The Origin and Detection of High-Redshift Supermassive Black Holes

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Abstract. Supermassive black holes (SMBHs) are common in local galactic nuclei, and SMBHs as massive as several billion solar masses already exist at redshift $z = 6$. These earliest SMBHs may arise by the combination of Eddington-limited growth and mergers of stellar-mass seed BHs left behind by the first generation of metal-free stars, or by the rapid direct collapse of gas in rare special environments where the gas can avoid fragmenting into stars. In this contribution, I review these two competing scenarios. I also briefly mention some more exotic ideas and how the different models may be distinguished in the future by $LISA$ and other instruments.

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INTRODUCTION

The discovery of very bright quasars, with luminosities $\geq 10^{47} \text{ erg s}^{-1}$, at redshift $z \simeq 6$ in the Sloan Digital Sky Survey (SDSS) suggests that some SMBHs as massive as a few $\times 10^9 \text{ M}_\odot$ already existed when the universe was less than 1 Gyr old (see, e.g., ref. [1] for a review). The presence of these SMBHs presents a puzzle. Metal–free stars, with masses $\sim 100 \text{ M}_\odot$, are expected to form at redshifts as high as $z \sim 25$ [2, 3, 4], and leave behind remnant BHs with similar masses [5]. However, the natural time-scale, i.e. the Eddington time, for growing these seed BHs by $\geq 7$ orders of magnitude in mass is comparable to the age of the universe (e.g. ref.[6]). This makes it difficult to reach $10^9 \text{ M}_\odot$ without a phase of rapid (at least modestly super–Eddington) accretion, unless a list of optimistic assumptions are made in hierarchical merger models, in which multiple seed BHs are allowed to grow without interruption, and to combine into a single SMBH [7, 8, 9, 10, 11, 12, 13, 14, 15].

An alternative class of explanations involves yet more rapid gas accretion or collapse [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. In this family of models, primordial gas collapses rapidly into a SMBH as massive as $10^4 - 10^6 \text{ M}_\odot$, either directly, or possibly by accreting onto a pre–existing smaller seed BH [27], or going through the intermediate state of a very massive star [17], a dense stellar cluster [28, 29], or a “quasistar” [30]. These so–called “direct collapse” models involve metal–free gas in relatively massive ($\geq 10^8 \text{ M}_\odot$) dark matter halos at redshift $z \gtrsim 10$, with virial temperatures $T_{\text{vir}} \gtrsim 10^4 \text{K}$. The gas that cools and collapses in these halos must avoid fragmentation, shed angular momentum efficiently, and collapse rapidly.
GROWTH FROM STELLAR-MASS SEEDS

Several authors have worked out the growth of SMBHs from stellar–mass seeds, by following the build-up of dark matter (DM) halos, and using simple prescriptions to track the formation of seed BHs, their subsequent growth by accretion, and their mergers. This can be done either semi–analytically [6, 31, 7, 10], using Monte-Carlo realizations of the DM merger trees [8, 9, 11, 15], or based on cosmological hydrodynamics simulations [13, 12, 14].

The uncertainties about the statistics of the DM halo merger trees are essentially negligible, since DM halo formation has been directly resolved in numerical simulations at the relevant low masses (down to $\sim 10^6 \, M_\odot$) and high redshifts (out to $z \approx 30$). The accuracy of the merger trees is limited mainly by the $5\%$–$10\%$ uncertainty in the normalization of the primordial power spectrum, $\sigma_8 h^{-1}$, and by the need to extrapolate the primordial power spectrum 2–3 orders of magnitude below the spatial scales on which it has been directly constrained.\footnote{In models in which the small-scale power is suppressed, such as warm dark matter, this extrapolation can dramatically reduce the number of high-redshift halos, making it much harder to form the seeds of the $z = 6$ SMBHs [32].}

