Supermassive black hole formation by cold accretion shocks in the first galaxies

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ABSTRACT

We propose a new scenario for supermassive star (SMS: $\gtrsim 10^5 M_\odot$) formation in shocked regions of colliding cold accretion flows near the centres of the first galaxies. Recent numerical simulations indicate that assembly of a typical first galaxy with virial temperature $T_{\text{vir}} \gtrsim 10^4 K$ proceeds via cold and dense flows penetrating deep to the centre, where supersonic streams collide with each other to develop a hot ($\sim 10^4 K$) and dense ($\sim 10^4 \text{ cm}^{-3}$) shocked gas. The post-shock layer first cools by efficient Ly$\alpha$ emission and contracts isobarically until $\lesssim 8000$ K. Whether the layer continues its isobaric contraction depends on the density at this moment: if the density is high enough to excite $H_2$ rovibrational levels collisionally ($\gtrsim 10^4 \text{ cm}^{-3}$), enhanced $H_2$ collisional dissociation suppresses the gas from cooling further. In this case, the layer fragments into massive ($\gtrsim 10^5 M_\odot$) clouds, which collapse isothermally ($\sim 8000$ K) by Ly$\alpha$ cooling without subsequent fragmentation. As an outcome, SMSs are expected to form and eventually evolve into the seeds of supermassive black holes (SMBHs). By calculating the thermal evolution of the post-shock gas, we delimit the range of post-shock conditions for SMS formation, which can be expressed as $T \gtrsim 6000 K (n_H/10^4 \text{ cm}^{-3})^{-1}$ for $n_H \gtrsim 10^4 \text{ cm}^{-3}$ and $T \gtrsim 5000$–6000 K for $n_H \gtrsim 10^3 \text{ cm}^{-3}$, depending somewhat on the initial ionization degree. We found that metal enrichment does not affect the above condition for metallicity below $\gtrsim 10^{-3} Z_\odot$ if metals are in the gas phase, while condensation of several per cent of metals into dust decreases this critical value of metallicity by an order of magnitude. Unlike the previously proposed scenario for SMS formation, which postulates extremely strong ultraviolet radiation to quench $H_2$ cooling, our scenario here naturally explains SMBH seed formation in the assembly process of the first galaxies, even without such strong radiation.

Key words: stars: formation – stars: Population III – galaxies: formation – galaxies: nuclei – dark ages, reionization, first stars – early Universe.

1 INTRODUCTION

The discovery of high-$z$ quasars has demonstrated the existence of supermassive black holes (SMBHs) of $\sim 10^6 M_\odot$ at the age of the Universe, $\lesssim 1$ Gyr (e.g. Fan 2006; Willott et al. 2007; Mortlock et al. 2011). As an origin for such SMBHs, seed black hole (BH) formation as a remnant of Population III stars ($M_{\text{seed}} \sim 100 M_\odot$) and subsequent growth by merger and gas accretion have been studied by a number of authors (e.g. Haiman & Loeb 2001; Volonteri, Haardt & Madau 2003; Li et al. 2007). Even with the Eddington accretion rate $M_{\text{Edd}} = L_{\text{Edd}}/c^2$, where $L_{\text{Edd}}$ is the Eddington luminosity and $c$ is the speed of light, the growth time $t_{\text{grow}} = 0.05 \ln (M_{\text{BH}}/M_{\text{seed}})$ Gyr becomes as great as the age of the Universe at $z \gtrsim 6$ ($\gtrsim 0.8$ Gyr): seed BHs are thus required to keep growing at the Eddington rate. However, negative feedback by growing BHs prevents such efficient accretion (Alvarez, Wise & Abel 2009; Milosavljević, Couch & Bromm 2009; Jeon et al. 2011).

As a solution to this, the alternative possibility of massive seed BH formation by the direct collapse of supermassive stars (SMSs: $\gtrsim 10^5 M_\odot$) has been considered by some authors. Specifically, SMS formation in massive haloes ($T_{\text{vir}} \gtrsim 10^4 K$) irradiated with strong far-ultraviolet (FUV) radiation has often been studied (e.g. Bromm & Loeb 2003; Regan & Haehnelt 2009a,b; Shang, Bryan & Haiman 2010). Since the $H_2$ molecule, the main coolant in primordial gas, is photodissociated with strong FUV radiation in the Lyman and Werner bands, clouds under such an environment collapse isothermally at $\sim 8000$ K through Ly$\alpha$ cooling without fragmentation, if they are massive enough with $\gtrsim 10^5 M_\odot$. As an outcome of such collapse, SMSs are expected to form. A massive seed BH as a remnant of SMS collapse reduces the growth time to $10^5 M_\odot$ within $0.46$ Gyr and mitigates the growth-time problem by a big margin. This scenario, however, has a serious drawback: for this...
mechanism of SMS formation to work, extremely strong FUV radiation \( L_{\text{FW}}^{\text{21}} \gtrsim 10^{-2} \cdots 10^3 \) (in units of \( 10^{-21} \text{erg s}^{-1} \text{cm}^{-2} \text{Hz}^{-1} \text{sr}^{-1} \)) is required (Omukai 2001; Bromm & Loeb 2003; Shang et al. 2010), while the fraction of haloes irradiated with such intense FUV fields with \( L_{\text{FW}}^{\text{21}} \gtrsim 10^3 \) is estimated to be \( \lesssim 10^{-6} \) at \( z \sim 10 \) (Dijkstra et al. 2008), i.e., only extremely rare haloes satisfy the condition for SMS formation. Moreover, if high-energy components, such as cosmic rays or X-rays, are present along with the FUV radiation, their ionization effect promotes \( \mathrm{H}_2 \) formation and then strongly suppresses SMS formation (Inayoshi & Omukai 2011). Although the above scenario might be still viable considering the rarity of high-

\( z \) SMBHs, it is worthwhile exploring another possibility.

