SUPERMASSIVE POPULATION III SUPERNOVAE AND THE BIRTH OF THE FIRST QUASARS

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ABSTRACT

The existence of supermassive black holes as early as \( z \sim 7 \) is one of the great, unsolved problems in cosmological structure formation. One leading theory argues that they are born during catastrophic baryon collapse in \( z \sim 15 \) protogalaxies that form in strong Lyman–Werner UV backgrounds. Atomic line cooling in such galaxies fragments baryons into massive clumps that are thought to directly collapse to \( 10^2-10^3 \, M_\odot \) black holes. We have now discovered that some of these fragments can instead become supermassive stars that eventually explode as thermonuclear supernovae (SNe) with energies of \( \sim 10^{55} \text{erg} \), the most energetic explosions in the universe. We have calculated light curves and spectra for supermassive Pop III SNe with the Los Alamos RAGE and SPECTRUM codes. We find that they will be visible in near-infrared all-sky surveys by \textit{Euclid} out to \( z \sim 10-15 \) and by \textit{WFIRST} and \textit{WISH} out to \( z \sim 15-20 \), perhaps revealing the birthplaces of the first quasars.

Key words: black hole physics – cosmology: theory – early universe – galaxies: formation – galaxies: high-redshift – hydrodynamics – radiative transfer – stars: early-type – supernovae: general

Online-only material: color figures

1. INTRODUCTION

One model for the origin of supermassive black holes (SMBHs), which have now been found at \( z \sim 7 \) or less than a Gyr after the big bang (Mortlock et al. 2011), is catastrophic baryon collapse in protogalaxies that form in strong Lyman–Werner (LW) UV backgrounds at \( z \sim 15 \) (Wise et al. 2008; Regan & Haehnelt 2009; Shang et al. 2010; Agarwal et al. 2012; see also Bromm & Loeb 2003; Johnson & Bromm 2007; Djorgovski et al. 2008; Milosavljević et al. 2009; Alvarez et al. 2009; Lippai et al. 2009; Tanaka & Haiman 2009; Li 2011; Park & Ricotti 2011, 2012, 2013; Johnson et al. 2012, 2013c; Whalen & Fryer 2012; Latif et al. 2013a, 2013b; Choi et al. 2013; Reisswig et al. 2013). In this scenario, the primitive galaxy is built up by mergers between halos and by accretion in the vicinity of nearby LW UV sources that completely suppress star formation in the halos without evaporating them (Wolcott-Green et al. 2011; see also Johnson et al. 2008, 2009; Greif et al. 2008, 2010; Jeon et al. 2012; Pawlik et al. 2011, 2013; Wise et al. 2012 about recent numerical models of primaeval galaxies). When the galaxy reaches \( \sim 10^8 \, M_\odot \), its virial temperature crosses the threshold for atomic hydrogen line emission and its baryons begin to rapidly cool and collapse. Infall rates at the center of the galaxy can be enormous: \( 0.1-1 \, M_\odot \, \text{yr}^{-1} \), or 1000 times those in which the first stars form at \( z \sim 25 \) (Bromm et al. 1999, 2002; Abel et al. 2000, 2002; Nakamura & Umemura 2001; O’Shea & Norman 2007, 2008; Wise & Abel 2007; Yoshida et al. 2008; Turk et al. 2009; Stacy et al. 2010; Clark et al. 2011; Smith et al. 2011; Greif et al. 2011, 2012; Susa 2013; Hirano et al. 2013; for recent reviews on Pop III star formation, see Glover 2013; Whalen 2012).

Numerical simulations show that the baryons can shed angular momentum via the “bars within bars” instability on multiple spatial scales and collapse into an isothermal atomically cooled disk. The most recent models show that such disks can either feed a single massive central object or fragment into several slightly smaller ones (Regan & Haehnelt 2009; D. J. Whalen et al., in preparation). In Figure 1 we show the formation and fragmentation of such a disk at the center of a \( 10^8 \, M_\odot \) halo in a strong LW background at \( z \sim 15 \) in an adaptive mesh refinement (AMR) simulation done with Enzo.\textsuperscript{10} The recent discovery of a \( 10^9 \, M_\odot \) black hole (BH) in a quasar at \( z \sim 7 \) (Mortlock et al. 2011) favors SMBH seed formation by direct baryon collapse in LW protogalaxies over the creation of BHs by Pop III stars at \( z \sim 25 \) (Whalen & Fryer 2012; Johnson et al. 2013c).

The evolution of the fragments depends on their masses at birth and subsequent accretion histories (see Ohkubo et al. 2009, for studies of Pop III stellar evolution under ongoing accretion at much lower rates). One possibility is that the fragment forms a supermassive star (Fuller et al. 1986). In most cases these stars collapse directly to BHs. Another possibility is that the core of the star becomes a BH whose radiation supports the upper, convective layers of the star against collapse. The result is a “quasi-star” that appears to an external observer to be a large, cool star that is powered by a BH at its center rather than by a fusion core (Begelman et al. 2006, 2008; Begelman 2010; Volonteri & Begelman 2010). There is some question as to whether a quasi-star could be stable because a jet from the BH could rupture the upper layers of the star and destabilize its
envelope, but the final result would be the same: a $10^4$–$10^5 M_\odot$ SMBH seed.

