\text{LW}} = 0.3$) representing the number fraction of halos irradiated within log $J_{\text{LW}} \rightarrow \log J_{\text{LW}} + \Delta \log J_{\text{LW}}$. From higher redshifts down to $z \approx 30$, the mean value of $J_{\text{LW}}$ in the pdf increases owing to a large number of clustered source halos with $m_{ac,z}$ and the $J_{\text{LW}}$ distribution peaks around $\approx 270$ at $z \approx 25$. Toward lower redshifts, the target halo mass becomes higher than the typical mass of source halos. Therefore, the abundance of sources is hardly boosted by the clustering effect (Iliev et al. 2003). Moreover, the LW intensity is diluted by the cosmic expansion, lowering the mean value. While the dispersion of the pdf is larger at higher redshifts, reflecting the diversity of the progenitor mass, the pdf peaks at $J_{\text{LW}} \approx 60$ by $z = 10$ when all the $10^4$ trees converge to the high-$z$ quasar host.

We note that our model does not consider LW radiation produced from DM minihalos with $m < m_{ac,z}$, where H$_2$ is the only coolant to induce star formation. However, strong LW background radiation in the overdense region likely suppresses its formation. Therefore, the histogram shown in Figure 3 counts the lower bound of the LW background intensity.

### 3.2. Thermal and Dynamical Evolution of Gas Clouds in the High-$z$ Quasar Hosts

In this section we focus our analysis on the gas properties in the main progenitors along the three representative merger
trees. In Figure 4, we show the evolution of gas density (left panels) and temperature (right panels) at the central core as a function of redshift. In order to examine the impact of baryonic streaming motion, for each merger tree we assume two different $v_{bsm}$ values, i.e., $v_{bsm} = 1\sigma$ (top panels), and $2\sigma$ (bottom panels). Each curve corresponds to the representative case highlighted in Figure 1. Along with the three evolutionary tracks, we denote the epochs when the parent halo mass exceeds $M_h = 10^6 M_\odot$, $10^7 M_\odot$, and $3 \times 10^7 M_\odot$ in the left panels, and when the LW background intensity first crosses $J_{LW} = 1, 10, 100$ and 1000 are marked in the right panels. When the halo mass grows faster and/or the streaming velocity is higher, gas collapse is significantly delayed owing to pressure (thermal + kinetic) support of the gas cloud. This effect makes the gas enter the atomic-cooling stage at lower densities ($H^{-}H_2$ and $H^{-}H$ cases) owing to strong LW irradiation before the onset of gravitational collapse.

For the lowest-mass case (blue curve, tree id 1), the gas density gradually increases with the halo mass in the early stage ($z > 30$), where the gas cloud is supported by thermal and turbulent pressure against its self-gravity and DM gravitational force. After the halo mass reaches $\sim 10^6 M_\odot$, the cloud becomes gravitationally unstable owing to its low temperature and collapses over one freefall timescale at $z \approx 28$. The gas temperature remains at $T \lesssim 10^3 K$ owing to $H_2$ cooling, under a modest level of LW intensity ($J_{LW} \sim 1$) at $z > 35$. In addition to LW radiation, the gas is heated by four major merger events around $z = 31-34$, but the dynamical heating rate does not overcome the $H_2$ cooling rate in this case.

For the intermediate-mass case (orange curve, tree id 2), the evolution begins from a redshift higher than in the previous case. In this case, the gas temperature is substantially higher as a result of the combination of merger heating and intense LW irradiation with $J_{LW} \lesssim 100$ before the cloud gravitationally collapses, the level of LW intensity is not strong enough to suppress $H_2$ formation in the dense region ($\gtrsim 10^2$ cm$^{-3}$), where $H_2$ reforms owing to its self-shielding effect. As a result of efficient $H_2$ cooling, the gas temperature drops down to $T \approx 10^3 K$ in the collapsing stage.

