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THE FIRST H II REGIONS IN THE UNIVERSE

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ABSTRACT

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1. INTRODUCTION

Numerical simulations predict that the first stars in the universe appear at $z \sim 20 - 30$ in cosmological minihalos of masses $\gtrsim 10^5 M_\odot$. The original models imply that they are $100 - 500 M_\odot$ due to large central accretion rates mediated by inefficient H₂ cooling (Bromm et al. 1999, 2001; Nakamura & Umemura 2001; Abel et al. 2000, 2002), but more recent surveys extend their minimum masses down to $20 - 30 M_\odot$ (O'Shea & Norman 2007, 2008; Wise & Abel 2007c). Population III stars synthesized the first heavy elements and, with their high surface temperatures (10^5 K) and ionizing emissivities (10^{50} s^{-1}), began to ionize the early intergalactic medium (IGM). The surprise 2003 discovery of large free electron fractions at high redshifts by the Wilkinson Microwave Anisotropy Probe (*WMAP*) suggested that the universe began to be ionized much earlier than previously thought and launched a series of studies on cosmological reionization (Ciardi, Ferrara, Marri, & Raimondo 2001; Haiman & Holder 2003; Cen 2003; Somerville & Livio 2003; Barkana & Loeb 2004; Sokasian, Abel, Hernquist, & Springel 2003; Ciardi, Ferrara, & White 2003). The models relied heavily on estimates of UV escape fractions from the first stars, motivating the first radiation hydrodynamical calculations of ionizing UV breakout from star-forming halos in one dimension (Whalen et al. 2004; Kitayama et al. 2004).

The dark matter minihalos in which the first stars are born exhibit large central baryon densities of $\gtrsim 10^6 \text{ cm}^{-3}$ that decrease as $\sim r^{-2.2}$ in radius. Whalen et al. (2004) and Kitayama et al. (2004) find that the ionization front (I-front) of the star executes an early transition to D-type but then rapidly reverts to R-type as it descends the density gradient. Breakout usually occurs on timescales of a few hundred kyr followed by complete ionization of the halo and final H II region radii of 2.5 - 5 kpc. The steep density gradients in the now ionized and isothermal gas become sharp pressure gradients that drive what was once the core of the halo outward in a strong shock at $30 - 40 \text{ km s}^{-1}$, ten times the escape velocity of the halo. The shock sweeps up more than half the baryons in the halo into a dense shell 100 - 200 pc in radius by the end of the life of the star. Line-driven winds, which

create similar shells around high mass stars in the galaxy today, are not thought to be important in the metal-free atmospheres of primeval stars (Kudritzki 2000; Baraffe, Heger, & Woosley 2001; Vink, de Koter, & Lamers 2001). UV escape fractions, defined as the ratio of the number of photons that escape the halo to the number produced, vary with stellar mass but typically exceed 80%.

Alvarez et al. (2006) performed three-dimensional calculations of UV breakout from Population III stars which, along a given line of sight, match semi-analytical I-front tracking to self similar solutions of champagne flows in H II regions (Shu et al. 2002). The first radiation hydrodynamical calculations in realistic three-dimensional halos derived from cosmological initial conditions were done by Abel et al. (2007), who implemented monoenergetic adaptive raytracing techniques for ionizing UV transfer in the Enzo adaptive mesh refinement (AMR) code. In addition to finding UV escape fractions and ionized core shocks that are consistent with the one-dimensional models, their models show how density inhomogeneities in the halo corrugate the I-front. Photons preferentially exit into low density voids but are trapped by dense filaments, leading to the classic 'butterfly' H II region morphology seen in the first numerical simulations of quasar ionization fronts (Abel, Norman, & Madau 1999).