In this paper, we propose a new scenario for SMS formation in the post-shock gas of cold accretion flows in the forming first galaxies. Recent numerical simulations of galaxy formation have revealed that, in haloes with virial temperature \( T_{\text{vir}} \gtrsim 10^4 \) K, the shock position does not stay at the virial radius and shrinks inside owing to efficient Ly\( \alpha \) cooling, and the accreting cold gas penetrates deep to the centre through dense filamentary flows (Birnboim & Dekel 2003; Kereš et al. 2005; Dekel & Birnboim 2006; Dekel et al. 2009; Bromm & Yoshida 2011). The supersonic flows collide each other and the resultant shock develops a hot and dense \((10^4 \cdots 10^5 \text{cm}^{-3})\) gas near the centre (Wise & Abel 2007; Greif et al. 2008; Wise, Turk & Abel 2008). By studying the thermal evolution of the shocked gas, we have found that, if the post-shock density is high enough for \( \mathrm{H}_2 \) rovibrational levels to reach local thermodynamic equilibrium (LTE), efficient collisional dissociation suppresses \( \mathrm{H}_2 \) cooling and the gas cannot cool below several thousand K. Massive clouds with \( \gtrsim 10^3 \) \( M_{\odot} \) formed by fragmentation of the post-shock layer subsequently collapse isothermally at \( \sim 8000 \) K through Ly\( \alpha \) cooling. Without further fragmentation, monolithic collapse of the clouds results in SMS formation. Note that, unlike the previous SMS formation mechanism, strong FUV radiation is not required in our scenario. Similar analysis has also been carried out by Safranek-Shrader, Bromm & Milosavljević (2010), who studied the fragmentation of the cold-stream shocked layer considering the effects of radiation fields and chemical enrichment, but for a single post-shock condition \((4 \times 10^3 \text{cm}^{-3}, 1.1 \times 10^4 \) K and equilibrium chemical abundances).

The organization of this paper is as follows. In Section 2, we describe the model for calculation of thermal evolution in the shocked gas. In Section 3, we present our results and clarify the conditions for isothermal collapse leading to SMS formation in terms of post-shock density and temperature. The effects of metal enrichment are also considered here. In Section 4, we analyse thermal processes in the shocked gas and discuss the reason for the bifurcation of thermal evolution in more detail. Finally, we summarize our study and present some discussion in Section 5.

2 MODEL

In this section, we describe our model for calculation of thermal evolution in hot and dense shocked regions formed by the collision of cold accretion flows in the first galaxies.

2.1 Evolution in the post-shock layer

We consider the thermal evolution in the post-shock layer under the assumption that the flow is steady and plane-parallel. Since the post-shock temperature is as high as the virial temperature of the first-galaxy-forming haloes \((T_{\text{vir}} \gtrsim 10^4 \) K), cooling by Ly\( \alpha \) emission is efficient early on. The post-shock flow is compressed almost isobarically as long as the gas cools effectively (e.g. Shapiro & Kang 1987). Within the steady-state approximation, the conservation of mass and momentum leads to the following relationships between the density \( \rho_0 \), pressure \( p_0 \) and flow velocity \( v_0 \) just behind the shock and those in the post-shock flow \( \rho, p \) and \( v \):

\[
\rho v = \rho_0 v_0, \tag{1}
\]

\[
\rho v^2 + p = \rho_0 v_0^2 + p_0. \tag{2}
\]

Along this flow, we solve the energy equation

\[
dE/dr = p + E \frac{d\rho}{\rho} - \Lambda_{\text{net}}, \tag{3}
\]

where \( E \) is the internal energy per unit volume, \( d/dr \) is the Lagrangian time derivative and \( \Lambda_{\text{net}} \) is the net cooling rate per unit volume. Assuming a strong shock and neglecting thermal pressure in the pre-shock flow, \( p_0 \sim 3 \rho_0 H_0^2 \) is satisfied just behind the shock front. Thus, we approximate the right-hand side of equation (2) by \( 4\rho_0 H_0^2 \). The cooling term \( \Lambda_{\text{net}} \) includes radiative cooling by \( \mathrm{H}, \mathrm{H}_2 \) and HD and cooling/heating associated with chemical reactions. We solve the chemical reactions of primordial gas among the following 14 species; \( \mathrm{H}, \mathrm{H}_2, \mathrm{e}^-, \mathrm{H}^+, \mathrm{H}^0, \mathrm{H}^+, \mathrm{He}, \mathrm{He}^+, \mathrm{He}^{++}, \mathrm{D}, \mathrm{HD}, \mathrm{D}^+, \mathrm{HD}^+ \) and \( \mathrm{D}^- \). We adopt the same coefficients for the cooling/heating and chemical reactions as in Inayoshi & Omukai (2011), except for omitting radiative/cosmic-ray ionization and dissociation in this calculation. In studying the effects of metal enrichment, we add cooling by the fine-structure-line emission of \( \mathrm{C}_2 \) and \( \mathrm{O}_2 \) to the primordial processes described above. Assuming the fraction of metals depleted to dust grains to be the same as in Galactic interstellar gas, we set the number fractions of \( \mathrm{C} \) and \( \mathrm{O} \) nuclei in the gas phase with respect to \( \mathrm{H} \) nuclei to \( x_{\text{C},\text{gas}} = 0.927 \times 10^{-4} (\text{Z} / 2) \) and \( x_{\text{O},\text{gas}} = 3.568 \times 10^{-4} (\text{Z} / 2) \) (Pollack et al. 1994). We follow Hollenbach & McKee (1989) in calculating the cooling rates of \( \text{C}_2 \) and \( \text{O}_2 \). We curtail the \( \text{C} \) and \( \text{O} \) chemistry by simply assuming that all \( \text{C} \) and \( \text{O} \) are in the states \( \text{C}_2 \) and \( \text{O}_2 \), respectively, from the following consideration: with lower ionization energy (11.26 eV) than \( \text{H} \) atoms, \( \text{C} \) is photoionized by weak background radiation and in the state of \( \text{C}_2 \), while \( \text{O} \) is in ionization equilibrium with \( \text{H} \) and almost neutral for \( \lesssim 8000 \) K, where \( \text{O}_2 \) cooling is important. Molecular cooling of metals (e.g. \( \text{CO} \) and \( \text{H}_2 \text{O} \)) is not included since its cooling is not important in the temperature range relevant for the bifurcation of thermal evolution \((\gtrsim 10^3 \) K).

