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MASTER'S THESIS

Origins of Supermassive Black Holes

The influence of magnetic fields and turbulence on the formation of seed black holes

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Kapteyn Astronomical Institute University of Groningen February 15, 2013



Far-long ago, in a distant space-time, a n0thing exploded over eons, rippling into the here-now.

Title page image & quote: 'Cosmic Calendar' by Olena Shmahalo; see it in motion at OlenaShmahalo.com

Abstract

The 'seeds' of the SMBHs with masses of $\sim 10^9 M_{\odot}$ observed already at $z \sim 6$ may have formed through the direct collapse of primordial gas in $T_{\rm vir} \gtrsim 10^4 \, {\rm K}$ halos, whereby the gas must stay hot $(\sim 10^4 \text{ K})$ in order to avoid fragmentation. In this context, the implications of magnetic fields and turbulence in the post-recombination Universe and during the gravitational collapse of a halo are explored, as well as the effects of a UV radiation background. Using a one-zone model, the evolution of a cloud of primordial gas is followed from its initial cosmic expansion through turnaround, virialization and collapse up to a density of $10^7 \,\mathrm{cm}^{-3}$. It was found that, in halos without any significant turbulence, the critical magnetic field for which H₂ never becomes an important coolant due to strong ambipolar diffusion heating is $\sim 13 \,\mathrm{nG}$ (comoving), quite large compared to the current upper limits on the mean primordial field (~1 nG). Magnetic fields $\gtrsim 0.5 \,\mathrm{nG}$ but smaller than $B_0^{\mathrm{crit},\mathrm{H}_2}$ result in an increased fragment mass and accretion rate onto the central object, due to an increase in gas temperature. However, the existence of a critical field depends crucially on the scaling of the magnetic field with density. Therefore, it is very important to correctly model this relationship. In turbulent halos, initial fields $\gtrsim 0.5 \,\mathrm{nG}$ will decay rather than being amplified by the small-scale dynamo, due to the existence of a saturation field $B_{\rm max}$. The moderating effect of the turbulence causes the gas in halos with a different B_0 to converge to approx. the same evolutionary track, so they become practically indistinguishable. SMBH seeds are likely to form in massive turbulent halos, $M \gtrsim 10^{11} M_{\odot}$, as their strong turbulent heating will keep the gas hot. Furthermore, it was found that in halos with no significant turbulence, the critical UV background intensity for keeping the gas hot is lowered by a factor ~ 10 for $B_0 \sim 2 \,\mathrm{nG}$ as compared to the zero-field case, and lowered even more for stronger fields. In turbulent halos, $J_{21}^{\rm crit}$ is found to be a factor ~ 10 lower compared to the zero-field-zero-turbulence case, and the stronger the turbulence (more massive halo and/or stronger turbulent heating) the lower J_{21}^{crit} . The reduction in J_{21}^{crit} is particularly important, since it exponentially increases the number of halos exposed to a supercritical radiation background.

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CHAPTER 1_

INTRODUCTION

1.1 The Formation and Growth of Seed Black Holes

Many present-day galaxies are observed to host supermassive black holes (SMBHs) in their center, with black hole masses ranging from 10^6 to $10^{9.5} M_{\odot}$. Dynamical estimates suggest that, across a wide range, the central black hole mass equals about 0.1% of the mass of the spheroidal component of the host galaxy (Magorrian relation; Magorrian et al. 1998). This and other correlations between the black hole mass and the properties of the host galaxy point to a common root or co-evolution between galaxies and their central black hole.

Several very bright quasars, with bolometric luminosities $\geq 10^{47} \,\mathrm{erg \, s^{-1}}$, have been detected already at z > 6, when the Universe was less than a tenth of its current age. These high-redshift quasars are very rare, with a space density of the order of $\sim 1 \,\mathrm{Gpc^{-3}}$, and have only been found in large surveys, such as the Sloan Digital Sky Survey (SDSS), or the smaller-area but deeper CFHQS and UKIDSS surveys. This suggests that some SMBHs with masses of $\simeq 10^9 \, M_{\odot}$ already existed less than 1 Gyr after the Big Bang (Fan 2006). It is possible that these bright quasars represent only the tail of the mass distribution, which would imply that large numbers of massive black holes might have existed at that time.

Explaining how such massive SMBHs could have assembled so soon after the Big Bang presents quite a challenge. The main questions concern how and when the 'seeds' of these SMBHs formed and how their subsequent growth proceeded. In the following section, the main possibilities for the formation of such seed black holes are discussed (for a detailed review, see e.g. Volonteri 2010; Haiman 2012). A diagram which summarizes these pathways in high-redshift galaxies is shown in Figure 1.1

1.1.1 Remnants of Pop III stars

Perhaps the most 'natural' scenario assumes that SMBHs grow from the remnants of the first stars. The first stars are expected to form in so-called minihalos or molecular cooling



Figure 1.1 – Summary of the possible pathways to massive black hole formation in DM haloes with $T_{\rm vir} \gtrsim 10^4$ K: via a stellar seed black hole, via a very massive or quasi star (also called the direct collapse scenario), or via runaway collisions in a nuclear star cluster (Regan & Haehnelt 2009).

halos, with halo masses of $\approx 10^6 M_{\odot}$ and in which cooling is possible through molecular hydrogen, at redshifts of $\sim 20 - 50$ (Tegmark et al. 1997; Abel et al. 2002; Bromm et al. 2002). The first generation of stars, or Population III stars, form out of metal-free gas, or slightly metal-enriched gas with a metallicity less than the critical metallicity at which the transition to Pop II stars occurs, which is thought to lie approximately in the range of $10^{-6} \leq Z/Z_{\odot} \leq 10^{-4}$, but probably also depends on the dust present (Schneider et al. 2002, 2006) and the background UV radiation (Aykutalp & Spaans 2011). Because cooling in low-metallicity gas is not very efficient, the cloud is expected not to fragment much, if at all, and this would result in a mode of star formation that is more top-heavy than the current Pop II/I star formation. Among Pop III stars, a distinction can be made between the first and second generation, termed Pop III.1 and Pop III.2, respectively (McKee & Tan 2008). Pop III.1 stars have a primordial composition, while Pop III.2 stars have been affected by the radiation of previously formed stars; once the gas has been partially ionized, HD cooling can become important, reducing the characteristic star formation mass. This characteristic mass is set by the typical excitation energy of the H_2 (for Pop III.1) and HD (for Pop III.2) cooling lines, which are 512 K and 150 K, respectively.

JEANS MASS AND FRAGMENTATION

For a (part of a) gas cloud to collapse, gravity has to overcome the internal pressure. The internal pressure is most commonly dominated by gas pressure, but both magnetic and turbulent pressure could also be important, depending on the situation. By equating the internal and gravitational energy of the matter-filled region, an (approximate) critical mass can be found, above which clouds are unstable to collapse; this is the Jeans mass. For the mentioned pressure sources, the Jeans mass scales as follows:

$$\int c_{\rm s}^3 \rho_{\rm m}^{-1/2}$$
 for gas pressure, (1.1)

$$M_{\rm J} \propto \begin{cases} v_{\rm A}^3 \rho_{\rm m}^{-1/2} & \text{for magnetic pressure,} \\ v_{\rm turb}^3 \rho_{\rm m}^{-1/2} & \text{for turbulent pressure,} \end{cases}$$
(1.2)

$$_{\rm urb}\rho_{\rm m}^{-1/2}$$
 for turbulent pressure, (1.3)

where $c_{\rm s} \propto (\gamma T)^{1/2}$ is the sound speed, $v_{\rm A} \propto B \rho_{\rm m}^{-1/2}$ is the Alfvén speed, $v_{\rm turb}$ is the turbulent velocity, and $\rho_{\rm m}$ is the matter density. Hence, the smaller the mass of the cloud, the larger its size, the higher its temperature, and the stronger its magnetic field and turbulence, the more stable it will be against gravitational collapse and thus less likely to fragment.

The final fate of these stars as a function of their initial mass is given in Figure 1.2. Low-metallicity stars with masses in the range $\sim 25 - 140 M_{\odot}$ are expected to form black holes directly, with $M_{\rm BH} \sim 10 - 50 \, M_{\odot}$ (Zhang et al. 2008). The problem with these light black holes is that they might not be dynamically stable within the center of their host; they might move around due to interactions with stars of similar mass, rather than settling at the center of the potential well. Stars with masses in the range $\sim 140 - 260 M_{\odot}$ are predicted to explode as pair-instability supernovae, and leave no remnant behind. And still more massive stars, with masses in excess of $\sim 260 M_{\odot}$, are also expected to form black holes, with masses at least half of the initial stellar mass, $M_{\rm BH} \sim 100 - 600 M_{\odot}$ (Bond et al. 1984; Fryer et al. 2001). These would be good seed black holes candidates. However, the shape of the initial mass function of Pop III stars is still an unsolved problem, and it is not known if Pop III stars actually have masses above the threshold ($\sim 260 M_{\odot}$) for the formation of these intermediate mass black holes.



Figure 1.2 – Initial-final mass function of non-rotating, metal-free stars. The x-axis shows the initial stellar mass and the y-axis shows both the final mass of the collapsed remnant (*thick black curve*) and the mass of the star when the event begins that produces that remnant (*thick gray curve*). Since no mass loss is expected for metal-free stars before the final stage, the gray curve is approximately the same as the line of no mass loss (*dotted line*) (Heger & Woosley 2002).

1.1.2 Stellar-dynamical processes

Once 'normal', Pop II stars are being formed, a new way of forming seed black holes becomes possible, at redshifts $\sim 10 - 20$. This first episode of efficient star formation can favor the formation of very compact nuclear star clusters, where stellar collisions can occur in a runaway fashion and finally lead to the formation of a very massive star (VMS; the growth of which should be much more efficient at low metallicity), which possibly leaves a black hole behind with a mass in the range $\sim 10^2 - 10^4 M_{\odot}$ (see e.g. Begelman & Rees 1978; Devecchi & Volonteri 2009)).

1.1.3 Direct collapse

Another group of scenarios suggests that seed black holes formed via the direct collapse of metal-free (or very metal-poor) gas in halos with $T_{\rm vir} \gtrsim 10^4$ K, at redshifts $\sim 5 - 10$, resulting in a seed black hole with a mass of $\sim 10^4 - 10^5 M_{\odot}$ (see e.g. Haehnelt & Rees 1993; Loeb & Rasio 1994; Eisenstein & Loeb 1995; Bromm & Loeb 2003; Koushiappas et al. 2004; Begelman et al. 2006; Lodato & Natarajan 2006). Efficient gas collapse only happens if fragmentation of the gas cloud into smaller clumps is suppressed. This can occur if the gas in the halo is kept hot (and thus the Jeans mass high) due to inefficient cooling, so if the formation of H₂ is inhibited, as otherwise H₂ cooling will lower temperatures to ~ 200 K and thereby the Jeans mass, leading to fragmentation. In these systems, the gas can then only cool through atomic hydrogen until it reaches $T_{\rm gas} \approx 4000$ K. At this point the cooling function of atomic hydrogen drops by a few orders of magnitude and contraction proceeds nearly adiabatically.

Avoiding fragmentation

Several mechanisms have been suggested to suppress H_2 cooling and thus prevent fragmentation. The main one of these mechanisms requires a critical level of Lyman-Werner radiation ($h\nu = 11.2 - 13.6 \text{ eV}$) to photo-dissociate the H_2 molecules and keep their abundance very low. The critical intensity needed to suppress H_2 in the massive halos where direct gas collapse could occur is large compared to the expected cosmic UV background at the relevant redshifts; $J_{21}^{\text{crit}} = 10^3 - 10^5$. However, the cosmic UV background fluctuates and its distribution has a long bright-end tail, due to the presence of a close luminous neighbor. Halos irradiated by such intensities would be a small subset of all halos ($\sim 10^{-6}$) where the background intensity exceeds the critical intensity and H_2 is effectively photo-dissociated (Dijkstra et al. 2008).

Another mechanism leading to the destruction of H_2 is the trapping of Lyman-alpha photons: for roughly isothermally collapsing gas at $T_{\rm vir} \gtrsim 10^4$ K, line trapping of Ly α photons causes the equation of state to stiffen, which makes it more difficult for the gas to fragment. This happens because the time required for the Ly α photons to escape from the medium becomes larger than the free-fall time of the gas, which prevents the gas from cooling. H_2 is naturally destroyed in these systems by collisional dissociation, because of the high gas temperature resulting from the Ly α trapping. The black holeto-baryon mass fraction found in this way is close to the Magorrian relation observed in galaxies today (Spaans & Silk 2006).

Yet another mechanism proposes that the dissipation of a sufficiently strong magnetic field, mainly through ambipolar diffusion, can heat the gas in the halo to $\sim 10^4$ K. The high temperature then causes the H₂ to be destroyed by collisional dissociation (similar to what happens through Ly α trapping), and thus fragmentation can be avoided. Sethi et al. (2010) find that a critical magnetic field of $B_0 \simeq 3.6$ nG (comoving) is necessary to obtain sufficient heating. This is somewhat higher than the upper limits on a possible primordial magnetic field as currently found from various methods (see section 1.2.1). However, it could still be realized in the rare $\gtrsim (2-3)\sigma$ regions of the spatially fluctuating magnetic field; these regions could contain a sufficient number of halos to account for the bright $z \sim 6$ quasars, but they probably cannot account for the much more numerous quasar black holes at somewhat lower masses. Finally, it has been suggested that fragmentation could be intimately related to angular momentum redistribution within a system; thus, highly turbulent systems would be less prone to fragmentation. This means that efficient gas collapse could proceed also in metal-enriched galaxies at later cosmic times (Begelman & Shlosman 2009).

Angular momentum transport

If fragmentation can be suppressed and the gas is able to cool, it will contract until rotational support halts the collapse. Usually, this will happen before a black hole has been created; instead a disk will form. The radius of the disk can be estimated as $r_{\text{disk}} = \lambda r_{\text{vir}}$, where λ is the dimensionless spin parameter: $\lambda = \frac{J|E|^{1/2}}{GM^{5/2}}$, with J the angular momentum of the halo, a result of tidal interactions with neighboring halos, and with E and M the total energy and mass of the halo, respectively. The spin parameter λ represents the amount of rotational support available in a system, and peaks around ~0.04 (Bullock et al. 2001). Additional mechanisms for angular momentum transport (discussed further down) are required to further condense the gas and eventually form a black hole.

It has been suggested that a black hole could form from low angular momentum material, either in halos that have very little angular momentum (Eisenstein & Loeb 1995), or from only the material in the low angular momentum tail of the distribution, which should exist for every halo (including the ones that can cool efficiently), implying that every one of them should contain gas that ends up in a high-density disk (Koushi-appas et al. 2004). However, both scenarios still require substantial angular momentum transport in order for a central massive object to form.

The redistribution of angular momentum can occur via runaway, global dynamical instabilities, such as the 'bars-within-bars' mechanism (Shlosman et al. 1989; Begelman et al. 2006). A self-gravitating gas cloud becomes bar-unstable when the level of rotational support exceeds a certain threshold. A bar can transport angular momentum outwards on a dynamical timescale, via gravitational and hydrodynamical torques. This allows the disk to shrink, and if the gas is able to cool, the instability will increase and the process cascades.

It has also been suggested that angular momentum can be redistributed by local, rather than global, instabilities. The stability of a self-gravitating disk can be evaluated using the Toomre parameter Q; $Q = \frac{c_s \kappa}{\pi G \Sigma}$, where c_s is the sound speed, κ is the epicyclic frequency (the frequency at which a radially displaced fluid parcel will oscillate), G is the gravitational constant and Σ is the surface density. When Q approaches a critical value, of order unity, the disk will become gravitationally unstable. If this destabilization is not too violent, it will lead to mass infall instead of fragmentation (Lodato & Natarajan 2006). Such an unstable disk develops non-axisymmetric spiral structures, which effectively redistribute the angular momentum, leading to mass inflow. This process stops when enough mass is transported to the center to stabilize the disk; this sets an upper limit to the mass of the seed black hole.

Final stages

For all these scenarios, the typical mass of the gas accumulated within the central few parsecs is of the order of $\sim 10^4 - 10^5 M_{\odot}$. This gas may directly collapse into a black hole, or fragment to form a dense stellar cluster which evolves into a black hole (see section 1.1.2), or go through an intermediate stellar stage. As the gas flows in, it becomes optically thick; radiation pressure may then temporarily balance gravity, forming a supermassive star (SMS, with a mass $\gtrsim 5 \times 10^4 M_{\odot}$). The evolution of a SMS depends on whether nuclear reactions are taken into account, and whether the star has a fixed mass or grows via accretion during its evolution.

A SMS of fixed mass, supported by radiation pressure, is thought to evolve as an n = 3 polytrope and finally collapse into a black hole containing most of the stellar mass (see e.g. Hoyle & Fowler 1963; Baumgarte & Shapiro 1999; Saijo et al. 2002; Shibata & Shapiro 2002).

If the mass accretion rate is high ($\sim 1 M_{\odot} \text{ yr}^{-1}$), the outer layers of the SMS cannot thermally relax. In this case, it is not well-described by an n = 3 polytrope, but will have a more complex structure with a convective core surrounded by a convectively stable envelope that contains most of the mass. The core will burn up its hydrogen, and subsequently collapses into a black hole with a mass of a few M_{\odot} . The black hole accretes material from the massive, radiation-pressure-supported envelope; the resulting structure is termed a 'quasistar' (Begelman et al. 2006, 2008; Begelman 2010). The key feature of this configuration is that the accretion is limited by the Eddington limit (see equation 1.4) for the entire quasistar, rather than that appropriate for just the black hole. Eventually, the radiation from the black hole will unbind the envelope.

