Beyond $J_{\text{crit}}$: a critical curve for suppression of H$_2$–cooling in protogalaxies

J. Wolcott-Green, Z. Haiman and G. L. Bryan*

Department of Astronomy, Columbia University, 550 West 120th Street, MC 5246, New York, NY 10027, USA

ABSTRACT

Suppression of H$_2$-cooling in early protogalaxies has important implications for the formation of supermassive black holes seeds, the first generation of stars, and the epoch of reionization. This suppression can occur via photodissociation of H$_2$ (by ultraviolet Lyman–Werner [LW] photons) or by photodetachment of H$^-$, a precursor in H$_2$ formation (by infrared [IR] photons). Previous studies have typically adopted idealised spectra, with a blackbody or a power–law shape, in modeling the chemistry of metal-free protogalaxies, and utilised a single parameter, the critical UV flux, or $J_{\text{crit}}$, to determine whether H$_2$-cooling is prevented. This can be misleading, and that independent of the spectral shape, there is a critical curve in the $(k_{\text{LW}}, k_{\text{H}^-})$ plane, where $k_{\text{LW}}$ and $k_{\text{H}^-}$ are the H$_2$-dissocation rates by LW and IR photons, which determines whether a protogalaxy can cool below $\sim 1000$ Kelvin. We use a one-zone model to follow the chemical and thermal evolution of gravitationally collapsing protogalactic gas, to compute this critical curve, and provide an accurate analytical fit for it. We improve on previous works by considering a variety of more realistic Pop III or Pop II-type spectra from population synthesis models and perform fully frequency-dependent calculations of the H$_2$-photodissociation rates for each spectrum. We compute the ratio $k_{\text{LW}}/k_{\text{H}^-}$ for each spectrum, as well as the minimum stellar mass $M_\ast$, for various IMFs and metallicities, required to prevent cooling in a neighboring halo a distance $d$ away. We provide critical $M_\ast/d^2$ values for suppression of H$_2$-cooling, with analytic fits, which can be used in future studies.

Key words: cosmology: theory – early Universe – galaxies: formation – molecular processes – stars: Population III

1 INTRODUCTION

It has long been known that the cooling of metal–free, primordial gas, from which the first generation of stars form in the first protogalaxies, is dominated by H$_2$ molecules (Saslaw & Zipoy [1967]). Furthermore, the abundance of H$_2$ molecules in an early protogalaxy is sensitive to radiation impinging on the galaxy, and can be regulated by the early ultraviolet (UV) background in the Lyman-Werner bands (Haiman et al. 1997). For unusually soft spectra, infrared (IR) radiation can also play a role, through the photodetachment of the H$^-$ ions, the main catalyst for H$_2$ formation in primordial gas (e.g. Omukai [2001]). Recent simulations have suggested that the first stars may not be as massive as had previously been thought (e.g. Greif et al. 2011). In the extreme case that the typical first-generation stars had masses as low as a few M$_\odot$, the IR radiation from these low-mass stars would dominate radiative feedback and H$_2$ chemistry in protogalaxies in the early Universe (Wolcott-Green & Haiman 2012). In recent years, the suppression of H$_2$ cooling via radiative feedback has attracted a lot of attention, in the context of forming massive black hole seeds in the early universe. Observations of high-redshift quasars reveal that supermassive black holes (SMBHs) with masses of $\sim 10^9$ M$_\odot$ have already formed as early as redshift $z \sim 7$ (Mortlock et al. 2011). A promising way to form such early massive SMBHs is to begin with a massive (say, $\sim 10^5$ M$_\odot$) seed BH at redshift $z \gtrsim 10$. This massive seed can then grow further by accretion, and reach $10^9$ M$_\odot$ by redshift $z \sim 7$. In particular, in contrast to starting with a stellar-mass BH, the accretion rate then need not exceed the value implied by the Eddington limit.