The most important – and still rather uncertain – ingredients of this 'stellar seed' scenario can be summarized as follows. (i) What is the threshold mass (or virial temperature, $T_{\text{seed}}$) for early DM halos in which Pop III stars can form? A reasonable guess is $T_{\text{seed}} = \text{few} \times 100$ K, which allows molecular H$_2$–cooling [33, 34]. (ii) In what fraction ($f_{\text{seed}}$) of these halos do seed BHs form? This is a more difficult question, since various feedback processes (due to radiation, metal pollution, or mechanical energy deposition) could suppress Pop III star formation in the vast majority of early low–mass halos. The answer also depends on the IMF of Pop III stars, since whether the stars leave a BH remnant or explode as pair-instability SNe depends on their masses. (iii) What is the time–averaged accretion rate of the seed BHs? This is conveniently parameterized by a duty cycle $f_{\text{duty}}$, defined as the fraction of the mass accretion rate that would produce the Eddington luminosity, if $\epsilon \approx 10\%$ of the rest mass was converted to radiation (so that $f_{\text{duty}} = 1$ is the fiducial Eddington rate). The expectation is that $f_{\text{duty}}$ is less than unity due to radiative feedback (but in practice, if the accretion is radiatively inefficient, or if the radiation is trapped or is beamed and “leaks out”, then $f_{\text{duty}}$ could exceed unity). (iv) Finally, what happens when DM halos merge? The simplest and most optimistic assumption is that the BHs to promptly coalesce, as well. However, even if dynamical friction on the DM is efficient, it is possible that, due to the radiation of its parent star, the remnant BHs are no longer embedded in dense enough gas to allow this. Furthermore, even if the BHs coalesce, the merged binary BH can be ejected from the shallow potential wells ($\sim 1\, \text{km/s}$) of the early halos by the gravitational “kick”, and effectively lost. This depends on the recoil speed, which depends strongly on the mass ratio and on the spin vectors of the two BHs.

In Figure 1, we show SMBH mass functions at $z = 6$, illustrating the impact of the above assumptions, taken from a recent example of the Monte Carlo merger tree approach [15]. The mass functions were constructed from the merger histories of $\approx 10^5$
DM halos with masses $M > 10^8 M_\odot$ at redshift $z = 6$. A robust conclusion for a model to produce enough $z = 6$ SMBHs is that $f_{\text{duty}} \gtrsim 0.6$ — namely the $\approx 100 M_\odot$ stellar seed BHs must accrete near the Eddington rate nearly all the time. The initial BH occupation fraction also has to be $f_{\text{seed}} \gtrsim 10^{-3}$. Finally, if the initial seeds are rare ($f_{\text{seed}} = 10^{-3} - 10^{-2}$), then gravitational kicks do not have a big impact, and it makes little difference to the SMBH mass function whether spins are aligned or randomly oriented. This is because in this case, the few “lucky” seeds that form earliest already have a chance to grow by $\gtrsim$ two orders of magnitude in mass before encountering their first merger. The masses of the two BHs at the merger are then very unequal ($q = M_1 / M_2 \lesssim 0.01$), making kick velocities too low ($\sim 1 \text{km/s}$; irrespective of the spins) to lead to ejection.

An important additional issue is that in those models that satisfy the SDSS constraint on the SMBH abundance (upper right corners in Figure 1, marked in red), the massive end of the SMBH mass function is extremely steep. This prediction is not surprising, as the most massive SMBHs reside in few $\times 10^{12} M_\odot$ halos, which probe the $5\sigma$ tail of the halo mass function at $z = 6$ (and there are indeed $\approx 10^6$ times as many few $\times 10^9 M_\odot$ halos, which host $\sim 10^6 M_\odot$ BHs). It does mean, however, that the total mass density in SMBHs with masses above $\gtrsim 10^5 M_\odot$ BHs (shown by the numbers in the upper right corners in Figure 1) are overpredicted by a factor of $10^2 - 10^3$. The mass density of such SMBHs at $z \approx 0$ is inferred to be several $\times 10^3 M_\odot \text{Mpc}^{-3}$, and the expectation is that most ($\gtrsim 90\%$) of this mass was accreted well after $z = 6$ [35]. Some strong feedback is
FIGURE 2. Temperature evolution of a metal-free cloud, irradiated by a strong UV flux. The models solve for the chemical and thermal evolution, but assume a pre-imposed density evolution, based on the spherical collapse model. Various cases are shown, with UV intensities at the Lyman limit of $J_{21} = 0, 1, 10, 100$ and $10^3$, in the usual units of $10^{-21}$ erg cm$^{-2}$ sr$^{-1}$ s$^{-1}$ Hz$^{-1}$ (solid and dashed curves; see the legend in the panel). Each blue dotted line corresponds to a different constant Jeans mass. The gas is heated adiabatically until a density of $n \approx 10^9 - 10^{10}$ cm$^{-3}$, at which $\text{H}_2$-cooling becomes efficient and cools the gas to a few $\times 100$ K. However, there exists a critical flux, with a value between $J_{21} = 10^2$ and $10^3$, above which $\text{H}_2$-cooling is disabled (adapted from ref. [28]).