1.1.4 Primordial black holes

Another possibility is that SMBHs grew from primordial black holes, which may have formed in the early Universe by many different processes; however, it is still highly uncertain whether they exist at all (for a review, see Carr 2003). The general idea is that if the overdensity in a certain region of space is large enough, the whole region can collapse into a black hole, with a mass roughly equal to the mass within the particle horizon at the redshift of formation. The possible black hole masses range from the Planck mass up to $10^5 M_{\odot}$. However, primordial black holes with an initial mass smaller than $\sim 5 \times 10^{14}$ g are expected to have been evaporated due to Hawking radiation within a current Hubble time. For larger masses, constraints on the mass range and distribution have been found from various observations, including microlensing techniques and distortions of the cosmic microwave background, limiting the black hole mass to below $\sim 10^3 M_{\odot}$ (for more on constraints, see Carr et al. 2010).

1.1.5 From seed to SMBH

Once a seed black hole is formed, it must grow rapidly within a short timespan to explain the observed high-redshift quasars. Mass accretion at the Eddington rate causes a black hole to increase in mass over time as

$$M_{\rm BH}(t) = M_{\rm BH}(0) \exp\left(\frac{1-\epsilon}{\epsilon} \frac{t}{t_{\rm Edd}}\right),\tag{1.4}$$

where $t_{\text{Edd}} = 0.45 \text{ Gyr}$ and ϵ is the radiative efficiency. This means that, for a 'standard' efficiency of ~0.1, it takes a $10^2 M_{\odot}$ seed at least ~0.81 Gyr and a $10^5 M_{\odot}$ seed at least ~0.46 Gyr to grow into a $10^9 M_{\odot}$ black hole. A larger radiative efficiency of 0.2 increases the growing time to ~1.81 Gyr for a $10^2 M_{\odot}$ seed and to ~1.03 Gyr for a $10^5 M_{\odot}$ seed. However, the black hole might not accrete at the Eddington rate the whole time, since the accretion rate could be limited by several different factors, both 'external' and 'internal' effects. On one hand, the external conditions relate to the amount of gas available for accretion. The constant availability of gas in the halo during the accretion period could require halos to merge, since episodes of star formation and feedback from supernovae might deplete the gas. On the other hand, the internal effects relate to feedback from the radiative output produced by the accreting black hole itself (see e.g. Pelupessy et al. 2007; Johnson & Bromm 2007; Milosavljević et al. 2009; Park & Ricotti 2011; Spaans et al. 2012).

The fact that seed black holes may not constantly accrete at or near the Eddington limit due to these effects is especially an issue for the Pop III remnant scenario, since this amount of accretion is likely necessary for these light seeds to grow into SMBHs in the available time. However, it has been proposed that these seeds might experience super-Eddington accretion for a short period of time, which could be a result of inefficient radiative losses due to the trapping of photons in the accretion disk (see e.g. Begelman 1979; Volonteri & Rees 2005).

It is also possible that high-accretion rate events can trigger the formation of collimated outflows (jets) that do not cause feedback in the vicinity of the black hole, but will deposit their kinetic energy at large distances. All in all, the interplay between all of these effects, and thus the black hole accretion history, are still poorly understood.

1.2 Primordial Magnetic Fields

In models and simulations of the first stars and galaxies, it is often assumed that magnetic fields are not yet present. However, this is not necessarily true, since a variety of mechanisms exist for generating magnetic fields early in the Universe, both before and after recombination (for a review, see e.g. Widrow et al. 2012). Unfortunately, there is no direct observational evidence, so the nature of the primordial magnetic field, if it exists at all, remains unknown. However, observations of strong magnetic fields in galaxies at intermediate redshift (e.g. Bernet et al. 2008) and of coherent magnetic fields on supercluster scales (Kim et al. 1989) suggest that in order for such fields to exist, a primordial seed field may be necessary. It would explain how the galactic dynamo (see further down) was able to generate the strong fields in relatively little time, and why the magnetic field in our own Galaxy has alternating directions in the arm and inter-arm regions (e.g. Han 2008).

1.2.1 Seed field generation

Such seed fields may have been generated during inflation or phase-transitions. Quantum fluctuations in the electromagnetic field during inflation may give rise to large-scale magnetic fields, similar to how large-scale structure in the Universe is thought to result from the amplification of linear density perturbations that originated as quantum fluctuations during inflation (Turner & Widrow 1988). After inflation, the early Universe has been predicted to go through a series of phase-transitions, in which the nature of particles and fields changed in fundamental ways. The electromagnetic and weak nuclear forces became distinct during the electroweak phase transitions at 10^{-12} s after the Big Bang (the electroweak unification energy is $\sim 246 \,\text{GeV}$), while the quark-gluon plasma became locked into hadrons (baryons and mesons) during the quark-hadron phase transition at $t = 10^{-6}$ s. Both of these transitions had the potential to generate strong magnetic fields, since they involved the release of an enormous amount of energy, and since they involved charged particles which could drive electromagnetic currents, and hence fields (e.g. Baym et al. 1996; Quashnock et al. 1989; Sigl et al. 1997). Several issues with these scenarios, and ways around them, have been discussed at length in the literature. Inflation-produced fields may be severely diluted by the expansion of the Universe to negligible levels. Fields generated from phase transitions after inflations will have a very small coherence length, due to the small size of the Hubble scale at that time, so the effective field strength on galactic scales is likely negligible. This can be remedied if the field has a non-zero helicity; then magnetic field energy can be efficiently transferred from small to large scales in an inverse cascade (e.g. Frisch et al. 1975; Brandenburg et al. 1996). But even if these fields are uninteresting on galactic scales, they may still have an effect on for example the thermodynamics of the post-recombination Universe.

Magnetic fields may also have been generated after recombination, originating from a battery process: any force that acts differently on positive and negative charges will drive currents, and hence generate magnetic fields. One such mechanism is the Biermann battery (Biermann 1950). For a given pressure gradient, the electrons tend to get accelerated much more than the ions, since their mass is much smaller. This generates an electric field, and if this field has a curl, then according to Faraday's law of induction a magnetic field can arise. Vorticity is generated when the density and pressure (temperature) gradients are not parallel to each other; such a situation can arise in various ways, for example in shocks. Seed fields of the order of 10^{-19} G are expected from this mechanism. The Biermann battery is expected to operate in many different astrophysical settings, such as during structure formation (e.g. Kulsrud et al. 1997), in the intergalactic medium (IGM) during reionization (Subramanian et al. 1994; Gnedin et al. 2000), in stars, and in active galactic nuclei (AGN).

Any force that acts differently on electrons and ions can give rise to magnetic fields; this includes for example radiation pressure, since electrons are more strongly coupled with the radiation field. This kind of battery is thought to have been important during reionization, for example; Langer et al. (2003) found that it gives rise to $\sim 10^{-11}$ G seed fields at 1 Mpc, assuming $z_{\rm ion} \sim 7$.

Seed fields formed by a battery in stars or accretion disks can be rapidly amplified by dynamo effects (see further) because of the relatively short dynamical timescales of these objects. The strong magnetic fields generated this way can then be expelled from the object, into the interstellar medium (ISM) by supernovae and stellar winds, and into the IGM by AGN jets, providing yet another source of seed fields.

Constraints

As mentioned, for the very early Universe there are no direct observations showing the presence of magnetic fields. However, many attempts at deriving upper limits on the field strength are to be found in the literature. Various methods have been used, yielding different results; e.g. using Big Bang nucleosynthesis (Grasso & Rubinstein 1996, who find an upper limit of $\leq 1 \mu$ G), using reionization observations (Schleicher & Miniati 2011, who find an upper limit of $\leq 2 - 3$ nG), using Faraday rotation (e.g. Pogosian et al. 2011), and using the cosmic microwave background (CMB) power spectrum (e.g. Yamazaki et al. 2010, who find an upper limit of ≤ 3 nG at 1 Mpc (comoving)). The tightest limit so far comes from the CMB trispectrum, which might be a more sensitive probe than the CMB bispectrum and all modes in the CMB power spectrum, and has been found to be ≤ 1 nG on Mpc scales, and perhaps even sub-nG (Trivedi et al. 2012).

1.2.2 Magnetic field amplification

Several mechanisms exist for amplifying an existing magnetic field. In the case of a collapsing halo, the most important ones are gravitational compression, the small-scale turbulent dynamo, the large-scale dynamo in protostellar and galactic disks, and the magneto-rotational instability (MRI).

Gravitational compression

Gravitational compression increases the magnetic field as $B \propto \rho_{\rm b}^{\alpha}$ when the field is coupled to the gas. Gravitational compression under spherical symmetry leads to an increase with $\alpha = 2/3$. If the collapse proceeds preferentially along one axis, for example because of rotation or strong magnetic fields, the scaling is closer to $\alpha = 1/2$. In realistic cases, often intermediate values are found (e.g. Machida et al. 2006; Banerjee et al. 2009; Schleicher et al. 2009; Hocuk et al. 2012). It has for example been suggested that α should depend on the ratio between the thermal and magnetic Jeans mass as $\alpha = 0.57 \left(M_{\rm J}/M_{\rm J}^{\rm B}\right)^{0.0116}$, so that the scaling relation flattens for strong magnetic fields (Machida et al. 2006; Schleicher et al. 2009).

Large-scale dynamos & the MRI

The process where kinetic energy is converted into magnetic energy is generally referred to as a dynamo (for an extensive review on dynamo theory, see Brandenburg & Subramanian 2005, and references therein). Turbulent flows with significant amounts of kinetic helicity act as large-scale dynamos, also referred to as mean-field dynamos. ("Helicity" describes the property that rising turbulent eddies in the northern (southern) hemisphere expand and twist clockwise (counterclockwise) to conserve angular momentum, while falling turbulent eddies twist counterclockwise (clockwise).) Shear flows, such as found in galactic and protostellar disks because of differential rotation, are potential candidates for producing large-scale dynamo action. These dynamos show large-scale spatial (and in the case of the solar dynamo, also temporal) coherence. One such mechanism is the $\alpha\Omega$ dynamo, where the Ω effect refers to a distortion of poloidal magnetic field lines into toroidal components by shear, so that the toroidal magnetic field is amplified, and where the α effect closes the dynamo loop by generating poloidal fields from the toroidal fields, if the velocity field is complex enough. The turbulence required for such dynamos can be provided by the magneto-rotational (or Balbus–Hawley) instability (Balbus & Hawley 1991). The combination of radially decreasing angular velocity in a rotating disk and a minimal magnetic field strength is required to drive the MRI (Tan & Blackman 2004). The vertical stratification then provides the turbulence with the helicity that is required to drive a large-scale dynamo, but the MRI itself may also exponentially amplify the magnetic field.

Small-scale dynamos

Non-helical turbulent flows can act as small-scale dynamos, which produce disordered, random magnetic fields that are correlated on scales of the order of or smaller than the forcing scale of the flow (originally proposed by Kazantsev 1968). These dynamos typically have larger growth rates than large-scale dynamos, and are able to operate also in situations where the turbulent flow lacks helicity and persistent shear. The magnetic field amplification results from the random stretching and folding of the field lines by the turbulent random flow. This process can be illustrated by the stretch-twist-fold model (e.g. Zeldovich et al. 1983). First, a closed flux rope gets stretched to twice its length



Figure 1.3 – A schematic illustration of the stretch-twist-fold dynamo (Brandenburg & Subramanian 2005).

while preserving its volume, as in an incompressible flow (A \rightarrow B in Figure 1.3). The rope's cross-section then decreases by a factor two, and because of magnetic flux freezing the magnetic field must increase by a factor two. Next, the rope is twisted into a figure '8' (B \rightarrow C in Figure 1.3) and then folded (C \rightarrow D in Figure 1.3) so that now there are two loops, with their fields pointing in the same direction and together occupying a similar volume as the original loop. Hence, the flux through this volume has doubled. The last step consists of merging the two loops into one (D \rightarrow A in Figure 1.3), through small diffusive effects. This is important to render the whole process irreversible. The

merged loops are now topologically the same as the original loop, but with the field strength doubled.

During gravitational collapse, turbulence is generated by the release of gravitational energy and the infall of accreted gas on the inner, self-gravitating core. This means that, in the context of star and galaxy formation, a strong tangled magnetic field may be generated already during the collapse phase by the small-scale dynamo (Schleicher et al. 2010). It is thought that this dynamo mechanism could provide the minimal fields required for the excitation of large-scale dynamos to build the observed galactic-scale fields. For the formation of seed black holes, it implies that the existence of an accretion disk may cause the magnetic field to be further amplified (by a large-scale dynamo and/or the MRI) which provides additional stability and hence reduces fragmentation.

TURBULENCE

"Big whirls have little whirls that feed on their velocity, and little whirls have lesser whirls, and so on to viscosity."

— L.F. Richardson, 1922

Turbulent flows may be viewed as made of a hierarchy of eddies, which are loosely defined as coherent patterns of velocity, vorticity and pressure, over a wide range of length scales, superimposed upon a mean flow. Most of the turbulent energy is contained in the largest scales; these eddies obtain energy from the mean flow and also from each other. The energy cascades from these large scales to smaller scales by an inertial and essentially inviscid mechanism; these intermediate scales are therefore referred to as the 'inertial range'. At a certain point, the eddies are small enough for molecular viscosity, and hence dissipation, to become important. The scale where the energy input from the downward cascade is in exact balance with the energy drain from viscous dissipation is the Kolmogorov length scale, and thus the smallest scale in the spectrum. Each of these length scales is also characterized by a velocity, $v \propto l^{\beta}$, and a timescale, $t_{\rm ed} = l/v$, the eddy turnover time. The dependence of the velocity on the length scale through β is determined by the nature of the turbulence.

Kolmogorov turbulence describes a situation where the gas is incompressible and is thus applicable in particular for subsonic turbulence. In this case, the velocity scales with $\beta = 1/3$. On the other hand, turbulence in the presence of shocks, where the gas is quite strongly compressed, is best described by Burgers turbulence; in this case, the velocity scales with $\beta = 1/2$. However, in realistic turbulence intermediate values are expected, since it has been found from numerical simulations that turbulence always contains both rotational and compressional components (e.g. Federrath et al. 2010).

1.3 This Work

In this work, the focus lies on how the 'seeds' of these SMBHs could have formed and how massive these seeds were. Of particular interest are seed black holes formed through the direct collapse scenario, for which the gas in the halo must stay hot ($\sim 10^4$ K). In this context, the implications of magnetic fields and turbulence in the post-recombination Universe and during the gravitational collapse of a halo are explored, using an analytical one-zone model. The effects of a UV radiation background are also considered. The analytical model and all its components are described in detail in Chapter 2; Chapter 3 contains a brief overview of the numerical code and the input parameters; the results from the simulation are presented in Chapter 4, and discussed in Chapter 5, as well as some suggestions for future work. Finally, the conclusions can be found in Chapter 6.

CHAPTER 2______ THE ANALYTICAL MODEL

The evolution of a cloud of primordial gas is followed from its initial cosmic expansion to a high-density core, using a one-zone model, in which the physical variables involved are regarded as those at the center of the cloud. In this chapter, the various physical ingredients of the model will be discussed in detail.

2.1 Cosmology

The model is set up using standard cosmology, so it assumes a ACDM Universe which is approximately flat, and with cosmological parameters as given by WMAP7 (NASA/ WMAP Science Team 2011). At the redshifts under consideration, the contribution from radiation to the energy density of the Universe is negligible compared to the contributions from matter and the cosmological constant, and can be ignored. The values of the relevant parameters today are as follows:

$$H_0 = 70.4 \,\mathrm{km \, s^{-1} \, Mpc^{-1}},\tag{2.1}$$

$$\rho_{\rm c,0} = 9.9 \times 10^{-30} \,\mathrm{g \, cm^{-3}},$$
(2.2)

$$\Omega_{\rm b,0} = 0.046,\tag{2.3}$$

$$\Omega_{\rm DM,0} = 0.226,$$
 (2.4)

$$\Omega_{\Lambda,0} = 0.728.$$
 (2.5)

Here, H_0 is the Hubble constant today, $\rho_{c,0}$ is the mean energy density in the Universe today (which is equal to the critical density today), and $\Omega_{b,0}$, $\Omega_{DM,0}$ and $\Omega_{\Lambda,0}$ are respectively the baryon, dark matter and dark energy densities today, relative to $\rho_{c,0}$. The relative total matter density today is given by the sum of the baryon and dark matter densities and denoted as $\Omega_{m,0}$.

The evolution with redshift of the Hubble parameter, the cosmic time, and the tem-

perature of the cosmic microwave background (CMB) are calculated as

$$H(z) = H_0 \left(\Omega_{\rm m,0} (1+z)^3 + \Omega_{\Lambda,0} \right)^{1/2}, \qquad (2.6)$$

$$t_{\rm u}(z) = \frac{2}{3H_0\sqrt{\Omega_{\Lambda,0}}} \ln\left(\frac{1+\cos\phi}{\sin\phi}\right),\tag{2.7}$$

where
$$\phi = \arctan\left(\sqrt{\frac{1-\Omega_{\Lambda,0}}{\Omega_{\Lambda,0}}}(1+z)^{3/2}\right),$$
 (2.8)

$$\frac{dt}{dz} = -\frac{1}{H(z)(1+z)},$$
(2.9)

$$T_{\rm CMB} = 2.725(1+z) \,\,{\rm K}.$$
 (2.10)

2.2 Density Evolution

2.2.1 Co-evolution until turnaround

Initial perturbations in the mean cosmic density are assumed to grow by gravitational instability. According to the spherical collapse model for a top-hat overdensity, it will reach maximum expansion and then turn around and collapse into virial equilibrium when its radius is approximately half of the maximum expansion radius. During the initial phase, and roughly until shells start to cross each other near the virial radius, the gas pressure is negligible compared to the gravitational force, so the shells of gas and dark matter move in a similar manner.