For the highest-mass case (green curve, tree id 3), the gas temperature quickly rises to $T \approx 10^4 K$ owing to frequent
mergers. Owing to the clustering effect of the massive parent halo, the LW intensity reaches $J_{LW} \gtrsim 10^3$ at $z \simeq 47$, prominently higher than those seen in the less massive cases. Although the H$_2$ self-shielding becomes more effective as the central density increases up to $\gtrsim 10^4$ cm$^{-3}$, the gas collapses, keeping a nearly constant temperature of $T \approx 8000$ K. Inside the dense and warm region, H$_2$ is collisionally dissociated and its radiative cooling does not alter the thermal evolution.

In cases where $v_{bhm} = 2 \sigma$, the gas property evolution is shown in the bottom panels of Figure 4. Overall, the collapse of gas clouds is delayed owing to kinetic energy injection to the gas concentrated at the halo center. When the cloud begins to collapse, the corresponding halo masses reach $M_h \simeq (3.5, 4.2, 5.9) \times 10^7 M_\odot$. For comparison, the collapse halo masses are $M_h \simeq (0.24, 2.1, 2.2) \times 10^7 M_\odot$ for $v_{bhm} = 1 \sigma$. The delay effect is more remarkable for the lower-mass cases because the halo circular velocity is lower than the effective sound speed boosted by injection of turbulence and streaming motion. As the gas collapse proceeds, H$_2$ forms efficiently in the modest $J_{LW}$ environment, and eventually its cooling reduces the gas temperature in the low- and intermediate-mass cases.

3.3. The Statistical Properties of the High-$z$ Quasar Progenitors

As noted in Section 3.2 and Figure 4, depending on the main cooling processes inducing star formation, the evolutionary tracks of the gas clouds embedded in the main progenitors of high-$z$ quasar hosts are classified into three cases: (i) H$_2$ cooling, (ii) initial H Ly$\alpha$ cooling followed by H$_2$ cooling after a short isothermal collapse, and (iii) H Ly$\alpha$ cooling when temperature is kept above 8000 K by compression along a wide density range. In Figure 5, we present the number count of merger trees for the three types with different baryonic streaming velocities, denoted as (i) H$_2$, (ii) H Ly$\alpha$, and (iii) H Ly$\alpha$. Without the streaming velocity, 74% of the trees experience gas collapse via H$_2$ cooling, while the rest (26%) form atomically cooling gas clouds (cases H Ly$\alpha$ and H Ly$\alpha$).

With nonzero streaming motion ($v_{bhm} = 0$), nearly all cases enter the atomic-cooling stage because the halo mass reaches $m_{ac,x}$ via mergers owing to the significant delay effect. As the streaming velocity increases, the gas mass becomes higher at the onset of gravitational collapse, and thus the compressional heating rate during the collapse stage is higher owing to the accumulation of kinetic energy. Therefore, the number of trees where gas isothermally collapses with $T \approx 8000$ K (case H--H) increases monotonically from 14% to 27% with increasing streaming velocity from $v_{bhm} = 1 \sigma$ to $3 \sigma$.

In Figure 6, we show the distributions of the halo virial temperature (top panels) and LW background intensity (middle panels) for the three types of gas collapse. For each case, the values of $T_{\text{vir}}$ and $J_{LW}$ are measured at the epoch when the gas cloud first enters its unstable stage. In contrast to cases with $v_{bhm} = 0$, where gas collapse is led by H$_2$ cooling in less massive halos with $T_{\text{vir}} \approx 10^3$--$10^4$ K, the streaming velocity delays the cloud collapse until after the halo grows across the atomic-cooling threshold of $T_{\text{vir}} \gtrsim 10^4$ K. The virial temperature for the H--H cases is generally higher than that for the H--H cases, and the mean value of $T_{\text{vir}}$ for each case increases with larger streaming velocity. This trend is more clearly shown in the distributions of $J_{LW}$, namely, the mean LW background intensity for the H--H cases is $(J_{LW}) \gtrsim 10^3$, which is $\approx 10$ times higher than that for the H--H cases. The higher value of $J_{LW}$ is mainly caused by the delay of gas collapse until the halo mass becomes massive enough to be exposed by a larger number of LW source halos. In addition, compressional heating in collapsing clouds is stronger with larger $v_{bhm}$, and the minimum LW intensity required to keep isothermal collapse is extended to lower values.