therefore needed to eliminate this significant overprediction. Possible candidates for this are radiative feedback internal to halos, which maintains the “$M - \sigma$ relation” in ultra-high redshift, low mass halos, or the termination of Pop III star formation, at redshifts as high as $z \sim 20$, due to Lyman Werner radiation or metal pollution.

Finally, it is worth emphasizing that the mass accretion rate corresponding to the Eddington limit – for the fiducial radiative efficiency of $\varepsilon \equiv L/mc^2 = 0.1$ for converting mass to radiation – would need to be exceeded only by a factor of a $\sim$ few to make the growth from stellar seeds much easier. Radiative feedback is usually expected to lead to sub–Eddington rates (e.g. [36]), and in spherical symmetry, the accretion was recently to shown to be episodic, with $f_{\text{duty}} \approx 0.3$ [37]. However, modestly exceeding the Eddington rate is certainly plausible in theory; density inhomogeneities can allow radiation to leak out of low density regions while most of the accreting matter can be contained in high density regions. For example, magnetized radiation dominated accretion disks are subject to a “photon bubble” instability that nonlinearly appears to lead to strong density inhomogeneities (e.g. [38]). Nevertheless, observations have so far not revealed systems that sustain super–Eddington accretion for extended periods; it would then still have to be explained why the $z \approx 6$ quasar BHs have this unique behaviour.
GROWTH BY RAPID DIRECT COLLAPSE

An appealing alternative idea is to produce, say, a $10^5 M_\odot$ SMBH “directly” – i.e. much faster than this would take under Eddington–limited accretion from a stellar seed. This would clearly be helpful to explain the high-redshift SMBHs, and many authors (listed in the Introduction) proposed this may be possible using metal–free gas in relatively massive ($\gtrsim 10^8 M_\odot$) dark matter halos at redshift $z \gtrsim 10$, with virial temperatures $T_{\text{vir}} \gtrsim 10^4 K$.

The gas that cools and collapses in these halos must avoid fragmentation, shed angular momentum efficiently, and collapse rapidly. These conditions are unlikely to be met, unless the gas remains “warm”, i.e. at temperatures $T_{\text{vir}} \sim 10^4 K$. In recent numerical simulations, Shang et al. [26] found that the gas in such halos, when collapsing in isolation, forms $H_2$ efficiently, and cools to temperatures of $T \sim 300 K$. Although no fragmentation was seen, the gas is expected to ultimately fragment on smaller scales that have not yet been resolved [39]. More importantly, even if fragmentation was avoided, the cold gas was found to flow inward at low velocities, near the sound speed of $\sim 2-3 \text{ km s}^{-1}$, with a correspondingly low accretion rate of $\sim 0.01 M_\odot \text{ yr}^{-1}$. This results in conditions nearly identical to those in the cores of lower-mass minihalos; extensive ultra–high resolution simulations had concluded that the gas then forms a single $\sim 100 M_\odot$ star [2, 3, 4] or perhaps a massive binary [39], rather than a supermassive star or BH.

There have been at least three different ideas on how to avoid $H_2$–cooling and keep the gas warm. One is for the gas to “linger” for a sufficiently long time at $10^4 K$ that it collapses to a SMBH, even before $H_2$ has a chance to reduce the temperature. For a sufficiently high space– and column–density of neutral hydrogen, the absorption of trapped Lyman $\alpha$ photons can be followed by collisional de–excitation, rather than the resonant scattering of the Lyman $\alpha$ photon, effectively trapping much of the cooling radiation. This could lead to such lingering and to SMBH formation – analogous to opacity–limited fragmentation in colder gas in the context of star formation [20, 25].