The density of an overdense region that collapses and virializes at a certain redshift $z_{\rm vir}$ is calculated from the equation of motion of a bound shell collapsing under the influence of gravity:

$$\ddot{r} = -\frac{GM}{r^2}.\tag{2.11}$$

The solution is given by the following parametric system of equations, where r is the radius of the cloud and t is the time (Peebles 1993):

$$\int r(\theta) = r_{\rm vir}(1 - \cos\theta) \tag{2.12}$$

$$\begin{cases} t(\theta) = \frac{t_{\text{ta}}}{\pi} (\theta - \sin \theta), \qquad (2.13) \end{cases}$$

where $r_{\rm vir}$ is the radius at virialization:

$$r_{\rm vir} \approx \frac{r_{\rm max}}{2} = \left[GM \left(\frac{t_{\rm c}}{2\pi} \right)^2 \right]^{1/3}, \qquad (2.14)$$

which depends on the total mass M of the cloud; and $t_{\rm ta}$ is the age of the Universe at the time of turnaround. From Equation 2.13, a relation between the redshift and the parameter θ can be found:

$$1 + z_{\rm ta} = (1+z) \left(\frac{\theta - \sin\theta}{\pi}\right)^{2/3}.$$
 (2.15)

The parameter θ is chosen in such a way that turnaround occurs when $\theta = \pi$ and virialization when $\theta = 3\pi/2$. For a given z, Equation 2.15 can be solved to find the corresponding θ . The evolution of the total matter overdensity in the cloud (including both baryonic and dark matter) can then be calculated as function of θ :

$$\frac{\rho}{\rho_{\rm u}} = \frac{9}{2} \frac{(\theta - \sin \theta)^2}{(1 - \cos \theta)^3}.$$
(2.16)

At the moment of turnaround (z_{ta}) , when the halo decouples from the background, the gas decouples from the dark matter and becomes self-gravitating, so that the evolution of the dark matter and baryonic matter proceeds in different ways.

2.2.2 Decoupled evolution

Dark matter

The dark matter density continues to evolve according to the spherical collapse model until virialization. Afterwards, the density within the halo stays constant at $\rho_{\text{DM,vir}}$.

$$\rho_{\rm DM}(\theta) = \frac{9\pi^2}{2} \left(\frac{1+z_{\rm ta}}{1-\cos\theta}\right)^3 \Omega_{\rm DM,0} \rho_{\rm c,0}, \qquad \text{where } \theta \in \left[\pi, \frac{3\pi}{2}\right], \tag{2.17}$$

$$\rho_{\rm DM,vir} = \frac{9\pi^2}{2} \left(1 + z_{\rm ta}\right)^3 \Omega_{\rm DM,0} \rho_{\rm c,0} = 8\rho_{\rm DM}(z_{\rm ta}).$$
(2.18)

The baryon density will quickly start to overwhelm that of the extended virialized dark matter halo.

Baryonic matter

Any effects due to rotation are neglected for simplicity. The baryonic matter collapse, starting from the moment of turnaround, is expected to proceed like the Larson-Penston similarity solution (for the isothermal case; Larson 1969; Penston 1969), as generalized to polytropic cases by Yahil (1983). According to this solution, the cloud consists of two parts: a central core region and an envelope. The central core region has a flat density distribution ($\rho \approx constant$), whereas the density in the envelope decreases outwards as $\rho \propto r^{-2/(2-\gamma)}$, with γ the adiabatic index. The size of the central flat region is roughly given by the local Jeans length:

$$\lambda_{\rm J} = c_{\rm s} \sqrt{\frac{\pi}{G\rho_{\rm m}}},\tag{2.19}$$

which corresponds to a Jeans mass, where a cloud with a larger mass will be unstable to collapse:

$$M_{\rm J} = \frac{\pi}{6} \rho \lambda_{\rm J}^3 = \frac{4\pi^4 c_{\rm s}^3}{3(4\pi G)^{3/2} \rho_{\rm m}^{1/2}}$$
(2.20)

$$\simeq 2M_{\odot} \left(\frac{c_{\rm s}}{0.2\,{\rm km\,s^{-1}}}\right)^3 \left(\frac{n_{\rm b}}{10^3\,{\rm cm^{-3}}}\right)^{-1/2},$$
 (2.21)

with $c_{\rm s} = \sqrt{\frac{\gamma k_{\rm B}T}{\mu m_{\rm H}}}$ the sound speed in the central region and $\rho_{\rm m}$ the total matter density in the central region. The radius of the central region is chosen to be $r_{\rm c} = \lambda_{\rm J}/2$. The collapse in the core proceeds approximately at the free-fall rate, although additional heat input, for example due to magnetic energy dissipation, may delay gravitational collapse. An arbitrary factor η is introduced with which to regulate this delay. The mean baryonic density evolution in the central part is described by

$$\frac{\mathrm{d}\rho_{\mathrm{b}}}{\mathrm{d}t} = \eta \frac{\rho_{\mathrm{b}}}{t_{\mathrm{ff}}},\tag{2.22}$$

where $t_{\rm ff}$ is the free-fall time, which is a function of the (mean) total matter density and is calculated as

$$t_{\rm ff} = \sqrt{\frac{3\pi}{32G\rho_{\rm m}}} \approx 0.54 \frac{1}{\sqrt{G\rho_{\rm m}}}.$$
(2.23)

The conversion to number density is done as follows:

$$n_{\rm b} = \frac{\rho_{\rm b}}{\mu m_{\rm H}},\tag{2.24}$$

where μ is the mean molecular weight (see section 2.3.3) and $m_{\rm H}$ is the mass of a hydrogen atom.

Virialization

Virialization is assumed to occur when the overdensity compared to the cosmic background reaches a certain value, $\rho/\rho_{\rm u} = \Delta_{\rm c}$. An approximate value for $\Delta_{\rm c}(z)$ in a flat Universe is given by (Bryan & Norman 1998)

$$\Delta_{\rm c}(z) = 18\pi^2 + 82\left(\Omega_{\rm m}(z) - 1\right) - 39\left(\Omega_{\rm m}(z) - 1\right)^2.$$
(2.25)

This is generally approximated as $\Delta_c \approx 200$ for the virialization redshifts of interest.

Initially, the gas heats up to the virial temperature of the halo, as the infalling material is shock heated. When the cooling time becomes shorter than the dynamical time, it starts to cool and collapse. Because cooling through Lyman-alpha photons is very efficient, the gas cannot virialize by gaining internal energy, so it has to increase its kinetic energy in order to reach virial equilibrium. As a result, the gas becomes turbulent during virialization. Virialization drives turbulence even in the cold flow regime of galaxy formation for halo masses below $10^{12} M_{\odot}$ (Wise & Abel 2007).

The expressions for the virial parameters are as follows (Barkana & Loeb 2001):

$$r_{\rm vir} = 0.784 \left(\frac{M}{10^8 h^{-1} M_{\odot}}\right)^{1/3} \left(\frac{\Omega_{\rm m}}{\Omega_{\rm m}(z)} \frac{\Delta_{\rm c}}{18\pi^2}\right)^{-1/3} \left(\frac{1+z}{10}\right)^{-1} h^{-1} \,\rm kpc, \tag{2.26}$$

$$v_{\rm vir} = \sqrt{\frac{GM}{r_{\rm vir}}} = 23.4 \left(\frac{M}{10^8 h^{-1} M_{\odot}}\right)^{1/3} \left(\frac{\Omega_{\rm m}}{\Omega_{\rm m}(z)} \frac{\Delta_{\rm c}}{18\pi^2}\right)^{1/6} \left(\frac{1+z}{10}\right)^{1/2} \,\rm km \, s^{-1}, \quad (2.27)$$

$$T_{\rm vir} = \frac{\mu m_{\rm H} v_{\rm vir}^2}{2k_{\rm B}} = 2 \times 10^4 \left(\frac{\mu}{0.6}\right) \left(\frac{M}{10^8 h^{-1} M_{\odot}}\right)^{2/3} \left(\frac{\Omega_{\rm m}}{\Omega_{\rm m}(z)} \frac{\Delta_{\rm c}}{18\pi^2}\right)^{1/3} \left(\frac{1+z}{10}\right) \,\,{\rm K}.$$
(2.28)

The virial velocity will be important later on for calculating the turbulent energy, as will be explained in section 2.4.2.

To give an idea of the values of these parameters, an atomic cooling halo (with $M = 10^9 M_{\odot}$) which virializes at z = 10 has $r_{\rm vir} \approx 3.2 \,\rm kpc$, $v_{\rm vir} \approx 3.7 \times 10^6 \,\rm cm/s$ and $T_{\rm vir} \approx 4.9 \times 10^4 \,\rm K$; while a molecular cooling halo (with $M = 10^6 M_{\odot}$) which virializes at z = 20 has $r_{\rm vir} \approx 320 \,\rm pc$, $v_{\rm vir} \approx 3.7 \times 10^5 \,\rm cm/s$ and $T_{\rm vir} \approx 1.0 \times 10^3 \,\rm K$.

2.3 Chemical Network

The species that are included in the chemical network of this model are H, H⁺, H⁻, H₂, H₂⁺, and e⁻. HD or other molecules involving deuterium are not included; since there is little initial ionization, their abundance is expected to be low and thus HD cooling will not contribute significantly. Reactions with He are not taken into account, but it is considered in the calculation of the mean molecular mass. The He mass fraction is taken to be ~0.248 (corresponding to an abundance $x_{\text{He}} \approx 0.0825$) and stays constant throughout the time integration. The fractional abundances of H, H₂ and e⁻ are explicitly followed during the integration (abundances relative to the total hydrogen density, $n_{\text{H}} = \frac{X_{\text{H}}\rho_{\text{b}}}{m_{\text{H}}}$, where X_{H} is the hydrogen mass fraction), and their initial values are taken to be

$$x_{\rm e} = 2 \times 10^{-3}, \tag{2.29}$$

$$x_{\rm H_2} = 10^{-20}$$
 (basically 0), (2.30)

$$x_{\rm HI} = 1 - x_{\rm e} - 2x_{\rm H_2}.\tag{2.31}$$

The reactions that were assumed to be most important, and thus used in the model, are the following (Shang et al. 2010):

(9)	$\mathrm{H} + \mathrm{e}^- \longrightarrow \mathrm{H}^- + \gamma$	$(\mathrm{H}^{-} \text{ formation})$
(10)	${\rm H} + {\rm H}^- \longrightarrow {\rm H}_2 + {\rm e}^-$	$(H_2 \text{ formation})$
(13)	$\mathrm{H^-} + \mathrm{H^+} \longrightarrow 2 \mathrm{H}$	
(15)	$\rm H_2 + H \longrightarrow 3 H$	$(\mathrm{H}_2 \text{ collisional dissociation})$
(17)	$\mathrm{H}_{2} + \mathrm{H}^{+} \longrightarrow \mathrm{H}_{2}^{+} + \mathrm{H}$	
(18)	$\rm H_2 + e^- \longrightarrow 2 H + e^-$	
(19)	$\mathrm{H^-} + \mathrm{e^-} \longrightarrow \mathrm{H} + 2 \mathrm{e^-}$	
(20)	$\mathrm{H^-} + \mathrm{H} \longrightarrow 2 \mathrm{H} + \mathrm{e^-}$	
(21)	$\mathrm{H^-} + \mathrm{H^+} \longrightarrow \mathrm{H_2^+} + \mathrm{e^-}$	
(25)	${\rm H}^- + \gamma \longrightarrow {\rm H} + {\rm e}^-$	$(\mathrm{H^{-}\ photo-dissociation})$
(28)	${\rm H}_2 + \gamma \longrightarrow 2 {\rm H}$	$(H_2 \text{ photo-dissociation})$

The reaction rates can be found in appendix A of Shang et al. (2010), numbered as above.

2.3.1 Evolution of the electron fraction

The evolution of the fractional abundance of electrons, x_e , is given by the following equation (Peebles 1993; Sethi et al. 2008):

$$\frac{\mathrm{d}x_{\mathrm{e}}}{\mathrm{d}t} = \left[\beta_{\mathrm{e}}x_{\mathrm{HI}}\exp\left(-\frac{h\nu_{\alpha}}{k_{\mathrm{B}}T_{\mathrm{CMB}}}\right) - \alpha_{\mathrm{e}}x_{\mathrm{e}}^{2}n_{\mathrm{H}}\right]C + \gamma_{\mathrm{e}}(T)x_{\mathrm{HI}}x_{\mathrm{e}}n_{\mathrm{H}},\qquad(2.32)$$

where

$$\nu_{\alpha} = \frac{c}{\lambda_{\alpha}} = \frac{c}{1216 \,\text{\AA}},\tag{2.33}$$

$$\alpha_{\rm e} = 2.6 \times 10^{-13} \left(\frac{T}{10^4 \,\rm K}\right)^{-0.8} \,\rm cm^3 \,\rm s^{-1}, \tag{2.34}$$

$$\beta_{\rm e} = \alpha_{\rm e} \frac{(2\pi m_{\rm e} k_{\rm B} T_{\rm CMB})^{3/2}}{(2\pi\hbar)^3} \exp\left[-\frac{3.4\,{\rm eV}}{k_{\rm B} T_{\rm CMB}}\right],\tag{2.35}$$

$$C = \frac{1 + K\Lambda x_{\rm HI} n_{\rm H}}{1 + K(\Lambda + \beta_{\rm e}) x_{\rm HI} n_{\rm H}},$$
(2.36)

$$K = \frac{\lambda_{\alpha}^{3}}{8\pi} H(z)^{-1},$$
(2.37)

$$\Lambda = 8.22458 \,\mathrm{s}^{-1}.\tag{2.38}$$

In the equation for the evolution of the electron fraction, the first term represents the recombination and photo-ionization of the primordial plasma, the second term is the collisional recombination term and the third term represents collisional ionization (H + $e^- \rightarrow H^+ + 2e^-$). Here, ν_{α} is the frequency of the Ly α resonance photons, α_e is the rate coefficient for case B recombinations of atomic hydrogen (which takes into account that direct recombination into the ground state does not lead to a net increase in the number of neutral hydrogen atoms, since the emitted photon is able to ionize other hydrogen atoms in the neighborhood), and β_e is the rate coefficient for ionizations from excited states of atomic hydrogen. The Ly α resonance photons reduce the net recombination at $z \gtrsim 800$ considerably larger than it would have been if C was unity. For $z \lesssim 800$, $C \simeq 1$. C depends on Λ , the two-photon decay rate ($2s \rightarrow 1s$) (rate from Goldman 1989). For further details, see Peebles (1993).

The first term rapidly decreases, and after this recombination process has been suppressed by cosmic expansion only the second term will be important in decreasing the electron fraction. The collisional ionization term is expected to be an important source of electrons when the temperatures become comparable to 10^4 K (which is expected to occur due to the dissipation of magnetic and turbulent energy). The collisional ionization rate γ_e can be found in appendix A of Shang et al. (2010), under reaction number (1).

2.3.2 Evolution of the molecular hydrogen fraction

The evolution of the fractional abundance of molecular hydrogen, x_{H_2} , is given by the following equation (Sethi et al. 2010):

$$\frac{\mathrm{d}x_{\mathrm{H}_2}}{\mathrm{d}t} = k_{\mathrm{m}} x_{\mathrm{e}} x_{\mathrm{HI}} n_{\mathrm{H}} - k_{\mathrm{des}} x_{\mathrm{H}_2} n_{\mathrm{H}}, \qquad (2.39)$$

where

$$k_{\rm m} = \frac{k_9 k_{10} x_{\rm HI} n_{\rm H}}{k_{10} x_{\rm HI} n_{\rm H} + k_{\gamma} + (k_{13} + k_{21}) x_{\rm e} n_{\rm H} + k_{19} x_{\rm e} n_{\rm H} + k_{20} x_{\rm HI} n_{\rm H} + k_{25}}, \quad (2.40)$$

$$k_{\rm des} = k_{15}x_{\rm HI} + k_{17}x_{\rm p} + k_{18}x_{\rm e} + k_{28}\frac{f_{\rm sh}}{n_{\rm H}},$$
(2.41)

$$k_{\gamma}(T_{\rm CMB}) = 4 \left(\frac{m_{\rm e}k_{\rm B}T_{\rm CMB}}{2\pi\hbar^2}\right)^{3/2} \exp\left[-\frac{0.754\,{\rm eV}}{k_{\rm B}T_{\rm CMB}}\right] k_9(T_{\rm CMB})\,.$$
(2.42)

Here, $k_{\rm m}$ is the net rate of formation of H₂ through the H⁻ channel, $k_{\rm des}$ is the net destruction rate of H₂, and k_{γ} is the destruction rate of H⁻ by CMB photons. The subscript number of the other rate coefficients refers to the corresponding reaction as listed above.

For column densities that are large enough, molecular hydrogen can shield itself from radiation in the Lyman-Werner bands. The self-shielding factor $f_{\rm sh}$ is given by Draine & Bertoldi (1996) as

$$f_{\rm sh} = \min\left[1, \left(\frac{N_{\rm H_2}}{10^{14}\,{\rm cm}^{-2}}\right)^{-3/4}\right],$$
 (2.43)

where the local column density is commonly approximated as

$$N_{\rm H_2} \approx x_{\rm H_2} n_{\rm H} \frac{\lambda_{\rm J}}{2}.$$
(2.44)

According to Shang et al. (2010), this approximation agrees within a factor ~ 10 with the H₂ column densities obtained from non-local integrations, and becomes increasingly better for larger densities.

Radiation background

A sufficiently intense UV radiation background can either directly photo-dissociate H_2 (in the Lyman-Werner bands, within the photon energy range 11.2 eV to 13.6 eV, via the two-step Solomon process: $H_2 + \gamma \longrightarrow H_2^* \longrightarrow 2 \text{ H}$), or photo-dissociate the intermediary H^- (photon energies $\gtrsim 0.76 \text{ eV}$). The relevant criterion for suppressing H_2 formation, and thus molecular hydrogen cooling, is that the photo-dissociation timescale is shorter than the H_2 formation timescale. Generally, $t_{\text{diss}} \propto J^{-1}$ and $t_{\text{form}} \propto \rho^{-1}$, so the condition $t_{\text{diss}} = t_{\text{form}}$ yields a critical intensity that increases linearly with density, $J^{\text{crit}} \propto \rho$. The intensity is written as J_{21} , which denotes the specific intensity just below 13.6 eV, in the units of $10^{-21} \text{ erg cm}^{-2} \text{ sr}^{-1} \text{ sr}^{-1} \text{ Hz}^{-1}$. The expected level of the cosmic UV background in the Lyman-Werner bands near reionization of the Universe is (Bromm & Loeb 2003)

$$J_{\rm bg} \approx \frac{1}{f_{\rm esc}} \frac{hc}{4\pi} \frac{N_{\gamma} X_{\rm H} \rho_{\rm b, bg}}{m_{\rm H}}, \qquad (2.45)$$

or

$$J_{21} \approx 400 \left(\frac{N_{\gamma}}{10}\right) \left(\frac{f_{\rm esc}}{0.1}\right)^{-1} \left(\frac{1+z}{11}\right)^3, \qquad (2.46)$$

where $f_{\rm esc}$ is the escape fraction of ionizing radiation from star-forming halos and N_{γ} is the average number of ionizing photons per baryon required to reionize the Universe. In molecular cooling halos, with virial temperatures $<10^4$ K, the critical intensity is expected to be small compared to the UV background intensity; in larger, atomic cooling halos, with virial temperatures $\geq 10^4$ K, the critical intensity is expected to be much larger, mainly because the gas can cool through atomic hydrogen, reach high densities, and become self-shielding against Lyman-Werner radiation.