Next, we consider the condition for gravitational instability during isobaric compression of the post-shock layer, and thus for fragmentation. For isobaric compression, the dynamical time \( t_{\text{dyn}}(\equiv \rho/(d\rho/dt)) \), which characterizes thermal evolution, is approximately equal to the cooling time

\[
t_{\text{cool}} = \left( \frac{3}{2} m_{\text{H}} k_B T \right) / \Lambda_{\text{net}}, \tag{4}
\]

where \( m_{\text{H}} \) is the number density of \( \text{H} \) nuclei and \( T \) is the temperature. On the other hand, the growth time-scale for gravitational instability is given by the free-fall time (e.g. Larson 1985)

\[
t_{\text{ff}} = \sqrt{\frac{32}{3\pi G \rho}}. \tag{5}
\]

As long as the cooling is effective enough and so \( t_{\text{cool}} \ll t_{\text{ff}} \), the post-shock layer continues to be compressed isobarically. However, once cooling becomes ineffective and \( t_{\text{cool}} \) exceeds \( t_{\text{ff}} \), the contraction of the layer halts and a dense layer begins to develop inside the post-shock region. For example, since the growth rate of baryonic mass in haloes of \( \sim 10^4 M_{\odot} \) at \( z \sim 10 \) is \( \sim 4 \times \ldots\)
2.2 Evolution after fragmentation

After fragmentation, the cloud collapses owing to self-gravity and its evolution cannot be modelled as a steady flow any more. Density evolution in a cloud collapsing by self-gravity is described by the Penston–Larson self-similar solution (Penston 1969; Larson 1969), which has a density profile with a flat core of Jeans scale and an envelope with power-law density distribution \( \rho(\rho) \propto \rho^{-2} \). The density in the central core roughly increases over the free-fall timescale. We here calculate the evolution in the central core using a one-zone model, where the density evolution is given by

\[
\frac{d\rho}{dt} = \frac{\rho}{t_f}. \tag{6}
\]

Namely, after the condition for fragmentation (\( t_{cool} \gtrsim t_f \)) is satisfied, we switch the density evolution described by equations (1)–(2) to that described by equation (6) in our calculation and solve equation (3) for this density evolution.

When the collapse proceeds significantly and the cloud becomes optically thick, radiative cooling becomes ineffective due to photon-trapping. We assume the radius of the core to be half a Jeans length,

\[
R_c = \frac{\lambda_1}{2} = \sqrt{\frac{\pi k_B T}{G \rho \mu m_H}}, \tag{7}
\]

where \( \mu \) is the mean molecular weight. Since we consider the core of the collapsing cloud, the column density of the \( i \)th species is given by \( N_i = x_i n_R R_c \), where \( x_i \) is its concentration. Using this value, we estimate the optical depth and the reduction rate of radiative cooling as in Inayoshi & Omukai (2011).

2.3 Initial conditions

According to numerical simulations of the first galaxy formation (e.g. Greif et al. 2008; Wise et al. 2008), the pre-shock number density and temperature of cold flows and the shock velocity are typically \( 10^3 \) cm\(^{-3} \), \( 200 \) K and 20 km s\(^{-1} \), respectively, which correspond to the post-shock density \( 4 \times 10^3 \) cm\(^{-3} \) and temperature 9000 K. With these fiducial values in mind, we carry out calculations for a wide range of initial number densities and temperatures: \( 10^2 \) cm\(^{-3} \) \( < n_{H_0} < 10^3 \) cm\(^{-3} \) and 3000 K \( < T_0 < 10^5 \) K. Since \( H_2 \), the main coolant below 8000 K, forms through the electron-catalysed reactions

\[
H + e^- \rightarrow H^- + \gamma, \tag{8}
\]

the initial ionization degree \( x_{e,0} \), along with the initial \( H_2 \) concentration \( x_{H_2,0} \), is an important quantity for the subsequent thermal evolution. In reference to the results of Kang & Shapiro (1992), who studied the chemical abundances in pre-shock gas considering photoionization and dissociation by UV radiation emitted from the shock, we regard \( x_{e,0} \sim 10^{-2} \) and \( x_{H_2,0} \sim 10^{-6} \) as the typical ionization degree and molecular fraction, respectively. However, since cold accretion flows are far denser (\( \sim 10^3 \) cm\(^{-3} \)) than the range Kang & Shapiro (1992) assumed (\( \lesssim 10^{-2} \) cm\(^{-3} \)), electron recombination as well as shielding of the UV photoionization/dissociation probably lower the pre-shock ionization degree \( x_{e,0} \) and elevate the molecular fraction \( x_{H_2} \) from those values. Taking this uncertainty into account, we study cases with a wide range of initial ionization degree and \( H_2 \) fraction: \( 10^{-5} \leq x_{e,0} \leq 10^{-1} \) and \( 10^{-6} \leq x_{H_2,0} \leq 10^{-3} \).

3 RESULTS

In this section, we present our results for thermal evolution after the gas experiences a cold accretion shock. We first consider the case of primordial gas and then discuss the effects of small metal enrichment.

3.1 Primordial-gas case

In Fig. 1, we show the temperature evolution of primordial gas for four post-shock conditions, indicated by two open and two filled circles. We here set the initial ionization degree and molecular fraction to \( x_{e,0} = 10^{-2} \) and \( x_{H_2,0} = 10^{-6} \), respectively. First, we consider the cases from the open-circle initial conditions in Fig. 1, the temperature evolution of which is shown by dashed lines. In the lower initial-density case \( (n_{H_0}, T_0) = (5 \times 10^2 \text{ cm}^{-3}, 3.6 \times 10^4 \text{ K}) \), the temperature evolution of primordial gas after heating by a cold accretion shock for initial ionization degree \( x_{e,0} = 10^{-2} \) and \( H_2 \) fraction \( x_{H_2,0} = 10^{-6} \) is shown by the two thin solid lines. These two evolutionary tracks are calculated by the density evolution of equation (6) from the initial conditions and show the temperature evolution after overtaking the shock by cold accretion flows are far denser (\( \sim 10^3 \) cm\(^{-3} \)) than the range Kang & Shapiro (1992) assumed (\( \lesssim 10^{-2} \) cm\(^{-3} \)), electron recombination as well as shielding of the UV photoionization/dissociation probably lower the pre-shock ionization degree \( x_{e,0} \) and elevate the molecular fraction \( x_{H_2} \) from those values. Taking this uncertainty into account, we study cases with a wide range of initial ionization degree and \( H_2 \) fraction: \( 10^{-5} \leq x_{e,0} \leq 10^{-1} \) and \( 10^{-6} \leq x_{H_2,0} \leq 10^{-3} \).