Numerical experiments with ionization fronts in idealized H and He density profiles approximating those of cosmological halos reveal that they are prone to two types of violent dynamical instabilities (Whalen & Norman 2008a,b). One occurs when the shocked neutral shell of a D-type ionization front radiatively cools and collapses into a cold dense layer that is subject to Vishniac overinstabilities (Vishniac 1983). Radiation behind the front opportunistically streams through cracks in the shell, shooting ahead of the main front as 'fingers' of ionized gas (Garcia-Segura & Franco 1996). They rapidly become nonlinear, completely breaking the shell up into dense clumps of gas. This kind of instability is thought to be common in the galaxy today, where metal fine structure lines efficiently cool shocked gas in D-type I-fronts. The other type of instability appears when a density perturbation is advected across an R-type I-front, causing it to become dimpled. The sides of the dimple become D-type first due to the lower fluxes associated with the larger angles of incidence of photons there. The wall of the dimple abruptly slows as its tip continues forward as R-type, elongating the dimple into a jet that fragments and crumples into a turbulent flow (Williams 1999). This is known as a shadow instability and does not require any kind of radiative cooling in the shocked ambient gas swept up by the front.

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Whalen & Norman (2008a) show that atomic line cooling by H and He alone is too weak to incite Garcia-Segura instabilities in primordial ionization fronts. However, the hard UV spectra that create cosmological H II regions also form H₂ in the outer layers of the I-front, as first pointed out by Ricotti et al. (2001). Enough molecular hydrogen can survive the LW component of the spectrum to cool and fracture the shocked shell as metals do in galactic I-fronts. Both Garcia-Segura and shadow instabilities may be important in cosmological H II regions because they can form persistent clumps that reduce UV escape fractions and later become enriched by primordial supernova remnants, perhaps efficiently cooling and becoming Jeans unstable to collapse into new stars.

Multifrequency UV transport is necessary to fully capture these phenomena for two reasons. First, the profile of the spectrum governs the structure of the I-front, and to recover the true width of the front and rates of H₂ production in its outer layers, all energies above the ionization edge of H at which there are significant numbers of photons must be included. Furthermore, UV flux below 13.6 eV can attack H₂ and its key intermediaries. Photons with energies greater than 0.255 eV photodetach H⁻ and Lyman-Werner (LW) photons from 11.18 - 13.6 eV photodissociate H₂. Thus, while ionizing flux above 13.6 eV manufactures H₂ in the I-front, UV below this threshold regulates its formation and cannot be neglected. Second, shadow instabilities in primordial I-fronts become fully manifest only in the high ionized gas temperatures of hard UV spectra (compare Figures 7 and 8 of Whalen & Norman 2008a), which can be found from first principles only by sampling photon rates across many energy bins. What most distinguishes cosmological I-front transport at high redshifts from H II regions in the galaxy today is the manner in which photons of many energies couple strongly to both primordial chemistry and hydrodynamics. This interdependence introduces a variety of characteristic timescales to self-consistent UV transport, as we review later.

Since single stars are thought to form in cycles within a given halo as gravitational mergers assemble halos into the first primitive galaxies, accurate H II region models are key to simulations of protogalaxy formation (Johnson et al. 2007; Yoshida et al. 2007; Wise & Abel 2007b). Greif et al. (2007) apply ionization equilibrium arguments to ray tracing in the smooth particle hydrodynamics code GADGET to construct approximate H II regions as initial conditions for primordial supernova explosions. Wise & Abel (2007a) utilize their adaptive ray tracing scheme in Enzo to compute the formation of H II regions *in situ* as a key component to stellar feedback in preliminary attempts at *ab initio* first galaxy formation. The recent proliferation of radiative transfer methods in large-scale structure formation codes attests to the importance of cosmological ionization fronts on many spatial scales and over many epochs of time (Iliev et al. 2006).

