FEEDBACK FROM GALAXY FORMATION: PRODUCTION AND PHOTODISSOCIATION OF PRIMORDIAL H$_2$

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ABSTRACT

We use one-dimensional radiative transfer simulations to study the evolution of H$_2$ gas-phase (H$^-$ catalyzed) formation and photodissociation regions in the primordial universe. We find a new positive feedback mechanism capable of producing shells of H$_2$ in the intergalactic medium (IGM), which are optically thick in some Lyman-Werner bands. While these shells exist, this feedback effect is important in reducing the H$_2$ dissociating background flux and the size of photodissociation spheres around each luminous object. The maximum background opacity of the IGM in the H$_2$ Lyman-Werner bands is $\tau_{H_2}$ $\approx$ 1–2 for a relic molecular fraction $x_{H_2}$ = $2 \times 10^{-6}$, about 6 times greater than that found by Haiman, Abel, & Rees. Therefore, the relic molecular hydrogen can decrease the photodissociation rate by an order of magnitude. The problem is relevant to the formation of small primordial galaxies with masses $M_{DM}$ $\lesssim$ 10$^8$ $M_\odot$ that rely on molecular hydrogen cooling to collapse. Alternatively, the universe may have remained dark for several hundred million years after the birth of the first stars, until galaxies with virial temperature $T_{vir}$ $\gtrsim$ 10$^4$ K formed.

Subject headings: cosmology: theory — galaxies: formation — intergalactic medium

1. INTRODUCTION

Many recent observations point to a flat geometry and a significant cold dark matter (CDM) content. Recent measurements of the cosmic microwave background (CMB) anisotropies (de Bernardis et al. 2000; Lange et al. 2001; Tegmark, Zaldarriaga, & Hamilton 2000), large-scale structure (Hamilton & Tegmark 2000), Ly$\alpha$ power spectrum (Croft et al. 1999; McDonald et al. 2000), and distances of high-redshift supernovae (SNe) (Perlmutter et al. 1998; Riess et al. 1998; Garnavich et al. 1998) are all consistent with a flat CDM model of the universe, in which about $\frac{1}{3}$ the total energy density of the universe is dark matter (DM) and $\frac{2}{3}$ is "vacuum energy." Big bang nucleosynthesis fits to the observed D/H abundances suggest a small baryon density, with closure parameter $\Omega_b h^2$ $\approx$ 0.02 (Burles & Tytler 1998).

Thus, the baryons are a small fraction of the DM. In the linear phase of structure formation, the baryons simply trace the DM perturbations on large scales.

In CDM cosmologies, low-mass DM virialized objects form first. Larger halos form later from the merger of smaller subunits (hierarchical scenario). Since the gas temperature prior to reionization is about 100 K, the gas can collapse in objects with $M_{DM}$ $> 10^4$–$10^5$ $M_\odot$. Low-mass DM halos will then produce the first luminous objects (Population III) if the baryons collapsed into the DM potential wells and heated to the virial temperature can dissipate their internal energy support. The lack of metals in the primordial universe makes molecular hydrogen the only coolant below $T$ $\sim$ 10$^4$ K. Therefore, unless some H$_2$ is formed, the baryons cannot cool in shallow DM potential wells with $M_{DM}$ $\lesssim$ 10$^8$[(1 + z)/10]$^{-2/3}$ $M_\odot$, corresponding to a virial temperature $T_{vir}$ $\lesssim$ 10$^4$ K. The formation of H$_2$ occurs mainly through the chemical reaction

$$H + H^- \rightarrow H_2 + e^- .$$

Together with a similar reaction (H$^+$ + H $\rightarrow$ H$_2$ + H$^+$), this is the only possibility for virialized objects with $T_{vir}$ $\lesssim$ 10$^4$ K to cool and eventually form stars (Lepp & Shull 1984). Despite the fact that the physics is much simpler, theoretical models of the formation and fate of Population III objects must confront the lack of observational constraints and uncertainties on initial conditions. The fate of the Population III objects is still unresolved or at least controversial. The main complications of the model are the feedback processes between luminous objects and the formation and destruction of H$_2$ that can affect star formation on both local (interstellar medium [ISM]) and large (intergalactic medium [IGM]) scales.

Molecular hydrogen is photodissociated by photons with energies between 11.1 and 13.6 eV (Lyman-Werner bands) through the two-step Solomon process (Stecher & Williams 1967). Thus, the radiation from the first stars (or quasars) could dissociate H$_2$ before the IGM is reionized (negative feedback). The H$^-$ formation process instead relies on the abundance of free electrons. A positive feedback is therefore possible in a gas partially ionized by an X-ray background or direct flux of Lyman continuum radiation. Depending on the relative importance of the positive/negative feedback, star formation could be triggered or suppressed after the formation of the first stars.

Understanding the star formation history at high redshift is important for modeling the metal enrichment of the IGM. It may also influence IGM reionization if, as pointed out in Ricotti & Shull (2000), the contribution to the Lyman continuum (Lyc) emissivity in the IGM at high redshift is dominated by low-mass galactic objects. The contribution to the emissivity from these objects is important because their spatial abundance is higher and because the fraction, $\langle f_{Lyc} \rangle$, of Lyc radiation that escapes from a low-mass galaxy halo is larger than for more massive objects.

Tegmark et al. (1997) used a simple collapse criterion, that the gas cooling time must be less than the Hubble time, to determine the minimum H$_2$ fraction a virialized object must have in order to collapse. This minimum mass is a
decreasing function of the virialization redshift and is somewhat dependent on the cooling function used. Tegmark et al. (1997) found a minimum mass of $M_{DM} \sim 10^{7} M_{\odot}$ at $z \sim 30$ using the Hollenbach & McKee (1979) molecular cooling function. Abel et al. (1998) and Fuller & Couchman (2000) instead found a minimum mass an order of magnitude smaller using Lepp & Shull (1984) and Galli & Palla (1998) cooling functions, respectively. Objects of these masses can form around redshift $z \sim 30$ from 3 $\sigma$ perturbations of the initial Gaussian density field. More realistic models (Omukai & Nishi 1998; Nakamura & Umemura 1999) confirm this basic result.

Abel, Bryan, & Norman (2000) and Bromm, Coppi, & Larson (1999) used high-resolution numerical simulations to study the formation of the first stars. Abel et al. (2000) used three-dimensional adaptive mesh refinement (AMR) simulation with dynamic range about $2 \times 10^{2}$ to follow the collapse of the first objects starting from cosmological initial conditions (standard CDM cosmology). They found an approximately spherical protogalaxy of $10^{6} M_{\odot}$ with a collapsing core of $\sim 100 M_{\odot}$.

Similar results have been found by Bromm et al. (1999) using smoothed particle hydrodynamics (SPH) simulations starting from ad hoc initial conditions. For some initial conditions and larger halo masses they could form disk protogalaxies with more than one star formation region. Unfortunately, without taking into account radiative transfer effects and SN explosions, it was not possible to determine the size of the initial mass function (IMF) of the first stars. Local effects of UV radiation on star formation have been studied with semianalytical models (Omukai & Nishi 1999; Glover & Brand 2001). The main result is that massive stars are effective in suppressing cooling in small protogalaxies, but star formation can continue in larger galaxies. If the ISM is clumpy, star formation is not suppressed in the denser clumps.