The fragment could instead collapse quasistatically with intermittent nuclear burning without ever entering the main sequence. If it has enough angular momentum a black hole accretion disk (BHAD) system might form at its center. In this case most of the fragment eventually falls into the BH, perhaps with the formation of a strong wind that drives nuclear burning in the disk and blows some heavy elements out of the clump. However, if infall onto the fragment is heavy during its collapse it may be difficult to form a standard, geometrically thin accretion disk because this would require photon leakage times (radiative cooling times) to be shorter than the accretion (inflow) times, an ordering of time scales that is unlikely under these circumstances.

If a supermassive star forms in these conditions its radiation may not halt accretion and it too may evolve under heavy infall over its entire life (Johnson et al. 2012). In contrast, lower-mass Pop III stars usually disperse baryons from their halos (Whalen et al. 2004; Kitayama et al. 2004; Alvarez et al. 2006; Abel et al. 2007; Wise & Abel 2008; Whalen & Norman 2008b, 2008a). Other mechanisms for massive fragmentation and SMBH seed formation have been proposed, such as the suppression of gas cooling by primordial magnetic fields (Sethi et al. 2010) and cold accretion shocks (Inayoshi & Omukai 2012).

We have found that for a narrow range of mass around $55,000 M_\odot$, atomically cooled fragments can settle into stable nuclear burning and become supermassive stars with lifetimes of $\sim 2$ Myr (A. Heger & K.-J. Chen, in preparation). These stars die as extremely energetic thermonuclear supernovae (SNe), with energies of $\sim 10^{55}$ erg, or 100 times those of $65$–$260 M_\odot$ Pop III PI SNe (Rakavy & Shaviv 1967; Barkat et al. 1967; Heger & Woosley 2002; Bromm et al. 2003; Kitayama & Yoshida 2005; Gal-Yam et al. 2009; de Souza et al. 2011a; Vasiliev et al. 2012; see also Montero et al. 2012). Such events would be the most energetic explosions in the cosmos, and their detection could reveal the birthplaces of SMBHs created by direct collapse, since LW protogalaxies are the only environments known to form such massive clumps at $z \sim 15$. Could such SNe be discovered by existing or future observatories? Whalen et al. (2013b, 2013f) recently found that $140$–$260 M_\odot$ Pop III PI SNe will be detected in the near-infrared (NIR) out to $z \gtrsim 30$ by the James Webb Space Telescope (JWST; Gardner et al. 2006) and to $z \sim 15$–$20$ in all-sky surveys by the Wide Field Infrared Survey Telescope (WFIRST) and the Wide Field Imaging Surveyor for High Redshift (WISH) (see also Wise & Abel 2005; Scannapieco et al. 2005; Fryer et al. 2010; Kasen et al. 2011; Hummels et al. 2012; Pan et al. 2012a, 2012b; Whalen et al. 2013a, 2013c; de Souza et al. 2013). However, supermassive SNe might occur in very dense accretion envelopes that quench their luminosities at early times, when the greatest fraction of their flux is redshifted into the NIR. It is not clear if explosions could be detected.

We present numerical simulations of light curves, spectra and NIR signals of $55,500 M_\odot$ Pop III SNe at $7 < z < 30$ done with the Los Alamos RAGE and SPECTRUM codes. We consider only the observational signatures of these events, and defer detailed discussion of progenitor evolution, explosive nucleosynthesis and multidimensional mixing to A. Heger & K.-J. Chen (in preparation). The effects of these explosions on the protogalaxies that host them are examined in Johnson et al. (2013b), Whalen et al. (2013d), and Whalen et al. (2013e). In Section 2 we review our numerical methods for evolving the star, its explosion, and the propagation of the blast through the star and its envelope. In Section 3 we examine blast profiles, light curves and spectra for the SN in the source frame, and calculate detection thresholds as a function of redshift for these emissions. In Section 5 we conclude by discussing complementary detection strategies for the formation of SMBH seeds via direct collapse.

2. NUMERICAL METHOD

We calculate light curves and spectra in three stages. First, we evolve the $55,500 M_\odot$ zero-metallicity star from the beginning of the main sequence through collapse, explosive nuclear burning, and the expansion of the shock to the edge of the star in the Kepler code. In a parallel calculation we map the Kepler profile of the star onto a two-dimensional (2D) AMR mesh in the CASTRO code and evolve it through the same stages as in
our Kepler model. Next, we spherically average mass fractions from the final CASTRO profile onto a one-dimensional (1D) spherical-coordinate grid in Radiation Adaptive Grid Eulerian (RAGE) along with final density, velocity and energy profiles from the Kepler calculation. This is done to approximate how mixing in the interior of the star prior to shock breakout affects explosion spectra at later times. We evolve the shock through the surface of the star and into the surrounding medium with RAGE until it dims below observability. Finally, we post process our RAGE profiles with the SPECTRUM code to calculate light curves and spectra.