Alternatively, $H_2$–cooling may be disabled if the gas is exposed to an intense UV flux $J$, either directly photo–dissociating $H_2$ (in the Lyman–Werner bands near a photon energy of $\sim 12 \text{ eV}$) or photo–dissociating the intermediary $H^-$ (at photon energies $\gtrsim 0.76 \text{ eV}$). Requiring the photo-dissociation timescale, $t_{\text{diss}} \propto J^{-1}$, to be shorter than the $H_2$–formation timescale, $t_{\text{form}} \propto \rho^{-1}$, generically yields a critical flux that increases linearly with density, $J_{\text{crit}} \propto \rho$. Since the gas in halos with $T_{\text{vir}} \gtrsim 10^4 K$ can cool via atomic Lyman $\alpha$ radiation and lose pressure support, it inevitably collapses further. As a result, in these halos, the critical flux is high, $J_{\text{crit}} \approx 10^2 - 10^5$, depending on the assumed spectral shape (ref. [26]; see also refs. [40, 17] who found similar, but somewhat higher values). The existence of this critical flux is illustrated in Figure 2, using a one-zone model in which the density evolution is approximated by spherical collapse. Figure 3 shows the radial structure of a $10^8 M_\odot$ halo, at the time of its collapse, when illuminated at various intensities, taken from three–dimensional simulations with the AMR code Enzo. These profiles clearly show that when the UV flux exceeds a critical value, the core of the halo is prevented from cooling to low temperatures.

The 3D simulations also provide an estimate of the mass of the central “object”
FIGURE 3. The results of adaptive mesh refinement (AMR) simulations of a primordial halo, with a total mass of a few $10^7$ M$_\odot$, collapsing at redshift $z \approx 10-15$, exposed to various UV background fluxes. The four panels show snapshots of the spherically averaged profile of the particle number density, gas temperature, e$^-$ fraction and H$_2$ fraction at the time of the collapse of the core for several different values of the UV background intensity $J_{21}$, as labeled. The existence of a critical flux, here with a value between $J_{21} = 30$ and $10^2$, above which H$_2$–cooling is disabled, is evident (adapted from ref.[26]).

(star or SMBH) that ultimately forms at the core of the halo, based on the measured profile of the mass accretion rate. This is illustrated in Figure 4. In particular, when the flux exceeds the critical value, and the gas remains warm, the collapse is significantly delayed. However, when the gas ultimately does collapse, it accretes toward the center at the sound speed ($c_s \approx 10\text{km/s}$), leading to a mass accretion rate of $\dot{M} \approx 1\text{M}_\odot\text{yr}^{-1}$. This is much higher than in the case of cold ($c_s \sim 1\text{km/s}$) gas in halos with efficient H$_2$ cooling (the simulations reveal $\dot{M} \propto c_s^3$, as expected in self–gravitating gas).

Importantly, the critical flux is high – likely significantly exceeding the expected level of the cosmic UV background at high redshifts. Therefore, only a small subset of all $T_{\text{vir}} \gtrsim 10^4\text{K}$ halos, which have unusually close and bright neighbors, may see a sufficiently high flux. However, given the strong clustering of early halos, there is a sufficient number of these close halo pairs to account for the abundance of the $z = 6$ quasars [41]. A more significant challenge to this idea is that in order to avoid fragmentation, the gas in these halos must also remain essentially free of any metals and dust [28]. This requirement could be difficult to reconcile with the presence of a nearby, luminous galaxies.

ALTERNATIVE MODELS

Since both of the “standard” scenarios discussed above require some optimistic assumptions, it is interesting to consider some more exotic possibilities.

It is commonly believed that the magnetic fields permeating galaxies such as the Milky Way arose by the amplification of a much weaker large–scale seed field. Weak
FIGURE 4. The local accretion timescale $t_{\text{acc}}$ as a function of the enclosed gas mass $M_{\text{gas}}$, in the same halo depicted in Figure 3, illuminated with different intensities, as labeled. In the halos exposed to a supercritical flux ($J_{21} = 10^2$ and $10^3$), the mass accretion rate, $\dot{M} \approx 1 \, M_\odot \, \text{yr}^{-1}$, is nearly $10^3$ times higher than in halos whose gas cools via H$_2$ ($J_{21} \lesssim 10$). At the center of the brightly illuminated halos, $\approx 10^5 M_\odot$ of gas accumulates within a Kelvin-Helmholtz time of $\approx 10^5$ yr, possibly leading to the formation of a SMBH with a comparable mass (adapted from ref.[26]).