Here, two different UV spectra are considered. They are both Planck spectra with a blackbody temperature of either $T_* = 10^4$ or 10^5 K (denoted by T4 and T5, respectively). The softer of these spectra is meant to approximate the mean spectrum of a normal (present-day) stellar population (Pop II), whereas the higher temperature case is closer to the harder spectrum expected to be emitted by the first generation of massive, metal-free stars (Pop III) (Tumlinson & Shull 2000; Bromm et al. 2001; Schaerer 2002).

In molecular cooling halos, the critical value has been estimated at $J_{21} \approx 0.1$ (e.g. Mesinger et al. 2009). In atomic cooling halos with $T_{\rm vir} \approx 10^4$ K the critical value has been estimated at $J_{21} \leq 10^3$ for T4 backgrounds and $J_{21} \gtrsim 10^5$ for T5 backgrounds (Omukai 2001; Bromm & Loeb 2003). Shang et al. (2010) have estimated the critical value in atomic cooling halos with $T_{\rm vir} \geq 10^4$ K at $30 < J_{21} < 300$ for T4 backgrounds and at $10^4 < J_{21} < 10^5$ for T5 backgrounds. These values are a factor of 3-10 lower than previous estimates, probably due to the higher H₂ collisional dissociation rate used.

These UV backgrounds are incorporated in the reaction rates of reactions 25 and 28 as follows:

$$k_{25} = 10^{-10} \alpha J_{21}, \quad \alpha(T4) = 2000, \quad \alpha(T5) = 0.1,$$

 $k_{28} = 10^{-12} \beta J_{21}, \quad \beta(T4) = 3, \qquad \beta(T5) = 0.9.$

2.3.3 Mean molecular weight

The mean molecular weight μ is calculated as follows:

$$n_{\rm b} = n_{\rm e} + n_{\rm p} + n_{\rm HI} + n_{\rm H_2} + n_{\rm He}$$
 with $n_{\rm e} = n_{\rm p}$ (2.47)

$$= \frac{1}{m_{\rm H}} \left(2\rho_{\rm p} + \rho_{\rm HI} + \frac{\rho_{\rm H2}}{2} + \frac{\rho_{\rm He}}{4} \right) \qquad \text{with } n_i = \frac{\rho_i}{A_i m_{\rm H}}$$
(2.48)

$$= \frac{\rho_{\rm b}}{m_{\rm H}} \left(2X_{\rm p} + X_{\rm HI} + \frac{X_{\rm H2}}{2} + \frac{X_{\rm He}}{4} \right) \qquad \text{with } X_i = \frac{\rho_i}{\rho_{\rm b}}$$
(2.49)

$$= \frac{\rho_{\rm b}}{m_{\rm H}} \left(2x_{\rm e} + x_{\rm HI} + x_{\rm H_2} + x_{\rm He} \right) X_{\rm H} \qquad \text{with } x_i = \frac{\lambda_i}{A_i X_{\rm H}}$$
(2.50)

$$\equiv \frac{\rho_{\rm b}}{\mu m_{\rm H}},\tag{2.51}$$

$$\Rightarrow \mu = \left[\left(2x_{\rm e} + x_{\rm HI} + x_{\rm H_2} + x_{\rm He} \right) X_{\rm H} \right]^{-1}, \qquad (2.52)$$

where X_i is the mass fraction of species *i* and A_i is the atomic mass number. The difference between the proton and neutron mass is neglected here. The above assumes that He has recombined completely, and also that it is never ionized, which is reasonable given the temperatures reached in this model. For a primordial hydrogen and helium mixture of gas with $X_{\rm H} \approx 0.75$ and $X_{\rm He} \approx 0.25$, $\mu \approx 1.23$ for a fully neutral (atomic) gas and $\mu \approx 0.59$ for a fully ionized gas (with He doubly ionized), in units of the proton mass.

2.4 Magnetic Field Evolution

Several mechanisms act to increase and decrease the magnetic field strength, B. Here, gravitational compression and the small-scale dynamo can amplify the magnetic field, while ambipolar diffusion and decaying MHD turbulence will decrease the field. The evolution of the magnetic field energy $E_{\rm B} = B^2/8\pi$ is calculated as

$$\begin{cases}
2\alpha \frac{\dot{\rho}_{\rm b}}{\rho_{\rm b}} E_{\rm B} - L_{\rm AD} - L_{\rm MHDT} & z \ge z_{\rm ta},
\end{cases}$$
(2.53)

$$\frac{\mathrm{d}E_{\mathrm{B}}}{\mathrm{d}t} = \begin{cases} 2\alpha \frac{\dot{\rho_{\mathrm{b}}}}{\rho_{\mathrm{b}}} E_{\mathrm{B}} - L_{\mathrm{AD}} & z_{\mathrm{ta}} > z \ge z_{\mathrm{vir}}, \end{cases}$$
(2.54)

$$\left(2\left(\frac{B}{B}\right)_{\rm SSD}E_{\rm B}\qquad z_{\rm vir}>z.$$
(2.55)

Here, the density-dependent term represents the gravitational compression, with α the compression index depending on the collapse symmetry, L_{AD} is the ambipolar diffusion rate, L_{MHDT} is the rate of decaying MHD turbulence and $(\dot{B}/B)_{SSD}$ is the growth rate of the field as induced by the small-scale dynamo. More about these various mechanisms can be found in the following sections.

In analogy to the gas pressure, the magnetic pressure also sets a characteristic scale for collapse; the magnetic Jeans mass and scale, given by

$$M_{\rm J}^{\rm B} = \left(\frac{5}{18G}\right)^{3/2} \left(\frac{3}{4\pi}\right)^2 B^3 \rho_{\rm m}^{-2}$$
(2.56)

$$\simeq 2M_{\odot} \left(\frac{v_{\rm A}}{0.2\,{\rm km\,s^{-1}}}\right)^3 \left(\frac{n_{\rm b}}{10^3\,{\rm cm^{-3}}}\right)^{-1/2},\tag{2.57}$$

$$\lambda_{\rm J}^{\rm B} = \left(\frac{6M_{\rm J}^{\rm B}}{\pi\rho_{\rm m}}\right)^{1/3},\tag{2.58}$$

where $v_{\rm A}$ is the Alfvén speed.

The cloud will only be able to collapse if its mass is larger than both $M_{\rm J}$ and $M_{\rm J}^{\rm B}$, and the relevant Jeans scale is found by taking the maximum of $\lambda_{\rm J}$ and $\lambda_{\rm J}^{\rm B}$. For $B_0 \gtrsim 1 \,\mathrm{nG}$, the magnetic Jeans scale is larger and thus more restrictive, which means that the minimum halo mass required for collapse is raised to $M \approx 5 \times 10^8 (B_0/1 \,\mathrm{nG})^3 M_{\odot}$ (Sethi & Subramanian 2005; Sethi et al. 2008).

2.4.1 Gravitational compression

Detailed models for magnetic energy dissipation via Ohmic and ambipolar diffusion show that the magnetic field is frozen into the gas unless it is very strong. In order for the cloud to collapse, the magnetic energy density needs to be less than the gravitational energy density of the cloud core; from this criterion it can be found that the initial field strength should satisfy $B \lesssim 10^{-5} (n_{\rm b}/10^3 \,{\rm cm}^{-3})^{0.55}$ G (Maki & Susa 2004, 2007).

If the flux-freezing condition applies, the magnetic field depends on the density as $B \propto \rho_{\rm b}^{\alpha}$. Gravitational compression under spherical symmetry leads to an increase in the magnetic field strength with $\alpha = 2/3$. If the collapse proceeds preferentially along one

axis, for instance because of rotation or strong magnetic fields, the scaling is closer to $\alpha = 1/2$. In realistic cases, often intermediate values are found (Machida et al. 2006; Banerjee et al. 2009; Schleicher et al. 2009; Hocuk et al. 2012).

2.4.2 Small-scale dynamo

Turbulence may act to amplify weak magnetic fields due to random stretching and folding of the magnetic field lines in a turbulent random flow; this is the small-scale dynamo mechanism. During gravitational collapse, turbulence is generated by the release of gravitational energy and the infall of accreted gas on the inner, self-gravitating core. It is assumed that gas is continually falling in, so the turbulence will not decay but is constantly replenished. However, this depends on the ambient gas reservoir; in a 2D or 3D setting the accretion process may be more complicated, with e.g. clumpy or intermittent accretion. It has been shown that the injection scale of such accretiondriven turbulence is close to the size of the system under consideration; hence close to the local Jeans length $\lambda_{\rm J}$ (Klessen & Hennebelle 2010; Federrath et al. 2011).

Numerical simulations showed that such turbulence is subsonic in the first star-forming molecular cooling halos, and highly supersonic in the halos with virial temperatures larger than 10^4 K. It also appears that the order-of-magnitude of the turbulent velocity does not change during the collapse (Greif et al. 2008; Wise & Abel 2007; Wise et al. 2008). For accretion-driven turbulence, the turbulent velocity on the injection scale is expected to be comparable to the (free-fall) velocity of the infalling gas, and for a roughly isothermal density profile, the free-fall velocity is independent of radius. Hence, while the injection scale changes during the collapse, the injected velocity is assumed to stay the same and is approximately equal to the virial velocity ($v_{in} \approx v_{vir} \approx \text{constant}$). On scales smaller than the injection scale, the turbulent velocity is expected to scale as $v \propto l^{\beta}$, with $\beta = 1/3$ for Kolmogorov turbulence and $\beta = 1/2$ for Burgers turbulence. Kolmogorov turbulence describes a situation where the gas is incompressible and is thus applicable in particular for subsonic turbulence, whereas Burgers turbulence describes turbulence in the presence of shocks, where the gas is quite strongly compressed. In simulations of realistic turbulence one typically finds power laws in between both cases.

The magnetic field on a scale l typically grows exponentially on the eddy turnover time $t_{\text{ed}} = l/v$, where v is the turbulent velocity on the scale l:

$$v = v_{\rm in} \left(\frac{l}{\lambda_{\rm J}}\right)^{\beta},\tag{2.59}$$

with $v_{\rm in}$ the velocity injected on the Jeans scale $\lambda_{\rm J}$. However, the magnetic field will not continue to grow indefinitely, but rather it will saturate when the magnetic energy corresponds to a fraction $Rm_{\rm cr}^{-1}$ of the kinetic energy. $Rm_{\rm cr}$ is the critical magnetic Reynolds number; for $Rm = vl/\eta > Rm_{\rm cr}$ (with η the magnetic diffusivity), the equation for dynamo growth predicts exponential growth of the magnetic field on the eddy turnover time. The maximum magnetic field strength is thus given by (Subramanian & Barrow 1998)

$$B_{\rm max} = \left(\frac{4\pi\rho_{\rm b}v^2}{Rm_{\rm cr}}\right)^{1/2}.$$
(2.60)

This equation roughly describes the behavior of $B_{\rm max}$, however, the exact value of the saturation field strength is still somewhat uncertain. The critical magnetic Reynolds number also appears to be somewhat uncertain; Schleicher et al. (2010) cite a value of ~60, while Haugen et al. (2004b) and Schober et al. (2012b) find that the value that $Rm_{\rm cr}$ increases with compressibility. Haugen et al. (2004a, b) found $Rm_{\rm cr} \approx 35$ for subsonic turbulence and $Rm_{\rm cr} \approx 70$ for supersonic turbulence, at a magnetic Prandtl number of about unity; while Schober et al. (2012b) found $Rm_{\rm cr} \approx 107$ for Kolmogorov turbulence and $Rm_{\rm cr} \approx 2718$ for Burgers turbulence, in the limit of large magnetic Prandtl numbers. The stretch-twist-fold dynamo process works best in a purely rotational turbulent velocity field; therefore, the dynamo is expected to be more easily excited in Kolmogorov turbulence.

Once the magnetic field B on a scale l becomes larger than the saturation value B_{max} , it is no longer amplified by the small-scale dynamo; however it is still amplified by gravitational compression ($\propto \rho^{2/3}$). It can thus in principle increase above the saturation level (which only increases $\propto \rho^{1/2}$), but in this case it is subject to turbulent decay. On a given scale, this decay will probably also happen on the eddy turnover time. As a result, the value of the magnetic field tends to stay close to the saturation value on that scale.

The growth rate of the magnetic field due to the small-scale dynamo is thus given as (following the prescription of Schleicher et al. 2010)

$$\left(\begin{array}{cc} \alpha \frac{\dot{\rho}_{\rm b}}{\rho_{\rm b}} + t_{\rm ed}^{-1} & B < B_{\rm max}, \end{array} \right)$$
(2.61)

$$\left(\frac{\dot{B}}{B}\right)_{\rm SSD} = \begin{cases} \frac{\dot{B}_{\rm max}}{B_{\rm max}} & B = B_{\rm max}, \end{cases}$$
(2.62)

$$\left(\alpha \frac{\dot{\rho}_{\rm b}}{\rho_{\rm b}} - t_{\rm ed}^{-1} \quad B > B_{\rm max}.$$
 (2.63)

The most important contribution to the total magnetic energy comes from the integral scale, the scale on which the magnetic field is largest. Schleicher et al. (2010) have shown that in an atomic cooling halo, the integral scale increases very rapidly to the maximum scale on which the magnetic field is coherent after the start of the simulation. For this reason, here only the evolution of the magnetic field at this scale of maximal coherence is followed. Since the magnetic field is distorted by the gravitational collapse, the largest possible coherence length is always smaller than the Jeans length by some factor f_d . The exact value of this factor is uncertain and will be a free parameter in the model; the fiducial value is 0.1. The resistive scale lies well below this value. So the integral scale is calculated as:

$$l_{\rm int} = f_{\rm d} \max\left(\lambda_{\rm J}, \lambda_{\rm J}^B\right) \tag{2.64}$$

2.4.3 Ambipolar diffusion

Ambipolar diffusion is important in a mostly neutral medium where a tangled magnetic field is present. The Lorentz force then acts on only a small fraction of the gas (the ionized component) and this generates a velocity difference between the ions and neutrals. This

relative velocity gets damped by ion-neutral collisions and thus results in the dissipation of magnetic field energy. The ambipolar diffusion heating rate is given as (Shang et al. 2002; Pinto et al. 2008; Pinto & Galli 2008; Schleicher et al. 2008a)

$$L_{\rm AD} = \frac{\eta_{\rm AD}}{4\pi} |(\nabla \times \mathbf{B}) \times \mathbf{B}/B|^2, \qquad (2.65)$$

where

$$\eta_{\rm AD} = \frac{\rho_{\rm n} B^2}{4\pi \gamma_{\rm AD} \rho_{\rm b}^2 \rho_{\rm i}},\tag{2.66}$$

$$\rho_{\rm n} = \rho_{\rm HI} + \rho_{\rm H_2} + \rho_{\rm He}, \qquad (2.67)$$

$$\rho_{\rm i} = \rho_{\rm H^+},\tag{2.68}$$

$$\gamma_{\rm AD} = \frac{\frac{1}{2} x_{\rm HI} \langle \sigma v \rangle_{\rm H^+, \rm HI} + \frac{2}{3} x_{\rm H_2} \langle \sigma v \rangle_{\rm H^+, \rm H_2} + \frac{4}{5} x_{\rm He} \langle \sigma v \rangle_{\rm H^+, \rm He}}{m_{\rm H} (x_{\rm H} + 2x_{\rm H_2} + 4x_{\rm He})}.$$
 (2.69)

Here, $\eta_{\rm AD}$ is the AD resistivity, $\rho_{\rm n}$ and $\rho_{\rm i}$ are the neutral and ionized mass densities, respectively, $\gamma_{\rm AD}$ is the ion-neutral coupling coefficient, σ is the cross-section for the collisions between ions and neutrals, and v is the ion-neutral relative velocity. Collisions with electrons are neglected here, as their contribution is suppressed by a factor $m_{\rm e}/m_{\rm H}$.