2.1. Kepler

We determine the internal structure of the star at the time of the explosion by evolving it from the beginning of the main sequence to the onset of collapse in the 1D stellar evolution code Kepler (Weaver et al. 1978; Woosley et al. 2002). The SN begins when the core of the star begins to contract and initiates explosive burning in the O and Si layers (Heger & Woosley 2002, 2010; Joggerst & Whalen 2011; Chen et al. 2011). The non-rotating star, which is resolved with 1148 mass zones, lives for 1.69 Myr and then dies as blue giant with a radius of $1.33 \times 10^{13}$ cm, similar to those of the $Z$-series stars in Whalen et al. (2013f) even though they are $\sim 200$ times as massive. The mass of the He core at the time of the explosion is $2.67 \times 10^4 M_{\odot}$.

This treatment is approximate for several reasons. First, we do not model the pre-main sequence evolution of the star or its growth from much lower masses. Instead, the star is initialized at the beginning of the main sequence in our evolution calculations. Second, we exclude the ongoing accretion under which the star may evolve over its lifetime, which might alter its final properties. Third, we do not include stellar rotation, which could lower the mass at which the star explodes (Chatzopoulos & Wheeler 2012; Chatzopoulos et al. 2013). Rotation may also broaden the mass range for which supermassive fragments can actually become stars by supporting them against collapse and enabling stable nuclear burning. Finally, we do not include radiative feedback from the star on inflow, which could regulate its growth rates. However, in some cases luminosity from the star terminates accretion (Johnson et al. 2012) so our assumption that the star has a constant mass would be valid. The evolution of massive primordial clumps and supermassive stars under ongoing accretion will be the focus of future studies.

2.2. CASTRO

At the beginning of central collapse we map our Kepler profiles onto a 2D axisymmetric grid in CASTRO (Almgren et al. 2010) and then evolve the SN through collapse and explosive burning, halting the simulation when the shock reaches the edge of the star. CASTRO (Compressible ASTROphysics) is a multidimensional Eulerian AMR code with an unsplit Godunov hydrodynamics solver. Energy production is calculated with a 19 isotope network up to the point of oxygen depletion in the core and with a 128 isotope quasi-equilibrium network thereafter. We evolve mass fractions for the same 15 even numbered isotopes that are predominantly synthesized by PI SNe. Radiation transport is not required in these models because the mean free paths of photons prior to breakout are so short that they are simply advected through the star by the fluid flow. We include the contribution of photons to the gas pressure in the equation of state (EOS). Our models include energy deposition due to radioactive decay of $^{56}$Ni in the ejecta as described by Equation (4) in Joggerst et al. (2010) although, as we discuss below, this explosion produces very little $^{56}$Ni, unlike $140-260 M_{\odot}$ Pop III PI SNe.

Mapping an explosion profile from a 1D Lagrangian coordinate mesh in mass to a 2D mesh in space can lead to violations in conservation of mass and energy. Linear interpolations in radius can also fail to resolve key features of the original profile, such as the structure of the core of the star and its temperature profile. Failure to properly map temperature features can be especially problematic because nuclear burn rates are highly sensitive to them during the explosion. To avoid these difficulties, we port Kepler profiles to CASTRO with the new conservative mapping scheme of Chen et al. (2011). This approach conserves mass and energy while reproducing all the features of the original profile over a broad dynamical range in space. The CASTRO root grid is $256^2$ with a resolution of $2.0 \times 10^{10}$ cm and up to two levels of AMR refinement (a factor of four increase in resolution).

The star explodes with an energy of $7.74 \times 10^{54}$ erg. Explosive burning begins in the O and Si layers and is done by $\sim 100$ s. The SN creates only trace amounts of $^{56}$Ni, $\sim 2.25 \times 10^{-8} M_{\odot}$, unlike Pop III PI SNe that form up to $50 M_{\odot}$ of $^{56}$Ni. The core of the SMS does not burn all the way to $^{56}$Ni like in PI SNe, and the little that is formed is at the edge of the He layer. As shown in Figure 2, the shock heavily mixes the interior of the star by the time it reaches the surface, in contrast to Pop III PI SNe that exhibit little mixing (Joggerst & Whalen 2011). The mixing is driven by fluid instabilities that are seeded during collapse and then amplified by explosive burning rather than by the formation of a reverse shock and the subsequent appearance of Rayleigh–Taylor instabilities at later times, as in $15-40 M_{\odot}$ Pop III SNe (Joggerst et al. 2010). Mixing is important to SN spectra because it can determine the order in which emission and absorption lines appear over time. Mass fractions for the various elements are realistically distributed in radius and angle in CASTRO when the shock breaks out of the star. Spherically averaging them prior to mapping them into RAGE therefore allows us to capture how mixing governs the order in which lines later appear in the spectra over time even though our RAGE models are 1D. We halt the CASTRO run when the shock is $\sim 100$ photon mean free paths $\lambda_p$ from the edge of the star:

$$\lambda_p = \frac{1}{\kappa_{Th} \rho},$$

where $\kappa_{Th}$ is the opacity due to Thomson scattering from electrons (0.288 gm$^{-1}$ cm$^2$ for primordial gas) and $\rho$ is the density just beyond the shock inside the star.