The photodissociating UV radiation can affect the $H_{2}$ abundance over large distances if the IGM is optically thin in the Lyman-Werner bands. Haiman & Loeb (1997) and Haiman et al. (2000) computed self-consistently the rise in the dissociating UV background (UVB) using the Press-Schechter formalism for sources of radiation. They found that $H_{2}$ in the IGM had a negligible effect on the buildup of the UVB because of its small optical depth $\tau_{HI} \approx 0.1$ and because the photodissociation regions around the first luminous objects overlap at an early stage. Therefore, the negative feedback of the UVB suppresses star formation in small objects. However, if the first objects are miniquasars, the produced X-ray background is strong enough to cancel out the UVB negative feedback, and reionization could be produced by small objects. Contrary to the Haiman et al. (2000) result, Ciardi, Ferrara, & Abel (2000a) found no negative feedback from the UVB. They estimated the mean specific intensity of the continuum background at $z = 20$ in the $912-1120$ Å Lyman-Werner bands, $J_{\nu} \sim 10^{-27}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$.$^{1}$ This value is 4 orders of magnitude smaller than the value found by Haiman et al. (2000). Even if the photodissociation regions overlap by $z = 25$, only at $z \lesssim 15$ does the UVB become the major source of radiative feedback. At higher redshifts, direct flux from neighboring objects dominates the local photodissociation rate (Ciardi et al. 2000b).

Machacek, Bryan, & Abel (2001) included the feedback effect of the photodissociating UV background in three-dimensional AMR simulations of the formation and collapse of primordial protogalaxies. They used a box of 1 Mpc$^{3}$ comoving volume and resolution in the maximum refinement zones of about 1 pc comoving. Their results confirm that a photodissociating background flux of $F_{LW} \gtrsim 5 \times 10^{-24}$ ergs s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ delays the cooling and star formation in objects with masses in the range $10^{5}-10^{7} M_{\odot}$. They also provided an analytical expression for the collapse mass threshold, for a range of UV fluxes.

The simple observation that star formation in our Galaxy can trigger further star formation in a chainlike process (McCray & Kafatos 1987) suggests that positive feedback effects could be important also at high redshift. Haiman, Rees, & Loeb (1996) found that UV irradiation of a halo can enhance the formation of $H_{2}$ and favor the collapse of the protogalaxies. Ferrara (1998) estimated that the formation of $H_{2}$ behind shocks produced during the blow-away process of Population III can replenish the relic $H_{2}$ destroyed inside the photodissociation regions around those objects. Finally, it has been noticed that positive feedback is possible if the first objects emit enough X-rays (Haiman et al. 2000; Oh 2001; Venkatesan, Giroux, & Shull 2001).

In this paper we explore a new positive feedback effect that could be important in regulating star formation in the first galaxies. Ahead of the ionization front, a thick shell of several kiloparsecs of molecular hydrogen (with abundance $x_{H_{2}} = n_{H_{2}}/(n_{H} + n_{e}) \lesssim 10^{-4}$) forms because of the enhanced electron fraction abundance in the transition region between the H II region and the neutral IGM. This shell, which we call a positive feedback region (PFR), can be optically thick in the $H_{2}$ Lyman-Werner bands, depending on the source turn-on redshift $z_{\tau}$, luminosity, and escape fraction $\langle f_{esc} \rangle$ of ionizing radiation. We find that the photodissociation spheres around single objects are smaller than in previous calculations where the effects of the PFRs and $H_{2}$ self-shielding have been neglected. PFRs could also be important in calculating the buildup of the dissociating background. A self-consistent calculation of feedback effects on star formation, including the new feedback process discussed in this study, will be the subject of a subsequent paper. We will use a three-dimensional cosmological simulation with radiative transfer, in order to understand what regulates the star formation at high redshift.

This paper is organized as follows. In § 2 we describe chemical and cooling/heating processes included in the radiative transfer code. In § 3 we discuss some representative simulations and find analytical formulae that fit the simulation results. In § 4 we use this analytical relationship to constrain the parameter space where negative or positive feedback occurs. In § 5 we discuss the opacity of the IGM to the photodissociating background. We summarize our results in § 6.

Throughout this paper, when we talk about “small halos,” we refer to objects with virial temperatures $T_{vir} \lesssim 10^{4}$ K that rely on the presence of molecular hydrogen in order to collapse. Conversely, “large halos” are objects with $T_{vir} \gtrsim 10^{5}$ K that can cool down and collapse even if $H_{2}$ is completely depleted. The cosmological model we adopt is a flat $\Lambda$CDM model with density parameters $(\Omega_{\Lambda}, \Omega_{0}, \Omega_{b}) = (0.7, 0.3, 0.04)$ and Hubble constant $H_{0} = 70$ km s$^{-1}$ Mpc$^{-1}$. Thus, the baryon density is $\Omega_{b} h^{2} = 0.0196$, compatible with D/H inferences from big bang nucleosynthesis (Burles & Tytler 1998).
2. RADIATIVE TRANSFER IN THE PRIMORDIAL UNIVERSE

We use one-dimensional radiative transfer simulations to investigate the evolution of H$_2$ photodissociation regions in the primordial universe. We are interested in studying the evolution of the abundances and ionization states of hydrogen, helium, and molecular hydrogen around a single ionizing/dissociating source that turns on at redshift $z_t$. Hubble expansion and Compton heating/cooling are also included.

2.1. One-Dimensional Nonequilibrium Radiative Transfer

The radiative transfer equation in an expanding universe in comoving coordinates has the following form:

$$\frac{1}{c} \frac{\partial J_\nu(R)}{\partial t} + \frac{1}{c} \frac{\partial J_\nu(R)}{\partial R} - \frac{H}{c} \left[ \frac{\partial J_\nu(R)}{\partial \ln \nu} - 3J_\nu(R) \right] = \epsilon_\nu - \kappa_\nu J_\nu(R) ,$$

(2)

where $J_\nu(R)$ (ergs s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$) is the specific intensity and $a = (1 + z_{em})/(1 + z_{abs})$, with $z_{em}$ and $z_{abs}$ the emission and absorption redshifts and $\epsilon_\nu$ and $\kappa_\nu$ the emissivity and absorption coefficients.

If the scale of the problem is smaller than the horizon size, $c/H$, and $| \partial J_\nu/R \partial \ln \nu | \sim J_\nu$ (true in the case of continuum radiation), we can neglect the cosmological terms. In § 2.4 we show that we can also use the classical radiative transfer equation for lines if we account for the cosmological redshift of the radiation (or line cross sections). Finally, if the emission and absorption coefficients do not change on timescales shorter than a light crossing time, $(L/c)$, we can solve at each time step the stationary classical radiative transfer equation. For the case of a single point source, the solution is the attenuation equation

$$J_\nu(R) = \frac{J_\nu(0)}{R^2} \exp \left[ - \tau_\nu(R) \right] ,$$

(3)

where

$$\tau_\nu(R) = \sum_i n_i(r) \sigma_i(v) dr ,$$

(4)

with $n_i$ the number density and $\sigma_i$ the absorption cross section of species $i$.

2.2. Chemistry and Initial Conditions

We solve the time-dependent equations for the photochemical formation/destruction of eight chemical species (H, H$^+$, H$^-$, H$_2$, H$_2^+$, He, He$^+$, He$^{++}$), including the 37 main processes relevant to determine their abundances (Shapiro & Kang 1987). We use ionization cross sections from Hui & Gnedin (1997) and photodissociation cross sections from Abel et al. (1997).

The energy equation is

$$\frac{d\epsilon_a}{dt} = \Gamma - \Lambda ,$$

(5)

where $\epsilon_a = (3kT/2)n_H[1 + x(\text{He}) + x_e]$, with $n_H$ the hydrogen number density and $x(\text{He})$ and $x_e$ the helium and electron fractions, respectively. Note that $n_H$ is a function of time because of the Hubble expansion. In addition, $x_e$ is time dependent.