The momentum transfer rate coefficients for these species (calculated for zero drift velocity, which is a good approximation in the absence of shocks) are given by (Pinto & Galli 2008)

$$\langle \sigma v \rangle_{\rm H^+, H} = 0.649 \, T^{0.375} \times 10^{-9} \, \rm cm^{3} \, s^{-1},$$
 (2.70)

$$\langle \sigma v \rangle_{\mathrm{H^+,H_2}} = \left[1.003 + 0.050 \log\left(\frac{T}{\mathrm{K}}\right) + 0.136 \log\left(\frac{T}{\mathrm{K}}\right)^2 \right]$$

$$(2.71)$$

$$-0.014 \log \left(\frac{T}{K}\right)^{3} \times 10^{-9} \text{ cm}^{3} \text{ s}^{-1},$$

$$(1.424 + 7.428 \times 10^{-6} \text{ Tr} - 6.724 \times 10^{-9} \text{ Tr}^{2}) \times 10^{-9} \text{ cm}^{3} \text{ s}^{-1} \qquad (2.72)$$

$$\langle \sigma v \rangle_{\rm H^+, He} = (1.424 + 7.438 \times 10^{-6} T - 6.734 \times 10^{-9} T^2) \times 10^{-9} \rm \ cm^3 \ s^{-1}.$$
 (2.72)

To estimate the differential operator in Equation 2.65 we adopt an intuitive approach, so that for a given average magnetic field B with coherence length $l_{\rm B}$ the ambipolar diffusion heating rate can be calculated as

$$L_{\rm AD} \approx \frac{\eta_{\rm AD}}{4\pi} \frac{B^2}{l_{\rm B}^2} \tag{2.73}$$

$$\approx \frac{\rho_{\rm n}}{16\pi^2 \gamma_{\rm AD} \rho_{\rm b}^2 \rho_{\rm i}} \frac{B^4}{l_{\rm B,AD}^2}.$$
(2.74)

The coherence length $l_{\rm B}$ is in principle a free parameter, which depends on the generation mechanism of the magnetic field and its evolution afterwards. However, it is constrained through the fact that in the pre-recombination Universe ($z \gtrsim 1000$) tangled magnetic fields are strongly damped by radiative viscosity on scales smaller than the Alfvén damping scale ($l_{\rm min} = 2\pi/k_{\rm max}$), where $k_{\rm max}$ (comoving) is given by (Jedamzik et al. 1998; Subramanian & Barrow 1998)

$$k_{\rm max} \simeq 235 \,{\rm Mpc}^{-1} \left(\frac{B_0}{10^{-9} \,{\rm G}}\right)^{-1} \left(\frac{\Omega_{\rm m,0}}{0.3}\right)^{1/4} \left(\frac{\Omega_{\rm b,0} h^2}{0.02}\right)^{1/2} \left(\frac{h}{0.7}\right)^{1/4},$$
 (2.75)

with $B_0 = B/(1+z)^2$ the comoving magnetic field strength. Since fluctuations of the magnetic field may be present on larger scales as well, the heating rate is initially estimated using the minimum value

$$l_{\rm B,AD} = l_{\rm B,min} = \frac{2\pi}{k_{\rm max}(1+z_{\rm init})} \left(\frac{n_{\rm b}}{n_{\rm b,init}}\right)^{-1/3}.$$
 (2.76)

However, while this may be valid initially, the formation and collapse of the halo will most likely affect the coherence length of the magnetic field, when the field is frozen into the gas. In this case, the length scale for ambipolar diffusion will be estimated as the minimum of Equation 2.76 and the integral scale (Equation 2.64).

Another mechanism for magnetic energy dissipation, Ohmic dissipation, could be present. However, Schleicher et al. (2009) verified that ambipolar diffusion is always the dominant mechanism, and so Ohmic dissipation is neglected here.

2.4.4 Decaying MHD turbulence

In the expanding Universe, magnetic fields which vary on length scales smaller than the magnetic Jeans scale (see Equation 2.58) can induce decaying magnetohydrodynamical (MHD) turbulence. Non-linear interactions between different modes causes the magnetic field to decay by an energy cascade to smaller and smaller spatial scales, and through subsequent dissipation, independent of the exact viscous mechanism of dissipation. The prescription of Sethi & Subramanian (2005) is adopted for calculating the heating rate due to decaying MHD turbulence:

$$L_{\rm MHDT} = \frac{B_0(t)^2}{8\pi} \frac{3m}{2} \frac{[\ln(1+t_{\rm d}/t_{\rm i})]^m H(t)}{[\ln(1+t_{\rm d}/t_{\rm i}) + \ln(t/t_{\rm i})]^{m+1}},$$
(2.77)

where t is the cosmological time at redshift z, t_i the time where decay starts, i.e., after the recombination epoch when velocity perturbations are no longer damped by the large radiative viscosity; it is assumed that this time corresponds to a redshift $z_i = 1000$, and t_d is the dynamical timescale (the physical decay timescale for the turbulence), which may be approximated as the Alfvén crossing time associated with the smallest surviving scales in the magnetic spectrum, k_{max} : $t_d = l_{\text{B,min}}/v_A$, where $v_A = B/\sqrt{4\pi\rho_b}$. For a magnetic field power spectrum with power law index n, the decay index m is given as $m = \frac{2(n+3)}{n+5}$. The magnetic field power spectrum is assumed to be nearly scale invariant (scale invariance implies that n = -3) with n chosen as n = -2.9. This choice will however not influence the results significantly.

This prescription is only valid during the expansion phase; however, its contribution to the heating rate and magnetic field dissipation becomes very small and can safely be ignored during further evolution.

2.5 Temperature Evolution

The evolution of the temperature, T, is given by the following equation (Peebles 1993; Sethi & Subramanian 2005; Glover & Abel 2008; Schleicher et al. 2009):

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\gamma - 1}{\rho_{\mathrm{b}}} \left[T \frac{d\rho_{\mathrm{b}}}{dt} + \frac{\mu m_{\mathrm{H}}}{k_{\mathrm{B}}} \left(L_{\mathrm{heat}} - L_{\mathrm{cool}} \right) \right] + k_{\mathrm{iC}} x_{\mathrm{e}} \left(T_{\mathrm{CMB}} - T \right), \qquad (2.78)$$

where

$$\gamma = \frac{5 + 5x_{\rm He} + 5x_{\rm e} - 3x_{\rm H_2}}{3 + 3x_{\rm He} + 3x_{\rm e} - x_{\rm H_2}} \simeq 5/3, \tag{2.79}$$

$$k_{\rm iC} = \frac{8\sigma_{\rm T}a_{\rm R}T_{\rm CMB}^4}{3m_{\rm e}c\,(1+x_{\rm He}+x_{\rm e})}.$$
(2.80)

Here, γ is the adiabatic index, $\sigma_{\rm T}$ is the Thomson scattering cross section, and $a_{\rm R}$ is the radiation constant, related to the Stefan-Boltzmann constant σ as $a_{\rm R} = \frac{4\sigma}{c}$. The first term in the temperature evolution equation is the adiabatic heating/cooling rate due to collapse/expansion, the second term incorporates various other heating and cooling volume rates, $L_{\rm heat}$ and $L_{\rm cool}$, which will be discussed in more detail further on, and the third term represents Compton heating/cooling, where the CMB photons interact by (inverse) Compton scattering with the electrons in the gas and the gas is either heated up or cooled down, depending on the CMB temperature.

2.5.1 Cooling

Two cooling mechanisms are assumed, effective in their respective regimes: atomic hydrogen cooling and molecular hydrogen cooling:

$$L_{\rm cool} = L_{\rm HI} + L_{\rm H_2}.$$
 (2.81)

The volume rates (in units of $\operatorname{erg} \operatorname{cm}^{-3} \operatorname{s}^{-1}$) for these cooling processes are as follows:

$$L_{\rm HI} = 7.9 \times 10^{-19} \left[1 + \left(\frac{T}{10^5 \,\rm K}\right)^{1/2} \right]^{-1} \exp\left(-\frac{118\,348}{T}\right) x_{\rm e} x_{\rm HI} n_{\rm H}^2, \tag{2.82}$$

$$L_{\rm H_2} = \frac{L_{\rm H_2, LTE}}{1 + L_{\rm H_2, LTE}/L_{\rm H_2, n \to 0}} x_{\rm HI} x_{\rm H_2} n_{\rm H}^2.$$
(2.83)

In the low-density limit, the cooling rate per H₂ molecule (in units of erg cm³ s⁻¹) is given by the sum of the cooling rates due to collisional de-excitations, and can be approximated over the range $10 \text{ K} \leq T \leq 10^4 \text{ K}$ as (Galli & Palla 1998)

$$L_{\rm H_2,n\to 0} = \det\left[-103.0 + 97.59\log T - 48.05\left(\log T\right)^2 + 10.80\left(\log T\right)^3 - 0.9032\left(\log T\right)^4\right].$$
 (2.84)

Collisional de-excitation of excited H_2 becomes competitive with radiative de-excitation at fairly low gas densities $(n_b \approx 10^4 \text{ cm}^{-3})$, and so as the number density increases, the cooling rate of H_2 quickly reaches its local thermodynamic equilibrium (LTE) value. The critical density for this transition is given by (Glover & Abel 2008)

$$n_{\rm cr,H_2} = dex \left[4.845 - 1.3 \log T_4 + 1.62 (\log T_4)^2 \right] {\rm cm}^{-3},$$
 (2.85)

with $T_4 = \frac{T}{10^4 \text{ K}}$. In the LTE limit, the level populations become independent of the gas density, and the cooling rate per H₂ molecule is largely determined by the magnitude of the transition probabilities. Since these are small, the LTE cooling rate is also small; it is given by

$$L_{\rm H_2,LTE} = \sum_{i,j>i} A_{ji} E_{ji} f_j, \qquad (2.86)$$

where A_{ji} is the radiative de-excitation rate (transition probability) for a transition from level $j \rightarrow i$, E_{ji} is the corresponding energy of the transition, and f_j is the fraction of H_2 molecules in level j so that $\sum_j f_j$, computed assuming LTE, and these summed over all bound levels i and over all bound levels j with energies greater than i.

Hollenbach & McKee (1979) have fitted an analytical form to the LTE equation (in units of erg cm⁻³ s⁻¹) which is accurate to better than a factor 2, where $L_{\text{H}_2,\text{LTE}}^{rot}$ and $L_{\text{H}_2,\text{LTE}}^{vib}$ are the cooling coefficients for rotational LTE in v = 0 and vibrational LTE in v = 0, 1, 2:

$$L_{\rm H_2,LTE} = \left(L_{\rm H_2,LTE}^{rot} + L_{\rm H_2,LTE}^{vib} \right) n_{\rm H}^{-1},$$
(2.87)

where

$$L_{\rm H_2,LTE}^{rot} = \left(\frac{9.5 \times 10^{-22} T_3^{3.76}}{1 + 0.12 T_3^{2.1}}\right) \exp\left[-\left(\frac{0.13}{T_3}\right)^3\right] + 3 \times 10^{-24} \exp\left(-\frac{0.51}{T_3}\right), \quad (2.88)$$

$$L_{\rm H_2,LTE}^{vib} = 6.7 \times 10^{-19} \exp\left(-\frac{5.86}{T_3}\right) + 1.6 \times 10^{-18} \exp\left(-\frac{11.7}{T_3}\right),\tag{2.89}$$

with $T_3 = \frac{T}{10^3 \text{ K}}$.

2.5.2 Heating

Two additional heating sources are present: dissipation of magnetic and turbulent energy. Ambipolar diffusion and decaying MHD turbulence are considered as mechanisms for dissipating magnetic field energy, and energy dissipation from turbulence driven by accretion onto the central core is also taken into account:

$$\int L_{\rm AD} + L_{\rm MHDT} \qquad z \ge z_{\rm ta}, \tag{2.90}$$

$$L_{\text{heat}} = \begin{cases} L_{\text{AD}} & z_{\text{ta}} > z \ge z_{\text{vir}}, \end{cases}$$
(2.91)

$$L_{\rm AD} + L_{\rm ADT} \qquad z_{\rm vir} > z.$$
 (2.92)

The ambipolar diffusion heating rate (L_{AD}) can be found from Equation 2.65 and the heating rate from decaying MHD turbulence (L_{MHDT}) can be found from Equation 2.77. The heating rate from the dissipation of accretion-driven turbulence (L_{ADT}) is described in the next section.

Dissipation of accretion-driven turbulence

As mentioned before, turbulence is generated during gravitational collapse by the infall of accreted gas on the central core, and is continually replenished, assuming a steady accretion rate. Part of the turbulent energy will go to driving the small-scale dynamo, and part of it will be transferred from large eddies (large scales) to smaller ones in a cascade process, until it is dissipated at by viscosity at small enough scales. Within this range of scales, the turbulence has self-similar properties. The exact dissipation scale, whether set by molecular viscosity or ambipolar diffusion, is not very important here; only the rate at which energy is dissipated into heat, which does not depend on the scale. The rate (per unit mass) at which energy is injected into the system is (Shu 1992)

$$\epsilon_{\rm in} = \frac{E_{\rm in}/m}{t_{\rm ed}(\lambda_{\rm J})} = \frac{1}{2} \frac{v_{\rm in}^2}{\lambda_{\rm J}/v_{\rm in}} = \frac{v_{\rm in}^3}{2\lambda_{\rm J}}.$$
 (2.93)

The volume heating rate from accretion-driven turbulence (ADT) can then be estimated as

$$L_{\rm ADT} = f_{\rm t} \rho_{\rm b} \epsilon_{\rm in}, \qquad (2.94)$$

where f_t is the fraction of the injected energy that is dissipated, which will be a free parameter in the model. It has a maximum at $\sim 1 - Rm_{cr}^{-1}$, since a fraction of the turbulent energy will go into amplifying the magnetic field, but could also be less if the energy is dissipated more slowly.



The model code is written using MATLAB[®] (2009b, The MathWorks Inc., Natick, Massachusetts). It is divided up into three parts: evolution from initial state to turnaround, from turnaround to virialization, and from virialization to end state. In each part, a system of differential equations describing the evolution of the electron fraction, the molecular hydrogen fraction, the temperature, the magnetic field energy, and the density (except in the first part) is integrated over time. The equations are written in logarithmic form, and are integrated using the *ode15s* solver, a multi-step method that can solve stiff ordinary differential equations. This is a variable order solver based on the numerical differentiation formulas (NDFs). It can be set to use the backward differentiation formulas (BDFs, also known as Gear's method), but the latter are usually less efficient.

The model is initialized at a redshift of 800 (z_{init}) . The dissipation of magnetic fields into the IGM after recombination can significantly influence its temperature and ionization, so this early start provides the proper initial conditions for subsequent collapsing halos.

The integration is stopped when the density reaches $n_{\rm b} \approx 10^7 \,{\rm cm}^{-3}$. The model is not equipped to deal with higher densities; this would require the inclusion of additional physical processes, such as for example three-body interactions which increase the H₂ formation rate, Li chemistry as Li⁺ becomes the main charge carrier at densities of $\sim 10^8 \,{\rm cm}^{-3}$ (Glover & Savin 2009), etc.

3.1 Input Parameters

The code takes the following parameters as input:
Collapse parameters				
Name	Default value	Info		
M	$10^9 M_{\odot}$	halo mass		
$z_{ m vir} \ \eta$	10 1	delays collapse if $\eta < 1$		

 ${\bf Table \ 3.1-Input \ parameters \ related \ to \ the \ collapse \ and \ their \ default \ values}$

Radiation background parameters				
Default value	Info			
0 0	indicates the UV bg to be used (none, T4 or T5 spectrum) radiation intensity just below 13.6 eV			
1	E Default value))			

 ${\bf Table} ~ {\bf 3.2-Input} ~ {\bf parameters} ~ {\bf related} ~ {\bf to} ~ {\bf the} ~ {\bf radiation} ~ {\bf background} ~ {\bf and} ~ {\bf their} ~ {\bf default} ~ {\bf values}$

Turbulence parameters				
Name	Default value	Info		
β	1/3	1/3 for Kolmogorov, $1/2$ for Burgers turbulence		
$Rm_{\rm cr}$	60	critical magnetic Reynolds number		
$v_{ m in}$	$v_{ m vir}$	injected velocity at the Jeans scale		
$f_{ m d}$	0.1	maximum fraction of $\lambda_{\rm J}$ allowed for the integral scale		
$f_{ m t}$	0.1	dissipated fraction of the injected turbulent energy		

Table 3.3 – Input parameters related to turbulence and their default values

Magnetic field parameters					
Name	Default value	Info			
$\begin{array}{c} B_{0,\mathrm{init}} \\ \alpha \\ n \end{array}$	1 nG 2/3 -2.9	initial comoving magnetic field strength power law index of dependence of B on $\rho_{\rm b}$ magnetic power spectrum index			

Table 3.4 – Input parameters related to the magnetic field and their default values



The figures below are divided into two parts: a left-hand side where the density decreases with time from left to right, representing the expansion phase, and a right-hand side where the density increases with time from left to right, representing the collapse phase. The dotted line in the right-hand part indicates when virialization occurs.

4.1 Model Without Turbulence

To better understand the effects of turbulence, the model is first integrated without turbulent heating and without the small-scale dynamo. In Figure 4.1 the evolution of the physical magnetic field strength is shown for fiducial values of the parameters as listed in Section 3.1, and different initial comoving field strengths B_0 , where $B_0 =$ $B/(1+z_{\rm init})^2$. The resulting time-evolution of the physical quantities for an initial comoving field strength of zero is virtually the same as for $B_0 = 0.01 \,\mathrm{nG}$, since the dissipation of such a small field does not alter the thermal evolution; therefore the zero-field case is not shown in the figures. In order to see the effects of ambipolar diffusion on the magnetic field strength more clearly, B is scaled with the density as $Bn_{\rm b}^{-\alpha}$ (where $\alpha = 2/3$, unless mentioned otherwise) so that a straight horizontal line indicates that ambipolar diffusion did not decrease the field strength significantly, as is shown in Figure 4.2. It can be seen that ambipolar diffusion decreases the magnetic field strength during the expansion phase in the cases where B_0 is 1 nG or less, and further decreases the field strength during the collapse also for the cases where B_0 is 10 nG or less. The dissipation during expansion is particularly important when B_0 is less than $0.5 \,\mathrm{nG}$. However, during collapse, in the case where $B_0 = 0.01 \,\mathrm{nG}$ the field strength does not decrease much anymore. During the expansion phase, the difference occurs because for stronger fields, the dissipation of only a small fraction of their energy causes such an increase in the gas temperature and ionization fraction that ambipolar diffusion becomes less efficient. The differences in dissipation strength during the collapse phase are mainly a result of the dissipation scale changing between $2\pi/k_{\rm max}(n_{\rm b})$ (Equation 2.75) and the integral scale (Equation 2.64). The evolution of the different scales for $B_0 = 1 \,\mathrm{nG}$ can be seen in Figure 4.7.



Figure 4.1 – Without turbulence – Evolution of the physical magnetic field strength with baryonic density for several different initial comoving field strengths.



Figure 4.2 – Without turbulence – Evolution of the magnetic field strength scaled with the baryonic density for several different initial comoving field strengths.