Figure 1. The temperature evolution of primordial gas after heating by a cold accretion shock for initial ionization degree \( x_{e,0} = 10^{-2} \) and \( H_2 \) fraction \( x_{H_2,0} = 10^{-6} \). The evolutionary tracks are shown with dashed and dash–dotted lines for four combinations of initial temperature and density, indicated by two open and two filled circles. From low-density or low-temperature initial conditions (dashed lines starting from open circles), the temperature decreases below \( 10^3 \) K owing to \( H_2 \) and HD cooling. On the other hand, from dense and hot initial conditions (dash–dotted lines from filled circles) the clouds do not cool below \( 10^3 \) K and subsequently collapse almost isothermally by H atomic cooling. The triangle symbol on each track indicates the epoch during which the post-shock layer fragments by gravitational instability. The thick solid line, the domain above which is hatched, divides the initial conditions leading to these two different types of thermal evolution. The two thin solid lines show the temperature evolution by H atomic cooling (upper) and \( H_2 \) and HD cooling (lower), respectively. These two evolutionary tracks are calculated by the density evolution of equation (6) from the initial conditions and show the temperature evolution after overtaking the shock by cold accretion flows are far denser (\( \sim 10^3 \) cm\(^{-3} \)) than the range Kang & Shapiro (1992) assumed (\( \lesssim 10^{-2} \) cm\(^{-3} \)), electron recombination as well as shielding of the UV photoionization/dissociation probably lower the pre-shock ionization degree \( x_{e,0} \) and elevate the molecular fraction \( x_{H_2} \) from those values. Taking this uncertainty into account, we study cases with a wide range of initial ionization degree and \( H_2 \) fraction: \( 10^{-5} \leq x_{e,0} \leq 10^{-1} \) and \( 10^{-6} \leq x_{H_2,0} \leq 10^{-3} \).

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post-shock gas cools by Lyα emission and is compressed isobarically. Although Lyα cooling becomes inefficient below 8000 K, enough H₂ for cooling has already been formed by this time, which enables a further temperature decrease. HD is formed abundantly for \( T \leq 1500 \) K, the cooling of which eventually lowers the temperature to \( \sim 50 \) K. At this point, without efficient coolant any more, \( t_{\text{cool}} \) becomes longer than \( t_{\text{ff}} \). Clouds with Jeans mass of several times \( 10M_\odot \) are produced by gravitational instability. Also, in the case of lower initial temperature (\( 10^5 \) cm\(^{-3}\), \( 3.3 \times 10^5 \) K), abundant H₂ is formed immediately. Cooling by H₂ and then by HD allows the temperature to plummet isobarically until \( \sim 100 \) K, where the fragmentation mass-scale of a few \( 10M_\odot \) is imprinted. In both cases, temperature evolution after fragmentation converges to the well-known track for clouds collapsing by self-gravity and cooling by H₂ and HD (lower thin solid line: Uehara & Inutsuka 2000; Nagakura & Omukai 2005).

Next, we see the two cases starting from the filled-circle initial conditions in Fig. 1, the evolutionary tracks of which are indicated by the dash–dotted lines. In the higher initial temperature case (\( 10^4 \) cm\(^{-3}\), \( 3.6 \times 10^5 \) K), the gas cools isobarically until 8000 K as in the open-circle cases. At \( \sim 8000 \) K, however, the density exceeds \( \sim 10^5 \) cm\(^{-3}\), the critical density for H₂ to reach LTE. For higher density, H₂ is rapidly dissociated collisionally from the excited rovibrational levels, and thus sufficient H₂ for cooling is never formed. Consequently, the gas cannot cool below \( \sim 8000 \) K, and massive clouds with \( \gtrsim 10^4 M_\odot \) are formed by fragmentation. Also, in the case of initial temperature somewhat lower than 8000 K (\( 2 \times 10^5 \) cm\(^{-3}\), \( 5 \times 10^5 \) K), H₂ cooling is suppressed by collisional dissociation and fragmentation occurs immediately, producing massive clouds with \( \gtrsim 10^4 M_\odot \), the temperature of which increases to 8000 K by compressional heating in the course of gravitational collapse. In both cases, the massive clouds thereafter collapse almost isothermally by Lyα cooling until very high density (\( \sim 10^{16} \) cm\(^{-3}\)), where the cloud becomes optically thick to H\(^\alpha\) bound–free absorption (Omukai 2001). Such isothermally contracting clouds do not fragment in the later phase and thus collapse monolithically to SMSs, which eventually evolve to the seeds of SMBHs (Bromm & Loeb 2003; Shang et al. 2010).

As seen above, the behaviour of thermal evolution can be classified into two types. The thick solid line in Fig. 1 corresponds to the boundary of initial conditions, above or below which the subsequent thermal evolution bifurcates. Namely, the post-shock conditions above the boundary (the hatched region) lead to isothermal evolution at \( \sim 8000 \) K, while those below it result in isobaric temperature decrease until \( \lesssim 100 \) K. The boundary on the low-density side (\( n_{\text{H}_0} \lesssim 10^4 \) cm\(^{-3}\)) can be fitted as

\[
T_0 \gtrsim 8 \times 10^3 \left( \frac{n_{\text{H}_0}}{7 \times 10^3 \text{ cm}^{-3}} \right)^{-1} \text{ K.} \tag{9}
\]

This means that, after isobaric cooling to 8000 K, if the density exceeds the H₂ critical value for LTE (\( \sim 10^4 \) cm\(^{-3}\)) then the gas cannot continue further isobaric compression and starts isothermal collapse. For higher densities, \( n_{\text{H}_0} \gtrsim 10^4 \) cm\(^{-3}\), the boundary is given by

\[
T_0 \gtrsim 5 \times 10^3 \left( \frac{n_{\text{H}_0}}{10^5 \text{ cm}^{-3}} \right)^{-0.1} \text{ K.} \tag{10}
\]

In Section 4, we discuss physical processes determining the location of the boundary in more detail.