2.3. RAGE

We evolve the shock through the surface of the star and its envelope with the Los Alamos National Laboratory (LANL) radiation hydrodynamics code RAGE (Gittings et al. 2008). RAGE is a multidimensional AMR code that couples second order conservative Godunov hydrodynamics to gray or multigroup flux-limited diffusion (FLD) to model strongly radiating flows, RAGE utilizes the LANL OPLIB atomic opacity database (Magee et al. 1995) and can evolve multimaterial flows with a variety of EOSs. We employ the same physics as in Frey et al. (2013): multispecies advection, gray FLD radiation transport with two-temperature (2T) physics and LTE opacities, energy deposition from the radioactive decay of $^{56}$Ni, and an ideal gas

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EOS. 2T physics better captures shock breakout, when radiation and matter temperatures can be out of equilibrium. We advect mass fractions for 15 elements, the even numbered elements predominantly synthesized by PI SNe.

As in Whalen et al. (2013f), we include the self-gravity of the ejecta in our simulations. Because so much mass is packed into such a small volume in the star, its initial potential energy is close to the energy released in the explosion and must be included to obtain the kinetic energy and luminosity of the shock at early times. As a test of our recent implementation of self-gravity in RAGE we evolved the SN from just before shock breakout to $2.9 \times 10^6$ s in both RAGE and Kepler. As we show in Figure 3, the two density profiles are essentially identical at the latter time. The minor differences at the center are attributable to differences between the hydrodynamics schemes of the two codes.

We spherically average densities, velocities, specific internal energies (erg gm$^{-1}$), and species mass fractions from CASTRO onto a 200,000 zone 1D spherical mesh in RAGE. Since radiation energy densities are not explicitly evolved in Kepler, we initialize them in RAGE as

$$E_{\text{rad}} = a T^4,$$

where $a = 7.564 \times 10^{-15}$ erg cm$^{-3}$ K$^{-4}$ is the radiation constant and $T$ is the gas temperature. Also, because gas energies in Kepler include contributions from the ionization states of atoms, we construct the specific internal energy from $T$ with

$$E_{\text{gas}} = C_V T,$$

where $C_V = 1.2472 \times 10^8$ erg K$^{-1}$ is the specific heat of the gas.

At the beginning of the simulation we resolve the region from the center of the grid to the edge of the shock in the velocity profile with 100,000 zones. We allow up to five levels of refinement during the initial mapping of the profile but turn off AMR during the simulation. Our grid ensures that the photosphere of the shock is always resolved since failure to do so can lead to underestimates of luminosity during post processing. The radius of the shock in our setup is $1.3 \times 10^{13}$ cm and our first grid has a resolution of $1.3 \times 10^9$ cm with an outer boundary at $2.6 \times 10^{13}$ cm.

We set reflecting and outflow boundary conditions on the fluid and radiation variables at the inner and outer boundaries of the grid, respectively. At the beginning of the simulation, Courant times are short due to high temperatures, large velocities and small cell sizes. To minimize execution times and to accommodate the expansion of the SN, we periodically regrid the profiles onto a larger mesh as the explosion grows. At each regrid we allocate 100,000 zones out to either the edge of the shock (pre-breakout) or the radiation front (post-breakout). In the latter case we take the radius at which the radiation temperature falls to the wind temperature (0.01 eV) to be the edge of the front. The inner boundary is always at the origin and the outer boundary of the final, largest mesh in our simulations is $1.0 \times 10^{18}$ cm. We again permit up to five levels of refinement during the initial regridding of the profile but disable AMR during the simulation.

### 2.4. Circumstellar Envelope

We consider explosions in two kinds of envelope: low-mass outflows (SMS1) and massive inflows like those that grew the star to such large masses in such short times (SMS2). For diffuse outflows we adopt the usual power-law density profile for a wind.
at a constant velocity:

$$\rho_W(r) = \frac{\dot{m}}{4\pi r^2 v_W}. \quad (4)$$

Here, $\dot{m}$ is the mass loss rate associated with the wind and $v_W$ is the wind speed. The mass loss rate is calculated from the total mass loss $M_{\text{tot}}$ and the main sequence lifetime of the star $t_{\text{MSL}}$:

$$\dot{m} = \frac{M_{\text{tot}}}{t_{\text{MSL}}}. \quad (5)$$

Pop III stars are not thought to lose much mass over their lives because there are no metals in their atmospheres to drive winds (Kudritzki 2000; Baraffe et al. 2001; Vink et al. 2001; Krúčka & Kubát 2006), so we set $M_{\text{tot}} = 0.1 M_\odot$ and $v_W = 1000 \text{ km s}^{-1}$.