The temperature evolution is shown in Figure 4.3. The thermal evolution for the $B_0 = 0.01 \,\mathrm{nG}$ case is found to be nearly identical to the zero-field case. For $B_0 = 0.1 \,\mathrm{nG}$, heat input from ambipolar diffusion during the expansion phase eventually increases the temperature above the temperature of the CMB, and for stronger fields the temperature is significantly increased, up to $\gtrsim 10^4 \,\mathrm{K}$ for $B_0 = 3 \,\mathrm{nG}$ and above. At that temperature, the cooling is dominated by atomic hydrogen cooling (as opposed to molecular hydrogen cooling at lower temperatures) which is very effective. Another effect of this high temperature is that collisional ionization becomes efficient at increasing the ionization degree, which is shown in Figure 4.4; the ionization fraction increases with increasing magnetic field strength. This increased ionization renders ambipolar diffusion less efficient, which also prevents a further increase in temperature, as can be seen from the heating and cooling rates shown in Figure 4.6 for an initial magnetic field of $B_0 = 1 \,\mathrm{nG}$. The H₂ fraction is shown in Figure 4.5. During the expansion phase, the higher ionization fraction results in an enhanced H_2 fraction at turnaround, compared to the zero-field case. However, the H₂ fraction only increases with increasing magnetic field strength up to $B_0 = 1 \text{ nG}$; at $B_0 = 3 \text{ nG}$ it is closer to the zero-field case again and then keeps increasing for increasing initial field strength once more. This is related to the high temperatures reached in those cases, which facilitates efficient collisional dissociation of H^- and H_2 .

During the collapse phase, the thermal evolution becomes more complicated. After turnaround, the H₂ fraction oscillates and evolves quite differently for different initial magnetic field strengths, as a result of the competition between collisional dissociation of H₂ and increased H₂ formation due to the enhanced electron fraction. This situation stabilizes approximately at a density of $\sim 1 \text{ cm}^{-3}$; now the H₂ fraction is larger for a larger initial magnetic field (except in the case where $B_0 = 13 \text{ nG}$), and increases only slightly further with increasing density. As a result of the enhanced H₂ fraction, the stronger molecular hydrogen cooling now allows the halo with the stronger magnetic field to cool to a temperature below that of a less magnetized halo for a brief period, but then ambipolar diffusion heating begins to increase the temperature again, due to the gas becoming increasingly more neutral.

Note that for the zero-field case and for initial fields smaller than 1 nG the gas temperature increases adiabatically after turnaround, and when sufficient H_2 is formed for efficient cooling and the temperature decreases again. The central temperature is smaller than the virial temperature of the host halo, which is $\sim 10^4$ K. This occurs because the innermost region starts to cool and collapse during the adiabatic compression and does not experience the virialization shock.

For initial fields in the range $3 - 12 \,\mathrm{nG}$, something interesting happens at high densities; the heating from ambipolar diffusion is so strong that at a certain point an instability forms. The molecular hydrogen cooling cannot compensate for the strong heating anymore, and the temperature suddenly increases. Then atomic hydrogen cooling takes over and stabilizes the temperature at ~8000 K. At the same time, collisional dissociation of H₂ becomes dominant over H₂ formation processes and the H₂ fraction drops steeply. However, when the temperature increases, also the ionization fraction increases strongly and this again aids the formation of H₂. Some molecules reform, but the high temperature and density prevent it from becoming an important coolant again, and the gas temperature stays high. The smallest B_0 for which an instability as described above occurs, in this case 3 nG, will be referred to as $B_0^{\rm crit,inst}$, the critical field strength for forming an instability. For an even stronger initial magnetic field, $B_0 = 13 \text{ nG}$, H_2 never becomes an important coolant as it cannot form fast enough. Ambipolar diffusion heating, which is the main heating process, is balanced by atomic hydrogen cooling at all times during the collapse, and thus the gas stays hot. The smallest B_0 for which this occurs will be referred to as B_0^{crit,H_2} , the critical field strength for which H_2 cooling never becomes efficient. The problem with these large fields, however, is that the magnetic Jeans mass becomes large compared to the halo mass, and thus the halo will likely not collapse at all.



Figure 4.3 – Without turbulence – Evolution of the gas temperature with baryonic density for several different initial comoving field strengths.



Figure 4.4 – Without turbulence – Evolution of the electron fraction with baryonic density for several different initial comoving field strengths.



Figure 4.5 – Without turbulence – Evolution of the H_2 fraction with baryonic density for several different initial comoving field strengths.



Figure 4.6 – Without turbulence – Evolution of the heating and cooling rates from various processes (as labeled) for an initial comoving field strength of 1 nG.



Figure 4.7 – Without turbulence – Evolution of various scales in the cloud for an initial comoving field strength of 1 nG. The top black line represents the diameter of the spherical cloud, the blue dotted line shows the scale associated with k_{\max} as it evolves with density, the red and green dash-dot lines represent the thermal and magnetic Jeans length, respectively, and the purple solid line is the integral scale.



Figure 4.8 – Without turbulence – Evolution of the heating and cooling rates from various processes (as labeled) for an initial comoving field strength of 13 nG.



Figure 4.9 – Without turbulence – Evolution of various scales in the cloud (as labeled) for an initial comoving field strength of $13 \,\mathrm{nG}$.

4.2 Model With Turbulence

When taking turbulence into account, this picture becomes quite different. In Figure 4.10 the magnetic field strength is shown as scaled with density for different initial comoving field strengths B_0 , and with fiducial values used for the other parameters, as listed in Section 3.1. The evolution until approximately virialization is identical to the model without turbulence, but changes when gas starts falling in onto the inner, virialized core. The accretion-driven turbulence quickly brings the magnetic field strength to $B_{\rm max}$ through the small-scale dynamo effect (see Equation 2.60), either by amplifying smaller fields or by draining energy from larger fields. The convergence to $B_{\rm max}$ occurs within a factor ~3 in density. $B_{\rm max}$ evolves as $\propto n_{\rm b}^{1/2}$, which is slower than the increase from gravitational compression alone ($\propto n_{\rm b}^{2/3}$), and is thus represented by a falling line. The amplification of small fields does however mean that their dissipation will not be negligible, and the $B_0 = 0.01$ nG case will no longer approximate the zero-field case.

Figure 4.11 shows the thermal evolution of the gas; the thick black line represents the zero-field case. As stated above, the evolution until virialization is the same as described for the model without turbulence, since turbulent effects are not yet important. After virialization, the peak in the temperature curve is shifted to lower densities for $B_0 = 0.01 \,\mathrm{nG}$ compared to the zero-field case, and shifts to higher densities for stronger fields, until for $B_0 = 0.5 \,\mathrm{nG}$ the evolution is almost equal to the zero-field case; for still stronger fields the peak shifts to lower densities again. The peak in the temperature results from a peak in the ambipolar diffusion heating. It is strong for small fields because even though all the different initial field strengths get amplified to the same value $B_{\rm max}$, the scale on which the dissipation occurs in the model is not equal, and smaller for smaller fields, resulting in more heating. For $B_0 = 0.5 \,\mathrm{nG}$, this AD heating peak is less strong than the turbulent heating, which is why it closely resembles the zero-field case. For larger fields the diffusion scale changes to the integral scale which is now the smallest, so the AD peak becomes important again and the evolution shifts away from the zero-field case. The different heating and cooling processes are shown in Figure 4.14, and the different scales are shown in Figure 4.15, both for an initial field of 1 nG. The general order of curves is preserved through the rest of the evolution, with the highest temperature in the zero-field case and the lowest for the largest B_0 . The same order is also visible in the evolution of the electron fraction (Figure 4.12) and of the H_2 fraction (Figure 4.13; except just after virialization, where collisional dissociation briefly becomes important due to the high temperatures). This order occurs because now the heating from dissipation of accretion-driven turbulence dominates over the ambipolar diffusion heating resulting from $B_{\rm max}$, no matter what the dissipation scale is. Molecular hydrogen cooling can easily keep up with the turbulent heating, since it does not increase very steeply with density (it grows roughly as $\propto n_{\rm b}^{3/2}$, while the H₂ cooling rate grows as $\propto n_{\rm b}^2$), and then initially higher temperatures mean an elevated ionization fraction, which facilitates the formation of H_2 , so that owing to the increased H_2 fraction the initially hotter halo will cool down to lower temperatures. The differences however decrease at increasingly higher densities. Thus, the system has little dependence on its initial history; the turbulence causes this 'memory' to be lost.

In the zero-field case, the turbulent heating increases the temperature above the zero-field-zero-turbulence case, but is at a density of $10^7 \,\mathrm{cm}^{-3}$ only higher by less than

a factor two. And for an initial magnetic field of 1 nG, the temperature at that density is even slightly lower for the turbulent halo. The same happens for larger fields, and no temperature instabilities occur. Thus, it seems that turbulence stabilizes the collapse thermodynamics.



Figure 4.10 – With turbulence – Evolution of the magnetic field strength scaled with the baryonic density for several different initial comoving field strengths.



Figure 4.11 – With turbulence – Evolution of the gas temperature with baryonic density for several different initial comoving field strengths.



Figure 4.12 – With turbulence – Evolution of the electron fraction with baryonic density for several different initial comoving field strengths.



Figure 4.13 – With turbulence – Evolution of the H_2 fraction with baryonic density for several different initial comoving field strengths.



Figure 4.14 – With turbulence – Evolution of the heating and cooling rates from various processes (as labeled) for an initial comoving field strength of 1 nG.



Figure 4.15 – With turbulence – Evolution of various scales in the cloud (as labeled) for an initial comoving field strength of 1 nG.

4.3 Effects of Various Parameters

In this section the effects of varying parameters other than the initial magnetic field are explored. All parameters that are not being varied are fixed at their fiducial values as listed in Section 3.1, unless mentioned otherwise.

4.3.1 Halo mass

The main result of increasing the mass is that the infall velocity, and hence the turbulent velocity, increases, which adds significantly more turbulent heating. Heating by ambipolar diffusion also increases, because $B_{\rm max}$ is larger for larger turbulent velocities, but is always much less than turbulent heating. In massive enough halos, the turbulent heating is so strong that molecular hydrogen cannot form fast enough to become an important coolant, so the cooling is dominated by atomic hydrogen and the temperature of the halo stays around $\sim 10^4$ K. This happens for halos with a mass between $10^{10} M_{\odot}$ and $10^{11} M_{\odot}$ and higher, as can be seen from Figure 4.16. If the dissipated fraction of the injected turbulent energy is increased, then this transition occurs at smaller halo masses (e.g. between $10^9 M_{\odot}$ and $10^{10} M_{\odot}$ for $f_{\rm t} = 0.25$). However, if either the dissipated fraction or the fraction of the kinetic energy that is turned into turbulent energy is decreased, then the transition only occurs at larger halo masses (e.g. between $10^{11} M_{\odot}$ and $10^{12} M_{\odot}$ for $f_{\rm t} = 0.01$ or for $v_{\rm in} = 0.5 v_{\rm vir}$).

When turbulence is unimportant, the only effect of increasing the halo mass is that

the halo radius increases, which changes the ambipolar diffusion scale at large initial fields; however, the difference in heating is small and thus the mass has little effect on the thermal evolution of the halo.



Figure 4.16 – With turbulence – Evolution of the gas temperature with baryonic density for several different halo masses.

4.3.2 Delayed collapse

Setting the parameter η to a value smaller than 1 slows the collapse; the effect of this is that virialization happens at a lower density, but the overall shape of the temperature evolution curve does not change significantly for a turbulent halo. When turbulent effects are not important, the increased timespan causes the magnetic field strength to be decreased significantly due to ambipolar diffusion, so that at a certain point there will be less AD heating than at that same density in the fiducial model. This causes the halo to cool down to lower temperatures, ~200 K. However, high densities are only reached at z < 6, which might not leave enough time for the seed black hole to grow into a SMBH. A forced collapse may also be possible; in this case, virialization happens at a higher density, but again the overall thermal evolution does not change much for a turbulent halo. When turbulent effects are not important, the temperature is somewhat increased, which results in an instability (such as discussed in 4.1) occurring already for B_0 between 1 - 2 nG if $\eta = 2$.

4.3.3 Radiation background

The effect of the radiation background is to photo-dissociate H^- and H_2 , which results in higher destruction rates of H_2 ; more details can be found in Section 2.3.2. The radiation background is switched on at turnaround, $z \approx 15$; an earlier or slightly later turn-on is also possible, but does not change the results significantly, if at all.

The effects of different radiation intensities of a T4 background on the temperature, ionization fraction and H₂ fraction are shown in Figures 4.17, 4.18, and 4.19, respectively, for an initial field of 1 nG. However, the critical intensity does not depend on the initial field strength when turbulent effects are important. After the radiation background is turned on, H₂ is destroyed rapidly, because it cannot self-shield as the density is too low; this happens even for a low intensity of $J_{21} = 1$. The cooling is dominated by atomic hydrogen cooling, so the temperature is high and thus the ionized fraction becomes elevated. In the case where $J_{21} = 1$, molecular hydrogen succeeds in reforming and becomes the dominant coolant at a density of $\sim 10 \text{ cm}^{-3}$, but at higher intensities H₂ cannot reform fast enough to become an important coolant. The critical intensity for a T4 background is thus found to be $1 < J_{21} \leq 10$.



Figure 4.17 – With turbulence – Evolution of the gas temperature with baryonic density for a T4 background and several different UV intensities.

The effects of different radiation intensities of a T5 background on the temperature and H₂ fraction are shown in Figures 4.20 and 4.21, respectively. The results are similar to those for the T4 background, only higher radiation intensities are needed to prevent H₂ from forming fast enough to become the dominant coolant. The critical intensity for a T5 background is found to be $10^3 < J_{21} \le 10^4$.



Figure 4.18 – With turbulence – Evolution of the electron fraction with baryonic density for a T4 background and several different UV intensities.



Figure 4.19 – With turbulence – Evolution of the H_2 fraction with baryonic density for a T4 background and several different UV intensities.



Figure 4.20 – With turbulence – Evolution of the gas temperature with baryonic density for a T5 background and several different UV intensities.



Figure 4.21 – With turbulence – Evolution of the H_2 fraction with baryonic density for a T5 background and several different UV intensities.

If turbulence is unimportant, the critical intensity is higher due to the difference in heating. For the zero-field case, the critical intensity is $10 < J_{21} \leq 10^2$ for a T4 background and $10^4 < J_{21} \leq 10^5$ for a T5 background. Similar results are found for an initial magnetic field of 1 nG, as can be seen from Figures 4.22 and 4.23. However, if the initial magnetic field is increased to 2 nG, H₂ never becomes an important coolant for a T4 background with $J_{21} = 10$, and for $J_{21} = 1$ an instability (such as discussed in 4.1) occurs at high densities, where much of the H₂ is suddenly destroyed and thus the gas stays hot afterwards. For a T5 background with the same initial field, a similar instability occurs for $J_{21} = 10^4$, while with an initial field of 3 nG the H₂ fraction is never large enough for significant cooling at this intensity. Thus, when turbulence is not important, a larger initial magnetic field decreases the critical intensity required to keep the gas in the halo around a temperature of ~10⁴ K, as illustrated in Figure 4.24 (for a T4 background).



Figure 4.22 – Without turbulence – Evolution of the gas temperature with baryonic density for a T4 background and several different UV intensities.

4.3.4 Compressibility and critical magnetic Reynolds number

The critical magnetic Reynolds number $Rm_{\rm cr}$ has been found to increase with increasing compressibility, so with increasing β ; hence, these parameters should not be varied independently of each other. The result of increasing $Rm_{\rm cr}$ is that $B_{\rm max}$ decreases, and the result of increasing β is that the eddy turnover time becomes smaller, so saturation occurs faster. However, since magnetic heating is in nearly all cases less important than turbulent heating, varying β and $Rm_{\rm cr}$ will not change the results.



Figure 4.23 – Without turbulence – Evolution of the gas temperature with baryonic density for a T5 background and several different UV intensities.



Figure 4.24 – Without turbulence – Evolution of the gas temperature with baryonic density for a T4 background with $J_{21} = 1$ and several different initial magnetic field strengths.

4.3.5 Injected velocity

If the injected turbulent velocity is only a fraction of the virial velocity instead of equal to $v_{\rm vir}$, then the amount of turbulence in the halo is decreased, and thus the amount of turbulent heating as well as the saturation field strength will be lower. Since $B_{\rm max}$ is lower, also the ambipolar diffusion heating will be decreased. Hence the temperature (see Figure 4.25), electron fraction and H₂ fraction are all decreased. Decreasing $v_{\rm in}$ also results in a longer eddy turnover time. This latter effect becomes more noticeable for smaller fractions; for a while, the magnetic field will decrease more slowly because the turbulent decay becomes almost comparable to the amplification by gravitational compression, as shown in Figure 4.26. When lowering the injected velocity even further, below 3% of the virial velocity, turbulence will no longer be important as a heating and dynamo source and the results approach those from the model without turbulence.



Figure 4.25 – With turbulence – Evolution of the gas temperature with baryonic density for several different injected turbulent velocities.

4.3.6 Turbulent dissipation fraction

Increasing (decreasing) the turbulent dissipation fraction f_t results in a higher (lower) temperature, higher (lower) electron fraction and eventually higher (lower) H₂ fraction. The difference is however not very large, e.g. maximum ~350 K between $f_t = 0.01$ and 0.9. Even when the dissipated fraction is as low as 0.1%, the heating is still dominated by turbulence, independent of v_{in} . The cooling is always dominated by molecular hydrogen, even with a maximum amount of turbulent heating. Since turbulent dissipation does not influence the dynamo action, no value of f_t will result in convergence to the model



Figure 4.26 – With turbulence – Evolution of the magnetic field strength scaled with the baryonic density for several different injected turbulent velocities.

without turbulence, as was the case for small values of $v_{\rm in}$.

4.3.7 Integral scale

The integral scale is set as a fraction f_d of the dominant Jeans length, where the fiducial value is chosen to be 0.1. This fraction may, however, be larger, which affects both B_{max} and the ambipolar diffusion scale. When turbulence is important and for small to moderate initial magnetic fields, this does not change the evolution, since turbulent heating remains the most important heating source. Only for large f_d (close to unity) and large initial magnetic fields (e.g. 10 nG), ambipolar diffusion becomes the main heating source (also depending on the value of f_t , the dissipated fraction of the turbulence) and this introduces a critical magnetic field for which an instability occurs (such as described in 4.1), after which the gas in the halo stays hot.