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* E-mail: jemma@astro.columbia.edu; zoltan@astro.columbia.edu; gbryan@astro.columbia.edu

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A promising site for forming such massive BH seeds are in the nuclei of so-called atomic-cooling halos — i.e. dark matter halos with virial temperatures $T_{\text{vir}} \gtrsim 10^4$K, or masses of $\gtrsim$ few $\times 10^5M_\odot$. Assuming that the gas at the center of such a halo is metal-free (or with metallicity at most $\sim 10^{-4}$ of the solar value; Omukai et al. 2008), and also that H$_2$-cooling is disabled, the gas remains at temperatures near $10^5$K. This leads to accretion rates in the core of the halo as high as $\sim 0.1 - 1 M_\odot$yr$^{-1}$. Several works have argued that under these conditions, fragmentation and Population III star-formation may be avoided, and a massive seed BH is produced instead, either by direct collapse, or via an intermediate state of a supermassive star (Oh & Haiman 2002; Bromm & Loeb 2003; Regan & Haehnelt 2006; Spaans & Silk 2006; Begelman et al. 2006; Sugimura et al. 2014) have investigated the relative importance of $k_{\text{LW}}$—photodissociation rate, and from blackbodies ($T_k = 10^3 - 10^5$K). We also provide an updated criterion for determining whether H$_2$—cooling is suppressed, as a fitting formula for the critical curve.

The non-existence of a single $J_{\text{crit}}$, and its importance for time-evolving spectra from population synthesis models has also been pointed out recently by Agarwal & Khochfar (2015) and Agarwal et al. (2016). These studies, as well as Sugimura et al. (2014) have investigated the relative importance of $k_{\text{LW}}$ and $k_{\text{H}}$—from STARBURST99 and from blackbody spectra in suppressing H$_2$—cooling. We here improve on these studies by computing the H$_2$—photodissociation rate, summing over all relevant LW lines, rather than assuming that the spectrum is flat in the LW bands, or taking an average of the LW flux. We show that both previous approximations, though computationally efficient, introduce significant errors in the photodissociation rate compared to our full frequency-dependent calculation.

This paper is organised as follows: In §2 we describe the details of our numerical modeling, We present our results using a variety of STARBURST99 models in §3 along with an updated fitting formulae for both the critical curve and critical mass in stars. We briefly discuss the results and implications of our work for future studies, and offer our conclusions in §4.

2 MODELING

2.1 One-Zone Model

We use a one-zone model to follow the thermochemical history of primordial gas in a collapsing atomic cooling halo. This model has been shown to mimic the evolution found in three-dimensional hydrodynamical simulations very well (Shang et al. 2010, hereafter SBH10) and is described in detail in, e.g. Omukai et al. (2008). We briefly summarize the
model here and highlight a few important updates we made to the chemistry network.

The one-zone model prescribes a homologous spherical collapse, in which the dark matter evolution is that of a top hat overdensity with turnaround redshift \( z_{\text{ta}} = 17 \) and \( \rho_{\text{b,DM}} \) constant after virialization. The timescale of collapse is taken to be the free–fall time. Using the solver \textsc{lsodar}, we follow the thermal and chemical evolution of initially primordial gas, with nine chemical species included: \( \text{H}, \text{H}^+, \text{He}, \text{He}^+, \text{He}^{++}, \text{H}^- , \text{H}_2^+, \text{H}_2 \), and electrons. Deuterium species are not included, as they do not affect our results at the temperatures of interest here, which are too high for HD–cooking to be important. Compressional heating as well as photochemical heating and cooling processes are included as detailed in SBH10.

We have made several updates to the one–zone model, most of which have not been included in previous studies ([Agarwal et al. 2014], is an exception). We use the modified self–shielding expression provided by Wolcott-Green et al. (2011), which is more accurate for gas near the critical density, \( n \gtrsim 10^3 \text{ cm}^{-3} \). The impact of a non–LTE ro-vibrational distribution is discussed in \( \text{[3.7]} \) Wolcott-Green et al. (2011) showed that the column density approximation most often used in the one–zone model for the optically–thick \( k_{\text{LW}} \) overestimates shielding by about an order of magnitude in the density range of interest compared to 3D simulations. We therefore modify the column density as recommended in that study: \( N_{\text{H}_2} = 0.25 \times \lambda_{\text{Jeans}} \times n_{\text{H}_2} \), which is half of the commonly used value. Here \( \lambda_{\text{Jeans}} \) is the Jeans length and \( n_{\text{H}_2} \) is the number density of molecular hydrogen. Though this is a somewhat crude fix, it more closely matches the results for optically–thick gas found in 3D hydrodynamical simulations. One caveat should be noted here: in general, \( \text{H}_2 \) self–shielding behavior will depend on the shape of the incident spectrum, since the shape determines the relative weights of the LW transitions. However, in practice, we find that the self–shielding function for a given SB99 spectrum differs very modestly from that for a flat spectrum, with errors typically of order a few per cent for young bursts, and not larger than \( \lesssim 25 \) per cent for the spectra considered here.