In the main progenitors of high-$z$ quasar hosts, massive gas clouds form owing to the significant delay effect of cloud collapse by rapid halo mergers and intense LW irradiation from nearby star-forming galaxies. The mass accretion rate onto the central region of a gravitationally collapsing cloud is approximated as $\dot{M} \simeq M_{\text{gas}}/\tau_{\text{ff}}$, where $M_{\text{gas}}$ and $\tau_{\text{ff}}$ are the gas mass and freefall timescale at the onset of gravitational collapse, respectively. Since the cloud is supported by thermal and kinetic energy of the gas, the accretion rate can be written as $\dot{M} \propto c_{\text{ff}}^3 G$ (Larson 1969; Penston 1969, etc.), which depends only on the gas thermal and kinetic temperature (see below Equation (15)). In the bottom panels of Figure 6, we show the distributions of $M \equiv M_{\text{gas}}^3 G$, for which we adopt the minimum temperature value in the cloud collapse stage at $T \gtrsim 10^4$ K. The accretion rate is broadly distributed over $M \approx 3 \times 10^{-3} - 5 M_\odot$ yr$^{-1}$. The vertical line in the bottom panels indicates a reference value of $0.1 M_\odot$ yr$^{-1}$, above which the outer envelope of an accreting protostar is blown, due to rapid heat injection through mass accretion, and the emission of stellar ionizing photons is strongly suppressed. For $v_{bhm} = 1 \sigma$, the majority of the H--H cases yield $M \gtrsim 0.1 M_\odot$ yr$^{-1}$. With $v_{bhm} > 1 \sigma$, all the cases have sufficiently high accretion rates exceeding the reference value (see more discussion in Section 5).

4. Effects of Metal Enrichment

4.1. Critical Metallicity

Metal enrichment is considered to be a major obstacle in forming massive BH seeds through star formation because efficient radiative cooling via metal fine-structure lines will induce gas fragmentation and suppress the formation of massive stars. In order to quantify the critical metallicity, we
calculate the cooling rate by C II and O I, assuming that the number fractions of carbon and oxygen nuclei in the gas phase with respect to hydrogen nuclei are $x_{C, \text{gas}} = 0.927 \times 10^{-4} \left( \frac{Z}{Z_{\odot}} \right)$ and $x_{O, \text{gas}} = 3.568 \times 10^{-4} \left( \frac{Z}{Z_{\odot}} \right)$ (Pollack et al. 1994), and all the carbon and oxygen are in the form of C II and O I, respectively. This treatment is justified for warm gas with $T \approx 8000$ K (Omukai et al. 2008).

In Figure 7, we present the metal-line cooling rate (dashed) and heating rate associated with mergers and gravitational compression (solid) as a function of the density of gas embedded in the two representative progenitor halos (tree id 2 and 3) with $v_{bim} = 1\sigma$. In order to examine the cooling effect by metal lines against heating, the H$_2$ cooling is turned off, and metal-line cooling is calculated but not included in the thermal evolution. The metallicity for each case is set so that the cooling rate is marginally balanced with the heating rate at least once during the collapse phase. Namely, the critical metallicity is estimated as $Z_{\text{crit}} = 1.9 \times 10^{-3} Z_{\odot}$ (tree id 2) and $2.5 \times 10^{-3} Z_{\odot}$ (tree id 3), respectively. These values are higher than the critical metallicity of $Z_{\text{crit}} \sim 3 \times 10^{-4} Z_{\odot}$ (in the absence of dust) obtained by Omukai et al. (2008), where the effect of turbulence and merger heating is not included. Although the critical metallicity depends on the relative abundance of metals produced in SN ejecta, we use $Z_{\text{crit}} = 2 \times 10^{-3} Z_{\odot}$ as a reference value in the following discussion.