When turbulence is not important, increasing f_d results in a decreased critical magnetic field $B_0^{\text{crit},\text{H}_2}$; for e.g. $f_d = 1$, the initial magnetic field strength required to keep H_2 from being an important coolant is lowered from 13 nG to 9 nG, as can be seen from Figure 4.27. However, the critical field for which an instability occurs $(B_0^{\text{crit},\text{inst}})$ does not change. These effects result purely from a changed ambipolar diffusion scale; hence, it appears that the critical magnetic field $B_0^{\text{crit},\text{H}_2}$ is quite sensitive to the choice of the AD scale, whereas $B_0^{\text{crit},\text{inst}}$ is not.



Figure 4.27 – Without turbulence – Evolution of the heating and cooling rates from various processes (as labeled) for an initial comoving field strength of 9 nG, and where the integral scale is equal to the dominant Jeans length.

4.3.8 Gravitational compression index

Varying the the power law index α which defines how *B* depends on the density has no effect when turbulent effects are important. When turbulence is not important, a smaller α means that the growth of the magnetic field becomes less steep. This results in less ambipolar diffusion heating, and thus a lower ionized fraction, a lower H₂ fraction, and a lower temperature (see Figure 4.28) at densities above $\sim 1 \text{ cm}^{-3}$.



Figure 4.28 – Without turbulence – Evolution of the gas temperature with baryonic density for different values of α , the scaling between the density and the magnetic field strength.

4.3.9 Reaction rates for H₂

To estimate the impact of the choice of reaction rates used to calculate the formation and destruction of H_2 , another choice of rates is considered. The fiducial rates are the ones as listed in Shang et al. (2010), and the alternative rates have been taken from Schleicher et al. (2008b). The first set of alternate rates changes the rates k_9 , k_{10} , k_{13} , k_{17} , k_{18} , k_{21} (rates k_{15} , k_{19} and k_{20} are unchanged; the numbering of the rates follows Shang et al. 2010). The second set of alternate rates is similar to the first set, with the addition of rate k_{14} . This is the rate for the following reaction:

(14)
$$H_2 + e^- \longrightarrow H + H^-,$$
 (4.1)

which introduces an extra H_2 destruction term. The effect of the alternate rates on the H_2 fraction is shown in Figure 4.29; the amount of molecular hydrogen is kept low up to higher densities. The result of this is that there is not enough H_2 present for effective cooling. Thus, the main coolant is atomic hydrogen and the temperature is kept high up to higher densities, as shown in Figure 4.30, until enough H_2 is formed to take over the cooling process. However, the difference in temperature reached at the end of the integration run for the different sets of rates is negligible. This is the case for any strength of the initial magnetic field. Hence, in the case where turbulence is present (and not too strong, otherwise the lower H_2 fraction will not be enough to compensate for the turbulent heating), it seems that the choice of reaction rates is not crucial to the final outcome.



Figure 4.29 – With turbulence – Evolution of the H_2 fraction with baryonic density for different choices of H_2 formation and destruction rates.

However, when turbulent effects are not important, the strong heat input from ambipolar diffusion combined with a higher destruction rate leads to an overall lower H_2 fraction; the stronger the initial magnetic field, the lower the H_2 fraction. This significantly lowers the critical initial field strength required to keep the gas in the halo hot, B_0^{crit,H_2} . For the first set of alternate rates, H_2 never becomes an important coolant for an initial field between 5 and 6 nG, while for the second set of alternate rates, H_2 never becomes an important coolant for an initial field between 3 and 4 nG, as shown in Figure 4.31. For the fiducial rates, this happened only for an initial field between 12 and 13 nG. However, the critical field for the formation of an instability, $B_0^{\text{crit,inst}}$, stays at 3 nG, although the instability occurs at a slightly lower density for the first set of alternate rates (by a factor of ~0.8), and again at a slightly lower density for the second set (by a factor of ~0.5).



Figure 4.30 – With turbulence – Evolution of the gas temperature with baryonic density for different choices of H_2 formation and destruction rates.



Figure 4.31 – Without turbulence – Evolution of the gas temperature with baryonic density for several different initial comoving field strengths, for the second set of alternate H_2 formation and destruction rates.

CHAPTER 5_____ Discussion

The model shows that for halos affected by turbulence and/or magnetic fields, several possible scenarios exists, which lead to a dense, hot ($\sim 10^4$ K) collapsing gas cloud.

5.1 Without Turbulence

Halos that have no significant turbulence but include a magnetic field are thermally significantly affected by this field if it is initially larger than ~0.1 nG (comoving). For larger fields, $2 n G < B_0 \leq 3 n G$, an instability occurs at high densities after which the temperature stays close to ~10⁴ K. It is conceivable that this instability will occur also for smaller fields, but at a density that falls outside the range of this model. In fact, such an instability can also be seen in Schleicher et al. (2009, Figures 10 and 11), occurring for $B_0 = 1 n G$ at a density of ~10¹¹ cm⁻³. The situation where H₂ never becomes an important coolant and the gas temperature stays at ~10⁴ K only occurs for very large initial fields, $12 n G < B_0^{\text{crit}, \text{H}_2} \leq 13 n \text{G}$.

The density at which the instability occurs slightly depends on the reaction rates used for the formation and destruction of H_2 , but the initial magnetic field at which it occurs stays the same. However, the critical magnetic field for which the H_2 abundance is never high enough for efficient cooling, and thus for which the gas always stays at $\sim 10^4$ K once it has heated up, is significantly lowered by both alternate sets of rates (to $5 \text{ nG} < B_0^{\text{crit},H_2} \leq 6 \text{ nG}$ for the first set, and to $3 \text{ nG} < B_0^{\text{crit},H_2} \leq 4 \text{ nG}$ for the second set), and hence appears to be very sensitive to the choice of reaction rates. The same effect occurs ($B_0^{\text{crit,inst}} \sim \text{equal}$, $B_0^{\text{crit,H}_2}$ lower) when the ambipolar diffusion scale is increased to the size of the collapsing cloud, instead of a fraction thereof. The magnetic field for which an instability occurs thus seems to be fairly robust.

However, the density and magnetic field for which the instability occur also depend on the scaling of the magnetic field with the density; the shallower the slope, the stronger the magnetic heating needs to be for the gas to become hot. It has been suggested that the slope should depend on the magnetic Jeans mass, and thus on the field strength itself, so that a stronger field would mean a shallower slope (see 1.2.2). If this is the case, then the existence of the instability depends on how flat the scaling relation becomes; for shallow slopes no reasonable initial magnetic field is able to produce sufficient heating.

There is not yet a consensus on the strength of the mean primordial magnetic field. Upper limits of $\leq 2-3$ nG have been found by e.g. Yamazaki et al. (2010) and Schleicher & Miniati (2011), while Trivedi et al. (2012) find tighter limits of ≤ 1 nG or even smaller (see also Section 1.2.1). The probability of existence and magnitude of the magnetic fields required for creating an instability depends strongly on these upper limits. If we assume that the primordial magnetic field was generated by some mechanism in the early Universe with a strongly random distribution, then $\delta B \sim B$. Thus, if the mean primordial field is ~1 nG, then a 3 nG field would be reached by the ~3 σ upward fluctuations. The critical magnetic field for which the H₂ abundance never becomes high enough for efficient cooling is (in the fiducial model) rather large compared to these limits, and the probability that this scenario will occur is thus quite small, unless the actual reaction rates are closer to the alternate ones than to the fiducial ones.

The results for the model without turbulence are in reasonable agreement with the results of Schleicher et al. (2009) for $B_0 \leq 1 \,\mathrm{nG}$, which is the range of initial magnetic field strengths they considered. The results for the zero-field case (equivalent to $B \simeq 0.01 \,\mathrm{nG}$) correspond to the results for the zero metallicity case of Omukai et al. (2005), who also used a one-zone model. The results presented here are however quite different from the results by Sethi et al. (2010) (only the zero-field cases agree with each other), who did not encounter any instabilities and found a critical magnetic field $(B_0^{\mathrm{crit},\mathrm{H}_2})$ of 3.6 nG, which is much lower than what was found here. The main differences with their model seem to be the evolution of the density with time, and the way the ambipolar diffusion rate is calculated. Since the zero-field cases do agree, and the reaction rates for the evolution of the H₂ fraction that were used should be identical, the discrepancies are most likely an effect of the ambipolar diffusion rate.

5.2 With Turbulence

For turbulent halos, it was expected that the magnetic field would become amplified by the turbulent dynamo, and that this would lower the critical field strength. While fields up to ~0.5 nG are indeed amplified during collapse, larger fields will instead decay due to the existence of a saturation field $B_{\rm max}$, which depends on the amount of turbulent energy. This saturation field grows as $\propto n_{\rm b}^{1/2}$, which is slower than the increase from gravitational compression alone, $\propto n_{\rm b}^{\alpha}$, if $\alpha > 1/2$. Since the growth of the magnetic field with density is less steep, also the ambipolar diffusion heating grows less strongly. Even with the added turbulent heating, the total heating does not increase fast enough to trigger an instability or prevent the H₂ fraction from becoming large enough for efficient cooling. By the end of the integration run, the difference in temperature, electron fraction and H₂ fraction between the different initial magnetic field strengths is small, due to the moderating effect of the turbulence. However, the mean minimum temperature is ~2.5 times larger than for the zero-field case in a halo where turbulent effects are not important, due to the turbulent heating. While a stronger magnetic field does not change the results, the mass of the halo does make a difference. The gas temperature in a halo with mass $\sim 10^{11} M_{\odot}$ does stay close to $\sim 10^4$ K during collapse, owing to its strong turbulent heating. This could happen also at smaller (or possibly larger) masses, depending on the strength of the turbulence in that halo. A different set of reaction rates can change this transition mass, but they are not crucial to the results.

The choice of the integral scale also does not seem to be very important; when it is increased, ambipolar diffusion becomes more important as a heating source, but only for very large fields ($B_0 \simeq 10 \,\mathrm{nG}$ if the integral scale is equal to the relevant Jeans length) an instability occurs where the amount of H₂ cooling drops dramatically. Since the required fields are so large, this is not likely to occur.

The quick convergence of the magnetic field to B_{max} as found here agrees with the results of Schleicher et al. (2010) for atomic cooling halos, as well as the finding that the thermal pressure dominates over the magnetic pressure during the collapse. However, the ratio of magnetic to thermal pressure is found to be between 0.8 and 0.1 after virialization, which is a bit larger than what Schleicher et al. (2010) found (their maximum ratio is 0.5). In a three-dimensional configuration, the small-scale dynamo is expected to generate highly inhomogeneous fields, so the larger this ratio, the higher the chance that magnetic fields will be dynamically important locally.

5.3 With Radiation Background

The effects of a UV radiation background were also examined, as well as the possibility of a lower critical intensity when taking magnetic fields and turbulence into account. For a halo not influenced by turbulence or magnetic fields, the critical intensity was found to be $10^1 < J_{21}^{\text{crit}} \leq 10^2$ for a T4 background, and $10^4 < J_{21}^{\text{crit}} \leq 10^5$ for a T5 background. These limits are consistent with those found by Shang et al. (2010) and lower by a factor ~10 than previous estimates by e.g. Omukai (2001) and Bromm & Loeb (2003), likely due to the different H₂ dissociation rates used. For an initial magnetic field of 1 nG, these limits do not change; however, when the field is increased to 2 nG, for a T4 background an instability occurs already at $J_{21} = 1$, while for $J_{21} = 10$ the gas stays hot during the entire collapse phase. For a 2 nG field and a T5 background, an instability occurs already at $J_{21} = 10^4$. For a 3 nG field and a T5 background, this instability occurs already at $J_{21} = 10^3$, while for $J_{21} = 10^4$ the gas stays hot during the entire collapse phase. Thus, for halos that have an initial comoving magnetic field of ~2 nG the critical intensity required to suppress H₂ cooling is lowered by a factor ~10, and the stronger the field, the lower J_{21}^{crit} .

In a turbulent halo of $10^9 M_{\odot}$, the critical intensity was found to be $1 < J_{21}^{\text{crit}} \leq 10^1$ for a T4 background, and $10^3 < J_{21}^{\text{crit}} \leq 10^4$ for a T5 background; these are a factor ~10 lower than for a halo not influenced by turbulence or magnetic fields. Since this is due to the turbulent heating in such halos, larger halos and/or halos with stronger turbulent heating will have an even lower J_{21}^{crit} .

The fact that the values of J_{21}^{crit} that have been found here are smaller than previous estimates is quite important. The mean cosmic UV background is expected to have value around $J_{21}^{\text{bg}} \sim 40$ (Dijkstra et al. 2008), which is smaller than the critical intensities, especially in the case of a T5 background. However, the background will inevitably fluctuate spatially, and thus a fraction of all halos will be irradiated by an intensity exceeding J_{21}^{crit} . Then, the lower this critical intensity, the larger the fraction of halos which are suitable candidates for direct SMBH formation; e.g. according to the distribution proposed by Dijkstra et al. (2008), a decrease in J_{21}^{crit} from 10⁴ to 10³ means an increase in the fraction of irradiated $T_{\text{vir}} \approx 10^4$ K halos from negligibly small ($\leq 10^{-8}$) to $\sim 10^{-6}$ (see their Figure 2). For $J_{21}^{\text{crit}} \sim 10^2$, the halo fraction even increases to $\sim 10^{-3}$. With a sufficiently low J_{21}^{crit} , one could argue that this mechanism provided many, if not all, seeds for the SMBHs observed in galaxies today.

5.4 Fragmentation

In order to estimate the mass of the black hole seed, a criterion for when fragmentation occurs is required. It has been shown that the equation of state helps to determine how strongly self-gravitating gas fragments (e.g. Spaans & Silk 2000; Li et al. 2003). A fragmentation criterion can be formulated in terms of the polytropic exponent (or effective adiabatic index), which can be expressed as:

$$\gamma = \frac{\mathrm{d}\ln P}{\mathrm{d}\ln\rho_{\mathrm{b}}} \tag{5.1}$$

$$= 1 + \frac{\mathrm{d}\ln T}{\mathrm{d}\ln\rho_{\mathrm{b}}} \tag{5.2}$$

Roughly speaking, fragmentation occurs efficiently when $\gamma \lesssim 1$, i.e. during temperature drops, and (almost) stops when the equation of state stiffens, so when $\gamma \gtrsim 1$. Thus, the preferred mass scale of the fragments is set by the relevant Jeans mass at the density where the polytropic exponent increases above a threshold value $\gamma_{\rm frag} \approx 1$ after a temperature minimum. Of course, this only holds provided that the halo is massive enough to be able to collapse. In theory $\gamma_{\rm frag} = 1$ and fragmentation stops approximately when the gas becomes isothermal, but based on the simulations of Bromm & Loeb (2003), Omukai et al. (2008) argue for a threshold value slightly below unity, so that fragmentation does not occur during the atomic cooling phase, where γ has been found to be between 0.95 and 1. For this reason a fragmentation threshold of $\gamma_{\rm frag} = 0.95$ is adopted here.

5.4.1 Without turbulence

The evolution of the polytropic exponent in a halo without turbulence or magnetic fields (or with an initial magnetic field strength $\leq 0.01 \text{ nG}$) is quite simple, as can be seen in Figure 5.1. Initially, the temperature increases adiabatically and $\gamma \approx 5/3$, until enough molecular hydrogen is formed and the gas starts to cool. The temperature minimum occurs at a number density of $\sim 1.0 \times 10^3 \text{ cm}^{-3}$, which sets a fragment mass of $\sim 7.9 \times 10^3 M_{\odot}$. At the end of the simulation the polytropic exponent is decreasing again, but after comparison with the results of similar simulations that go up to higher densities (e.g. Omukai et al. 2008; Schleicher et al. 2009) it does not seem likely that another



Figure 5.1 – Evolution of the polytropic exponent γ with baryonic density for several different models. The top three plots show the results for the zero-field, 3 nG, and 13 nG case of the model without turbulence, respectively, while the bottom plot shows the results for the zero-field case of the model with turbulence. The dashed horizontal lines indicate $\gamma = 0.95$ and 1; the dotted vertical line indicates when virialization occurs.

fragmentation episode will occur, because eventually the fragments become completely opaque to their own cooling radiation and the collapse becomes approximately adiabatic.

For an initial field of 0.1 nG, the evolution of the polytropic exponent is rather similar to the zero-field case, but the temperature minimum is shifted to a lower density $(\sim 4.2 \times 10^2 \,\mathrm{cm}^{-3})$. As a result, the fragment mass is somewhat larger compared to the zero-field case, $M_{\text{frag}} \approx 1.2 \times 10^4 M_{\odot}$. A similar shift of the temperature minimum to an even lower density ($\sim 2.5 \times 10^2 \,\mathrm{cm}^{-3}$) occurs also for $B_0 = 0.5 \,\mathrm{nG}$. Here, the minimum temperature reached by the gas is increased compared to the zero-field case, which would result in a somewhat larger Jeans mass. However, at this point in the evolution, the magnetic Jeans mass dominates over the thermal Jeans mass, and thus the fragment mass is increased greatly, $M_{\rm frag} \approx 1.9 \times 10^6 M_{\odot}$. Near the end of the simulation, the polytropic exponent stays approximately constant at ~1.10. For $B_0 = 1 \text{ nG}$, the temperature drops more steeply at first, but the location of the minimum does not change much compared to the 0.5 nG case. However, since the magnetic field is stronger, the magnetic Jeans mass and thus the fragment mass will be larger, $M_{\text{frag}} \approx 5.2 \times 10^7 M_{\odot}$. For $B_0 = 3 - 10 \,\text{nG}$, the temperature also drops steeply at first, but the location of the minimum is close to that of the zero-field case. At this point, the magnetic Jeans mass dominates, and the fragment mass increases with increasing magnetic field; $\sim 3.5 \times 10^9 M_{\odot}$, $\sim 2.1 \times 10^{10} M_{\odot}$, and $\sim 2.5 \times 10^{11} M_{\odot}$ for $B_0 = 3 \,\mathrm{nG}$, $5 \,\mathrm{nG}$, and $10 \,\mathrm{nG}$, respectively. However, at the moment where the temperature instability occurs, the polytropic exponent shoots steeply up and down, thereby crossing the threshold value again. It is uncertain whether this will result in another fragmentation episode or not. However, it does not seem likely that fragmentation will occur, given that the time where $\gamma < \gamma_{\rm frag}$ is shorter than the free-fall time at that point, and thus the change happens too quickly for the system to be able to react. Afterwards, the gas becomes nearly isothermal with $\gamma \approx 0.99$. Finally, even for halos with $B_0 \gtrsim 13 \,\mathrm{nG}$ a (relative) temperature minimum occurs, albeit very shallow, at a density of $\sim 1.0 \times 10^{-1} \,\mathrm{cm}^{-3}$, which corresponds to a fragment mass of $\sim 2.2 \times 10^{11} M_{\odot}$. Afterwards, the gas becomes nearly isothermal with γ as above.