We have also updated some of the most important chemical rates which determine the \( \text{H}_2 \) abundance, based on the results of recent studies. These include the associative detachment rate (\( \text{H} + \text{H} \rightarrow \text{H}_2 + \epsilon \) [Kreckel et al. 2010]), and the mutual neutralization rate (\( \text{H}^- + \text{H}^+ \rightarrow 2\text{H} \) [Stenrup et al. 2009]). We have added several reactions to the one–zone chemistry network which have been shown to be important by, e.g. Glover (2015b). These include collisional dissociation of \( \text{H}_2 \) by neutral hydrogen through dissociative tunneling, the rate for which is provided by [Martin et al. 1996] and the ionization of atomic hydrogen by \( \text{H}^- \text{H}^+ \) collisions and \( \text{H}^- \text{He} \) collisions, using the rates from [Lenzen et al. 1991]. The radiative recombination rate for \( \text{H}^+ \) is the Case B rate from [Hui & Gnedin 1997] – appropriate for low–ionization fraction of gas collapsing in an atomic cooling halo (Glover 2015b) – rather than the Case A rate previously used in SBH10. We use the rate for radiative association from [Abel et al. 1997], rather than that from [Hutchins 1976] used by SBH10. The remainder of the chemistry network is the same as in SBH10 and provided in their Appendix.

### Table 1. Summary of \textsc{starburst99} model galaxy parameters

| Case | A | B | C | D | E |
|------|---|---|---|---|---|
| \( \alpha \) | 2.35 | 2.35 | 2.35 | 1 | 1 |

All assume a power-law IMF with exponent \( \alpha \) and mass limits given below in units of \( M_{\odot} \). Each IMF is run with metallicities \( Z = 0.001, 0.004, 0.008 \) \( Z_{\odot} \).

#### 2.2 Model Spectra

We use the publicly available population synthesis package \textsc{starburst99} ([Leitherer et al. 1999], hereafter SB99) to generate spectra with a range of metallicities, IMFs, and ages. We use the UV line spectra provided by SB99 (at 0.3 \text{˚A resolution}) for calculating the \( \text{H}_2 \)–photodissociation rate. Unfortunately, high–resolution spectra are not available for the full wavelength range required for all photochemical rates; therefore, for all continuum processes we use the SB99 spectra at lower resolution, which varies from \( 1\text{–}20 \) \text{˚A} over the relevant wavelengths.

We focus here on spectra for the SB99 “burst” models, in which a single population with specified mass, metallicity and IMF forms instantaneously and evolves over time, without any ongoing star formation. In the DCBH scenario, these are likely the most relevant, because the intense flux required for \( \text{H}_2 \)–cooling suppression must come from a very bright close neighbor, rather than from the cosmological background (see e.g. [Shang et al. 2010; Dijkstra et al. 2008; Ahn et al. 2009; Agarwal et al. 2012, 2014; Regan et al. 2014; Habouzit et al. 2016]). These studies show that the most likely candidates for DCBHs are within 1–2 kpc of a bright source. As pointed out by [Vishal et al. 2014], one promising scenario is that two atomic cooling (sub–)halos in very close proximity are nearly synchronised in their collapse, so that the first to form stars illuminates the other with a strong LW flux mostly from young, bright, massive stars. [Vishal et al. 2014] and [Regan et al. 2016] show that there are issues of photoevaporation if the collapsing DCBH candidate halo has been irradiated with a strong flux for \( \gtrsim 20 \) Myr; we therefore focus primarily on burst populations with ages up to 20 Myr.