4.2. Efficiency of Metal Enrichment

Throughout this paper, we do not consider the genetic pollution process through mergers of metal-rich minihalos, given that the star-forming efficiency is strongly suppressed by intense LW radiation in the overdense region. However, we note that this treatment is justified only when the “actual” LW intensity is as high as the average value shown in Figure 3.
Therefore, due to SN bubbles produced from one source halo, the gas metallicity in the target halo increases by

\[ \Delta Z \simeq \frac{m_{\text{ej}}}{m_{\text{sn},0}} \left( \frac{f_{\text{esc,m}}}{0.5} \right) \left( \frac{m}{M_\odot} \right) \left( \frac{5r_{\text{vir}}}{r_s} \right)^2, \]

where \( f_{\text{esc,m}} = 0.5 \) is motivated by 3D high-resolution hydrodynamical simulations of SN-driven galactic outflows (Li et al. 2017).

As discussed in Section 3.1, the LW intensity peaks when the target halo reaches the atomic-cooling threshold because (1) source halos with \( m_{\text{ac,z}} \) are the most abundant population in number and (2) two halos with comparable mass are strongly clustered. This circumstance will also maximize the efficiency of environmental enrichment. Assuming \( M_\text{hi} = m_{\text{ac,z}} \), we estimate

\[ N_e = \frac{n_{\text{hi}}}{0.4} \text{ (tree id 1), 6 (tree id 2), and 86 (tree id 3).} \]

As a result, the gas metallicity in the target halo is calculated as \( Z = N_e \Delta Z \simeq 9.3 \times 10^{-5} Z_{\odot} f_{\text{mix}} N_e \).

Therefore, we obtain the conditions where the environmental enrichment process affects the thermal evolution of gas in the target halo as

\[ N_e > 21.5 f_{\text{mix}}^{-1}. \]

Since \( f_{\text{mix}} \leq 1 \), the gas evolution in the main progenitor surrounded by \( \lesssim 21 \) nearby source halos within \( r_s \) is unlikely to be affected by metal-line cooling. On the other hand, if the mixing efficiency is as high as \( f_{\text{mix}} \gtrsim 0.25 \), metal enrichment will play an important role in changing the gas evolution in rapidly growing halos (tree id 3), reducing the number fraction of H–H collapse cases (see Figure 5).

Additionally, inhomogeneous density distributions inside the source halos and the nonsteady SFR that forms SNe in the earlier stage change the velocity and shape of expanding bubbles. Those effects could result in either an overestimation or underestimation of the bubble size. To discuss the efficiency of environmental enrichment precisely, we need to further study a variety of situations with different physical parameters, as well as the metal mixing efficiency \( f_{\text{mix}} \). We leave this to future work.

4.3. Dynamical Evolution of Metal-enriched Gas

We quantify the critical metallicity and discuss the impact of metal-line cooling on the thermal evolution of gas clouds. However, dynamical evolution of a collapsing cloud with \( Z \gtrsim Z_{\text{crit}} \) that is composed of a warm outer envelope \( (T \simeq 8000 \text{ K}) \) and a cool central core has not been fully understood; especially, long-term behavior of the mass inflow rate onto the central newly formed protostar is still uncertain. Recent cosmological simulations suggest that rapid mass inflows may occur even with metal
pollution above the critical metallicity in atomic-cooling halos (Regan et al. 2020a), but widespread star formation limits the final mass of the central star to \( \lesssim 10^7 M_\odot \) (Regan et al. 2020b). On the other hand, when the metallicity is lower than the critical value, the collapsing gas cloud fragments only at the central region and forms a compact disk, in which a vast majority of the clumps merge with the central protostar via inward migration (Inayoshi & Haiman 2014; Chon & Omukai 2020). As a result, the stellar growth is not quenched by metal pollution. Future work is needed to investigate the star formation in the overdense regions where high-\( z \) quasars form to quantify the impact of metal pollution on the gas dynamics.