We mention the effect of initial chemical composition on thermal evolution. In Fig. 2, we show the boundaries for SMS-forming conditions for different initial ionization degrees (\( 10^{-5} \leq n_{\text{e},0} \leq 10^{-1} \)). The positions of the boundaries are almost independent of \( n_{\text{e},0} \) for \( \gtrsim 10^5 \) cm\(^{-3}\), while the portions at \( \lesssim 10^4 \) cm\(^{-3}\) move to lower density with decreasing \( n_{\text{e},0} \). In particular, for \( n_{\text{e},0} = 10^{-3} \) this results in the spiky domain around 8000 K extending as low as \( \sim 3 \times 10^2 \) cm\(^{-3}\). With higher initial ionization degree, more H₂ is formed by electron-catalysed reactions (8), which results in a wider range of post-shock conditions for H₂ cooling, i.e. a smaller range for SMS formation. The boundary for \( n_{\text{e},0} \leq 10^{-2} \) asymptotically approaches that for higher \( n_{\text{e},0} \) at \( \gtrsim 3 \times 10^5 \) K, since the ionization degree jumps up immediately to \( \sim 10^{-1} \), even with a smaller initial value, by effective collisional ionization,

\[
\text{H} + \text{e}^+ \rightarrow \text{H}^+ + 2 \text{e}^-, \tag{11}
\]

in this temperature range. We also studied cases with different molecular fraction \( n_{\text{H}_2,0} = 10^{-6}, 10^{-5} \) and \( 10^{-3} \), and found that the boundaries for SMS formation are almost independent of \( n_{\text{H}_2,0} \). This is because, even with high initial value, H₂ is rapidly dissociated collisionally for \( \lesssim 10^4 \) cm\(^{-3}\) and its fraction reaches the equilibrium one, which is independent of initial value.

3.2 Metallicity effect

Next, we consider the cases with slight metal enrichment. In Fig. 3, we present the boundaries for SMS-forming initial conditions for various metallicities with \( 0 \leq Z \leq 2 \times 10^{-3} Z_\odot \). With some metals, cooling by fine-structure line emission of C II and O I can exceed that by H₂ and plays an important role in thermal evolution. With metallicities as low as \( Z \lesssim 5 \times 10^{-4} Z_\odot \), metal cooling does not affect thermal evolution around 8000 K and the boundary does not move from the primordial case. As seen in Section 3.1, not enough H₂ for cooling is formed from initial conditions hotter and denser than the boundary (i.e. the hatched region of Fig. 1) and only massive clouds are produced, which collapse isothermally thereafter. With increasing metallicity, metal-line cooling becomes able to make the gas cool below \( \sim 5000 \) K isobarically even without H₂. Once the temperature decreases and collisional dissociation becomes ineffective, abundant H₂ eventually forms and the gas cools to \( \lesssim 100 \) K. By this additional cooling, the boundary of the SMS-forming initial conditions moves to higher density. With metallicities as high as
Z \sim 10^{-3} Z_{\odot},\) the cooling rate by C II and O I becomes comparable to the compressional heating at \(\sim 8000\) K and \(\sim 10^{7}\) cm\(^{-3}\). Therefore, even without the help of H\(_2\) cooling metal cooling alone is able to lower the temperature to the range where H\(_2\) collisional dissociation is ineffective, and thus the boundary shifts to higher density.

In summary, for metallicity higher than the critical value \(Z_c \sim 10^{-3} Z_{\odot},\) the boundary density becomes far higher than the typical post-shock value for a cold accretion shock, \(\sim 10^{5}\) cm\(^{-3}\), and such an initial condition would be very difficult to realize. Thus the possibility of SMS formation is strongly reduced for higher metallicity. On the other hand, as long as \(Z < Z_c\), the range of initial conditions for SMS formation remains the same as in the primordial case.

### 4 MECHANISM FOR THE BIFURCATION OF THERMAL EVOLUTION

In this section, we explain what processes are responsible for the bifurcation of thermal evolution in the region where the cold accretion shock is thermalized and give a physical interpretation for the location of the bifurcation boundary for the post-shock conditions in Figs 1 and 2.

Efficient Ly\(_{\alpha}\) cooling drives the temperature in a hot gas rapidly to \(\sim 8000\) K, where its cooling rate is sharply cut off, as the atomic hydrogen is not excited for lower temperature. In Fig. 4, we show the cut-off temperature (dotted line) below which H\(_2\) takes over the role of dominant coolant. Thus, for post-shock gas to continue isobaric cooling below 8000 K, H\(_2\) cooling must become effective and keep the cooling time \(t_{\text{cool}}\) shorter than the free-fall time \(t_0\). The cooling time owing to H\(_2\) cooling is given by

\[
t_{\text{cool}} \approx \frac{(3/2)k_\text{cool}T}{L_{\text{H}_2}x_{\text{H}_2}},
\]

where \(L_{\text{H}_2} = \Lambda_{\text{H}_2}/(n_{\text{H}_2}x_{\text{H}_2})\) is the cooling rate per H\(_2\) molecule \((\text{erg s}^{-1})\) and has the density dependence \(L_{\text{H}_2} \propto (1 + n_{\text{H}_2}/n_\text{LTE})^{-1}\) \((n_{\text{H}_2,\text{LTE}} \sim 10^{4}\) cm\(^{-3}\) is the H\(_2\) critical density for LTE). In the conditions under consideration (below the dotted line in Fig. 4), the H\(_2\) fraction \(x_{\text{H}_2}\) is set by the equilibrium between the electron-catalysed formation reaction and collisional dissociation reaction, \(^1\) and so

\[
x_{\text{H}_2} = \frac{k_\text{form}}{k_\text{cd}} x_e,
\]

where \(k_\text{form} (H + e^- \rightarrow H^+ + \gamma)\) and \(k_\text{cd} (H_2 + H \rightarrow 3H)\) are reaction-rate coefficients for the indicated reactions, respectively. Note that \(k_\text{cd}\) depends on the fraction of H\(_2\) in excited states and thus on the density. The rate coefficient \(k_\text{cd}\) significantly increases with density near the H\(_2\) critical density \(n_{\text{H}_2,\text{crit}}\), which results in the rapid decrease of \(x_{\text{H}_2}\) by effective collisional dissociation at \(\gtrsim 10^7\) cm\(^{-3}\).