We summarize the IMF parameter choices for our SB99 models in Table 1. Each IMF is run at three different metallicities from \( Z/Z_{\odot} = 0.05 – 0.4 \), though for the direct collapse model, the lower end of the range is more likely to be relevant, as the DCBH halo must be nearly pristine (see, e.g. [Omukai et al. 2008]), and is less likely to remain so with a highly enriched near neighbor.

The specific luminosities at the Lyman limit (\( L_{13.6} \) in units erg s\(^{-1} \) Hz\(^{-1} \) M\(_{\odot}^{-1} \)) output by SB99 are converted to \( J_{21} \) by:

\[
J_{21} = \frac{M_\ast}{16\pi^2d^2} \times \frac{L_{13.6}}{10^{-21}},
\]

where \( M_\ast \) is the total stellar mass of the SB99 burst galaxy and \( d \) is the distance from the illuminating halo.

In Figure 1 we show an example SB99 spectrum with metallicity \( Z/Z_{\odot} = 0.05 \) at \( t = 10 \) Myr, as well as T4 and T5 blackbodies normalised to have the same luminosity at the Lyman limit. The frequencies of the \( \text{H}_2 \) LW transitions are
also shown for reference. As this figure illustrates, the SB99 spectrum is much closer to T5 than to T4. We calculate the frequency–dependent optically–thin H$_2$ photodissociation rate for each of the SB99 models using the data from Abgrall et al. (1993) to obtain the frequency–dependent Lyman–Werner absorption cross–sections $\sigma_{v',J',v,J}(\nu)$.

The total H$_2$–photodissociation rate depends on the ro-vibrational distribution of molecules, $f_{v',J}$:

$$k_{\mathrm{LW}} = \sum_{v,J} k_{\mathrm{diss},v',J} f_{v',J},$$

which in general can depend on the detailed thermochemical history of the collapsing cloud. For simplicity, we assume all molecules are in the ground vibrational state with a Boltzmann distribution at the Lyman limit. Red (dotted) vertical lines show the Lyman-Werner band transitions (arbitrary units). We show the spectra in the energy range of interest, from the H$^+$ photodetachment threshold, 0.76 eV, to the Lyman limit, 13.6 eV. The SB99 spectrum is much closer to T5 than to T4.

2.3 H$_2$–Photodissociation Rate

We calculate the frequency–dependent optically–thin H$_2$ photodissociation rate for each of the SB99 models using the high–resolution UV spectra. Photodissociation occurs via the two–step Solomon process (Solomon 1965; see also Field et al. 1968; Stecher & Williams 1967), in which H$_2$ molecules are electronically excited by absorption of Lyman–Werner photons (900–1100 Å). Following excitation, $\sim$ 15% of molecules are dissociated in subsequent radiative decay to the vibrational continuum of the electronic ground state, while all others return to a bound state via radiative cascade.

The rate of photodissociation of molecules from initial ro-vibrational state $(v,J)$ is

$$k_{\mathrm{diss},v',J} = \sum_{v,J'} \frac{\nu_{v',J'}}{\nu_{v,J}} \int f_{\mathrm{diss},v',J'} \, d\nu,$$

where $f_{\mathrm{diss},v',J'}$ is the fraction of molecules that are dissociated from the excited state $(v',J')$, provided by Abgrall et al. (2000). The “pumping rate” of H$_2$ from the ground state $(v,J)$ to $(v',J')$ is:

$$\zeta_{v,J,v',J'} = \int_{\nu_{\mathrm{min}}}^{\nu_{\mathrm{max}}} 4\pi \sigma_{v,J,v',J}(\nu) \frac{J_\nu}{\hbar \nu} \, d\nu,$$

where $J_\nu$ is the specific intensity of the SB99 spectra in the usual units and $\hbar$ is Planck’s constant. The limits of integration are from $\nu_{\mathrm{min}} = 11.16$ eV to $\nu_{\mathrm{max}} = 13.6$ eV. We use the data from Abgrall et al. (1993) to obtain the frequency–dependent Lyman–Werner absorption cross–sections $\sigma_{v,J,v',J}(\nu)$.