Despite steady progress in numerical models of the first H II regions, their true structure remains unsolved. First and foremost, none of the calculations proceed from the true initial conditions of UV breakout, which are set by accretion geometries and radiation flows well into the main sequence of the star and have never been simulated. If primordial accretion disks are long-lived they could

collimate ionizing radiation into bipolar flows above and below the plane of the disk that are very different from the isotropic fluxes and unpreprocessed halos assumed in studies to date. Second, the models rely on the on-the-spot (OTS) approximation (Osterbrock 1989), in which ionizing photons due to recombinations to the ground state are assumed to be reabsorbed in their grid point of origin. This is done to eliminate the radiative transfer of diffuse photons that would exhaust most algorithms. However, Ritzerveld (2005) has shown that in H II regions with large central densities, such as those of the first stars, the photon budget at large radii is actually dominated by reprocessed radiation. Recombination radiation could therefore blunt shadowing and profoundly alter the morphology of the H II region as well as modify the propagation speed of the I-front. Diffuse photons might also dampen instability growth at larger scales by eroding the neutral H and He between ionized fingers of gas.

At present, no calculations in realistic three-dimensional halo profiles properly model the structure of the I-front or its breakup due to H₂ cooling because they rely on a single energy or at most 2 - 3 energy groups to avoid the higher cost of a full multifrequency approach. Abel et al. (2007) and Wise & Abel (2007a) find protuberances in their H II regions that they ascribe to dynamical instabilities, but it is difficult to distinguish these structures from those that would form from simple density inhomogeneities in the halo without first performing tests in idealized profiles. Another issue is that the most recent models lack any prescription for the self-shielding of H₂ formed in the I-front from LW photons. As a result, they overestimate H₂ destruction in the dense layer of D-type fronts, potentially excluding Garcia-Segura instabilities that might otherwise have arisen there. The degree to which clumps of dense gas form and survive in halos therefore remains uncertain. Finally, the standard in early cosmological H II region simulations has been to assume that stellar luminosities and spectral profiles remain constant over the life of the star. In reality, both can vary significantly over the main sequence, modulating the advance and structure of the front. Rapid rotation also leads to equatorial cooling in primordial stars, with angle-dependent fluxes that have yet to be included in H II region calculations.

We present the next generation of H II region calculations for the first stars. We import three-dimensional halo baryon profiles computed from cosmological initial conditions with the Enzo AMR code into the ZEUS-MP radiation hydrodynamics code and photoionize them with time-dependent stellar fluxes and spectra, obtained from the stellar evolution code KEPLER. ZEUS-MP has been modified to perform nine-species primordial H and He gas chemistry together with photon-conserving multifrequency UV transport that includes augmented H₂ self-shielding functions for LW photodissociation. The intent of our study is to analyze I-front instability growth and clumping in primordial minihalos, evaluate UV breakout and escape fractions, and compute the circumstellar environments of supernova explosions. Realistic initial conditions for Population III supernovae (SN) are perhaps the most important of these goals because metal mixing in relic H II regions could lead to prompt star formation that might significantly alter global photon production

rates at high redshifts and has never been studied.

While our simulations do not address all the shortcomings in previous models, they are a clear step forward in understanding the true structure of the first H II regions in the universe and how primordial SN explosions evolve within them. In § 2 we describe the ZEUS-MP radiative transfer (RT), nonequilibrium rate equations for primordial chemistry, and time integration scheme by which chemistry and radiation are solved self-consistently with hydrodynamics. Garcia-Segura instabilities in I-fronts in spherically-averaged three dimensional Enzo halo profiles are examined in § 3, where we also evaluate the effect of additional H₂ cooling channels on shock fragmentation. H II region breakout in actual three-dimensional Enzo halos is described in § 4 and in § 5 we conclude.

2. ZEUS-MP

ZEUS-MP is a massively-parallel Eulerian hydrocode with multifrequency UV photon-conserving radiative transfer (Whalen & Norman 2008a) self-consistently coupled to the nine-species primordial gas reaction network of Anninos et al. (1997) and Abel et al. (1997). The equations of fluid dynamics are