The cooling function $\Lambda$ includes H and He line and continuum cooling (Shapiro & Kang 1987) and molecular rovibrational cooling excited by collisions with H and H$_2$ (Martin, Schwarz, & Mandy 1996; Galli & Palla 1998). As mentioned above, adiabatic cosmic expansion cooling is also included. The heating term $\Gamma$ includes Compton heating/cooling and photoionization/photodissociation heating. We solve the system of ordinary differential equations for the abundances and energy equations, using a fourth-order Runge-Kutta solver. We switch to a semi-implicit solver (Gnedin & Gnedin 1998) when it is more efficient (i.e., when the abundances in the grid are close to their equilibrium values). Convergence analysis showed that a logarithmic grid with 400 cells in space and 400 cells in frequency (for the continuum flux) coordinates is sufficient to achieve convergence within a 10% error. The spectral range of the radiation is between 0.7 eV and 1 keV.

The primordial helium mass fraction is $Y_p = \rho(\text{He})/\rho_b = 0.24$, where $\rho_b$ is the baryon density, so that $x(\text{He}) = Y_p/4(1 - Y_p) = 0.0789$. The initial values at $z = z_i$ for the temperature and species abundances in the IGM are $T = 10^4$ K, $x_{H_2} = 2 \times 10^{-6}$, and $x_e \approx x_{H_2} = 10^{-5} / (\hbar c \Omega H_0^2) = 6.73 \times 10^{-4}$. The initial abundance of the other ions is set to zero. We explore two cases: (1) sources embedded in the constant density IGM and (2) sources inside a virialized halo. For case (2) we use initial conditions and a density profile to match the numerical simulation of Abel et al. (2000).

The density distribution of massive stars in the halo is crucial for determining $\langle f_{esc} \rangle$, the escape fraction of ionizing photons (Ricotti & Shull 2000). If all the stars are located at the center of the DM potential, it is trivial to find $\langle f_{esc} \rangle$ for a given baryonic density profile because the calculation is reduced to the case of a single Str"omgren sphere,

$$f_{esc} = 1 - \frac{4\pi z^2_{H_2}}{S_0} \int_0^\infty n_H(R) R^2 dR ,$$

(6)

where $z^2_{H_2} = 2.59 \times 10^{-13}$ cm$^3$ s$^{-1}$ is the case B recombination rate coefficient at $T = 10^4$ K and $n_H$ (cm$^{-3}$) is the hydrogen number density. Assuming that the gas profile is given by solving the hydrostatic equilibrium equation in a DM density profile (Navarro, Frenk, & White 1997) and that the LyC photon luminosity, $S_0$ (photon s$^{-1}$), is proportional to the baryonic mass of the galaxy, we find

$$f_{esc} = \begin{cases} 1 - 0.55f_\rho \left( \frac{1 + z^3}{\epsilon} \right) & \text{if } (1 + z) < 1.22 \left( \frac{\epsilon}{f_\rho} \right)^{1/3} , \\ 0 & \text{if } (1 + z) > 1.22 \left( \frac{\epsilon}{f_\rho} \right)^{1/3} . \end{cases}$$

(7)

Here $z$ is the collapse redshift of the halo, $S_0 = (1.14 \times 10^{49}$ s$^{-1})f_\rho (M_{DM}/10^6 M_\odot)$, $\epsilon$ is the star formation efficiency normalized to the Milky Way, and $f_\rho$ is the collapsed gas fraction (see Ricotti & Shull 2000 for details). We expect $f_\rho$ to be small since the DM potential wells of these objects are too shallow to hold photoionized gas. When $\langle f_{esc} \rangle$ is not zero, the number of photons absorbed is such that all the gas in the halo is kept ionized. Since we assume spherical symmetry, we can only place the source at the center of the halo. From the steep rise of $\langle f_{esc} \rangle$ in equation (7), it is clear that $\langle f_{esc} \rangle$ is essentially either 1 or 0 for the majority of the redshifts and star formation efficiencies. In a more realistic geometry, $\langle f_{esc} \rangle$ turns out to be small but not zero. We can make a more realistic calculation if we place the grid outside the virial radius in the constant density IGM and...
reduce the ionizing flux by a factor \( \langle f_{\text{esc}} \rangle \).\(^2\) The escape fraction from the halo can be estimated with more accurate calculations (Dove, Shull, & Ferrara 2000; Ricotti & Shull 2000) or left as a free parameter.

### 2.3. Photon Production

The spectral energy distribution (SED) of the source is assumed to be either a constant power law, \( F_{\nu} \propto \nu^{-\alpha} \), with \( \alpha = 1.8 \) for the case of a miniquasar (QSO), a constant (at \( t = 0 \)) SED from a population of metal-free stars for the Population III source (Tumlinson & Shull 2000), or an evolving SED of stars with metallicity \( Z = 0.001 \) (Leitherer et al. 1995) for the Population II source. We consider the two extreme cases of an instantaneous burst of star formation or continuous star formation.

In Figure 1 we show the SED of a zero-metallicity population for instantaneous star formation, in which \( 100 M_\odot \) of gas is converted into stars with a Salpeter IMF, a lower mass cutoff at \( M_{\text{low}} = 1 M_\odot \), and an upper cutoff at \( M_{\text{up}} = 100 M_\odot \). The solid line shows the nonevolved SED (at \( t = 0 \)). We also show the photoionization and photodissociation cross sections for \( \text{H}^- \) (dotted line), \( \text{H}_2 \) (dashed line), and \( \text{H}_2^+ \) (dot-dashed line). The \( \text{H}_2 \) photodissociation cross section in the Lyman-Werner bands is the average cross section of the lines between 11.2 and 13.6 eV according to Abel et al. (1997).

In Figure 2 we show the SED of the \( Z = 0.001 \) metallicity population with the same parameters as for the Population III in Figure 1. The lines show the SED at \( t = 1, 5, 10, \) and \( 100 \) Myr after the burst (Leitherer et al. 1995).

We have explored the effects of changing the IMF and mass cutoff. The main difference is that the Ly\(\alpha\) luminosity \( S_0 \) can change by as much as an order of magnitude for a steeper IMF (\( \alpha = 3.3 \)) or for a Salpeter IMF (\( \alpha = 2.35 \)) with \( M_{\text{up}} = 30 M_\odot \). The Ly\(\alpha\) luminosity at \( t = 0 \) generated by converging instantaneously \( 10^6 M_\odot \) of baryons into stars is \( S_0 \approx 10^{53} \) (photon s\(^{-1}\)) for the Population III SED and \( S_0 \approx 6 \times 10^{52} \) (photon s\(^{-1}\)) for the Population II SED. The specific flux from the object is \( F_\nu = L_\nu / 4\pi R^2 \) (ergs s\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\)), where \( L_\nu \) is the specific luminosity.

In Ricotti, Gnedin, & Shull (2001) we erroneously underestimated the specific intensity by a factor of \( 4\pi \) for the Population II and Population III SEDs. Therefore, the stated photon luminosities in those figures should be a factor of \( 4\pi \) bigger.