5. Discussion

5.1. Protostellar Mass and BH Mass Distribution

We apply the obtained mass accretion rate to estimate the final protostellar mass distribution at the end of star formation episodes. Due to the existing angular momentum at large scales, the rapidly accreted pristine gas settles into a disk, which becomes gravitationally unstable and thus results in fragmentation and clump formation (e.g., Oh & Haiman 2002). Most clumps can migrate inward and merge with the central protostar before forming stars (Inayoshi & Haiman 2014), yielding the accretion rate onto the stellar surface through the disk \( \dot{M}_* = \eta \dot{M}_s \), where \( \eta (\lesssim 1) \) denotes the conversion efficiency from the global accretion rate to that through the accretion disk. Hydrodynamical simulations find that mass accretion through the unstable disk proceeds episodically and the time-averaged value of the efficiency is \( \eta \approx 0.6 \) (Sakurai et al. 2016; D. Toyouchi et al., in preparation).

When the time-averaged accretion rate is higher than a critical rate, \( \dot{M}_s \gtrsim \dot{M}_{s,\text{crit}} \), the accreting star continues to expand its envelope with a lower surface temperature of \( T_{\text{eff}} \approx 5000 \) K, from which UV radiation hardly emits. As a result, stellar radiative feedback does not prevent the central star growing via mass accretion (Omukai & Palla 2001; Hosokawa et al. 2012, 2013; Schleicher et al. 2013; Sakurai et al. 2015, 2020; Haemmerlé et al. 2018). Since the value of \( \dot{M}_{s,\text{crit}} \) ranges from 0.01 to 0.04 \( M_\odot \) yr\(^{-1} \), depending on the treatment of the stellar evolution calculations and their boundary conditions (Hosokawa et al. 2013; Haemmerlé et al. 2018), we adopt the highest \( \dot{M}_{s,\text{crit}} = 0.04 M_\odot \) yr\(^{-1} \) as a reference value. This choice leads to a lower bound of the stellar/BH mass. With \( \dot{M}_s \gtrsim \dot{M}_{s,\text{crit}} \), the final stellar mass is determined either by its finite lifetime or by the onset of stellar collapse triggered by the general relativistic (GR) instability (Shibata et al. 2016; see a review by Woods et al. 2019 and references therein). The final mass is also affected by fuel supply through mass accretion onto the star. Woods et al. (2017) have investigated the final mass of stars accreting at a constant rate over \( \lesssim 0.01 - 10 M_\odot \) yr\(^{-1} \) (radiative feedback is neglected) and found that the final mass linearly increases with the accretion rate below \( \sim 0.03 M_\odot \) yr\(^{-1} \) but is saturated around \( \sim \) a few \( \times 10^5 M_\odot \) owing to the GR instability. The relation between the critical mass and accretion rate is fitted as

\[
\dot{M}_{s,\text{GR}} \approx \left[ 0.83 \log \left( \frac{\dot{M}_s}{M_\odot \text{ yr}^{-1}} \right) + 2.48 \right] \times 10^5 M_\odot \]  

at \( \dot{M}_s \gtrsim 0.1 M_\odot \) yr\(^{-1} \), which is used for our analysis.

On the other hand, when the stellar accretion rate is lower than the critical rate, \( \dot{M}_s \lesssim \dot{M}_{s,\text{crit}} \), the star evolves to the main-sequence stage and begins to emit strong ionizing radiation, quenching the stellar growth. Here, we simply consider that ionizing radiation from the star heats the disk surface and thus photoevaporation suppresses the accretion rate (McKee & Tan 2008; Hosokawa et al. 2011; Tanaka et al. 2013). This process becomes important when the ionization front reaches the stellar gravitational influence radius for ionized gas with a temperature of \( 2 \times 10^4 \) K, defined by

\[
R_{\text{inf},*} \equiv \frac{GM_*}{c_{\text{s,ion}}^2} \approx 0.17 \text{ pc} \left( \frac{M_*}{10^4 M_\odot} \right)^{1/2},
\]

and the ionized gas breaks out through the neutral infalling gas. The photoevaporation rate can be expressed as

\[
M_{\text{pe}} \approx 2.1 \times 10^{-2} M_\odot \text{ yr}^{-1} \left( \frac{\Phi_{\text{ion}}}{10^{52} \text{ s}^{-1}} \right)^{1/2} \left( \frac{R_{\text{disk}}}{0.1 \text{ pc}} \right)^{1/2},
\]

where \( \Phi_{\text{ion}} \) is the ionizing photon number flux and \( R_{\text{disk}} \) is the size of the accretion disk. The photon flux is approximated as \( \Phi_{\text{ion}} \approx 1.6 \times 10^{52} \) s\(^{-1} \) \( (M_*/10^5 M_\odot) \) in the range of \( 10^3 \lesssim M_*/M_\odot \lesssim 10^4 \) for main-sequence stars (Johnson et al. 2012).