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) \quad (1)$$

$$\frac{\partial \rho v_i}{\partial t} = -\nabla \cdot (\rho v_i \mathbf{v}) - \nabla p - \rho \nabla \Phi - \nabla \cdot \mathbf{Q} \quad (2)$$

$$\frac{\partial e}{\partial t} = -\nabla \cdot (e \mathbf{v}) - p \nabla \cdot \mathbf{v} - \mathbf{Q} : \nabla \mathbf{v} \quad (3)$$

where ρ , e , and the v_i are the mass density, internal energy density, and velocity components at each mesh point, and $p = (\gamma-1)e$ and \mathbf{Q} are the gas pressure and von Neumann-Richtmeyer artificial viscosity tensor (Hayes et al. 2006). The left hand side of each equation is updated term by term in operator-split and directionally-split substeps, with each new update acting upon the partially-evolved variable of the previous substep. Terms that represent forces acting on a fluid parcel are evolved in the ZEUS-MP source routines. Divergence terms that describe changes to a variable due to flow in or out from a mesh point are updated in the ZEUS-MP advection routines.

2.1. Nonequilibrium Primordial Chemistry

Nine additional continuity equations are evolved to advect H, H⁺, He, He⁺, He⁺⁺, H⁻, H₂⁺, H₂, and e⁻, which are assumed to have the same velocities. We solve these equations in the ZEUS-MP advection routines. The reaction network is composed of thirty reactions, each of which is represented by a term in the nonequilibrium rate equations of Anninos et al. (1997)

$$\frac{\partial \rho_i}{\partial t} = \sum_j \sum_k \beta_{jk}(T) \rho_j \rho_k + \sum_j \kappa_j \rho_j. \quad (4)$$

The β_{jk} are the rate coefficients of the reactions between species j and k that create (+) or remove (-) species i, and the κ_j are the ionization rates. The rate equations are recast in the backward difference formalism (BDF) and are sequentially updated in a semi-implicit manner

that is described in detail in section 2.3 of Whalen & Norman (2006). The reaction network is updated in a module that is operator-split from the hydrodynamics.

Truncation error prevents the continuity equations from guaranteeing charge and baryon conservation, which we enforce with the following constraints

$$\rho_b f_H = \rho_H + \rho_{H^+} + \rho_{H^-} + \rho_{H_2^+} + \rho_{H_2} \quad (5)$$

$$\rho_b (1 - f_H) = \rho_{He} + \rho_{He^+} + \rho_{He^{2+}} \quad (6)$$

$$m_H n_e = \rho_{H^+} - \rho_{H^-} + \frac{1}{2} \rho_{H_2^+} + \frac{1}{4} \rho_{He^+} + \frac{1}{2} \rho_{He^{2+}} \quad (7)$$

Baryon conservation is satisfied every hydrodynamical time step by assigning any error between the sum of the species densities and ρ_b , the primordial gas density, to the largest of the species densities to bring them into agreement with ρ_b . Total H and He species abundances are separately conserved to their cosmic values $f_H = 0.76$ and $1 - f_H = 0.24$ within ρ_b , respectively. Charge is separately conserved by setting the total electron abundance to the sum of the charged H and He species abundances.

2.2. H₂ Cooling Channels

We perform isochoric updates to the gas energy every time the reaction network is solved

$$\dot{e}_{\text{gas}} = \Gamma - \Lambda. \quad (8)$$

Here, Γ is the rate at which photons at all energies above the H ionization limit deposit heat into the gas and Λ is the sum of all the cooling rates, which includes collisional ionization and excitation of H and He, recombinations in H and He, inverse Compton scattering from the CMB, and bremsstrahlung emission.