We treat the massive infall envelope as a wind in reverse, with $\dot{m} = 0.01 M_\odot \text{ yr}^{-1}$ and an infall velocity $v_{\text{w}} = 5 \text{ km s}^{-1}$, in keeping with numerical simulations of baryon collapse in protogalaxies in strong LW backgrounds. This profile assumes that accretion is spherical when in reality it may occur in a disk, so it should be considered to be the densest envelope through which the SN shock might propagate. In both cases we take the wind to be 76% H and 24% He by mass. Rather than calculate the ionization state of the wind (Whalen & Norman 2006) we take it to be cold ($T = 0.01 \text{ eV}$) and neutral in all our models for simplicity. This assumption holds for dense envelopes, where semi-analytical studies have shown that ionizing UV photons cannot propagate more than a few dozen stellar radii from the star over its lifetime (Johnson et al. 2012; for studies on UV breakout from low-mass Pop III protostellar disks, see Omukai & Palla 2001; Omukai & Inutsuka 2002; Omukai & Palla 2003; Tan & McKee 2004; McKee & Tan 2008; Hosokawa et al. 2011, 2012; Stacy et al. 2012).

On the other hand, the compact blue progenitor, with a total luminosity of $3.5 \times 10^{42} \text{ erg s}^{-1}$ and $T_{\text{eff}} = 6.85 \times 10^4 \text{ K}$, likely ionizes the diffuse wind so the luminosities we calculate for that case are lower limits. We show initial RAGE density and velocity profiles for the shock, the star, and its envelope in Figure 4. The surface of the star is visible as the sharp drop in density at $\sim 1.4 \times 10^{13} \text{ cm}$. The fact that the accretion envelope has a density at the surface of the star that is seven orders of magnitude greater than that of the wind has important consequences for shock and radiation breakout, as we discuss below. In both cases we evolve the SN out to 3 yr.

### 2.5. SPECTRUM

We calculate spectra for the explosions with the LANL SPECTRUM code. SPECTRUM directly sums the luminosity of every fluid element in a SN profile to calculate the total flux escaping the ejecta along the line of sight for 14900 wavelengths. The procedure is described in detail in Frey et al. (2013) and accounts for Doppler shifts and time dilation due to the relativistic expansion of the ejecta. SPECTRUM also calculates the intensities of emission lines and the attenuation of flux along the line of sight with OPLIB opacities, so it captures limb darkening and absorption lines imprinted on the flux by intervening material in the SN ejecta and envelope.
As explained in Frey et al. (2013), densities, velocities, radiation temperatures, and mass fractions from the finest levels of refinement in the RAGE AMR hierarchy are extracted and ordered by radius into separate files, with one variable per file. These profiles can contain more than 200,000 radial zones, so limits on machine memory and time prevent us from using all of them to calculate a spectrum. We therefore map only a subset of the points onto the new grid. We first sample the radiation energy density profile inward from the outer boundary to find the position of the radiation front, which we define to be where $aT^4$ rises above $1.0 \text{ erg cm}^{-3}$. This energy density is intermediate to that of the cold wind and the radiation front. The radius of the $\tau = 25$ surface is then found by integrating the optical depth due to Thomson scattering inward from the outer boundary, where $\kappa_{\text{Th}} = 0.288 \text{ gm}^{-1} \text{ cm}^{2}$ for primordial H and He. This gives the greatest depth from which photons can escape from the ejecta because $\kappa_{\text{Th}}$ is the minimum total opacity.

To compute a spectrum, we interpolate the densities, temperatures, velocities and mass fractions we extract from RAGE onto a 2D grid in $r$ and $\mu = \cos \theta$ in SPECTRUM, whose inner and outer boundaries are zero and $10^{18}$ cm. The region from the center of the grid to the $\tau = 25$ surface is partitioned into 800 uniform zones in log radius. We allocate 6200 uniform zones in radius between the $\tau = 25$ surface and the edge of the radiation front. The wind between the front and the outer boundary is divided into 500 uniform zones in log radius, for a total of 7500 radial bins. The fluid variables in each of these new radial bins is mass averaged to ensure that SPECTRUM captures very sharp features in the original RAGE profile. The grid is discretized into 160 uniform zones in $\mu$ from $-1$ to 1. Our choice of mesh yields good convergence in spectrum tests, fully resolving regions of the flow from which photons can escape the ejecta and only lightly sampling those from which they cannot.

### 3. BLAST PROFILES, LIGHT CURVES, AND SPECTRA

We show velocity and gas temperature profiles at shock breakout for the SMS1 and SMS2 explosions in Figures 5 and 6. Before breakout, the SN cannot be seen by an external observer because photons from the shock are scattered by $e^-$ in the upper...
layers of the star. When the shock reaches the surface of the star it abruptly accelerates, as shown in the velocity profiles of Figures 5 and 6. The shock also releases a brief, intense pulse of photons into the envelope. This transient, which is mostly X-rays and hard UV, blows off the outer layers of the star, which detach from and accelerate ahead of the shock as we show at $8192$ and $8407$ s in the SMS1 velocities and at $8940$ and $1.02e04$ s in the SMS2 velocities. This effect is more pronounced in SMS1 because it is easier for the radiation front to drive a precursor into the diffuse wind than the dense infall. The advancing radiation front is visible as the flat plateau in gas temperature that extends from the outer edge of the shock into the surrounding medium. The temperature to which the radiation heats the gas falls as the shock expands, cools, and its spectrum softens (note that the temperature of the shock itself is much higher).