primordial magnetic fields, with strengths of up to $\sim 1 \text{nG}$, can be produced in phase transitions in the early universe, during inflation, or during the electroweak or QCD phase transitions. It has recently been shown that such a primordial magnetic field could produce a variant of the “direct collapse” scenario [42]. In particular, if the field is tangled, then ambipolar diffusion will provide an efficient new mechanism to heat the gas as it collapses in protogalactic halos. If the field has a strength above $|B| \gtrsim 3.6$ (comoving) nG, the collapsing gas is kept warm ($T \sim 10^4$ K) until it reaches the critical density $n_{\text{crit}} \approx 10^3 \text{cm}^{-3}$ at which the roto–vibrational states of H$_2$ approach local thermodynamic equilibrium. H$_2$–cooling then remains inefficient, and the gas temperature stays near $\sim 10^4$ K, even as it continues to collapse to higher densities. The critical magnetic field strength required to permanently suppress H$_2$–cooling is somewhat higher than upper limit of $\sim 2 \text{nG}$ from the cosmic microwave background (CMB). However, it can be realized in the rare $\gtrsim (2 - 3)\sigma$ regions of the spatially fluctuating B–field; these regions contain a sufficient number of halos to account for the $z \approx 6$ quasar BHs.

Another “exotic” idea is that the first Pop III stars may be powered by heating by dark matter annihilation, rather than by nuclear fusion [43]. Weakly interacting massive particles (WIMPs) can be such a heat source, as long as they reach sufficiently high density inside the first stars, and if the annihilation products are trapped inside the star.

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2 Because of the high magnetic Jeans mass, the magnetic pressure has significant dynamical effects, and can prevent gas collapse in halos with masses up to $M \gtrsim \text{few} \times 10^{10} M_\odot$. These are $\sim$100 times more massive than the DM halos in the “usual” direct collapse models.
FIGURE 5. The temperature evolution of a patch of the intergalactic medium is shown as it initially expands and then turns around and collapses to high density. The different curves correspond to different values of the assumed primordial magnetic field, as labeled. The gas evolves from the left to the right on this figure. The left panel shows the expanding phase, starting from an initial density of $\approx 100 \text{ cm}^{-3}$ (corresponding to the mean density at redshift $z \approx 800$) and ending at the turnaround just below $n = 10^{-2} \text{ cm}^{-3}$. The right panel follows the subsequent temperature evolution in the collapsing phase. The figure shows the existence of a critical magnetic field, with a value between $B = 3$ and 4 nG, above which $H_2$-cooling is disabled, and the gas temperature always remains near $10^4 \text{K}$ (adapted from ref.[42]).

Several authors have studied the impact of this additional heating mechanism on the structure and evolution of such “dark stars” [44, 45, 46, 47, 48, 44, 49, 50]. In particular, these stars can live much longer than “normal” Pop III stars, and because their radiation is soft, they can continue to accrete gas, as long as the dark matter heating persists, and grow to masses of up to $\sim 10^5 \text{M}_\odot$ [48, 49]. These stars are bright, and should be detectable directly by JWST [49].

**OBSERVATIONAL PROSPECTS**

In order to distinguish between the various proposed models discussed above, observations must be able to detect SMBHs with masses below $10^6 \text{M}_\odot$ beyond redshift $z \approx 10$. This requirement is satisfied by JWST (with a sensitivity of $\sim 10 \text{ nJy}$ at near-IR wavelengths) and also in the radio by EVLA and, ultimately, the proposed instrument SKA (with sensitivities of 1-10 $\mu$Jy at 1-10 GHz). These IR and radio data should also be able to provide at least a crude measure of their masses, but obtaining redshifts will be challenging.

The assembly of the earliest SMBHs will ultimately be best probed by the LISA satellite, which could detect $M < 10^4 \text{M}_\odot$ black holes beyond redshift $z \sim 20$, with a signal–to–noise ratio of S/N $> 30$ or better [51]. This should allow at least a crude determination of the masses and distances to these low–mass SMBHs, and to directly distinguish between the various proposed scenarios.
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