Furthermore, since \(x_{\text{H}_2}\) is proportional to \(x_e\), recombinations can also be a key reaction to determine \(t_{\text{cool}}\) \((\propto x_e^{-1})\) at \(\lesssim 8000\) K. Since the recombination time \(t_{\text{rec}} = 1/\alpha_{\text{rec}} n_e x_e\) \((\alpha_{\text{rec}}\) is the recombination-rate coefficient\)) has the same dependence on \(x_e\) as \(t_{\text{cool}}\), the ratio of these two time-scales becomes independent of \(x_e\) and is approximately given by

\[
t_{\text{cool}}/t_{\text{rec}} = \left(\frac{(3/2)n_n k_\text{cd}T}{L_{\text{H}_2}}\right) k_{\text{rec}}/k_\text{form} 
\]

\[
\simeq 0.9 \left(\frac{R_{\text{rec}}}{3000\text{kK}}\right)^0.9 \left(\frac{n_e}{10^4\text{cm}^{-3}}\right).
\]

The last expression above is valid for the density and temperature around \(t_{\text{cool}} \simeq t_{\text{rec}}\) and \(\gtrsim 10^7\) cm\(^{-3}\), and the large temperature dependence of equation (14) is due to that of \(k_\text{cd}\). In Fig. 4, we show the range of parameters satisfying \(t_{\text{cool}} > t_{\text{rec}}\) (the hatched region),

\(^1\) Only with high \(x_e \sim 10^{-1}\) does the charge-exchange reaction (H\(_2\) + H\(^+\) → H\(_2^+\) + H) become the main dissociation reaction of H\(_2\) at \(\lesssim 10^7\) cm\(^{-3}\). However, since the bifurcation boundary for \(x_e,0 = 10^{-1}\) is located at higher density \((\gtrsim 10^4\) cm\(^{-3}\)), the charge-exchange reaction does not have any influence on the location of the boundary. Thus, we adopt equation (13) even for \(x_e \sim 10^{-1}\).
where recombination effectively works during isobaric contraction. Note that the hatched region appears only at $10^5$ cm$^{-3}$, where $k_{\text{cd}}$ is significantly enhanced. On the other hand, the ionization degree is frozen during isobaric compression at a density lower than the hatched region, as $t_{\text{cool}} < t_{\text{rec}}$. Under constant $x_e$, the cooling time becomes shorter and shorter with decreasing temperature as $t_{\text{cool}} \propto T^{-0.7}$ (at $\approx 5000$ K) because collisional dissociation is strongly suppressed for lower temperatures. Thus, efficient H$_2$ cooling and the resultant isobaric evolution continue until $\sim 100$ K.

We first consider the cases with $x_{e,0} \gtrsim 10^{-4}$ and defer the discussion of lower ionization cases until later. As an example, in Fig. 4 we present the evolutionary tracks of shocked gas with $x_{e,0} = 10^{-2}$ for different initial temperatures (solid lines) and the bifurcation boundary of the SMS-forming initial condition (right dashed line). While the gas passes through the hatched region where $t_{\text{cool}} > t_{\text{rec}}$, the ionization degree and thus H$_2$ fraction fall rapidly. If such a gas runs out of H$_2$ before reaching the region where $t_{\text{cool}} < t_{\text{rec}}$, the condition for fragmentation $t_{\text{cool}} \gtrsim t_g$ is immediately satisfied and the clouds formed in this way collapse isothermally thereafter (the solid lines starting from the filled circles in Fig. 4). However, there is a small margin of the initial parameter range above the line $t_{\text{cool}} = t_{\text{rec}}$, from which the gas manages to maintain a small fraction of H$_2$ and can reach the region where $t_{\text{cool}} < t_{\text{rec}}$. In this case, the post-shock layer can continue isobaric contraction until $\sim 100$ K (the solid line starting from the open circle in Fig. 4). In summary, if the fragmentation condition $t_{\text{cool}} \gtrsim t_g$ is met in the range where $t_{\text{rec}} < t_{\text{cool}}$, the post-shock layer cannot cool further and clouds formed at this moment begin isothermal collapse. The set of initial conditions from which the evolutionary tracks meet the condition $t_{\text{cool}} = t_{\text{rec}}$ just on the line $t_{\text{cool}} = t_{\text{rec}}$ corresponds to the boundary for SMS formation in Fig. 1 in the high-density regime (i.e. equation 10). Note that the boundary given by equation (10) reflects the density–temperature relation of $t_{\text{rec}} = t_{\text{cool}}$, which is mainly determined by the temperature dependence of $k_{\text{cd}}$. Due to the strong dependence of $k_{\text{cd}}$ on temperature, H$_2$ is collisionally dissociated very efficiently for temperatures higher than given by equation (10). On the other hand, if the density is lower than the H$_2$ critical density $n_{\text{H}_2,0} (\approx 10^5$ cm$^{-3}$) after cooling isobarically to 8000 K, the gas continues further isobaric contraction to several 100 K by ineffective collisional dissociation of H$_2$. This explains the fact that the low-density side of the boundary of SMS-forming parameters in Fig. 1 (i.e. equation 9) corresponds to the isobaric contraction track with a density at $\approx 8000$ K of $\sim 10^4$ cm$^{-3}$.

Next, we consider the low-ionization cases with $x_{e,0} \lesssim 10^{-4}$. As seen in Fig. 4, the portion of the bifurcation boundary (left solid line) for $x_{e,0} = 10^{-5}$ is located in the region $t_{\text{rec}} > t_{\text{cool}}$, where $x_e$ is frozen during isobaric compression. Therefore, if the cooling condition $t_{\text{cool}} < t_g$ is initially satisfied in the post-shock layer, the gas continues to cool isobarically until $\lesssim 100$ K, where it produces $\sim 10^3 M_\odot$ fragments. Thus, the boundary of the SMS-forming condition is simply given by the requirement $t_g \lesssim t_{\text{cool}}$ for their initial values without the need for considering the recombination effect. The dot-dashed line in Fig. 4 presents the condition $t_g = t_{\text{cool}}$ for $x_e = 10^{-5}$ and in fact coincides with the boundary on the low-temperature side ($\lesssim 8000$ K).