The total H$_2$–photodissociation rate depends on the ro-vibrational distribution of molecules, $f_{v,J}$:

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2.4 Rate of H$^+$ Photodetachment

The rate of H$^+$ photodetachment is computed with the widely–used Shapiro & Kang (1987) fit for the cross-section $\sigma_{\nu,J}$. This is convolved with the flux from a blackbody or SB99 spectrum:

$$k_{\mathrm{H}^+} = 4\pi n_\mathrm{H} \int_{0.76 \, \mathrm{eV}}^{13.6 \, \mathrm{eV}} \sigma_{\nu,J} \frac{J_\nu}{\hbar \nu} \, d\nu.$$

Miyake et al. (2010) pointed out that a series of auto-detaching resonances above $\sim 11$ eV also contribute to the photodetachment rate; however, they find the additional suppression of the H$_2$ abundance is only $\lesssim 20$ per cent for blackbody spectra with $T_{\mathrm{BB}}$ up to $10^5$ K, and we therefore do not include these resonant contributions to the rate.

3 RESULTS AND DISCUSSION

3.1 Approximate Photodissociation Rates

Due to the computational expense of calculating the frequency–dependent H$_2$ photodissociation rate as described above, nearly all previous studies have instead derived an approximate rate by assuming that the (incident) flux across the LW bands is flat. With the flux at 13.6 eV specified by $J_{21}$ in the usual units, the optically–thin rate is then parameterised as

$$k_{\mathrm{LW}} = 1.39 \times 10^{-12} \beta J_{21}.$$  

By convention, the rate is calculated assuming a flat spectrum in the Lyman–Werner bands and $\beta$ is usually defined as the ratio of the flux at a single LW frequency to the flux at the Lyman limit, $\beta = J_{12}/J_{21}$. The most common choice is to define $J_{\mathrm{LW}}$ as the flux at 12.4 eV, the midpoint of the Lyman–Werner bands; we refer to this as $\beta_{\mathrm{flat}}$ (e.g. Shang et al. 2010). Alternatively, some studies define $J_{\mathrm{LW}}$ as the average flux in the LW bands (e.g. Agarwal & Khochfar 2015); we will refer to this as $\beta_{\mathrm{avg}}$:

$$\beta_{\mathrm{avg}} = \frac{1}{\Delta \nu_{\mathrm{LW}}} \int_{12.4 \, \mathrm{eV}}^{13.6 \, \mathrm{eV}} J_\nu \, d\nu.$$
These approximations save significant computational expense, avoiding integration over dozens or hundreds of LW lines, as described in the full rate calculation above. However, even in the idealised case of a $10^4 \text{K}$ blackbody spectrum, a non-zero slope of the spectrum in the LW bands can lead to errors in $k_{\text{LW}}$ of a factor of two compared to the rate if the spectrum is assumed flat at 12.4 eV. Hotter blackbody spectra are flatter in the LW bands so the errors are smaller, and only a few percent for $T_{\text{BB}} = 10^5 \text{K}$. For more realistic spectra, however, such as those from population synthesis codes like SB99, both the non-zero slope as well as absorption features – e.g. O IV $\lambda 1035$, Ly$\beta$, C II $\lambda 1036$, and LW lines themselves (Leitherer et al. 1999) – near the LW transition frequencies can cause the rate derived from $\beta_{\text{flat}}$ or $\beta_{\text{avg}}$ to deviate significantly from frequency dependent (“true”) rate.

In Figure 2 we show examples of SB99 spectra (high and low-resolution) in the LW bands, overlaid with the 76 LW transition strengths are shown in green. Because the absorption lines in the high-resolution spectrum overlap with the LW transition energies, significant errors can result from the assumption that the spectrum is flat in the LW bands, even when, as is the case here, the stellar population is relatively young and total absorption is modest.

In Figure 3, we show the ratio of the Lyman–Werner photodissociation rate, parameterised by the dimensionless parameter $\beta$ (eq. 5), from an approximate method ($\beta_{\text{approx}}$) to the full, frequency-dependent calculation ($\beta_{\text{calc}}$). In all cases the spectrum is the low-resolution UV from a starburst99 instantaneous burst with metallicity as indicated on the figure. The dissociation rate assuming either the average flux in the LW bands ($\beta_{\text{avg}}$) or a flat spectrum ($\beta_{\text{flat}}$) with $J_{\text{LW}} = J(12.4 \text{eV})$ both overestimate the “true” rate by a factor of 2 at 100 Myr after the burst and a larger factor for older bursts. This is due to the strong attenuation of the flux near the Lyman-limit (line blanketing), which is not captured by the approximations of flat spectra in the LW bands.