At breakout there are marked differences in the profiles of the two explosions as the shock plows into the envelope. In both cases the shock accelerates but then slows down as it crashes out into the surrounding envelope, although the deceleration is stronger in the dense infall. But the SMS1 shock reaches much higher peak velocities than the SMS2 shock. This is partly due to the greater inertia of the infall and partly because the radiation front more easily blows off the outermost layers of the star in the diffuse wind. The radiation front also advances more quickly into the diffuse wind than the accretion flow. On the other hand, when the shock breaks out into the dense envelope it heats it to much higher temperatures. This hardens the spectrum of the shock and raises the temperature of the surrounding gas to higher temperatures than in SMS1, $\sim 100$ eV instead of $\sim 50$ eV.

We show bolometric light curves for SMS1 and SMS2 in Figure 7. The light curve for SMS1 is similar to those of lower-mass Pop III PI SNe except that the explosion is approximately 40 times as luminous, as shown by the $z250$ light curve from Whalen et al. (2013f). SMS1 exhibits the classic breakout transient, whose width is related to the light-crossing time of the star but is somewhat broader due to radiation-matter coupling effects as discussed in Section 4.1 of Whalen et al. (2013f). Its light curve is similar in structure to that of $z250$, which is also the explosion of a compact blue giant. At early times the luminosity of SMS1 comes from the conversion of kinetic energy into thermal energy by the shock. Later, ejecta cooling (not $^{56}$Ni decay, since virtually none forms in these explosions) also contributes to its luminosity, in contrast to lower-mass PI SNe which are primarily powered by $^{56}$Ni at later times. As in the z-series PI SNe, there is a resurgence in luminosity at $\sim 10^7$ s that is again due to optical depth. At this time the $\tau = 1$ surface associated with the wavelength of peak emission in the spectrum has sunk to a hot layer deep in the ejecta, exposing it to the intergalactic medium and causing the SN to rebrighten.

Radiation breakout in SMS2 occurs far after shock breakout, at $\sim 3.0 \times 10^6$ s as we show in Figure 7. Radiation escapes the dense envelope much later because of its large optical depth, and when it happens it is gradual, as we show in Figure 8. Low-energy photons begin to leak out through the $\tau = 1$ surface for Thomson scattering at $\sim 2.6 \times 10^6$ s, and they are followed by more energetic photons by $5.6 \times 10^6$ s. At this point the shock is much cooler because of the large amount of $PdV$ work it must perform on the dense shroud as it expands, but this results in an extremely luminous event in the NIR, as we discuss below.

After radiation breakout the shock appears to flicker until $\sim 1.7 \times 10^7$ s. This is due to radiative cooling and the cyclic formation and dissipation of a reverse shock in the ejecta. As the shock plows up the envelope a reverse shock breaks free from the forward shock and is driven into the interior of the ejecta in the frame of the flow. As the reverse shock detaches and recedes from the forward shock, it loses pressure support to radiative cooling by emission lines in the shocked gas and retreats back toward the forward shock. As the forward shock continues to sweep up the envelope a reverse shock again forms and backsteps from the forward shock. The cyclic heating and cooling of shocked gas associated with the oscillation of the reverse shock, together with fluctuations in opacities associated with these temperature cycles, cause the variations in luminosity from $2.5 \times 10^6$ to $1.7 \times 10^7$ s. The period of oscillation is determined by cooling rates in the gas (Chevalier & Imamura 1982; Imamura et al. 1984; Anninos et al. 1997) and is independent of the mass swept up by the ejecta. Such ripples are also found in Lyman alpha emission by primordial SN remnants as they sweep up neutral gas in cosmological halos.

Figure 7. Bolometric luminosities for SMS1 and SMS2, together with the light curve for the $z250$ PI SN from Whalen et al. (2013f). (A color version of this figure is available in the online journal.)

Figure 8. Radiation breakout in SMS2: gas temperatures at $5.78e6$ s, $7.70e6$ s, and $1.02e7$ s.
on larger scales (note Figure 11 in Whalen et al. 2008c). The light curves of both SMS1 and SMS2 are easily distinguished from those of less massive Pop III PII SNe.

We show velocity and density profiles for both explosions at intermediate to late times in Figures 9 and 10. Multiple shocks are evident in the diffuse wind just ahead of the shock in the SMS1 run at earlier times but they mostly dissipate by 3 yr, although some structures are still visible in the velocity. These shocks are driven by the propagation of radiation through the low-density wind ahead of the shock rather than by the sweeping up of gas by the shock (indeed, the ejecta does not accumulate its own mass in ambient gas until it has grown to 6 pc). The formation of a strong reverse shock due to plowed-up gas can be seen in the SMS2 velocity profiles from $10^5$ s to $10^6$ s. By $10^7$ s the surrounding wind has become sufficiently diffuse that the propagation of radiation from the shock through it has created the same multiple shocks in it as in SMS1.

4. NIR LIGHT CURVES

We calculate NIR light curves from our spectra with the photometry code developed by Su et al. (2011). Each spectrum is redshifted prior to removing the flux that is absorbed by intervening neutral hydrogen along the line of sight using the method of Madau (1995). The spectrum is then dimmed by the required cosmological factors for a specified redshift. The least sampled data is linearly interpolated between the input spectrum and filter curve to model the light curve in a given filter.