5 CONCLUSION AND DISCUSSION

In this paper, we have proposed a new scenario for supermassive star (SMS) formation in the central hot and dense regions of the haloes formed by cold accretion shocks during the first galaxy formation. Since the gas cools effectively by Ly$\alpha$ emission in haloes with virial temperature $T_{\text{vir}} \gtrsim 10^4$ K, the location of the accretion shock does not stay at the virial radius but rather shrinks inward. The gas instead flows supersonically along cold and dense filaments to the central region of the first galaxy, where the flows collide with each other to produce hot ($\gtrsim 10^5$ K) and dense ($\gtrsim 10^3$ cm$^{-3}$) material by a shock (Birnboim & Dekel 2003; Kerei et al. 2005; Dekel & Birnboim 2006; Wise & Abel 2007; Greif et al. 2008; Wise et al. 2008; Dekel et al. 2009; Bromm & Yoshida 2011). We have calculated thermal evolution in such a hot and dense region formed by a cold accretion shock. For $\gtrsim 8000$ K, efficient Ly$\alpha$ cooling allows the post-shock gas to cool and contract isobarically at the value of the ram pressure from the shock front. To continue isobaric cooling below 8000 K, abundant H$_2$ needs to be formed and its cooling must be effective. If the density at $\approx 8000$ K is high enough ($\gtrsim 10^4$ cm$^{-3}$) to make the H$_2$ rovibrational levels reach LTE, the H$_2$ is dissociated effectively by the collisional reaction from excited levels, which suppresses cooling to lower temperature by H$_2$. At this epoch, gravitational instability of the post-shock layer produces massive fragments with $\gtrsim 10^5 M_\odot$, which subsequently collapse isothermally at $\approx 8000$ K by Ly$\alpha$ cooling. We have studied the thermal evolution of the post-shock gas for a wide range of initial conditions ($10^3$ cm$^{-3} < n_{\text{H}_2,0} < 10^5$ cm$^{-3}$ and $3000 K < T_0 < 10^5$ K) and have pinned down the conditions leading to isothermal collapse (the hatched region in Fig. 1): $T_0 > 6000 (n_{\text{H}_2,0}/10^3$ cm$^{-3})^{-1}$ K for $n_{\text{H}_2,0} \lesssim 10^3$ cm$^{-3}$ and $T_0 \gtrsim 5000–6000$ K for $n_{\text{H}_2,0} \gtrsim 10^4$ cm$^{-3}$, for pre-shock ionization degree $x_{e,0} = 10^{-2}$. Since H$_2$ is formed by electron-catalysed reactions (equation 8), the above condition depends somewhat on the initial ionization degree (see Fig. 2): for smaller $x_{e,0}$, the domain of initial conditions leading to isothermal collapse extends towards lower density. Those massive clouds continue isothermal collapse until very high density $\sim 10^{16}$ cm$^{-3}$, where they become optically thick to H$^-$ bound–free absorption (Omukai 2001). The clouds are supposed to collapse directly to SMSs without further fragmentation (e.g. Bromm & Loeb 2003; Regan & Haehnelt 2009a,b; Shang et al. 2010). Eventually, SMSs collapse through post-Newtonian instability, swallowing most of their material, to become seeds of SMBHs (Shibata & Shapiro 2002).

The first galaxies may be enriched with metals to some extent as well as dust dispersed by supernova (SN) explosions of the previous generations of stars. With high enough metallicity, the gas can cool to low temperature ($\sim 100$ K) by metal-line cooling alone even without H$_2$. In this case, SMS formation would be strongly suppressed. We have repeated the same analysis by considering cooling by Cu and O1 as well as metals. We have found that as long as the metallicity is lower than $Z_{\odot} \approx 10^{-3} Z_\odot$, the metal-line cooling does not change the condition for SMS formation from that in the primordial case (see Fig. 3). According to some cosmological simulations of the assembly of the first galaxies (Greif et al. 2010; Wise et al. 2012), the dense gas at the centre of galaxies is uniformly enriched to $\sim 10^{-3} Z_\odot$ by pair-instability SNe of massive Population III stars with $140 M_\odot \lesssim M \lesssim 260 M_\odot$. On the other hand, typical Population III stars have recently been considered to be less massive $\sim 40 M_\odot$ (Hosokawa et al. 2011; Stacy, Greif & Bromm 2011) and end their lives as ordinary core-collapse SNe. In this case, the resultant metallicity reduces by a factor of $\sim 10$ (Heger & Woosley 2002; Nomoto et al. 2006) and thus becomes lower than the critical metallicity for SMS formation that we estimated.