We evaluate the mass outflow rate owing to photoevaporation by setting \( R_{\text{disk}} \approx R_{\text{inf},*} \) as

\[
M_{\text{pe, min}} \approx 3.5 \times 10^{-2} M_\odot \text{ yr}^{-1} \left( \frac{M_*}{10^4 M_\odot} \right)
\]

which gives a lower bound for the rate because the outflow of ionized gas is mainly driven from larger radii (i.e., a larger surface area). Therefore, equating \( M_* = M_{\text{pe, min}} \), we obtain the feedback-regulated stellar mass as \( M_{s,\text{fb}} \approx M_{s,\text{pe}} \) or

\[
M_{s,\text{fb}} \approx 2.9 \times 10^3 M_\odot \left( \frac{M_*}{0.01 M_\odot \text{ yr}^{-1}} \right)
\]

at \( M_* \lesssim M_{s,\text{crit}} \), where \( t_{\text{pe}} (\approx 2.9 \times 10^8 \) yr) is the characteristic photoevaporation timescale (note that this expression is valid when the stellar lifetime is longer than \( t_{\text{pe}} \)). The final mass at the intermediate accretion rate (\( M_{s,\text{crit}} \lesssim M_* \lesssim 0.1 M_\odot \) yr\(^{-1} \)) is estimated by performing logarithmic interpolation.

In Figure 8, we show the mass distribution of massive BH seeds formed in the high-\( z \) quasar progenitor halos, calculated with the method described above (see also the bottom panels in Figure 6). Note that the number fraction from the different types of gas evolution is stacked at the same mass bin. Without the streaming motion (\( v_{\text{ram}} = 0 \); left panels), the BH mass is widely distributed from \( 500 M_\odot \) \( (250 M_\odot) \) to \( \gtrsim 2 \times 10^5 M_\odot \) for \( \eta = 0.6 \) (0.3, respectively) with a few peaks corresponding to the virial temperatures of halos when the BHs form by gas collapse. Overall, the cases with high accretion rates \( \dot{M}_s \) (H–H2 and H–H cases) are responsible for high-mass BH formation beyond \( \sim 10^7 M_\odot \), while the H2 case with lower accretion rates yields less massive BHs with \( < 10^4 M_\odot \). The number of BH seeds above \( 2 \times 10^5 M_\odot \) is limited because the GR instability induces direct collapse of accreting supermassive stars. The shape of the mass distribution at \( 10^5 \lesssim M_*/M_\odot \lesssim 10^5 \) depends on the accretion efficiency, namely, the smaller value of \( \eta = 0.3 \) yields a distribution skewed toward lower masses. With nonzero streaming motion (\( v_{\text{ram}} = 1 \sigma \); right panels), the less massive population with \( < 10^4 M_\odot \) decreases abruptly since nearly all the cases experience the atomic-cooling stage and thus the central stars
accrete at high rates without strong radiative feedback. We note that the BH mass distribution for higher streaming velocities is similar to that for \( v_{bsm} = 1 \sigma \), but their contribution to the total BH mass distribution is less important because regions with \( v_{bsm} \geq 2 \sigma \) are rarer.

As discussed in Section 4, the number fraction of the cases with highest mass accretion rates (H–H cases) would be reduced by the effect of line cooling via atomic carbon and oxygen, which are produced in nearby source halos through SNe and carried into the quasar main progenitor halos with interest. The level of reduction depends on the metal mixing efficiency in the main progenitor, namely, the enrichment effect could be neglected if the mixing efficiency is lower than \( \sim 20\% \). Nevertheless, the overall shape of the BH mass distribution still holds.