4.1. SMS1

NIR luminosities are plotted for SMS1 at $z = 7, 10, 15, 20$ and 30 in the left panel of Figure 11. The SN will be visible to JWST at all epochs for over 1000 days but falls below the photometry limit of WFIRST and WISH at $z \gtrsim 7$. If spectrum stacking extends the detection limit of WFIRST to AB magnitude 29 it could detect these explosions out to $z \sim 10$. SMS1 is quite luminous in the NIR, with peak magnitudes ranging from 27.5 at $z = 7$ to 29.5 at $z = 20$. These light curves exhibit far more variability than their redshifted bolometric light curves might suggest, eliminating any possibility that these events would be mistaken for high-redshift protogalaxies. This variation is due to the expansion and cooling of the fireball in the source frame.
The NIR profiles of SMS1 are easily distinguished from those of the \( u \)-series and \( z \)-series PI SNe at all redshifts (see Figures 10 and 11 of Whalen et al. 2013f). The SMS1 NIR light curves are similar in shape to those of \( z \)-series PI SNe, but the \( z \)-series luminosities are always several magnitudes dimmer at \( z > 7 \). The SMS1 light curves evolve with redshift as expected: they broaden as \( z \) increases and the optimum filter wavelength increases with redshift. The NIR luminosities rise more quickly than they decline so these events are most easily detected in their early stages, but they nonetheless exhibit enough variability at any stage to be found in multi-year baseline searches.

4.2. SMS2

We show NIR luminosities for SMS2 at \( z = 7, \, 10, \, 15, \, 20 \) and \( 30 \) in the right panel of Figure 11. They are quite different from those of SMS1. Consistent with radiation breakout from the shroud at \( \sim 20 \) days, no NIR signal is observed from these events until 100–150 days at \( z > 7 \). This explosion eventually becomes hundreds of times brighter in the NIR than SMS1, with peak AB magnitudes from 21 at \( z = 7 \) to 23 at \( z = 15 \). It is visible to \( JWST \) for 1000–3000 days out to \( z \sim 20 \) and to \( WFIRST \) and \( WISH \) for 1000 days out to \( z \sim 15–20 \). We also note that \( Euclid \), with a photometry limit of AB mag 24 at 2.2 \( \mu \)m, can detect SMS2 for \( \sim 1000 \) days at \( z = 10–15 \), the likely epoch of these events. The much higher NIR luminosities are due to the large radius of the fireball at radiation breakout and the relatively low temperature of the shock at this radius (\( \sim 10 \) eV) because of the \( PdV \) work the fireball must do against the dense envelope. These lower temperatures drive the redshifted peak of the shock’s spectrum into the NIR in the observer frame. The relative magnitudes of the three light curves are properly ordered in redshift. The ripples in luminosity have much shorter periods than those in the bolometric luminosity in Figure 7 and are likely due to opacity fluctuations in the shock.

In sum, SMS explosions in both diffuse winds and dense envelopes will be visible in \( JWST \) NIR deep fields out to \( z \gtrsim 30 \) but only the latter will be visible to all-sky NIR surveys by \( Euclid \), \( WFIRST \), and \( WISH \). But they will be visible at \( z \sim 15 \), which is when they likely begin to occur. The fact that these NIR profiles change considerably with circumstellar envelope suggests that they will be powerful probes of the environments of such explosions. It is worth noting that even fully shrouded explosions will be visible at the earliest epochs. The envelopes we have chosen should bracket those in which SMS PI SNe will occur, so the NIR signals of actual explosions may be intermediate to those of these two events. Given the massive infall rates required to form supermassive Pop III stars, it is unlikely these stars fully disperse their accretion envelopes in their lifetimes (Johnson et al. 2012), and so we expect their SN light curves to be closer to SMS2 than SMS1 in brightness. As noted earlier, both SMS1 and SMS2 are easily distinguished from low-mass Pop III PI SNe as well as core-collapse SNe (Whalen et al. 2013c) and Type IIn SNe (Moriya et al. 2010; Whalen et al. 2013a).

5. CONCLUSION

The discovery of supermassive Pop III PI SNe would confirm for the first time that massive fragments capable of collapsing to \( 10^8–10^9 \)\( M_\odot \) SMBH seeds do form in primeval galaxies at high redshift. Although the rate of such events remains unknown, it might be thought that they are very rare because supermassive fragments must fall into a relatively narrow mass range to actually become stars and because few protogalaxies form in LW backgrounds capable of fully sterilizing them of \( H_2 \). However, recent developments suggest that these processes were more frequent than previously thought.

First, new simulations indicate that the assembly of protogalaxies in strong LW backgrounds may have been relatively common, yielding higher rates of SMBH seed production than might naively be inferred from the number density of \( z \sim 7 \) quasars, \( \sim 1 \text{ Gpc}^{-3} \) (Agarwal et al. 2012). The sustained exponential growth required to reach such masses depended on the topology of cold flows over cosmic time (Di Matteo et al. 2012), so the scarcity of such flows may have governed the density of \( z \sim 7 \) quasars, not the rate of seed formation. Second, rotation could broaden the mass range over which supermassive...
stars encounter the pair instability by enhancing mixing and more rapidly building up massive He cores (Chatzopoulos & Wheeler 2012). Greater mass ranges imply larger event rates.