We here stress that our scenario naturally explains the formation of seed BHs in the conditions of first-galaxy formation without invoking extremely strong UV radiation as envisaged in the
previous scenario. The necessary condition for SMS formation in haloes with $T_{\text{vir}} \gtrsim 10^4$ K is isothermal collapse by atomic cooling as a result of the suppression of H$_2$ cooling in the entire density range. So far, as a mechanism to suppress H$_2$ cooling, photodissociation by FUV radiation has been considered. In this scenario, however, an extremely strong FUV intensity $J_{\text{FUV}} \gtrsim 10^7$–$10^9$ (in units of $10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$ sr$^{-1}$) is required to quench H$_2$ cooling (Omukai 2001; Bromm & Loeb 2003; Shang et al. 2010) and haloes irradiated by such intense radiation are extremely rare ($\lesssim 10^{-6}$ at $z \sim 10$; Dijkstra et al. 2008). Moreover, if external ionization by cosmic rays or X-rays, which promotes H$_2$ formation, is present as well, the FUV intensity needed for SMS formation is elevated. There would be little possibility ($\lesssim 10^{-6}$) of such an intense FUV field being realized in any haloes and thus SMS formation could be strongly suppressed (Inayoshi & Omukai 2011). On the other hand, in our scenario collisional dissociation, rather than photodissociation, suppresses H$_2$ cooling. Thus, even without FUV radiation, which has previously been considered to be indispensable, isothermal collapse and thus SMS formation can be realized as long as the right condition is met for the cold accretion shock. Note, however, this mechanism for SMS formation cannot operate in all first galaxies since SMBHs are rare objects. If we use the number density of haloes with mass $\sim 10^8$ M$_\odot$ at $z \sim 10$, $\sim 10$ Mpc$^{-3}$ (comoving) and assume each of them had a SMS of $\sim 10^5$ M$_\odot$, the predicted mass density of SMBHs $\sim 10^5$ M$_\odot$ Mpc$^{-3}$ (comoving) will exceed the total present-day BH mass density $\sim 3 \times 10^3$ M$_\odot$ Mpc$^{-3}$ estimated by Yu & Tremaine (2002). Therefore, our conditions for SMS formation would be satisfied only in a small fraction of first galaxies or else some other processes, e.g. turbulent fragmentation, lack of accreting material etc., suppress this mechanism from working to avoid the overproduction of BHs.

We here briefly discuss the effect of dust cooling, which has not been considered in this paper. If the depletion factor of metals to dust grains is as high as the present-day Galactic value $f_{\text{dust}} \approx 0.5$, the thermal evolution deviates from the isothermal one at $\gtrsim 10^6$ cm$^{-3}$ due to dust cooling, if the metallicity is higher than $Z_{\odot, \text{dust}} \approx 10^{-5}$ Z$_\odot$ (Omukai, Schneider & Haiman 2008). Although this critical metallicity $Z_{\odot, \text{dust}}$ is smaller than the critical value due to metal-line cooling $Z_{\odot} \approx 10^{-3}$ Z$_\odot$ by two orders of magnitude, the depletion factor in the first-galaxy-forming environment is highly uncertain. According to theoretical models of dust formation and destruction in the first SNe, typically only a few per cent of dust formed at the explosion survives, after being swept by the reverse shock, depending on the ambient density (Nozawa, Kozasa & Habe 2006; Bianchi & Schneider 2007). For example, with $f_{\text{dust}} \approx 0.05$, the critical metallicity becomes $Z_{\odot, \text{dust}} \approx 10^{-4}$ Z$_\odot$, which makes the constraint on metal pollution less severe. In any case, to predict whether isothermal collapse continues in spite of metal enrichment, we need more accurate knowledge of the depletion factor $f_{\text{dust}}$.

In this paper, we consider the hot and dense central regions resulting from shocks by cold accretion flows in the forming first galaxies. Likewise, a galaxy merging event drives inflows, creating a similar environment around the galaxy centre (e.g. Mayer et al. 2010). If the shocked region satisfies our post-shock criterion for H$_2$ collisional dissociation, SMS formation is expected in this case also. In merging galaxies, however, star formation and also metal enrichment are expected to have already proceeded significantly. Therefore, in the case of inflows by a galaxy merger, SMS formation is probably prohibited by the metal-cooling effect. The cold accretion shocks in the first galaxy formation would more easily provide suitable conditions for SMS formation. Recently, assuming seed BHs with $\sim 10^5$ M$_\odot$, Di Matteo et al. (2012) and Khandai et al. (2011) discussed their growth by cold accretion flows during the process of the first galaxy formation. Their results demonstrate that cold flows are less susceptible to feedback from growing BHs and a high accretion rate is maintained until the mass of the galaxy reaches $\gtrsim 10^{12}$ M$_\odot$, where the cold mode of accretion turns into the usual hot virialization mode. As a result, the BH is able to grow to $\gtrsim 10^9$ M$_\odot$ by $z \sim 6$.

Our scenario for SMS formation provides a mechanism for seeding BHs of $\sim 10^5$ M$_\odot$ in forming galaxies, which has been assumed in the studies of Di Matteo et al. (2012) and Khandai et al. (2011), while their results complementarily demonstrated that those seed BHs can in fact grow to SMBHs.

Finally, we remark on the remaining issues to be explored. In our scenario, the physical conditions in the post-shock gas (especially its density) are crucial for SMS formation. We have considered a range of density ($10^4$–$10^6$ cm$^{-3}$) and temperature (3000–10$^9$ K) as post-shock conditions. Currently, we only know the typical values of those parameters (Greif et al. 2008; Wise et al. 2008); we are still lacking knowledge of the relationship between post-shock conditions and formation conditions (i.e. mass, virialization epoch, etc.) of the first galaxies. In addition, our assumption that enough mass supply for Jeans instability is available through the streaming flow needs further investigation. Safranek-Shrader et al. (2010) evaluated the amount of accreted gas as $\sim 10^6$ M$_\odot$, which is inhomogeneously organized by turbulence (e.g. Wise & Abel 2007; Greif et al. 2008). Therefore, the outcome of the shocked material in most haloes could be numerous small subregions, rather than the massive layer envisaged in this paper. On the other hand, even if the turbulent motion dominates, a gravitational unstable cloud with $\sim 10^5$ M$_\odot$ could form in the centre and collapse subsequently (Wise et al. 2008). As a future project, we need to study in which haloes SMS-forming conditions are satisfied by way of realistic cosmological simulations, including e.g. molecular cooling and radiative and chemical feedback, to evaluate more quantitatively the feasibility of SMS formation in the first galaxies.

In this paper, we have supposed that for SMS formation massive clouds must collapse isothermally without fragmentation. In fact, three-dimensional hydrodynamical simulations by Bromm & Loeb (2003) confirmed that in some cases a cloud collapsing isothermally by atomic cooling does not experience fragmentation, at least in the range $\lesssim 10^6$ cm$^{-3}$, and consequently a supermassive clump forms at the centre. Even with some angular momentum, fragmentation resulted at most in a binary system in their calculation. However, depending on such initial conditions as degrees of rotation or turbulence, the clouds would fragment into less massive clumps during isothermal collapse. As a future study, researchers need to clarify the conditions under which clouds elude fragmentation by way of a three-dimensional hydrodynamical calculation.

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