5.4.2 With turbulence

When turbulence is taken into account, the differences between different initial field strengths are much smaller. In the zero-field case, the thermal evolution is quite different from the zero-field-zero-turbulence case, but the temperature minimum occurs at a similar density, $\sim 7.2 \times 10^2 \text{ cm}^{-3}$. The minimum temperature reached by the gas is however larger, which results in a larger fragment mass, $\sim 3.4 \times 10^4 M_{\odot}$. Afterwards, γ flattens off and stays approximately constant at ~ 1.08 . When a magnetic field is included, the location and value of the temperature minimum are very similar to the zero-field case, and at this point the thermal Jeans mass always dominates over the magnetic Jeans mass. Thus, the fragmentation behavior is nearly unchanged.

5.4.3 General fragmentation behavior

The fragmentation behavior is affected by the following factors: the minimum temperature, the location of the temperature minimum, the absence of a temperature minimum when the gas is cooled by atomic hydrogen and evolves (nearly) isothermally, and the magnetic Jeans mass (and thus the magnetic field strength) in the case where it dominates over the thermal Jeans mass. Of course, fragmentation does not occur when the fragment mass is larger than the mass of the halo.

When only one of these factors varies, it is easy to predict the outcome. For example, the minimum temperature increases with increasing injected velocity while the location of the minimum stays unchanged, as can be seen from Figure 4.25, as long as $v_{\rm in}$ is larger than 3% of the virial velocity. Since the magnetic Jeans mass is not important here, an increase in injected velocity thus means an increase in fragment mass.

However, when two or more of these factors change simultaneously, the result is not so straightforward. Both the minimum temperature and the density at which this minimum occurs are, for example, altered by a radiation background. The stronger the UV intensity, the higher the minimum temperature, which gives rise to higher fragment masses, but also the higher the density at which this minimum occurs, which gives rise to lower fragment masses if the thermal Jeans mass dominates. This is the case if turbulence is important or if the magnetic field is small. Because these two factors counteract, it becomes necessary to compute the fragment mass for each case. It turns out that the effect of the density is the strongest, and the fragment mass decreases with increasing UV intensity (but stays within the range $\sim 10^4 M_{\odot} \sim 10^5 M_{\odot}$), as long as molecular hydrogen cooling still becomes important. However, if the magnetic Jeans mass dominates, which occurs in halos where turbulence is not important and $B_0 \gtrsim$ $0.5 \,\mathrm{nG}$, the fragment mass actually does increase with increasing UV intensity, due to the effects of delayed molecular hydrogen formation on the magnetic field strength. For example, for $B_0 = 1 \,\mathrm{nG}$, the fragment mass increases from $\sim 5 \times 10^7 \,M_{\odot}$ without a radiation background, to $\sim 2 \times 10^8 M_{\odot}$ for a T5 background with $J_{21} = 10^4$.

Atomic cooling halos, in which the gas evolves nearly isothermally ($\gamma \approx 0.99$) once it has heated up to $\sim 10^4$ K, do not appear to go through a temperature minimum, see e.g. Figures 4.16 and 4.17. However, after the gas heats up, it cools down again by a small amount afterwards. This results in a dip in the polytropic exponent and thus the gas could become susceptible to fragmentation. Turbulent halos that cool through atomic hydrogen as a result of their large mass, or because they are exposed to a radiation background with an intensity larger than J_{21}^{crit} , could fragment around a density of $\sim 10^{-1}$ cm⁻³, which results in a fragment mass of $\sim 10^8 M_{\odot}$. For halos without significant turbulence in the presence of a supercritical radiation background, the density at which fragmentation could occur depends on the magnetic field strength, as halos with a stronger field heat up faster. In the zero-field case, the gas could fragment around a density of $\sim 10^2$ cm⁻³, which results in a fragment mass of $\sim 10^6 M_{\odot}$. For larger fields, fragmentation shifts to smaller densities, with a minimum density of $\sim 10^{-1}$ cm⁻³ corresponding to a fragment mass of $\sim 10^8 M_{\odot}$ if the thermal Jeans mass dominates, and larger but dependent on the magnetic field strength if the magnetic Jeans mass dominates.

5.4.4 When is the fragment mass largest?

The fragment mass is increased to $\sim 10^6 M_{\odot}$ or more (as opposed to the 'standard' $\sim 10^4 M_{\odot}$) for the parameter ranges described hereafter. A parameter range is denoted as "(T or NT, B_0 , J_{21}^{subcrit} or $J_{21}^{\text{supercrit}}$)", where T stands for halos with turbulence

and NT for halos without significant turbulence, B_0 has its usual meaning, and J_{21}^{subcrit} and $J_{21}^{\text{supercrit}}$ refer to whether the halo is exposed to a sub- or supercritical radiation background, respectively. A supercritical T4 (T5) radiation background is obtained, in a halo without significant turbulence, for $10 < J_{21} \leq 10^2$ ($10^4 < J_{21} \leq 10^5$) if $B_0 \lesssim 1 \,\text{nG}$, and for smaller J_{21} if B_0 is larger. In a turbulent halo, the critical intensity always lies in the range $1 < J_{21} \leq 10$ ($10^3 < J_{21} \leq 10^4$), independent of B_0 . For (NT, $0.5 \,\text{nG}, J_{21}^{\text{subcrit}}$), $M_{\text{frag}} \sim 10^6 \, M_{\odot}$, and for (NT, $> 0.5 \,\text{nG}, J_{21}^{\text{subcrit}}$) the fragment mass increases somewhat steeper than B_0^3 for larger B_0 . For (T, any, J_{21}^{subcrit}), the fragment mass is large ($\sim 10^8 \, M_{\odot}$) only when the halo is very massive ($\gtrsim 10^{11} \, M_{\odot}$, or $\gtrsim 10^{10} \, M_{\odot}$ if the turbulent energy dissipation fraction is increased from 10% to 25%). For (NT, $0, J_{21}^{\text{supercrit}}$), $M_{\text{frag}} \sim 10^6 \, M_{\odot}$, while for (NT, $\gtrsim 0.1 \,\text{nG}, J_{21}^{\text{supercrit}}$) the fragment mass is $\sim 10^8 \, M_{\odot}$ if the thermal pressure dominates, and larger but dependent on B_0 if the magnetic pressure dominates. For (T, any, $J_{21}^{\text{supercrit}}$), $M_{\text{frag}} \sim 10^8 \, M_{\odot}$.

In conclusion, the fragment mass is largest in halos without significant turbulence with the largest possible B_0 and exposed to supercritical background radiation, followed by the same type of halos but exposed to a subcritical background. The fragment mass in these halos does not depend on the mass of the halo itself, except of course that the halo must be more massive than the fragments (and that it must be able to start collapsing in the first place). Only turbulent halos that are very massive or that are exposed to a supercritical background (independent of B_0 , including the zero-field case) result in large fragment masses ($\sim 10^8 M_{\odot}$).

5.5 The Central Object

An order-of-magnitude estimate for the mass of the central object can be obtained when assuming that this object is a single (super-) massive star (SMS; see Section 1.1.3), using the following simple argument. At a certain radius, the mass accretion timescale $t_{\rm acc}$ equals the Kelvin-Helmholtz timescale $t_{\rm KH}$ for a protostar. This means that all the gas inside this radius will be incorporated into the protostar, while there is insufficient time to accrete the gas outside this radius (Abel et al. 2002, e.g.). For metal-free gas, the Kelvin-Helmholtz contraction timescale is approximately 10⁵ yr, with a relatively weak dependence on the protostellar mass (Schaerer 2002). The accretion rate in the self-similar collapse of a singular isothermal sphere is given by (Shu 1977):

$$\dot{M} = \frac{c_{\rm s}^3}{G},\tag{5.3}$$

and thus the accretion timescale is $t_{\rm acc} = GM/c_{\rm s}^3$. A similar result, differing only by a numerical factor of order unity, was also found by Shang et al. (2010) in their simulations of collapsing halos. Note that an isothermal sphere has a $\propto r^{-2}$ density profile and that deviations from this profile may increase \dot{M} if a central core is present. Setting $t_{\rm acc} = t_{\rm KH}$ results in a mass estimate that depends on the temperature as $\propto T^{3/2}$. Hence, for 'hot' halos with $T \sim 10^4$ K, the mass of the central object can be estimated as $\sim 5 \times 10^4 M_{\odot}$, as opposed to $\sim 200 M_{\odot}$ expected for $T \sim 300$ K. It must be noted that although the accretion rate for hot gas is higher, the gas collapse in a 'hot' halo will probably occur only after a significant delay, an effect seen in three-dimensional simulations (e.g. Shang et al. 2010). Assuming the seed black hole forms inside the halo around $z \sim 10$, the time available for accretion, so until $z \sim 6$, is ~0.5 Gyr. During this time, the seed may increase in mass by a factor ~2 × 10⁴ M_{\odot} at an e-folding time of ~0.05 Gyr, where the e-folding time is calculated as $\epsilon/(1-\epsilon)t_{\rm Edd}$ with $t_{\rm Edd} = 0.45$ Gyr, corresponding to Eddington-limited accretion with a radiative efficiency of $\epsilon \approx 0.1$. Hence, a ~5 × 10⁴ M_{\odot} seed black hole can grow into a ~10⁹ M_{\odot} SMBH by $z \sim 6$.

The amount of growth of course also depends on the reservoir of gas present for accretion. The fragment masses for atomic cooling halos in the case of small magnetic fields are generally less than $10^9 M_{\odot}$. However, the fragments may still merge and/or accrete gas from other fragments during their evolution. Even so, the regions in parameter space where the fragment mass is largest are the ones where SMBHs are most likely to form.

It is important to note that for the above scenario to occur, efficient redistribution of angular momentum is required, otherwise rotational support will halt the collapse. The mechanism responsible for angular momentum transport is unclear at this point, although several possible mechanisms have been suggested, e.g. redistribution by either global or local dynamical instabilities; see also Section 1.1.3. It is also possible that, in analogy with binary stars, a binary black hole forms, so that at least part of the angular momentum goes into their orbital motion.

5.6 Caveats

For future work, the model can still be improved upon in several ways. One has to keep in mind that a one-zone model such as this can only give an indication of critical values. A more realistic treatment of a collapsing halo would be obtained with a three-dimensional simulation, which is able to follow the evolution of the gas in the outer layers of the halo as well as in the center, and can account for non-spherical gas collapse. It would also be useful to follow the collapse up to higher densities, to have more certainty on whether the gas will or will not fragment again, and to see whether instabilities occur also for smaller magnetic fields and/or different scalings of the field with density. The collapse process itself has been simplified in that shocks have been ignored; once the velocity of the infalling gas becomes supersonic, shocks will occur which tend to slow the infall. It has also implicitly been assumed that the total mass of the halo stays constant, but this might not be accurate as gas flows could accrete onto the halo.

To better estimate the ambipolar diffusion rate, it would be necessary to explicitly calculate the integral in Equation 2.65. This is only possible if the power spectrum of the magnetic field is known, and the way it will be altered by for example the small-scale dynamo and gravitational compression. A more refined estimate of the ambipolar diffusion scale would also much improve the reliability of the results.

Furthermore, the treatment of turbulence and turbulent heating in this model is rather simplified. For example, a constant turbulent dissipation rate is assumed, which is not necessarily realistic.

Another assumption is that the gas stays metal- and dust-free. Especially for halos irradiated by a strong UV background, this may be difficult to justify, as the radiation

must come from one or more neighboring halos that have already formed stars.

When estimating the mass growth of the central object, it was assumed that the accretion is Eddington-limited. However, if the incoming gas flow is clumpy, super-Eddington accretion may be possible, enabling also lighter seed black holes to grow into the observed SMBHs.

An important factor to include in future work is feedback from the black hole on the surrounding gas. As has been shown by Spaans et al. (2012), X-ray flux from the BH in combination with a strong UV background can make it difficult for the seed black hole to accrete sufficient mass, as the strong X-ray radiation produced by accretion onto the BH tends to shut down the accretion for extended periods, thereby rendering the BH growth self-regulating.
CHAPTER 6.

Conclusions

The existence of supermassive black holes (SMBHs) with masses of $\sim 10^9 M_{\odot}$ at $z \sim 6$, as inferred from observations of very bright high-redshift quasars, presents a puzzle. In this work, the focus lies on how the 'seeds' of these SMBHs could have formed and how massive these seeds were. Of particular interest is seed BH formation through the direct collapse scenario, for which the gas in the halo is required to stay hot ($\sim 10^4$ K) to prevent fragmentation. In this context, the implications of magnetic fields and turbulence in the post-recombination Universe and during the gravitational collapse of a halo are explored, as well as the effects of a UV radiation background. Using a one-zone model, the evolution of a cloud of primordial gas is followed from its initial cosmic expansion through turnaround, virialization and collapse up to a density of 10^7 cm^{-3} .

It was found that in halos without any significant turbulence but with an initial comoving magnetic field between ~0.5 nG and ~12 nG, the fragment mass is increased from ~10⁴ M_{\odot} for the zero-field case to ~10⁶ M_{\odot} for $B_0 = 0.5$ nG, to ~5 × 10⁷ M_{\odot} for $B_0 = 1$ nG, and increasing for larger fields. This occurs because at the point of fragmentation, $n_{\rm b} \sim 10^{2-3} {\rm cm}^{-3}$, the magnetic Jeans mass dominates over the thermal Jeans mass.

For B_0 between ~3 nG and ~12 nG, an instability occurs at $n_b \gtrsim 10^5 \text{ cm}^{-3}$ which leads to strong H₂ dissociation and an increase in gas temperature to ~10⁴ K. Fragmentation at $n_b \sim 10^{2-3} \text{cm}^{-3}$ cannot be prevented in these cases, but the increased temperature enhances the accretion rate onto the central object for a self-similar collapse.

The critical magnetic field for which H_2 never becomes an important coolant is found to be ~13 nG, which is quite large compared to the current upper limits on the primordial magnetic field, ~1 nG comoving. However, the critical value is quite sensitive to the H_2 formation and destruction rates and the ambipolar diffusion scale; altering these may lower B_0^{crit,H_2} to more physically feasible values.

However, the existence of any critical magnetic field or instability depends crucially on the scaling of the magnetic field with the density. Therefore, it is very important to obtain a correct model for this relationship. In turbulent halos, initial fields $\gtrsim 0.5 \,\mathrm{nG}$ will decay rather than being amplified by the small-scale dynamo, because of the existence of a saturation field $B_{\rm max}$. This saturation field grows slower with density than a field would grow from gravitational compression alone ($\propto n_{\rm b}^{1/2}$ as opposed to $n_{\rm b}^{\alpha}$, if $\alpha > 1/2$). This results in the absence of any instability or critical magnetic field. The moderating effect of the turbulence causes the gas in halos with a different initial magnetic field to converge to approximately the same evolutionary track, so in the end they are practically indistinguishable from each other. However, the minimum temperature is increased compared to the zero-field-zeroturbulence case, which results in almost an order of magnitude larger fragment mass for a $10^9 M_{\odot}$ halo.

The ratio of magnetic to thermal pressure after virialization is found to be between 0.8 and 0.1. This implies that even though the thermal pressure dominates globally, locally magnetic fields may be dynamically important as the small-scale dynamo is expected to generate highly inhomogeneous fields in a three-dimensional setting.

A likely formation site for SMBH seeds are massive turbulent halos, $M \gtrsim 10^{11} M_{\odot}$ (also depending on the strength of the turbulence, if the fraction of turbulent heating is increased from 10% to 25%, then halos with $M \gtrsim 10^{10} M_{\odot}$ will stay hot as well). Their turbulent heating is so strong that molecular hydrogen cannot form fast enough to become an important coolant, and the cooling is dominated by atomic hydrogen.

Furthermore, it has been found that in halos with no significant turbulence, the critical UV background intensity for keeping the gas hot is lowered by a factor ~10 for $B_0 \sim 2 \,\mathrm{nG}$ as compared to the zero-field case, and lowered even more for stronger fields. In turbulent halos, J_{21}^{crit} is found to be a factor ~10 lower compared to the zero-field-zero-turbulence case, and the stronger the turbulence (more massive halo and/or stronger turbulent heating) the lower J_{21}^{crit} . The reduction in J_{21}^{crit} is particularly important, since it exponentially increases the number of halos exposed to a supercritical radiation background, and thus the number of possible sites for seed black hole formation.

Acknowledgments

First of all I would like to thank my supervisor Marco Spaans for his support, guidance and feedback, and of course for all the enlightening discussions we had.

Many thanks to all the helpful people on MATLAB Central and the T_EX Stack Exchange who were kind enough to help me out with all my MATLAB[®] and $I_{e}T_{E}X$ -related questions.

Thanks also to Olena, who allowed me to use her beautiful artwork on the title page of this thesis.

I would like to thank my fellow students at the Kapteyn Institute, for conversations and 'gezelligheid', and for not forgetting my name even after long periods of absence.

I also want to thank my family and friends, for their moral support and in particular for not asking me too much about when my thesis will finally be done.

Many thanks especially to my parents, for their continuing support and for attempting to understand what I was working on the whole time.

And last but not least I want to thank Daniel, for his never-ending encouragement and for putting up with me, and my cat Marley, for always managing to lift my spirits.

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