### 2.4. Radiative Transfer for the Lyman-Werner Bands

In Figure 3 we show a representative simulation after \( t \approx 16 \) Myr from a burst of a Population III object turning on at \( z_i = 19 \) with total Ly\(\alpha\) photon luminosity \( S_0 \approx 1.2 \times 10^{47} \) s\(^{-1}\). We find a shell of \( \text{H}_2 \) formation just in front of the \( \text{H}\alpha \) region that we call a PFR, where, in some cases, the abundance of \( \text{H}_2 \) is much higher than the relic abundance of \( x_{\text{H}_2} = 2 \times 10^{-6} \). Figure 4 shows the gas temperature as a function of the comoving distance from the source at \( t \approx 0.05, 1, \) and 22 Myr for the same object shown in Figure 3. Even if the temperature is \( T \approx 10^4 \) K in the PFR, collisional dissociation of \( \text{H}_2 \) is not very effective at the typical densities of the IGM or in the outer part of galaxy halos.

In other cases, we find that the column density of \( \text{H}_2 \) formed ahead of the ionization region is high enough (\( N \gtrsim 10^{14} \) cm\(^{-2}\)) that some Lyman-Werner bands are optically thick at line center. In order to include this effect properly, we solve the radiative transfer not only for the continuum

\[^2\text{For the sake of simplicity we simply reduce the ionizing flux by a factor } \langle f_{\text{esc}} \rangle \text{ without changing the SED of the source that, in a realistic case, should become harder. Indeed, as noted in § 3, in the simulations where the source is at the center of a halo the emerging ionizing photons are both reduced and harder.}\]
F. 3.-Abundances as a function of the comoving distance from the source at \( t = 100 \) Myr for a Population III object turning on at \( z_i = 30 \) with LyC photon luminosity \( S_\nu = 1.2 \times 10^{44} \) s\(^{-1}\). The \( \text{H}^+ \) and He\( ^{1+} \) ionization fronts are at \( R = 5 \) kpc, and just ahead of the fronts is the positive feedback region with an abundance \( x_{\text{H}_2} \approx 5 \times 10^{-4} \). The thick (thin) line shows including (excluding) line radiative transfer in Lyman-Werner bands.

Fig. 3.—Abundances as a function of the comoving distance from the source at \( t \approx 100 \) Myr for a Population III object turning on at \( z_i = 30 \) with LyC photon luminosity \( S_\nu = 1.2 \times 10^{44} \) s\(^{-1}\). The \( \text{H}^+ \) and He\( ^+ \) ionization fronts are at \( R = 5 \) kpc, and just ahead of the fronts is the positive feedback region with an abundance \( x_{\text{H}_2} \approx 5 \times 10^{-4} \). The thick (thin) line shows including (excluding) line radiative transfer in Lyman-Werner bands.

radiation but also in lines. Since the \( \text{H}_2 \) and H\( ^+ \) lines are very narrow (because the IGM temperature is \( T \approx 10 \) K [\( \Delta v \approx 10^{-6} \)]), we need extremely high spectral resolution in the frequency range of 10.2–13.6 eV. Fortunately, we only need to resolve 76 absorption lines longward of 912 Å [\( R(0) \), \( R(1) \), \( P(1) \)] Lyman lines and \( R(0) \), \( Q(1) \), \( R(1) \) Werner lines] arising from the \( J = 0 \) and 1 rotational levels of \( v = 0 \) in the \( \text{H}_2 \) ground electronic state. Thus, we only need high spectral resolution in the vicinity of the absorption lines. This limits the number of the frequency bins to just \( 3 \times 10^4 \) instead of \( \sim 10^6 \) for the uniform sampling. At densities \( n_H \lesssim 10 \) cm\(^{-3}\), the population of upper rotational or vibrational states of \( \text{H}_2 \) is negligible even at \( T = 10^4 \) K. We also include some H\( ^+ \) Lyman series resonance lines that are close in frequency to \( \text{H}_2 \) lines. For these lines we use a Voigt profile, since they are usually in the damping wing regime of the curve of growth. For the Lyman-Werner lines we use Gaussian profiles since the optical depth does not exceed a few. We redshift the specific flux according to the distance from the source, so that the maximum redshift of a line depends on the grid physical size. For our simulation the maximum frequency redshift is smaller than the distance of two consecutive Lyman or Werner line “triplets.” Therefore, we need to consider only a limited frequency range around each triplet. We resolve the frequency profile of each one of the 76 absorption lines in the Lyman-Werner bands with about 100 grid points if \( T \approx 10^4 \) K and with a few points if \( T \approx 10^5 \) K. Another complication arises from the fact that our spatial grid is logarithmic. Therefore, at a large enough distance from the source, the line can be redshifted several line widths inside each grid cell. We will show in § 5 that, for the simple case of constant density, temperature, and molecular abundance, the optical depth can be calculated analytically. The line profile, in this case, is similar to a top-hat function with \( \tau = x_{\text{H}_2} n_0(z) \sigma_{\text{asc},i} (v_i) / H(z) \) if \( v_i - \Delta v \leq v \leq v_i \) and zero otherwise, where \( \Delta v = H(z) \Delta \nu / \lambda_i \) (see Fig. 11 below). Here \( H(z) \) is the Hubble constant, \( \sigma = (\pi e^2 / m_e c) \) is the classical cross section, \( \sigma_{\text{asc},i} \) is the oscillator strength, and \( \lambda_i \) is the wave-

Fig. 4.—Gas temperature as a function of the comoving distance from the source at times \( t = 0.05 \), 1, and 22 Myr after a Population III object turns on at \( z_i = 19 \) with LyC photon luminosity \( S_\nu = 1.2 \times 10^{49} \) s\(^{-1}\).

Fig. 4.—Gas temperature as a function of the comoving distance from the source at times \( t = 0.05 \), 1, and 22 Myr after a Population III object turns on at \( z_i = 30 \) with LyC photon luminosity \( S_\nu = 1.2 \times 10^{44} \) s\(^{-1}\).
length of the $i$th line. In Figure 5 we show an example of the Lyman-Werner band spectrum emerging from the PFR after $t = 50$ Myr from the source turn-on. The source is a Population III object with Lyc photon luminosity $S_0 \approx 10^{43}$ s$^{-1}$ turning on at $z = 30$. Each panel shows the spectrum at progressively higher resolution.

3. RESULTS

3.1. Simulation Results

Preceding the ionization front, a thick shell of several kiloparsecs of molecular hydrogen (with $x_{\text{H}_2}$ up to $10^{-4}$) forms because of the enhanced electron fraction in the transition region from the H II region to the neutral IGM. This shell can be optically thick in some Lyman-Werner H$_2$ lines depending on the redshift, source luminosity, and escape fraction. This has two main consequences: (1) the photodissociation fronts around the sources slow down and their final radii are smaller than in the optically thin case, and (2) optically thick PFRs could reduce the intensity of the cosmological background in the Lyman-Werner bands.

In Figures 6, 7, and 8 we show the isocontours of log $x_{\text{H}_2}$ as a function of time and comoving distance from the source. The thick lines show the analytical fits for the position of the photodissociation, formation, and ionization fronts as a function of time. Figure 6a shows an example

![Fig. 6a](image1.png)

**Fig. 6a**—Contours of log $x_{\text{H}_2}$ as a function of time and comoving distance from the source. The thick lines show the analytical fits of the photodissociation front (D), ionization front (I), and formation region (F). (a) Example of negative feedback: Population II SED, $S_0 = 10^{40}$ s$^{-1}$, turn-on redshift $z_i = 29$. The source is at the center of baryonic halo with density profile $n \propto R^{-2}$. (b) Example of positive feedback: Population III SED, $S_0 = 10^{50}$ s$^{-1}$, turn-on redshift $z_i = 19$.