In this case, the effect of (modestly) over-estimating $\beta$ is counteracted by the smaller flux levels of the high-resolution spectra, and the upshot is the overall rate is underestimated by a factor of a few. We include the comparison only up to 20 Myr, after which the high-resolution UV spectra are no longer reliable (C. Leitherer, private communication).

3.2 Critical Curve

In general, $H_2$ dissociation, and therefore the thermal history, of gas in a primordial atomic cooling halo is controlled by two rates: $H_2$–photodissociation by LW photons ($k_{\text{LW}}$) and $H^-$–photodetachment by IR photons ($k_{\text{H-}}$), since $H^-$ is an intermediate in $H_2$ formation. While a threshold flux, $J_{\text{crit}}$, has most often been used to determine whether $H_2$–cooling should be suppressed, this can be misleading, and it

![Figure 2](image-url)

**Figure 2.** High- (red) and low-resolution (blue) spectra in the Lyman–Werner bands for a starburst99 model of an instantaneous burst with IMF A and $Z/Z_\odot = 0.05$ at 10 Myr. The Lyman–Werner transition strengths are shown in green. Because the absorption lines in the high-resolution spectrum overlap with the LW transition energies, significant errors can result from the assumption that the spectrum is flat in the LW bands, even when, as is the case here, the stellar population is relatively young and total absorption is modest.

![Figure 3](image-url)

**Figure 3.** Ratio of the Lyman–Werner photodissociation rate, parameterised by the dimensionless parameter $\beta$ (eq. 5), from an approximate method ($\beta_{\text{approx}}$) to the full, frequency-dependent calculation ($\beta_{\text{calc}}$). In all cases the spectrum is the low-resolution UV from a starburst99 instantaneous burst with metallicity as indicated on the figure. The dissociation rate assuming either the average flux in the LW bands ($\beta_{\text{avg}}$) or a flat spectrum ($\beta_{\text{flat}}$) with $J_{\text{LW}} = J(12.4 \text{eV})$ both overestimate the “true” rate by a factor of 2 at 100 Myr after the burst and a larger factor for older bursts. This is due to the strong attenuation of the flux near the Lyman-limit (line blanketing), which is not captured by the approximations of flat spectra in the LW bands.
requires the computation of \( J_{\text{crit}} \) specific to each spectrum. \( J_{\text{crit}} \) values have been estimated in the literature for idealised spectra with fixed shapes, such as a blackbody or power-law, but have then subsequently been adopted for different spectral shapes, without re-computing the appropriate \( J_{\text{crit}} \) values (e.g. \cite{Agarwal2012, Dijkstra2014}). For realistic, time-evolving spectra, such as those generated in population synthesis models, both \( k_{LW} \) and \( k_{H} \)- need to be re-computed and specified to determine whether \( H_2 \)-cooling is suppressed. Although a corresponding \( J_{\text{crit}} \) can be computed, as well, this, as we have emphasized, is unnecessary and misleading, and has led to erroneous assumptions in previous works. We therefore propose to replace the “critical flux” with the spectrum-independent “critical curve,” as shown in Figure 5.

The solid curve in Figure 5 shows the minimum combination of \( k_{LW} \) and \( k_{H} \) - required to keep the gas hot in our one-zone models. This curve results from the cooling behavior of the gas in our one-zone models, which follows the familiar bifurcated path: with a sufficiently strong radiation field, the \( H_2 \)-fraction remains too low for cooling to occur, and the gas is near the virial temperature of the halo throughout the initial stages of collapse (up to \( n \gtrsim 10^7 \text{ cm}^{-3} \)). Below the threshold, the \( H_2 \) fraction reaches \( \sim 10^{-3} \), cooling the gas to \( \sim \) a few \( \times 10^4 \text{K} \). On the critical curve in Figure 5, for all points above (rightward) of the curve, \( H_2 \)-cooling is suppressed, while for those below (leftward) of the curve, \( H_2 \)-cooling occurs and the gas temperature falls below \( 10^3 \text{K} \). The curve itself depends only on the details of the one-zone model, and does not depend on the shape of the irradiating spectrum. The location where each individual model spectrum falls relative to the critical curve does, however, depend on the spectral shape."