5.2. Subsequent BH Growth and Evolution

How do those massive seed BHs formed in overdense regions grow to be SMBHs that are observed as high-z quasars at \( z \approx 6–7 \)? In previous studies in the literature, the subsequent growth of their BHs via gas accretion and/or mergers and the required conditions have been discussed (e.g., Tanaka & Haiman 2009; Valiante et al. 2016). Recently, large-scale cosmological simulations have been exploring the evolution of SMBHs and the coevolution of their host galaxies, including various feedback processes due to SNe and active galactic nucleus activity with subgrid models. These simulations have generally found that massive seed BHs formed in protogalaxies hardly grow via gas accretion because dense, cold gas is expelled by energetic SN feedback associated with star formation. However, it is worth noting that most simulations in which SN feedback quenches BH growth have focused on “typical” atomic-cooling halos that will grow to \( \sim 10^{10–10^{11}} M_\odot \) by \( z \approx 6 \) (e.g., Habouzit et al. 2017; Latif et al. 2018; Smith et al. 2018).

On the other hand, as pointed out by Inayoshi et al. (2020), the progenitor halos of high-z quasar hosts with \( M_h \approx 10^{12} M_\odot \) at \( z \approx 6 \) form in rarer regions and have reached \( M_h \sim 10^9 M_\odot \) with deeper gravitational potential by the time when star formation takes place (\( z \approx 20–35 \)). In such massive halos, a large amount of cold gas is supplied to the nuclear region through filamentary structures of the proto-cosmic web (Di Matteo et al. 2012), and the seed BHs can be fed at high rates significantly exceeding the Eddington limit when the metallicity of inflowing gas is as low as \( \lesssim 0.01 Z_\odot \) (Toyouchi et al. 2021; see also Inayoshi et al. 2016). The critical halo mass required for the onset of rapid mass accretion exceeding the Eddington rate is \( M_h \approx 10^9 M_\odot \), almost independent of redshift. Most of the quasar progenitor halos of interest can reach this
mass threshold after the birth of seed BHs in $\sim 20-50 \, \text{Myr}$, within which intense starbursts would take place and form protogalaxies. Exploring the nature of BH growth embedded in such a protogalaxy is left for future investigations.

This process is a possible way to form IMBH populations. Observations of IMBHs in the local universe have the potential to constrain high-$z$ BH (seed) formation (see the review by Greene et al. 2020). Furthermore, if those IMBHs form binaries through galaxy mergers and dynamical processes during the cosmic history, the seed-forming channel also provides a significant number of gravitational-wave events (e.g., Chon et al. 2018; Hartwig et al. 2018; Regan et al. 2020), which will be detectable by space-based gravitational-wave detectors such as the Laser Interferometer Space Antenna (LISA; Amaro-Seoane et al. 2017) and Tianqin (Luo et al. 2016), as well as third-generation terrestrial instruments.

6. Summary

In this paper, we investigate a new scenario of the formation of heavy BH seeds through collapse of warm gas in massive halos that end up in quasar hosts at $z \approx 6-7$. In the highly biased, overdense regions of the universe, stronger halo clustering increases the frequency of halo mergers and boosts the mean intensity of LW radiation background produced from star-forming galaxies. Those effects are expected to increase the probability of massive seed formation because the conditions required for their formation (intense LW irradiation and violent merger heating) become less stringent than previously considered. Under such unique environments, we model the thermal and dynamical evolution of massive gas clouds along with $10^5$ merger trees of the main progenitors of high-$z$ quasar hosts using the Monte Carlo method. With those samples, we study the statistical properties of the progenitor halos of high-$z$ quasar hosts and massive seed BHs. Our major findings can be summarized as follows:

1. In the high-$z$ quasar-forming regions, DM halos are likely irradiated by strong LW radiation with intensity of $J_{\text{LW}} \approx 100-10^4$ (in units of $10^{-10} \, \text{erg} \, \text{s}^{-1} \, \text{cm}^{-2} \, \text{Hz}^{-1}$) from nearby star-forming galaxies at $z \lesssim 30$, and gas clouds in the halo interiors are heated by successive gaseous halo mergers. Suppression of H$_2$ cooling via LW irradiation/merger heating and injection of gas kinetic energy through halo mergers prevent gas collapse and delay prior star formation episodes.