A reasonable upper limit to SMS PI SN event rates are those of 140–260 $M_{\odot}$ Pop III PI SNe, which Whalen et al. (2013f) and others find to be $\sim 10^{-2}$ yr$^{-1}$ deg$^{-2}$ at $z \gtrsim 10$, which implies all-sky rates of up to $\sim 10^3$ yr$^{-1}$ (Wise & Abel 2005; Weinmann & Lilly 2005; O’Shea et al. 2005; Tornatore et al. 2007; Whalen et al. 2008a, 2010; Trenti et al. 2009; Greif et al. 2010; Maio et al. 2011; Hummel et al. 2012; Johnson et al. 2013a; Wise et al. 2012). Although actual SMS PI SN event rates may be well below this limit, precluding their detection by JWST, they will clearly be bright enough to appear in wide field campaigns. They might also be detected in present NIR all-sky surveys by the Subaru Hyper Suprime-Cam at $z \gtrsim 3$ but further calculations will be necessary to confirm this (e.g., Tominaoka et al. 2011; Tanaka et al. 2012; Moriya et al. 2013). Synchrotron emission from Pop III SNe at $z \gtrsim 10$ can be detected at 21 cm by existing observatories such as eVLA and eMerlin and future ones such as the Square Kilometre Array (SKA; Meiksin & Whalen 2013). SMS PI SN explosions in dense envelopes may likewise generate enough synchrotron emission to be discovered in radio surveys.

We note that the formation of somewhat less massive SMS stars ($\sim 10^4$–$10^5 M_{\odot}$) may lead to highly energetic ($E_{\gamma,iso} \sim 10^{55}$–$10^{57}$ erg s$^{-1}$) gamma-ray bursts (GRBs; Suwa & Ioka 2011; Nagakura et al. 2012; see also Whalen et al. 2008b; Mesler et al. 2012). They are characterized by extended prompt emission because of the large reservoirs that can drive the central engine and that are necessary for the GRB jet to puncture the large envelopes of such stars. The afterglows of very massive Pop III GRBs can appear in both current and future radio surveys by eVLA, eMerlin, and the SKA (de Souza et al. 2011b). They will also be visible in future all-sky NIR campaigns by WFIRST and WISH.

Given that most supermassive stars will still directly collapse to BH, could there be other ways of detecting SMBH seed formation in protogalaxies? Past studies have shown that collapsing supermassive stars become extremely luminous in thermal neutrino emission as the central BH forms, with energies of $\sim 10$ MeV (Fryer et al. 1986; Shi et al. 1998; Montero et al. 2012). The prospects for detecting such neutrinos depends on the initial mass and entropy of the core. Although the total energy emitted from these massive stars increases linearly with mass, the entropy of their cores also increases with mass. Higher entropies lead to larger proto-BHs with lower peak densities and lower temperatures. Fryer & Heger (2011) found that the neutrino luminosity does not increase much with mass for stars above 10,000 $M_{\odot}$. The mean electron neutrino energy for stars above 10,000 $M_{\odot}$ is below 6 MeV and the $\mu_+$ energy is not much higher. The collapse of such cores would be difficult to observe with neutrino detectors. However, if the core entropy is closer to that of a 1000 $M_{\odot}$ star, the luminosity peaks more dramatically. Although even for these cores the mean electron neutrino energy is $\sim 7$–8 MeV, the $\mu_+$ energy lies in the 20–30 MeV range and would be more easily detected after cosmological redshifting. More detailed calculations are needed to be certain, but these cores would likely contribute to the neutrino background in detectors such as IceCube. If the density profile of the collapsing star also imposes a unique spectrum on the neutrino flux, it would facilitate its extraction from noise.

As noted in the Introduction, collapse may also lead to the formation of a BHAD system without the creation of a star, with nuclear burning near the event horizon whose products could be expelled out into the halo by a jet (e.g., Surman et al. 2006, 2008). The nucleosynthetic signature of this process, which could be imprinted on stars that later form in the protogalaxy, depends on the temperature of the disk and hence the radius of the BH. It can therefore provide a diagnostic of the mass of the SMBH seed at birth, since massive BH with large event horizons burn at lower temperatures and yield chemical abundances that are distinct from those of smaller disks, which can burn all the way to Ni. Ancient, dim metal-poor stars bearing the ashes of this process could soon be discovered in ongoing surveys in the Galactic halo (e.g., Cayrel et al. 2004; Beers & Christlieb 2005; Frebel et al. 2005; Lai et al. 2008; Mackey et al. 2003; Smith & Sigurdsson 2007; Smith et al. 2009; Chiaki et al. 2013; Ritter et al. 2012). The collapse of a supermassive star could also emit gravity waves (GWs) that might be detected in existing or future GW facilities (e.g., Fryer et al. 2002; Fryer & New 2011). These multi-messenger events, together with the most energetic SNe in the universe, may soon herald the births of the first quasars.

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