For ease of comparison with previous studies, we have marked on the critical curve the positions of blackbodies of several different temperatures. It is worth noting that all blackbodies with temperatures \( \gtrsim 20,000 \text{K} \) lie in the flat portion of the curve, i.e. where photodissociation is the dominant mechanism for suppressing \( H_2 \)-cooling, while \( H^+ \)-photodetachment is only important for the coolest blackbodies considered, \( \sim 10^4 \text{K} \). While the T4 type has often been used in previous studies to approximate Pop II, the positions of the SB99 spectra on the critical curve underscore that it is not a good representation of Pop II; further, the increased fraction of mass in stars remains a problem for achieving \( H_2 \)-cooling suppression from populations with the softest (T4 type) spectra \cite{Wolcott-Green2012}.

The points in Figure 5 are the results of our one-zone model using individual SB99 spectra for the illuminating radiation field, each normalised with \( M_\odot / d^2 \) so as to coincide with the critical curve. SB99 bursts with all five IMFs and metallicities \( Z/Z_\odot = 0.05 - 0.2 \) are shown. While the SB99 spectra at early times (\( \lesssim 10 \text{Myr} \)) and low-metallicity (\( Z/Z_\odot = 0.05 \)) are comparable on the critical curve to higher metallicities, the IR radiation becomes important before 20 Myr for models with modest metallicities (\( Z/Z_\odot = 0.2 \)).

Our “critical curve” differs from that of \cite{Agarwal2014} due to our use of a reduced self-shielding column density, (see §2), as discussed above and in \cite{Wolcott-Green2012}.

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pairs without calculating individually the photodissociation and photodetachment rates. For two of our models (IMF A calculation in blue (solid), a fitting formula from a previous study shown in red (dashed), with the curve from our one–zone calculation in black (dot–dash). Our fitting formula (eq. 8) for the critical curve is

\[ k_{\text{crit}} = \frac{10^{-A}}{(1 + k_H/C)^B} \times \exp(-B \times k_H/C), \]  

\[ (8) \]

with A=9.05, B=0.95, C=1.6 \times 10^{-6}, and D=0.3. This fit is accurate to a few percent for \( k_{H^-} \lesssim 2 \times 10^{-6} \), corresponding to blackbody temperatures \( T_{BB} \gtrsim 12,000 K \) and the majority of SB99 results (which are leftward of that mark). It underestimates \( k_{LW} \) by a factor of two at \( k_{H^-} = 3 \times 10^{-6} \) (\( T_{BB} = 10^4 K \)).

### 3.3 Critical Star Formation in Illuminating Galaxy

In order to easily utilize our results in semi-analytic models and simulations of early structure formation, in Table 2 we provide the required stellar mass in an illuminating galaxy with a given IMF and metallicity, located at a distance \( d \) from an atomic cooling halo, to prevent \( H_2 \)–cooling:

\[ \left( \frac{M}{d^2} \right)_{\text{crit}} \]

This allows identification of DCBH candidate halo pairs without calculating individually the photodissociation and photodetachment rates. For two of our models (IMF A

| IMF | age (Myr) | \( Z = 0.001 \) | \( Z = 0.004 \) | \( Z = 0.008 \) |
|-----|-----------|---------------|----------------|----------------|
| A   | 6         | 0.917         | 0.994          | 1.07           |
|     | 10        | 1.96          | 2.36           | 2.74           |
|     | 20        | 6.31          | 7.99           | 9.59           |
| B   | 6         | 0.316         | 0.339          | 0.359          |
|     | 10        | 0.746         | 0.803          | 1.04           |
|     | 20        | 5.52          | 7.05           | 8.48           |
| C   | 6         | 0.84          | 1.27           | 3.12           |
| D   | 6         | 11.1          | 2.07           | 42.1           |
| E   | 2         | 1.29          | 3.47           | 1.01           |

Figure 7. Our fitting formulae for \( \left( \frac{M}{d^2} \right)_{\text{crit}} \) are shown (solid curves) with the data (triangles) from our one–zone model. In both cases we used IMF A for the SB99 spectra, with \( Z = 0.001 \) (0.008) shown in magenta (blue). The quadratic fit parameters are provided in § 5.3.