Previous studies (e. g. Abel et al. 2002; Whalen & Norman 2008a) have included only the collisional excitation of H₂ by H (Lepp & Shull 1983; Galli & Palla 1998). However, additional channels can come into play in warm or hot gas with a significant fractional ionization, such as we find in the gas shells driven by I-fronts in our simulations. Glover & Abel (2008) have recently shown that in gas with an elevated fractional ionization, collisional excitation of H₂ is actually dominated by H₂-H⁺ and H₂-e⁻ collisions, so these processes regulate molecular hydrogen cooling in gas at densities below the H₂ critical density. To properly account for these effects, we model H₂ cooling in our simulations with a new function based on the work of Glover & Abel (2008). This cooling function includes the collisional excitation of H₂ by H, He, H₂, protons and electrons using excitation rates derived from the calculations of Wrathmall & Flower (2007) and Wrathmall, Gusdorf & Flower (2007) for collisions with H, Flower & Roueff (1998) and Flower & Roueff (1999) for collisions with H₂, Flower, Roueff & Zeippen (1998) and Balakrishnan, Forrey & Dalgarno (1999) for collisions with He, Gerlich (1990) and Krstić (2002) for collisions with H⁺ and Draine, Roberge & Dalgarno (1983) for collisions with electrons. We assume a fixed ortho-to-para hydrogen ratio of 3:1, which is a good approximation at the temperatures of interest in our simulations (Glover & Abel 2008).

2.3. Photon-Conserving Radiative Transfer

We treat the star as a point source at the origin of a spherical polar coordinate mesh. We first partition its

total emission rate \dot{n}_γ of ionizing photons obtained from Table 4 of Schaerer (2002) into energy bins according to the number rate of a blackbody

$$\dot{n}_\gamma = \sum_{i=1}^n \dot{n}(\nu_i) \Delta\nu \propto \sum_{i=1}^n \frac{(\nu_i/c)^2}{e^{h\nu_i/kT} - 1} \Delta\nu, \quad (9)$$

where the sum is over $h\nu > 13.6$ eV. The emission rate for a particular bin is then

$$\dot{n}_{\gamma,j} = \dot{n}(\nu_j) \Delta\nu = \frac{\frac{(\nu_j/c)^2}{e^{h\nu_j/kT} - 1}}{\sum_{i=1}^n \frac{(\nu_i/c)^2}{e^{h\nu_i/kT} - 1}} \dot{n}_\gamma. \quad (10)$$

We convert this emission rate into a flux at the lower face of each central boundary zone that we transport out into the grid by solving the static approximation to the equation of radiative transfer

$$\nabla \cdot \mathbf{F} = -\chi \mathbf{F}_r, \quad (11)$$

where χ is the inverse mean path of the UV photons in the neutral gas at the bin energy

$$\chi = \left(\sum_{i=1}^m n_i \sigma_i \right)^{-1}. \quad (12)$$

Here, n_i is the number density of the species absorbing the photon in the i th reaction whose cross section is σ_i , and the sum is over all removal processes, which are summarized in Table 1. A simple integration yields the radial flux at the lower face of each zone on the grid:

$$F_i = \left(\frac{r_{i-1}}{r_i} \right)^2 F_{i-1} e^{-\tau} \quad (13)$$

where

$$\tau = \sum_{i=1}^m \sigma_i n_i (r_i - r_{i-1}), \quad (14)$$

is the total optical depth of the cell (the sum is again over all absorption processes). We compute fluxes only out to the maximum distance a photon could have traveled by the given time in the simulation to avoid superluminal fronts. Photon conservation mandates that the total number of absorptions in a grid zone must equal the number of photons that enter its lower face minus those that exit its upper face, which in spherical polar coordinates reduces to

$$N_{\text{abs}} = F_i (1 - e^{-\tau}) \times \frac{r_i^2 (\phi_{k+1} - \phi_k) (\cos \theta_j - \cos \theta_{j+1})}{h\nu}, \quad (15)$$

The absorption rate for a particular reaction is extracted from the total rate by:

$$N_i = \frac{1 - e^{-\tau_i}}{\sum_{j=1}^m (1 - e^{-\tau_j})} N_{\text{abs}} \quad (16)$$