2. Without baryonic streaming motion, 74% of the trees experience gas collapse led by H$_2$ cooling, while the rest (26%) form atomically cooling gas clouds that begin to collapse isothermally with $T \approx 8000 \, \text{K}$ via Ly$\alpha$ cooling. With a streaming velocity higher than the rms value, gas clouds for nearly all $10^4$ realizations of the merger trees enter the atomic-cooling stage.

3. The fraction of trees that host isothermal gas collapse is 14% and increases with streaming velocity, while the rest form H$_2$-cooled cores after short isothermal phases. However, this fraction is reduced by additional cooling via metal fine-structure lines when the collapsing gas could be enriched to $Z_{\text{crit}} \sim 2 \times 10^{-3} \, Z_{\odot}$, requiring efficient metal mixing $f_{\text{mix}} \gtrsim 0.25$. This high probability reflects that high-redshift quasar-forming regions likely provide such peculiar environments, which hardly occur in typical high-redshift star-forming regions.

4. The mass accretion rate onto a newly born protostar is distributed over $3 \times 10^{-3} \cdot 5 \, M_{\odot} \cdot \text{yr}^{-1}$, a large fraction of which exceeds the critical rate suppressing stellar radiative feedback. As a result, we expect a distribution of stellar masses (presumably BH masses) ranging from several hundred to above $10^5 \, M_{\odot}$.

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Appendix

The Critical Conditions for Collapse of an Isothermal Gas Cloud

In this appendix, we briefly describe the method of how to calculate the critical gas density at the center by solving the hydrostatic equation for an isothermal gas cloud (Equation (15)), where the gas pressure gradient force is balanced with the gas self-gravity and DM gravitational force. For demonstration purposes, in the left panel of Figure 9 we show the radial profiles of gas with an effective sound speed of $c_{\text{eff}} = 8.3 \, \text{km} \, \text{s}^{-1}$ (corresponding to $T = 10^4 \, \text{K}$ gas in the absence of turbulence) for different values of $\rho_0$ in a DM halo with $M_h = 6 \times 10^9 \, M_{\odot}$ at $z = 30$. As the central density increases, the density at the virial radius $\rho_{\text{gas}}(R_{\text{vir}})$ does not increase monotonically but has a local maximum value around $\rho_0 \approx 10^{-21} \, \text{g} \, \text{cm}^{-3}$. In general, the maximum value of $\rho_{\text{gas}}(R_{\text{vir}})$ can be found for a given combination of $M_h$, $z$, and $c_{\text{crit}}$. In the right panel of Figure 9, we present the relation between $\rho_{\text{gas}}(R_{\text{vir}})$ and $\rho_0$ for different halo masses ($z = 30$ and $c_{\text{eff}} = 8.3 \, \text{km} \, \text{s}^{-1}$ are fixed). As seen in the left panel, each curve has a local maximum and the maximum value decreases with $M_h$. The density value at the outer boundary ($\rho_{\text{ext}} = f_{\text{ext}}(\rho_0)$) weakly depends on $M_h$ and $z$ through the concentration factor $c_{\text{crit}}$, i.e., the three halos have $\rho_{\text{ext}} \approx 8 \times 10^{-25} \, \text{cm}^{-3}$, varying within 3%. For $M_h = 6 \times 10^9 \, M_{\odot}$, there exist two solutions where the boundary conditions are satisfied. Since the solution with the higher value of $\rho_0$ is not stable, we adopt the solution with the lower value of $\rho_0$ (see Ebert 1955; Bonnor 1958; Lynden-Bell & Wood 1968). As the halo mass increases to $M_h = 8 \times 10^9 \, M_{\odot}$ and $10^7 \, M_{\odot}$, there is no hydrostatic solution of the gas cloud. In our semianalytical model, we calculate the hydrostatic density profile that satisfies the boundary conditions at each time step and quantify the critical halo mass $M_{\text{crit}}$ above which the gas begins to collapse. We note that this method can be applied to a wide range of $c_{\text{eff}}$ and $z$ of interest in our paper.
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