Figure 8. The required ratio of stellar mass and squared-distance \( \left( \frac{M}{d^2} \right)_{\text{crit}} \) for a starburst galaxy to prevent \( H_2 \)–cooling in a neighboring atomic cooling halo, obtained from the one–zone model.

3.4 Importance of Level Populations

The most significant simplification we made in this study is to assume the ro-vibrational level populations of \( H_2 \) are well described by a Boltzmann distribution in the rotational levels \((J \geq 0–29)\) of the ground vibrational state \((v=0)\). Deviations from LTE can significantly affect the self–shielding behavior of \( H_2 \) and therefore change the critical curve shown in Figure 7. In the early phases of gravitational collapse of an atomic cooling halo, the \( H_2 \) in \( v=0 \) would not have reached equilibrium, since the critical densities are already \( n \sim 10^3 \sim 10^4 \) cm\(^{-3} \) for the first few rotational levels.

At the relevant temperatures for the early collapse, i.e. a few thousand Kelvin, high \( J \) states \((J \gtrsim 5–10)\) are negligibly populated, so this does not introduce significant errors in the optically–thin \( H_2 \)–photodissociation rate. As discussed in Wolcott-Green & Haiman (2011), however, the more levels
are populated, the less effective H\textsubscript{2} self-shielding becomes, so the optically-thick rate is more sensitive to the assumed distribution over ro-vibrational states. For example, in their study using the publicly available package CLOUDY to resolve level populations of H\textsubscript{2}, Richings et al. (2014) find differences compared to the optically-thick LTE rate of $\sim$ a factor of a few for $T_{\text{gas}} = 5000\text{K}$ and $n_{\text{tot}} = 10^2 \text{ cm}^{-3}$ at very high column densities, $N_{\text{H}_2} \gtrsim 10^{19} \text{ cm}^{-2}$ with much smaller errors at the relevant column densities for the early stages of collapse.

4 CONCLUSIONS

In most studies of the direct collapse black hole scenario, a single parameter $J_{\text{crit}}$ has been used to delineate the threshold flux above which H\textsubscript{2}–cooling is prevented in an atomic cooling–halo. However, this single-parameter assumption can be misleading, as the value of $J_{\text{crit}}$ depends on the spectral shape, and therefore needs to be re-computed for each incident spectrum. As long as the spectrum is assumed to have a fixed shape (in time), such as a blackbody or power-law, specifying the flux at a single frequency (e.g. the Lyman–limit) fixes all relevant photo-chemical rates. In a more general treatment, the ratio of the flux in the Lyman–Werner bands to that at the energies relevant for H\textsuperscript{-}photodetachment ($\sim 1–2\text{eV}$), is dependent on the details of the spectrum, which depend on the mass function,metallicity, and age of the irradiating galaxy. Although a new $J_{\text{crit}}$ could be computed for each case, we here emphasize that this is unnecessary, and advocate the use, instead of a two-dimension critical curve (Figure 5).

Using the population synthesis package STARBURST99 to generate realistic spectra, we investigated the relative importance of LW photodissociation and H\textsuperscript{-}photodetachment in suppressing the H\textsubscript{2} abundance and thereby preventing cooling below the virial temperature of a halo. Very few studies have used spectra from population synthesis modeling, and those that have (Sugimura et al. 2011, Agarwal & Khochfar 2013, Agarwal et al. 2010) relied on simplifications to derive a LW photodissociation rate, rather than performing a full, frequency–dependent calculation. We show in §3 that these simplifications overestimate the true photodissociation rate by a factor a few in the first $\sim 20\text{ Myr}$ of a burst.

We provide a fitting formula to the critical curve from our one–zone modeling (see Fig. 2 and Eq. 5), which includes important updates to the photochemical model and is accurate at the percent level. The resulting critical stellar masses (Table 2 and Figure 7) can be used directly in semi-analytic models and simulations of early structure formation.

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