TABLE 1
ZEUS-MP RADIATIVE REACTION PROCESSES

Rate	Reaction	Energy
k_{24}	$\text{H} + \gamma \rightarrow \text{H}^+ + \text{e}^-$	$h\nu > 13.6$ eV
k_{26}	$\text{He}^+ + \gamma \rightarrow \text{He}^{++} + \text{e}^-$	$h\nu > 54.4$ eV
k_{25}	$\text{He} + \gamma \rightarrow \text{He}^+ + \text{e}^-$	$h\nu > 24.6$ eV
k_{27}	$\text{H}^- + \gamma \rightarrow \text{H} + \text{e}^-$	$h\nu > 0.755$ eV
k_{28}	$\text{H}_2^+ + \gamma \rightarrow \text{H}^+ + \text{H}$	2.65 eV $< h\nu < 21$ eV
k_{29}	$\text{H}_2 + \gamma \rightarrow \text{H}_2^+ + \text{e}^-$	$h\nu > 15.42$ eV
k_{30}	$\text{H}_2^+ + \gamma \rightarrow 2\text{H}^+ + \text{e}^-$	30 eV $< h\nu < 70$ eV
k_{31}	$\text{H}_2 + \gamma \rightarrow 2\text{H}$	11.18 eV $< h\nu < 13.6$ eV

where the sum is over all processes and τ_i is the optical depth of the reaction. This rate is then converted into the rate coefficient required by the reaction network

$$k_i = \frac{N_i}{n_i V_{\text{cell}}}, \quad (17)$$

where n_i is the number density of the species absorbing the photon by the i th reaction. Since F_i is the flux associated with a single energy bin, we sum the k_i of all the bins to obtain the total reaction rate coefficient in the cell for the entire spectrum. In practice, we obtain good convergence in frequency when we allocate 40 uniformly spaced bins in energy from 0.255 to 13.6 eV and 80 logarithmically-spaced bins from 13.6 to 90 eV for a 10^5 K blackbody source. We adopt the on-the-spot (OTS) approximation by using case B recombination coefficients for H and He. The parallelization and load balancing of our radiation transport scheme, photon cross sections, and a multifrequency I-front test are described in detail in Whalen & Norman (2006, 2008a).

2.4. LW Photodissociation

The H_2 photodissociation component k_{31} is computed apart from the radiative transfer. We first construct the LW specific flux $\bar{F}(\nu)$ at a mesh point in s^{-1} ergs cm^{-2} Hz^{-1} by geometrically diluting its value at the center of the grid by r^{-2}

$$\bar{F}(\nu) = \frac{\int F(\nu) d\nu}{\Delta\nu} \frac{1}{r^2}. \quad (18)$$

The frequency range is 11.18 eV to 13.6 eV and total stellar luminosities from Table 3 of Schaerer (2002) are used to derive $F(\nu)$ for the blackbody spectrum of the star. We then attenuate this flux with the H_2 self-shielding function of eq. 37 in Draine & Bertoldi (1996), which includes a correction for thermal Doppler broadening, to calculate k_{31} (see also Abel et al. 1997)

$$k_{31} = 1.1 \times 10^8 \bar{F}(\nu) F_{\text{shield}}. \quad (19)$$

We adopt the thermally broadened function to approximate the effect of gas motion, assuming a temperature of 10,000 K for the Doppler correction as in Whalen & Norman (2008a). Although the use of thermal broadening as a proxy for flows in I-fronts is approximate, its inclusion reduces shielding at intermediate column densities, ensuring that the H_2 cooling in our simulations are conservative lower limits.

2.5. Time Integration Scheme

The non-equilibrium reaction network is a stiff set of differential equations that exhibits a range of disparate characteristic timescales in addition to the Courant time. The challenge to coupling UV radiation, chemistry, and hydrodynamics self-consistently is to evolve each on its own timescale without restricting the entire algorithm to the shortest timescale. Chemical reaction, photoionization, and recombination times are usually governed by the electron flow in the gas

$$t_{chem} = \frac{n_e}{\dot{n}_e}, \quad (20)$$

which is formulated to ensure that the fastest reaction operating at any place or time on the grid determines the maximum time by which the reaction network can

be accurately advanced. The time on which energy is deposited in the gas by ionizations or removed by cooling is usually shorter than for hydrodynamical processes alone, and is approximately

$$t_{heat} = \frac{e_{gas}}{\dot{e}_{rad}} \quad (21)$$

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