![Fig. 6b](image2.png)

![Fig. 7a](image3.png)

**Fig. 7a**—Same as Fig. 6. (a) QSO SED, $S_0 \approx 10^{51}$ s$^{-1}$, turn-on redshift $z_i = 19$. (b) Fossil H II region: Population II SED (instantaneous star formation law), $S_0 \approx 10^{49}$ s$^{-1}$, turn-on redshift $z_i = 14$.

![Fig. 7b](image4.png)
where positive feedback is unimportant. The emitting object has a Population II SED, \( S_0 \approx 10^{50} \text{ s}^{-1} \), and a turn-on redshift \( z_i = 30 \). The source is at the center of a baryonic halo with density profile \( n \propto R^{-2} \). Figure 6b instead shows an example where positive feedback is important. The source has Population III SED, \( S_0 \approx 10^{40} \text{ s}^{-1} \), and a turn-on redshift \( z_i = 20 \). The photodissociation front moves so slowly that the PFR shell gets close to it, producing an enhancement of H\(_2\) abundance instead of a depletion. In Figure 7a we show a QSO SED, \( S_0 \approx 10^{31} \text{ s}^{-1} \), and a turn-on redshift \( z_i = 20 \). The miniquasar produces fronts similar to the Population III object. In Figure 7b the source is a Population II object with an instantaneous burst of star formation. After \( t \approx 10^7 \) yr, when OB stars start to explode as SNe, the H II region recombines, triggering the formation of H\(_2\). Finally, Figure 8b shows the effect of including radiative transfer in the Lyman-Werner lines; the photodissociation front slows down considerably with respect to the optically thin case (Fig. 8a).

The UVB background affects these results in a simple way. The H\(_2\) abundance is \( x_{H_2} \propto 1/(F_s + F_{1,W}) \), where \( F_s \) and \( F_{1,W} \) are the fluxes in the Lyman-Werner band from the source and from the background, respectively. In the optically thin case \( F_s \approx 8.4 \times 10^{-22} R_{\text{crit}}(S_0/10^{49} \text{ s}^{-1}) \) (ergs s\(^{-1}\) cm\(^{-2}\) Hz\(^{-1}\)). Therefore, the background flux equals the source flux at a distance from the source \( R_{\text{crit}} \approx (8.4 \times 10^{-22}/F_{1,W})^{1/2}(S_0/10^{49} \text{ s}^{-1})^{1/2} \) kpc. At a distance \( R = 3R_{\text{crit}} \) the background flux will reduce our calculations of \( x_{H_2} \) by a factor of 10.

### 3.2. Analytical Fits

Let us introduce some relevant timescales. The collisional recombination timescales for neutral hydrogen and protons are \( t_{\text{H}} = t_{\text{rec}}(1 - x_e)/x_e \) and \( t_{\text{H},p} = t_{\text{rec}}/x_e \), respectively, where \( x_e \) is the electron fraction number density. Here we define \( t_{\text{rec}} = 1/[x_{H_2}^2 n_{H_2}] \), where \( x_{H_2}^2 = 2.59 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1} \) is the case B recombination coefficient at \( T = 10^4 \text{ K} \) and \( n_{H_2}(z) = (1.7 \times 10^{-7} \text{ cm}^{-3})(1 + z)^3 \) is the hydrogen number density for \( \Omega_b h^2 = 0.019 \). The age of the universe \( t_{\text{H}} \) and \( t_{\text{rec}} \) at the redshift \( z_i \) when the source turns on are

\[
\begin{align*}
    t_{\text{H}} & \approx \frac{2}{3} \frac{1}{H_0 \sqrt{\Omega_0}} (1 + z_i)^{-3/2} \\
    & = 538 \left( \frac{1 + z_i}{10} \right)^{-3/2} \text{ Myr}, \quad (8) \\
    t_{\text{rec}} & \approx \frac{1}{x_{H_2}^2 n_{H_2}(z)} = 720 \left( \frac{1 + z_i}{10} \right)^{-3} \text{ Myr}. \quad (9)
\end{align*}
\]

If the density of the IGM is constant and uniform, the radius \( R_f \) of the ionization front is

\[
R_f = \frac{1 - \exp \left( -\frac{t}{t_{\text{rec}}} \right)^{1/3}}{t_{\text{rec}}}, \quad (10)
\]

where \( R_s = [3S_0 t_{\text{rec}}(4 \pi n_{H_2}(z))^{1/3}] \) is the Strömgren radius and \( t \) is the time the source is on. The typical time for the H II region to reach the Strömgren radius in a nonexpanding IGM equals the H\(^+\) recombination time. A source turning on at redshifts \( z_i \lesssim 18 \), for which \( \lambda = t_{\text{H}}/t_{\text{rec}} \lesssim 2 \), produces an H II region that never reaches the Strömgren radius (Donahue & Shull 1987; Shapiro & Giroux 1987). In comoving coordinates, it expands forever because of cosmic dilution. This is true only if the source continues to shine with constant photon luminosity \( S_0 \). We therefore remind the reader of another typical timescale, namely, the time \( t_{\text{burst}} \approx 5 - 20 \text{ Myr} \) during which an instantaneous burst of star formation produces a substantial amount of ionizing photons.

Based on the simulations, we find analytical relationships that are good fits to the comoving front radii (radius of the ionization sphere, \( R_f \), radius of the photodissociation sphere, \( R_D \), and outer radius of the PFR, \( R_p \)), the peak H\(_2\) abundance \( x_{H_2}, F \), comoving thickness \( \Delta R_p \), and column density \( N_p \) of the PFR as a function of time. We also estimate the timescale, \( t_p \), on which a region in the IGM lies inside the PFR. These relations, without taking into account positive feedback, are shown in Figures 8a and 8b.
account line radiative transfer, are

\[ R_d = (16 \text{ kpc}) \left( \frac{1 + z}{10} \right) \beta S_{0.49} f_2(t) t^{1/2}, \]  
\[ R_f = (21 \text{ kpc}) \left[ S_{0.49} \langle f_{esc} \rangle f_1(t) \right]^{1/3}, \]  
\[ \Delta R_f = (5 \times 10^{-5} \gamma \text{ kpc}) \left( \frac{1 + z}{n_h(z)} \right) \beta (S_{0.49} \langle f_{esc} \rangle t)^{0.18}, \]  
\[ = (3.2 \gamma \text{ Mpc}) \left( \frac{1 + z}{10} \right)^{0.7} \left( \frac{S_{0.49} \langle f_{esc} \rangle t}{t_c^{0.466}} \right)^{0.18}, \]  
\[ \Delta R_f = \frac{\Delta R_f}{3}, \]

where \( S_{0.49} \) is the ionizing photon luminosity in units of \( 10^{49} \) (photon s\(^{-1}\)), \( \beta \) and \( \gamma \) are fitting parameters (Table 1) that depend on the SED of the object (\( \beta = \gamma = 1 \) for a Population III SED), and \( t \) is the time the source was on in Myr. \( \Delta R_f \) is the comoving thickness of the ionization front. The functions \( f_1(t) \) and \( f_2(t) \) are given by

\[ f_1(t) = \frac{(8.95 \times 10^5) \lambda}{(1 + z \hat{b})^3} \exp \left( \frac{\lambda}{t_c} \right) \]
\[ \times \left[ t_c E_2 \left( \frac{\lambda}{t_c}, \lambda \right) - E_2 \left( \lambda \right) \right] \text{ Myr}, \]  
\[ f_2(t) = 3 t f (1 - t e^{-1/3}) \text{ Myr}, \]

where \( t_c = 1 + t / t_{He} \), \( \lambda = t_{He} / t_{rec} \), and \( E_2(x) \) is the exponential integral of order \( n \) (Donahue & Shull 1987; Shapiro & Giroux 1987). Note that \( f_1(t) \sim t \) if \( t \leq t_{He} \) and \( f_2(t) \sim t \) if \( \lambda \leq 2 \) (i.e., \( z \leq 18 \)). Table 1 shows the normalization parameters \( \beta \) and \( \gamma \) and the ionizing photon luminosity \( S_{0.49} \) produced by an instantaneous burst of \( \sim 250 M_\odot \) of gas into stars for the SEDs from Population III, Population II (continuous star formation), and miniquasars.

Here the photodissociation front is defined as the locus where the molecular abundance is \( x_{H_2} = 10^{-6} \), half the relic \( H_2 \) fraction. In the optically thin regime, which is a good approximation in this case, the profile of the \( H_2 \) abundance inside the dissociation sphere is exponential: \( x_{H_2} = 2 \times 10^{-6} \exp \left[ - \ln (2) R / R_d \right] \). The photodissociation front slows down at \( t \geq t_{He} \), after the initial \( t^{1/2} \) expansion law. At late times the dissociation front approaches the maximum radius \( R_d = (340 z) \text{ kpc} \left( 1 + z / 10 \right)^{1/4} \beta S_{0.49}^{1/12} \), where \( \alpha = \left( 1 - (1 + z) z^{1/2} \right) 1/2 \). The relation \( (1 + z) = (1 + z) f_c^{-3} \) is used to relate time and redshift. The maximum thickness of the ionization front \( \Delta R_f = (7 \gamma \text{ Mpc} \) \left( 1 + z / 10 \right)^{0.43} \left( S_{0.49} \langle f_{esc} \rangle \right)^{0.18} \) is reached at \( t = 0.6 t_{He} \). When the ionization front is inside the halo with a density profile \( n \propto R^{-2} \), where \( R \) is the radius, we find \( \log R_f \propto (\log t)^2 \). The emerging spectrum in this case is

### Table 1

| Object        | \( S_{0.49} \) (250 \( M_\odot \) burst) | \( \beta \) | \( \gamma \) |
|---------------|---------------------------------|--------|--------|
| Population II | 2.8                            | 2.4    | 0.67   |
| Population III| 3.2                            | 1.0    | 1.0    |
| Quasar        |                                 | 0.8    | 1.17   |

The maximum value of \( x_{H_2,F} \), reached at \( t = (10 / 3) t_{He} \), is given by

\[ x_{H_2,F} = 5.9 \times 10^{-4} \left( \frac{1 + z}{10} \right)^{1/3} S_{0.49} \langle f_{esc} \rangle^{2/3}. \]

From equations (11)–(19) it is easy to derive useful relationships to quantify the importance of positive feedback as a function of the unknown free parameters. We will use these relationships in the next section. The ratio

\[ \frac{R_d}{R_f} = 0.76 \left( \frac{1 + z}{10} \right) \left( S_{0.49} \langle f_{esc} \rangle^{-1/3} \beta^{-1/2} S_{0.49}^{1/6} g(t) \right) \]

reaches the maximum value of

\[ \left( \frac{R_d}{R_f} \right)_{\text{max}} = 1.6 \left( \frac{1 + z}{10} \right)^{3/4} \left( S_{0.49} \langle f_{esc} \rangle^{-1/3} \beta^{-1/2} S_{0.49}^{1/6} \right) \]

at \( t \approx 0.9 t_{He} \), where the function \( g(t) = \left[ f_1(t) \right]^{1/2} \left[ f_2(t) \right]^{-1/3} \). The function has a maximum value of \( g = 0.75 t_{He}^{0.49} = 2.1(1 + z / 10)^{-1/4} \) at \( t = 0.9 t_{He} \).

It is also useful to estimate the \( H_2 \) column density \( N_F \) of the PFR and the timescale \( t_F \) on which a region in the IGM can be engulfed by the PFR:

\[ N_F \approx \frac{n x_{H_2,F} \Delta R_F}{1 + z} = (1.6 \times 10^{13} \text{ cm}^{-2}) \frac{\gamma}{\beta} \times \left( \frac{1 + z}{10} \right)^{2.6} \left( \frac{\langle f_{esc} \rangle}{S_{0.49}^{0.15} \text{c}} \right) \]
with the maximum value of

$$N_F^{\text{max}} = (9 \times 10^{14} \text{ cm}^{-2}) \frac{1}{\beta} \left(1 + z\right)^{1.3} \frac{\langle f_{\text{esc}} \rangle^{0.85}}{S_{0.49}^{0.15}}$$  \hspace{1cm} (24)$$

at $t \simeq 0.9t_{\text{ff}}$, and

$$t_F = \Delta R_F \left(\frac{dR}{dt}\right)^{-1} = \left(152t\right)\left(1 + z\right)^{0.7} \times \left(\frac{S_{0.49} \langle f_{\text{esc}} \rangle t^{-0.15}}{t_{\text{ff}}^{0.2}}\right).$$  \hspace{1cm} (25)$$

Finally, we derive the ratio $R_D/R_F = R_D/(R_I + \Delta R_F) = (R_D/R_I)(1 + \Delta R_F/R_I)^{-1}$ that gives us an idea of the fraction of the IGM volume in which the molecular hydrogen is destroyed:

$$R_D R_I = \frac{R_D}{R_I} \left[1 + 51\left(1 + z\right)^{0.7} \frac{S_{0.49} \langle f_{\text{esc}} \rangle t^{-0.15}}{t_{\text{ff}}^{0.2}}\right]^{-1},$$  \hspace{1cm} (26)$$

with the maximum value of

$$\left(\frac{R_D}{R_F}\right)^{\text{max}} = \frac{0.15 \beta^{1/2}}{\gamma} \left(\frac{\langle f_{\text{esc}} \rangle \left(1 + z\right)}{10}\right)^{-0.18} S_{0.49}^{0.18}$$  \hspace{1cm} (27)$$

at $t \simeq 0.9t_{\text{ff}}$.

4. DISCUSSION: NEGATIVE OR POSITIVE FEEDBACK?

In this section we use the analytical relationships found in § 3.2 to quantify the importance of the positive feedback as a function of the free parameters of the model. The free parameters are the Ly$\alpha$ escape fraction $\langle f_{\text{esc}} \rangle$, the star formation efficiency $\epsilon$ normalized to that in the Milky Way, and the collapsed gas fraction $f_g$. For a fixed cosmology, the ionizing photon luminosity is $S_0 = (1.14 \times 10^{46} \text{ s}^{-1}) \epsilon f_g (M_{\text{DM}}/10^6 M_\sun)$ (see Ricotti & Shull 2000 for details).

We quantify the importance of the positive feedback by showing in Figure 9 isocontours of constant ratio, $R_D/R_F$, of the photodissociation front radius to the formation front radius 10 Myr after the source turned on. Here the radius of the dissociation front $R_x$ is defined as the locus where the relic molecular abundance has dropped to $x_{H_2} = 10^{-8}$; therefore, it is smaller by a factor $\ln(200)/\ln(2) \approx 7.6$ with respect to the values given in the previous paragraph. Clearly, if $R_D/R_F < 1$, the dissociation region does not exist. Instead, the H$_2$ abundance could increase with respect to the relic value $x_{H_2} \approx 10^{-6}$ (for example, see Fig. 6b). Therefore, $R_D/R_F$ gives us an idea of the mean molecular abundance in the IGM and the opacity of the IGM to the photodissociating background.

We find that the existence of positive feedback depends crucially on $\langle f_{\text{esc}} \rangle$ and the SED of the first objects (Population III, Population II, or active galactic nucleus [AGN]). Figure 9 shows the parameter space where positive feedback is possible in the particular case of a Population III SED. The contour lines show $R_D/R_F$ as a function of redshift and mass of the halo. The shaded region shows the parameter space where $R_D/R_F < 1$, in which case the PFR fills up the region between the H II region and the photodissociation front. At small redshifts, the boundary of the shaded region is produced by the additional constraint that the H$_2$ abundance of the PFR has to be $x_{H_2} > 10^{-5}$. The choice of this value is somewhat arbitrary, but the main purpose is to show the H$_2$ abundance in the positive feedback region as a function of the redshift and halo mass. The thick solid line at the bottom is the minimum mass to collapse as a function of redshift according to the criteria of Abel et al. (1998). The two dashed lines show objects with virial temperatures of $T_{\text{vir}} = 10^4$ and $10^5$ K; protogalaxies that lie above $T_{\text{vir}} = 10^4$ K are not subject to negative/positive feedback because they can cool by H I line excitation (Ly$\alpha$). The minimum mass for collapse is calculated assuming that the object lies outside of a photodissociation region or a PFR and that the dissociating background is.

![Fig. 9a](image1.png)

**Fig. 9a.** Contours show $R_D/R_F$ for our standard model and cosmological parameters (§ 1). The shaded region ($R_D/R_F < 1$) shows the redshift and halo masses where positive feedback is dominant. The thick solid line shows the minimum mass needed to collapse according to Abel et al. (1998). Parameters are as follows: $\langle f_{\text{esc}} \rangle$ is the escape fraction, $\epsilon$ is the star formation efficiency normalized to the Milky Way, $f_g$ is the collapsed gas fraction, and $S_0 = (1.14 \times 10^{46} \text{ s}^{-1}) \epsilon f_g (M_{\text{DM}}/10^6 M_\sun)$. The dot-dashed lines show the collapse redshift of 1 and 3 $\sigma$ perturbations according to linear theory. (a) Population III SED, $\epsilon = 1$, $f_g = 1$, and $\langle f_{\text{esc}} \rangle = 0.2$. (b) Population III SED, $\epsilon = 1$, $f_g = 0.1$, and $\langle f_{\text{esc}} \rangle$ given by the analytical formula derived in Ricotti & Shull (2000).
negligible. The amount of H$_2$ formed in a just virialized object does not depend on the initial H$_2$ abundance, but it is sensitive to the electron fraction. For this reason, protogalaxies less massive than those found in the Abel et al. (1998) calculations can form inside a PFR. Finally, we note that the presence of PFRs will increase the opacity of the IGM in the Lyman-Werner lines, further decreasing the intensity of the dissociating UV background. All these effects have to be included in a three-dimensional cosmological simulation with radiative transfer in order to understand their global effect on structure formation and the star formation history.

5. IGM OPTICAL DEPTH IN THE LYMAN-WERNER BANDS

In this section we estimate the IGM optical depth in the Lyman-Werner bands that arises from the absorption in 76 narrow H$_2$ lines from $J = 0$ and 1 in $v = 0$ at different redshift. This calculation is analogous to the one in Haiman et al. (2000). We repeat it because we disagree with their technical analysis of H$_2$ line scattering and fluorescence. Haiman et al. (2000) assumed that only the fraction of absorptions that decay to the dissociating continuum remove photons from the UVB (about 11% of the time). For the other 89% of the absorptions, they assume that the Lyman-Werner photon is reemitted at the same frequency, with no net effect. This is not correct. Following the absorption in the Lyman or Werner bands, the molecule decays to a variety of rovibrational levels in the ground electronic state because the quadrupole transitions within the electronic excited state are much slower. The H$_2$ decays either to the $b^2Sigma^+_u$ (antibonding) state, which decays to the vibrational continuum (predisassociation), or to a bound vibrational rotational level in the electronic ground state ($X'Sigma^+_g$). At moderate UV intensities, the subsequent infrared cascade through the bound levels of the ground electronic state is entirely determined by the radiative decay rates (Black & Dalgarno 1976). From the cascade probabilities, Shull (1978) computed that a Lyman-Werner photon has a 14% probability, on average, to be reemitted at the same frequency. Approximately 12% of the absorption transitions dissociate and 74% fluoresce to excited ($v, J$) levels of $X'Sigma^+_g$. Roughly speaking, the probability to decay to one of the other 14 bound vibrational levels is about 6%. Therefore, only 14% of the time the Lyman-Werner photon is resonantly scattered following an absorption. The other 86% of the time, H$_2$ dissociates or the photon is split into infrared and less energetic (about 1 eV energy loss) UV photons that are removed from the Lyman-Werner bands right away or after a few absorptions.

Therefore, the H$_2$ optical depth of the IGM is given by

$$\tau_i(z_{ob}, z_{em}) = \frac{\pi e^2}{m_e c} \sum_{i=n_{h2}(v)} f_{asc,i}(1-f_{i,v'=0}) \times \left( \frac{z_{em}}{z_{ob}} \right) c \frac{dt}{dz} n_H(z') x_{H_2}(z') \phi(v', v_i),$$

where $z_{ob}$ and $z_{em}$ are the observer and emission redshifts, $v_i = v(1 + z_{em})/(1 + z_{ob})$, $n_H(z) = (1.12 \times 10^{-5} \text{ cm}^{-3}) \Omega_J^2 \hbar^2 (1 - Y_p) (1 + z)^3$ is the neutral H number density in the IGM, $\phi$ is the line profile, $f_{asc,i}$ is the oscillator strength, and $f_{i,v'=0}$ is the probability to decay to the ground vibrational level of the $X'Sigma^+_g$ state for the $i$th line calculated from Black & Dalgarno (1976). The maximum redshift interval a UV photon can travel before it is absorbed by a neutral atom corresponds to the redshift between two H $_1$ resonances in the higher Lyman series, the “dark screen” approximation of Haiman et al. (2000). Therefore, a photon is subject to the absorption from a subset of the 76 Lyman-Werner lines, $n_{h2}(v_i) \leq i \leq n_{h2}(v)$, where $n_{h2}(v)$ is the first Lyman-Werner line with frequency just above $v$ and $n_{h2}(v) > n_{h2}(v)$ is the Lyman-Werner line with frequency just below the next higher H $_1$ Lyman line with frequency greater than $v$.

It is possible to write an approximate analytical solution of equation (28), if we assume Gaussian line profiles,

$$\phi(v, v_i) = \frac{1}{\Delta \Gamma} \frac{1}{\sqrt{2\pi}} \exp\left[-\left(\frac{v - v_i}{\Delta \Gamma}\right)^2\right],$$

where $\Delta \Gamma = (\Gamma_i/2\pi) [(v - v_i)^2 + (\Gamma_i/2)^2]$, where $\Gamma_i = \gamma_i/2\pi$ and $\gamma_i = \sum_{j<i} (i \rightarrow j)$ is the natural width of the $i$th H $_1$ line. For a constant $x_{H_2} = 2 \times 10^{-6}$ molecular abundance, we have

$$\tau_i(z_{ob}, z_{em}) = 3.28 \times 10^{12} \frac{(1 + z_{ob})^{3/2}}{v} \sum_{n_{h2}(v)} f_{asc,i}(1-f_{i,v'=0}) \sqrt{\frac{v}{v_i}} \Phi(v_i),$$

where

$$\Phi(v) = \begin{cases} \frac{1}{\sqrt{\pi}} \arctan \left( \frac{v - v_i}{\Gamma_i} \right) - \arctan \left( \frac{v - v_i}{\Gamma_i} \right) & \text{for Lorentzian profile} \\ \frac{1}{2} \left( \text{erf} \left( \frac{v - v_i}{\Delta \Gamma} \right) - \text{erf} \left( \frac{v - v_i}{\Delta \Gamma} \right) \right) & \text{for Gaussian profile} \end{cases}$$

and $\text{erf}(x)$ is the error function. In Figure 10 we show the H$_2$ total optical depth (i.e., up to the maximum $z_{em}$ visible to the observer) of the IGM in the Lyman-Werner bands at redshifts $z = 30$ (solid line) and 15 (dashed line). The opacity

![Figure 10](image-url)
at energies less than Lyβ (hν < 12.09 eV) is produced by the H₂ Lyman lines. At energies higher than Lyβ, the H₂ Werner lines are also important. The maximum opacity that we find is τ ∼ 2, about 6 times higher than that found by Haiman et al. (2000). The background flux is thus reduced by an order of magnitude if we assume an average molecular fraction $x_{H_2} = 2 \times 10^{-6}$.

For the Gaussian line profile, the expression inside the square brackets of equation (30) tends to the asymptotic value in equation (31). The maximum optical depth of the ith line is therefore

$$\tau_{\text{max}}(z_{\text{ob}}) \approx x_{H_2} n_d(z = 0) \frac{c}{H_0} \frac{1 + z_{\text{ob}}}{v_i} \frac{12 \text{ eV}}{h v_i} \left( \frac{f_{\text{osc.}}}{10^{-2}} \right) \left( 1 + \frac{z_{\text{ob}}}{30} \right)^{3/2}. \quad (31)$$

In Figure 11 we show the optical depth through a constant density and molecular fraction gas for a single line. When the source redshift $z_{\text{em}}$ increases, the profile becomes wider and the optical depth tends to the asymptotic value $\tau_{\text{max}}$ in equation (31).

Finally, we calculate the total optical depth of the IGM as a function of distance from a single source. We also include in the calculation the Lyman series lines of H I, and we investigate the importance of the damping wings of the heavily saturated lines. The mean optical depth for photodissociation, $\langle \tau_{\text{GM}} \rangle$, can be calculated by solving the following equations:

$$k_{\text{diss}} = \text{const} \sum_{i=1}^{76} f_{\text{osc.}} I_{\text{diss}} \int d' \frac{J_{\nu}'}{h v'} \phi(v', v) \, , \quad (32)$$

$$k_{\text{diss}} \exp (-\langle \tau_{\text{GM}} \rangle) = \text{const} \sum_{i=1}^{76} f_{\text{osc.}} I_{\text{diss}} \int d' \frac{J_{\nu}'}{h v'} \phi(v', v) \times e^{-\langle \tau_{\text{GM}} \rangle (v' - z_{\text{em}}, z_{\text{ob}})} \, , \quad (33)$$

where $k_{\text{diss}}$ is the photodissociation rate and const = $4\pi x_{H_2} n_d(z_{\text{ob}}) \sigma$ with $\sigma = (\pi e^2/m_e c)$. Note that $\langle \tau_{\text{GM}} \rangle$ differs from $\tau$ in equation (29) since it includes the opacity of both H₂ and H I lines. In Figure 12 we show $\langle \tau_{\text{GM}} \rangle$ as a function of the comoving distance (and $z_{\text{ob}} < z_{\text{em}}$) from a source at $z_{\text{em}} = 30$. The solid line is calculated assuming a Voigt profile for the Lyman series hydrogen lines, therefore including the effect of line saturation. The dashed line is calculated neglecting line saturation. The insert is a zoom of the inner few Mpc, and the arrow indicates the distance at which the absorption lines are redshifted about one line width for gas at $T = 10^4$ K. Figures 5 and 12 both show clearly that the opacity at comoving distances from the source of less than 1 Mpc is produced in the PFR shell. The IGM opacity starts to be important around 10 Mpc. This reduces the photodissociation radius of the strongest sources at high redshift.

We remind the reader that all the calculations in this section assume a constant molecular fraction in the IGM of $x_{H_2} = 2 \times 10^{-6}$. In order to calculate a realistic average molecular fraction in the IGM as a function of the redshift,
we need to calculate the filling factor of the photodissociation regions, PFRs, and the H\textsubscript{2} formed inside relic H\textsubscript{II} regions. Only with a three-dimensional radiative transfer simulation will it be possible to treat self-consistently the aforementioned feedback effects.

6. DISCUSSION AND SUMMARY

The results of this work reinforce the possibility that the population of low-mass primordial galaxies (Population III) could exist, without being immediately suppressed by radiative feedback. A quantitative answer to this question has to be given by high-resolution cosmological simulations. Until the buildup of the dissociating background, local feedback effects regulate star formation. When the star formation is suppressed in a halo, it is reasonable to expect that H\textsubscript{II} regions start to recombine. The relic H\textsubscript{II} region, as shown in §3, produces new molecular hydrogen and perhaps a second burst of star formation. This is especially effective at high redshifts where the density of the IGM and protogalaxies is higher and the physical scales are smaller. Thus, at these redshifts, it is easier to believe that star formation is bursting rather than continuous. The picture that could emerge from numerical simulations is that H\textsubscript{II} regions and photodissociation regions in the IGM are short lived instead of continuously expanding, as in the reionization simulations of Gnedin (2000). This will have important effects on the distribution of the metals and the chemical evolution of galaxies.

In summary, our key results are as follows:

1. We have found a new positive feedback effect on the formation of H\textsubscript{2}. Each source of radiation produces a shell (PFR) of H\textsubscript{2} in front of the H\textsubscript{II} region with a thickness of several kiloparsecs and peak abundance $X_{H_2} \sim 10^{-4}$. The H\textsubscript{2} column density of the PFR is typically $N_f(H_2) \sim 10^{14} - 10^{15}$ cm$^{-2}$. Fossil H\textsubscript{II} regions, if they exist, are an important mechanism of H\textsubscript{2} production, both in the IGM and inside protogalaxies.

2. The PFR can be optically thick in the lines of the H\textsubscript{2} Lyman-Werner bands. The implication is twofold: (1) the photodissociation region around each single source is about 1.5 times smaller than in the optically thin case, and (2) the H\textsubscript{2} optical depth of the IGM increases. In a later paper we will calculate the IGM optical depth and the effect on the intensity of the photodissociating background by means of cosmological simulations.

3. We provide analytical formulae that fit the simulation results, in order to make a parametric study of the importance of positive feedback as a function of redshift. The most important parameters are $\langle f_{esc} \rangle$ and the SED of the sources (Population III, Population II, or AGN). If $\langle f_{esc} \rangle$ is not extremely small, PFRs have important effects on the opacity of the IGM to the H\textsubscript{2} photodissociating background and the size of photodissociation regions.

4. The background opacity of the IGM in the H\textsubscript{2} Lyman-Werner bands is about unity if $x_{HI} = 2 \times 10^{-6}$. Therefore, if the relic molecular hydrogen is not immediately destroyed, it can decrease the photodissociating background flux by about an order of magnitude.

The aforementioned results are the foundations on which we will construct a cosmological simulation in which these effects are treated self-consistently.

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